Supplementary Information for ***Acta Phys. -Chim. Sin.*** **2011**, *27* (3), 595-603

第一性原理方法预测水相核酸碱基及其代谢物的氧化还原电动势

李敏杰* 刘卫霞 彭淳容 陆文聪

(上海大学化学系, 上海 200444)

A First-Principles Method for Predicting Redox Potentials of Nucleobases and the Metabolites in Aqueous Solution

LI Min-Jie* LIU Wei-Xia PENG Chun-Rong LU Wen-Cong

(*Department of Chemistry, Shanghai University, Shanghai 200444, P. R. China*)

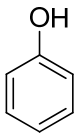
*Corresponding author. Email: minjieli@shu.edu.cn; Tel: +86-10-66133513.

Index

Part 1. The Cartesian Coordinates of compounds discussed in the text.

The Cartesian Coordinates of the 12 training set compounds.

No.1



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.134062	1.220373	0.000005
2	c	-1.860160	0.026776	0.000002
3	c	-1.172413	-1.192153	0.000001
4	c	0.222348	-1.224568	0.000004
5	c	0.939990	-0.023541	0.000007
6	c	0.263502	1.201478	-0.000014
7	o	2.309959	-0.111397	-0.000012
8	h	-2.946240	0.045209	0.000000
9	h	-1.725036	-2.128402	-0.000018
10	h	0.766681	-2.164209	0.000003
11	h	0.824780	2.134704	-0.000011
12	h	-1.652634	2.175874	0.000005
13	h	2.697545	0.777809	0.000088

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.291231	-1.241322	0.000004
2	c	-1.088644	-1.226986	0.000001
3	c	-1.787094	-0.000073	0.000000
4	c	-1.088624	1.226949	0.000001
5	c	0.291154	1.241488	0.000004
6	c	1.047190	0.000066	-0.000017
7	o	2.307381	-0.000094	0.000005
8	h	-2.873850	-0.000087	-0.000003
9	h	-1.646396	2.160036	0.000000
10	h	0.858145	2.167957	0.000005
11	h	0.858166	-2.167792	0.000005
12	h	-1.646394	-2.160091	0.000000

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.251431	0.242509	-0.000000
2	c	1.235415	-1.129863	0.000000
3	c	-0.006815	-1.831436	0.000000
4	c	-1.243816	-1.135628	0.000000
5	c	-1.254110	0.238003	-0.000000
6	c	-0.000000	0.941299	-0.000000
7	o	-0.084572	2.252878	-0.000000
8	h	-0.002694	-2.917714	0.000000
9	h	-2.175454	-1.692305	0.000000
10	h	-2.170896	0.819265	-0.000000
11	h	2.184998	0.799566	-0.000000
12	h	2.165877	-1.688954	0.000000
13	h	0.782119	2.707813	-0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	0.288812	1.214355	0.000004
2	c	-1.103237	1.203193	-0.000000
3	c	-1.832557	0.000059	-0.000003
4	c	-1.103162	-1.203394	-0.000000
5	c	0.288580	-1.214290	0.000004
6	c	1.078466	0.000236	0.000007
7	o	2.354255	-0.000177	-0.000008
8	h	-2.921426	-0.000082	-0.000007
9	h	-1.641372	-2.154615	-0.000003
10	h	0.834569	-2.157861	0.000006
11	h	0.833915	2.158441	0.000006
12	h	-1.641143	2.154579	-0.000003

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.268958	1.191703	-0.000073
2	c	1.120442	1.213463	-0.000015
3	c	1.848668	0.032532	0.000049
4	c	1.168776	-1.180722	0.000034
5	c	-0.216999	-1.216919	-0.000065
6	c	-0.936180	-0.026471	-0.000108
7	o	-2.286438	-0.113132	0.000089
8	h	2.924504	0.054903	0.000126
9	h	1.719665	-2.106049	0.000018
10	h	-0.747483	-2.154327	-0.000061
11	h	-0.830812	2.112519	-0.000010
12	h	1.630369	2.161937	0.000109
13	h	-2.699234	0.754563	0.000182

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	-1.039536	0.000007	-0.000036
2	c	-0.300563	1.242060	-0.000007
3	c	1.085145	1.226219	-0.000002
4	c	1.786020	-0.000008	-0.000003
5	c	1.085117	-1.226233	0.000011
6	c	-0.300577	-1.242051	0.000006
7	o	-2.288238	0.000006	0.000015
8	h	2.861750	-0.000026	0.000001
9	h	1.633407	-2.152232	-0.000040
10	h	-0.858181	-2.163200	0.000032
11	h	-0.858135	2.163228	0.000010
12	h	1.633434	2.152219	0.000069

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.000000	0.950913	0.000000
2	c	-1.249559	0.238164	0.000000
3	c	-1.221334	-1.129240	0.000000
4	c	0.015451	-1.826290	0.000000
5	c	1.245292	-1.121285	0.000000
6	c	1.256611	0.248305	0.000000
7	o	0.060481	2.221377	0.000000
8	h	0.017318	-2.901540	0.000000
9	h	2.171947	-1.666658	0.000000
10	h	2.162241	0.830590	0.000000
11	h	-2.168968	0.801789	0.000000
12	h	-2.142774	-1.683673	0.000000
13	h	-0.802377	2.685076	0.000000

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.039229	-0.000015	0.000274
2	c	-0.292300	-1.201307	0.000526
3	c	1.093512	-1.193369	-0.000196

4	c	1.809725	0.000032	-0.000287
5	c	1.093391	1.193383	-0.000253
6	c	-0.292372	1.201337	0.000654
7	o	-2.339122	-0.000065	-0.000595
8	h	2.886132	0.000110	-0.000108
9	h	1.622107	2.133358	-0.000175
10	h	-0.827037	2.138279	0.000337
11	h	-0.826894	-2.138290	0.000437
12	h	1.622300	-2.133304	-0.000035

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.268958	1.191703	-0.000073
2	c	1.120442	1.213463	-0.000015
3	c	1.848668	0.032532	0.000049
4	c	1.168776	-1.180722	0.000034
5	c	-0.216999	-1.216919	-0.000065
6	c	-0.936180	-0.026471	-0.000108
7	o	-2.286438	-0.113132	0.000089
8	h	2.924504	0.054903	0.000126
9	h	1.719665	-2.106049	0.000018
10	h	-0.747483	-2.154327	-0.000061
11	h	-0.830812	2.112519	-0.000010
12	h	1.630369	2.161937	0.000109
13	h	-2.699234	0.754563	0.000182

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.039536	0.000007	-0.000036
2	c	-0.300563	1.242060	-0.000007
3	c	1.085145	1.226219	-0.000002

4	c	1.786020	-0.000008	-0.000003
5	c	1.085117	-1.226233	0.000011
6	c	-0.300577	-1.242051	0.000006
7	o	-2.288238	0.000006	0.000015
8	h	2.861750	-0.000026	0.000001
9	h	1.633407	-2.152232	-0.000040
10	h	-0.858181	-2.163200	0.000032
11	h	-0.858135	2.163228	0.000010
12	h	1.633434	2.152219	0.000069

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.000000	0.950913	0.000000
2	c	-1.249559	0.238164	0.000000
3	c	-1.221334	-1.129240	0.000000
4	c	0.015451	-1.826290	0.000000
5	c	1.245292	-1.121285	0.000000
6	c	1.256611	0.248305	0.000000
7	o	0.060481	2.221377	0.000000
8	h	0.017318	-2.901540	0.000000
9	h	2.171947	-1.666658	0.000000
10	h	2.162241	0.830590	0.000000
11	h	-2.168968	0.801789	0.000000
12	h	-2.142774	-1.683673	0.000000
13	h	-0.802377	2.685076	0.000000

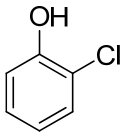
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.039229	-0.000015	0.000274
2	c	-0.292300	-1.201307	0.000526
3	c	1.093512	-1.193369	-0.000196
4	c	1.809725	0.000032	-0.000287
5	c	1.093391	1.193383	-0.000253
6	c	-0.292372	1.201337	0.000654

7	o	-2.339122	-0.000065	-0.000595
8	h	2.886132	0.000110	-0.000108
9	h	1.622107	2.133358	-0.000175
10	h	-0.827037	2.138279	0.000337
11	h	-0.826894	-2.138290	0.000437
12	h	1.622300	-2.133304	-0.000035

No.2



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.390731	-0.357016	0.000000
2	c	0.448543	-1.470429	-0.000000
3	c	1.832071	-1.289476	-0.000000
4	c	2.361046	0.006315	-0.000000
5	c	1.517827	1.115146	-0.000000
6	c	0.127656	0.946831	0.000000
7	o	-0.651147	2.062703	0.000000
8	cl	-2.142916	-0.569253	0.000000
9	h	2.488169	-2.154874	-0.000000
10	h	3.437320	0.154826	-0.000000
11	h	1.910730	2.127504	-0.000000
12	h	0.013818	-2.465071	-0.000000
13	h	-1.589766	1.805073	0.000015

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	-0.772587	-0.690259	-0.000000
2	c	-0.000000	0.559200	-0.000000
3	c	1.384438	0.549993	0.000000
4	c	2.076805	-0.671624	0.000000
5	c	1.381862	-1.903640	0.000000
6	c	0.006679	-1.920057	0.000000
7	cl	-0.868004	2.057070	-0.000000
8	o	-2.022726	-0.707038	-0.000000
9	h	3.163188	-0.663642	0.000000
10	h	1.942355	-2.834655	0.000000
11	h	-0.561069	-2.845810	-0.000000
12	h	1.930223	1.488534	0.000000

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.610606	-0.737734	-0.000000
2	c	-0.000000	0.583311	-0.000000
3	c	1.378017	0.697766	0.000000
4	c	2.161346	-0.468128	0.000000
5	c	1.568461	-1.769336	0.000000
6	c	0.205331	-1.908926	0.000000
7	cl	-1.032777	1.954302	-0.000000
8	o	-1.906874	-0.914263	-0.000000
9	h	3.243733	-0.376687	0.000000
10	h	2.208954	-2.645583	0.000000
11	h	-0.287993	-2.875626	0.000000
12	h	1.843599	1.677837	0.000000
13	h	-2.411395	-0.070699	-0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.809441	-0.694961	-0.000000
2	c	0.000000	0.510329	0.000000

3	c	1.389057	0.520457	0.000000
4	c	2.115689	-0.680407	0.000000
5	c	1.392850	-1.886641	0.000000
6	c	0.003769	-1.895921	-0.000000
7	cl	-0.850166	2.078571	-0.000000
8	o	-2.074820	-0.713442	-0.000000
9	h	3.203522	-0.668336	0.000000
10	h	1.931226	-2.836449	0.000000
11	h	-0.544313	-2.837345	-0.000000
12	h	1.909405	1.476817	0.000000

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.133644	0.943011	0.000055
2	c	-0.400379	-0.338591	0.000103
3	c	0.421629	-1.457280	0.000209
4	c	1.796103	-1.305190	0.000100
5	c	2.340281	-0.024538	-0.000158
6	c	1.519144	1.086856	-0.000179
7	cl	-2.135448	-0.559420	-0.000156
8	o	-0.596021	2.072403	0.000185
9	h	2.432087	-2.172617	0.000149
10	h	3.408352	0.108427	-0.000326
11	h	1.930000	2.082250	-0.000361
12	h	-0.022240	-2.438026	0.000359
13	h	-1.539937	1.925277	0.000562

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.024239	-1.919114	0.000000
2	c	-0.768711	-0.679670	0.000000

3	c	0.000000	0.554748	0.000000
4	c	1.384494	0.535612	0.000000
5	c	2.069003	-0.696983	0.000000
6	c	1.359818	-1.917157	0.000000
7	o	-2.009161	-0.678417	0.000000
8	cl	-0.849163	2.063730	0.000000
9	h	3.144571	-0.699346	0.000000
10	h	1.899407	-2.847879	0.000000
11	h	-0.592559	-2.833621	0.000000
12	h	1.935456	1.460159	0.000000

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.154245	-1.910123	0.000000
2	c	-0.644909	-0.713518	0.000000
3	c	0.000000	0.583654	0.000000
4	c	1.368089	0.647933	0.000000
5	c	2.138193	-0.538284	0.000000
6	c	1.516842	-1.811904	0.000000
7	o	-1.899927	-0.889632	0.000000
8	cl	-0.960657	2.005422	0.000000
9	h	3.210840	-0.463804	0.000000
10	h	2.120803	-2.701405	0.000000
11	h	-0.370410	-2.850539	0.000000
12	h	1.858119	1.606774	0.000000
13	h	-2.483516	-0.112677	0.000000

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.032750	-1.875749	0.000000
2	c	-0.785622	-0.670903	0.000000
3	c	0.000000	0.505575	0.000000
4	c	1.385494	0.493388	0.000000
5	c	2.079675	-0.705728	0.000000

6	c	1.346833	-1.891839	0.000000
7	o	-2.070100	-0.674849	0.000000
8	cl	-0.808908	2.070325	0.000000
9	h	3.155387	-0.713632	0.000000
10	h	1.861229	-2.839003	0.000000
11	h	-0.585114	-2.801762	0.000000
12	h	1.918950	1.429205	0.000000

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.133644	0.943011	0.000055
2	c	-0.400379	-0.338591	0.000103
3	c	0.421629	-1.457280	0.000209
4	c	1.796103	-1.305190	0.000100
5	c	2.340281	-0.024538	-0.000158
6	c	1.519144	1.086856	-0.000179
7	cl	-2.135448	-0.559420	-0.000156
8	o	-0.596021	2.072403	0.000185
9	h	2.432087	-2.172617	0.000149
10	h	3.408352	0.108427	-0.000326
11	h	1.930000	2.082250	-0.000361
12	h	-0.022240	-2.438026	0.000359
13	h	-1.539937	1.925277	0.000562

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.024239	-1.919114	0.000000
2	c	-0.768711	-0.679670	0.000000
3	c	0.000000	0.554748	0.000000
4	c	1.384494	0.535612	0.000000
5	c	2.069003	-0.696983	0.000000

6	c	1.359818	-1.917157	0.000000
7	o	-2.009161	-0.678417	0.000000
8	cl	-0.849163	2.063730	0.000000
9	h	3.144571	-0.699346	0.000000
10	h	1.899407	-2.847879	0.000000
11	h	-0.592559	-2.833621	0.000000
12	h	1.935456	1.460159	0.000000

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.154245	-1.910123	0.000000
2	c	-0.644909	-0.713518	0.000000
3	c	0.000000	0.583654	0.000000
4	c	1.368089	0.647933	0.000000
5	c	2.138193	-0.538284	0.000000
6	c	1.516842	-1.811904	0.000000
7	o	-1.899927	-0.889632	0.000000
8	cl	-0.960657	2.005422	0.000000
9	h	3.210840	-0.463804	0.000000
10	h	2.120803	-2.701405	0.000000
11	h	-0.370410	-2.850539	0.000000
12	h	1.858119	1.606774	0.000000
13	h	-2.483516	-0.112677	0.000000

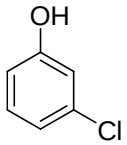
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.032781	-1.875751	0.000000
2	c	-0.785637	-0.670895	0.000000
3	c	0.000000	0.505573	0.000000
4	c	1.385493	0.493368	0.000000
5	c	2.079679	-0.705744	0.000000
6	c	1.346842	-1.891858	0.000000
7	o	-2.070115	-0.674824	0.000000
8	cl	-0.808888	2.070333	0.000000

9	h	3.155391	-0.713643	0.000000
10	h	1.861243	-2.839020	0.000000
11	h	-0.585157	-2.801756	0.000000
12	h	1.918962	1.429179	0.000000

No.3



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.183234	-0.898304	-0.000001
2	c	0.834261	0.056952	-0.000000
3	c	0.560471	1.423295	0.000000
4	c	-0.778766	1.829217	0.000000
5	c	-1.817464	0.900320	0.000000
6	c	-1.513956	-0.465788	-0.000001
7	cl	2.505911	-0.492305	-0.000000
8	o	-2.566010	-1.342449	-0.000002
9	h	1.368638	2.146411	0.000002
10	h	-1.011775	2.890689	0.000002
11	h	-2.857235	1.211259	0.000000
12	h	0.061411	-1.957224	-0.000002
13	h	-2.241321	-2.256506	0.000029

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.549753	-1.592341	0.000000
2	c	-0.954763	-0.194936	-0.000000

3	c	0.000000	0.795141	-0.000000
4	c	1.379089	0.488374	-0.000000
5	c	1.798148	-0.857300	0.000000
6	c	0.874414	-1.882462	0.000000
7	cl	-0.479245	2.485015	-0.000000
8	o	-1.407306	-2.512604	0.000000
9	h	2.106867	1.293319	-0.000000
10	h	2.862632	-1.075435	0.000000
11	h	1.170008	-2.927054	0.000000
12	h	-2.016719	0.025889	-0.000000

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.499113	-1.492976	0.000000
2	c	-0.951071	-0.157001	-0.000000
3	c	-0.000000	0.844225	-0.000000
4	c	1.409661	0.536472	-0.000000
5	c	1.841898	-0.796698	0.000000
6	c	0.909811	-1.816984	0.000000
7	cl	-0.458701	2.492148	-0.000000
8	o	-1.302831	-2.538495	0.000000
9	h	2.122982	1.355021	-0.000000
10	h	2.903609	-1.020888	0.000000
11	h	1.191130	-2.865667	0.000000
12	h	-2.011564	0.077200	-0.000000
13	h	-2.252707	-2.306459	0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.483826	-1.646558	-0.000000
2	c	-0.919053	-0.259657	-0.000000
3	c	0.000000	0.772465	-0.000000
4	c	1.387213	0.591449	0.000000
5	c	1.832028	-0.744895	0.000000

6	c	0.954092	-1.820796	0.000000
7	cl	-0.617634	2.469444	-0.000000
8	o	-1.305508	-2.615538	-0.000000
9	h	2.072280	1.432428	0.000000
10	h	2.907039	-0.934342	0.000000
11	h	1.328961	-2.843099	0.000000
12	h	-1.987153	-0.063269	-0.000000

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.504227	-0.464890	-0.000008
2	c	-0.183693	-0.894527	-0.000157
3	c	0.823492	0.056877	-0.000022
4	c	0.559425	1.412778	-0.000009
5	c	-0.771637	1.817118	0.000033
6	c	-1.801932	0.893964	0.000062
7	cl	2.485024	-0.488937	0.000031
8	o	-2.538095	-1.329326	-0.000105
9	h	1.358964	2.132020	0.000000
10	h	-1.002808	2.868406	-0.000071
11	h	-2.831318	1.209393	0.000047
12	h	0.049658	-1.946270	-0.000244
13	h	-2.243711	-2.244928	0.001178

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.881581	-1.877517	0.000000
2	c	-0.531312	-1.584365	0.000000
3	c	-0.956710	-0.201965	0.000000
4	c	0.000000	0.795071	0.000000
5	c	1.379668	0.503509	0.000000

6	c	1.803643	-0.842280	0.000000
7	o	-1.379229	-2.500206	0.000000
8	cl	-0.503511	2.464525	0.000000
9	h	2.099165	1.302968	0.000000
10	h	2.857574	-1.057483	0.000000
11	h	1.186136	-2.909948	0.000000
12	h	-2.010580	0.014471	0.000000

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.943261	-1.826198	0.000000
2	c	-0.463309	-1.520604	0.000000
3	c	-0.932736	-0.159857	0.000000
4	c	0.000000	0.836722	0.000000
5	c	1.392889	0.552457	0.000000
6	c	1.841159	-0.789127	0.000000
7	o	-1.259781	-2.507726	0.000000
8	cl	-0.507916	2.485244	0.000000
9	h	2.101558	1.362570	0.000000
10	h	2.897498	-0.989425	0.000000
11	h	1.237249	-2.862072	0.000000
12	h	-1.994584	0.029874	0.000000
13	h	-2.216483	-2.288635	0.000000

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.941135	-1.799872	0.000000
2	c	-0.461736	-1.603061	0.000000
3	c	-0.909271	-0.258974	0.000000
4	c	0.000000	0.778800	0.000000
5	c	1.371326	0.587220	0.000000
6	c	1.818540	-0.732500	0.000000
7	o	-1.294238	-2.590044	0.000000
8	cl	-0.617076	2.427493	0.000000

9	h	2.054956	1.416912	0.000000
10	h	2.879320	-0.923537	0.000000
11	h	1.317176	-2.810209	0.000000
12	h	-1.967214	-0.059876	0.000000

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.504227	-0.464890	-0.000008
2	c	-0.183693	-0.894527	-0.000157
3	c	0.823492	0.056877	-0.000022
4	c	0.559425	1.412778	-0.000009
5	c	-0.771637	1.817118	0.000033
6	c	-1.801932	0.893964	0.000062
7	cl	2.485024	-0.488937	0.000031
8	o	-2.538095	-1.329326	-0.000105
9	h	1.358964	2.132020	0.000000
10	h	-1.002808	2.868406	-0.000071
11	h	-2.831318	1.209393	0.000047
12	h	0.049658	-1.946270	-0.000244
13	h	-2.243711	-2.244928	0.001178

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.881581	-1.877517	0.000000
2	c	-0.531312	-1.584365	0.000000
3	c	-0.956710	-0.201965	0.000000
4	c	0.000000	0.795071	0.000000
5	c	1.379668	0.503509	0.000000
6	c	1.803643	-0.842280	0.000000
7	o	-1.379229	-2.500206	0.000000
8	cl	-0.503511	2.464525	0.000000

9	h	2.099165	1.302968	0.000000
10	h	2.857574	-1.057483	0.000000
11	h	1.186136	-2.909948	0.000000
12	h	-2.010580	0.014471	0.000000

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.943261	-1.826198	0.000000
2	c	-0.463309	-1.520604	0.000000
3	c	-0.932736	-0.159857	0.000000
4	c	0.000000	0.836722	0.000000
5	c	1.392889	0.552457	0.000000
6	c	1.841159	-0.789127	0.000000
7	o	-1.259781	-2.507726	0.000000
8	cl	-0.507916	2.485244	0.000000
9	h	2.101558	1.362570	0.000000
10	h	2.897498	-0.989425	0.000000
11	h	1.237249	-2.862072	0.000000
12	h	-1.994584	0.029874	0.000000
13	h	-2.216483	-2.288635	0.000000

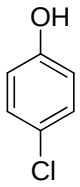
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.941135	-1.799872	0.000000
2	c	-0.461736	-1.603061	0.000000
3	c	-0.909271	-0.258974	0.000000
4	c	0.000000	0.778800	0.000000
5	c	1.371326	0.587220	0.000000
6	c	1.818540	-0.732500	0.000000
7	o	-1.294238	-2.590044	0.000000
8	cl	-0.617076	2.427493	0.000000
9	h	2.054956	1.416912	0.000000
10	h	2.879320	-0.923537	0.000000
11	h	1.317176	-2.810209	0.000000

12	h	-1.967214	-0.059876	0.000000

No.4



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.131413	-1.199778	-0.000002
2	c	0.265827	-1.209684	-0.000000
3	c	0.961322	-0.001997	-0.000000
4	c	0.275400	1.214832	0.000000
5	c	-1.118362	1.222476	0.000000
6	c	-1.824865	0.014855	-0.000001
7	cl	2.721760	-0.010023	-0.000000
8	o	-3.193701	0.089305	-0.000002
9	h	0.826670	2.149762	0.000000
10	h	-1.668826	2.158256	0.000000
11	h	-1.674965	-2.142863	-0.000002
12	h	0.805365	-2.151399	-0.000001
13	h	-3.576007	-0.802028	0.000029

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.000159	-1.924329	-0.000000
2	c	1.239884	-1.164036	0.000000
3	c	1.233761	0.213104	0.000000
4	c	-0.000000	0.899728	0.000000

5	c	-1.233743	0.212789	-0.000000
6	c	-1.239781	-1.164246	-0.000000
7	cl	-0.000327	2.641623	0.000000
8	o	0.000461	-3.181586	-0.000000
9	h	-2.159929	0.779251	-0.000000
10	h	-2.169052	-1.726207	-0.000000
11	h	2.169295	-1.725715	0.000000
12	h	2.159878	0.779691	0.000000

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.011157	-1.806549	-0.000000
2	c	-1.238058	-1.112080	-0.000000
3	c	-1.240985	0.259368	-0.000000
4	c	0.000000	0.966532	0.000000
5	c	1.245973	0.275060	0.000000
6	c	1.253754	-1.095549	-0.000000
7	cl	-0.014800	2.665003	0.000000
8	o	0.102167	-3.121151	-0.000000
9	h	2.172121	0.840389	0.000000
10	h	2.177212	-1.665971	-0.000000
11	h	-2.171625	-1.668913	-0.000000
12	h	-2.172475	0.816119	-0.000000
13	h	-0.762011	-3.578155	-0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.000710	-1.971983	0.000000
2	c	1.214331	-1.181426	-0.000000
3	c	1.212014	0.210790	-0.000000
4	c	-0.000000	0.908620	-0.000000
5	c	-1.212171	0.210257	0.000000
6	c	-1.213693	-1.181566	0.000000
7	cl	-0.000699	2.700980	-0.000000

8	o	0.000428	-3.245182	0.000000
9	h	-2.152351	0.760087	0.000000
10	h	-2.158919	-1.722756	0.000000
11	h	2.160346	-1.721235	-0.000000
12	h	2.152238	0.760529	-0.000000

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.814044	0.016756	0.000033
2	c	-1.127591	-1.189871	0.000049
3	c	0.260569	-1.199160	0.000049
4	c	0.951530	-0.002301	0.000032
5	c	0.274509	1.206825	0.000058
6	c	-1.109981	1.215847	0.000058
7	cl	2.703509	-0.012494	-0.000048
8	o	-3.161603	0.085595	-0.000185
9	h	0.818169	2.135871	0.000077
10	h	-1.648808	2.148122	0.000078
11	h	-1.670935	-2.121283	-0.000003
12	h	0.789884	-2.136452	-0.000004
13	h	-3.565078	-0.787189	0.000471

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.241083	-1.171940	0.000000
2	c	0.000038	-1.911648	0.000000
3	c	1.241140	-1.171919	0.000000
4	c	1.232944	0.212952	0.000000
5	c	0.000000	0.896467	0.000000
6	c	-1.232926	0.212875	0.000000
7	o	0.000040	-3.159196	0.000000

8	cl	-0.000062	2.634504	0.000000
9	h	-2.154742	0.767896	0.000000
10	h	-2.164746	-1.724830	0.000000
11	h	2.164813	-1.724791	0.000000
12	h	2.154740	0.768007	0.000000

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.262451	-1.099316	0.000000
2	c	0.015636	-1.817369	0.000000
3	c	-1.240823	-1.116482	0.000000
4	c	-1.234237	0.250928	0.000000
5	c	0.000000	0.949426	0.000000
6	c	1.242669	0.268973	0.000000
7	o	0.088380	-3.084720	0.000000
8	cl	-0.013490	2.666882	0.000000
9	h	2.162151	0.828424	0.000000
10	h	2.177833	-1.666434	0.000000
11	h	-2.156426	-1.686285	0.000000
12	h	-2.160553	0.799295	0.000000
13	h	-0.774884	-3.551213	0.000000

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.200421	-1.173096	0.000000
2	c	0.000345	-1.922148	0.000000
3	c	1.200978	-1.172824	0.000000
4	c	1.200021	0.211472	0.000000
5	c	0.000000	0.904372	0.000000
6	c	-1.199865	0.211139	0.000000
7	o	-0.000320	-3.216913	0.000000
8	cl	-0.000264	2.664247	0.000000
9	h	-2.134729	0.747005	0.000000
10	h	-2.139430	-1.702753	0.000000

11	h	2.140118	-1.702249	0.000000
12	h	2.134735	0.747603	0.000000

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.814044	0.016756	0.000033
2	c	-1.127591	-1.189871	0.000049
3	c	0.260569	-1.199160	0.000049
4	c	0.951530	-0.002301	0.000032
5	c	0.274509	1.206825	0.000058
6	c	-1.109981	1.215847	0.000058
7	cl	2.703509	-0.012494	-0.000048
8	o	-3.161603	0.085595	-0.000185
9	h	0.818169	2.135871	0.000077
10	h	-1.648808	2.148122	0.000078
11	h	-1.670935	-2.121283	-0.000003
12	h	0.789884	-2.136452	-0.000004
13	h	-3.565078	-0.787189	0.000471

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.241083	-1.171940	0.000000
2	c	0.000038	-1.911648	0.000000
3	c	1.241140	-1.171919	0.000000
4	c	1.232944	0.212952	0.000000
5	c	0.000000	0.896467	0.000000
6	c	-1.232926	0.212875	0.000000
7	o	0.000040	-3.159196	0.000000
8	cl	-0.000062	2.634504	0.000000
9	h	-2.154742	0.767896	0.000000
10	h	-2.164746	-1.724830	0.000000

11	h	2.164813	-1.724791	0.000000
12	h	2.154740	0.768007	0.000000

3.3 cation radical

Charge = 1 Multiplicity = 2

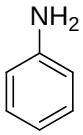
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.262451	-1.099316	0.000000
2	c	0.015636	-1.817369	0.000000
3	c	-1.240823	-1.116482	0.000000
4	c	-1.234237	0.250928	0.000000
5	c	0.000000	0.949426	0.000000
6	c	1.242669	0.268973	0.000000
7	o	0.088380	-3.084720	0.000000
8	cl	-0.013490	2.666882	0.000000
9	h	2.162151	0.828424	0.000000
10	h	2.177833	-1.666434	0.000000
11	h	-2.156426	-1.686285	0.000000
12	h	-2.160553	0.799295	0.000000
13	h	-0.774884	-3.551213	0.000000

3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.200421	-1.173096	0.000000
2	c	0.000345	-1.922148	0.000000
3	c	1.200978	-1.172824	0.000000
4	c	1.200021	0.211472	0.000000
5	c	0.000000	0.904372	0.000000
6	c	-1.199865	0.211139	0.000000
7	o	-0.000320	-3.216913	0.000000
8	cl	-0.000264	2.664247	0.000000
9	h	-2.134729	0.747005	0.000000
10	h	-2.139430	-1.702753	0.000000
11	h	2.140118	-1.702249	0.000000
12	h	2.134735	0.747603	0.000000

No.5



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.221663	1.209269	-0.004162
2	c	1.173417	1.204139	0.003215
3	c	1.884494	-0.000057	0.007631
4	c	1.173383	-1.204100	0.003204
5	c	-0.221803	-1.209271	-0.004277
6	c	-0.939147	0.000023	-0.007337
7	n	-2.338768	-0.000082	-0.076049
8	h	2.970781	-0.000051	0.014417
9	h	1.707098	-2.151608	0.006634
10	h	-0.762649	2.153695	-0.014083
11	h	1.707312	2.151527	0.006702
12	h	-2.790278	-0.836995	0.272940
13	h	-2.790375	0.837775	0.270509
14	h	-0.762608	-2.153787	-0.014419

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.301988	1.214749	0.000005
2	c	1.021380	-0.029870	0.000006
3	c	0.249330	-1.239788	-0.000006
4	c	-1.134610	-1.201009	0.000002
5	c	-1.811092	0.032412	0.000002
6	c	-1.082370	1.236196	-0.000007

7	n	2.357798	-0.136739	-0.000003
8	h	-2.897437	0.056667	0.000008
9	h	-1.610509	2.186441	-0.000007
10	h	0.793044	-2.179898	-0.000006
11	h	-1.703325	-2.127360	0.000009
12	h	2.776856	0.801438	0.000008
13	h	0.869024	2.143738	-0.000002

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.936585	-0.000001	-0.000204
2	c	-0.220081	-1.245595	-0.000237
3	c	1.155142	-1.231605	0.000008
4	c	1.854594	-0.000003	0.000249
5	c	1.155149	1.231602	0.000007
6	c	-0.220074	1.245599	-0.000239
7	n	-2.274341	0.000002	0.000207
8	h	2.940521	-0.000006	0.000623
9	h	1.708122	2.165545	0.000016
10	h	-0.773082	-2.180962	-0.000505
11	h	1.708111	-2.165551	0.000002
12	h	-2.809542	0.863872	0.000710
13	h	-2.809546	-0.863864	0.000711
14	h	-0.773070	2.180968	-0.000507

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.296366	1.198288	0.000000
2	c	1.062773	-0.033322	0.000000
3	c	0.243556	-1.227575	0.000008
4	c	-1.142490	-1.184772	-0.000005
5	c	-1.854261	0.034489	-0.000006
6	c	-1.094306	1.218613	0.000007
7	n	2.395523	-0.131914	-0.000006

8	h	-2.942378	0.057564	-0.000017
9	h	-1.605874	2.184422	0.000006
10	h	0.766125	-2.183524	0.000025
11	h	-1.696834	-2.126320	0.000002
12	h	2.792589	0.815548	-0.000011
13	h	0.847878	2.141377	0.000012

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.932503	-0.000014	-0.011072
2	c	-0.221055	1.200987	-0.006825
3	c	1.165789	1.195443	0.003963
4	c	1.873641	0.000022	0.009099
5	c	1.165826	-1.195430	0.004030
6	c	-0.221011	-1.200997	-0.006903
7	n	-2.327964	-0.000034	-0.080916
8	h	2.949706	0.000041	0.018101
9	h	1.694622	-2.133857	0.009155
10	h	-0.756809	2.136104	-0.013145
11	h	1.694569	2.133880	0.009156
12	h	-2.756864	-0.821693	0.301516
13	h	-2.756851	0.821822	0.301104
14	h	-0.756748	-2.136123	-0.013234

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.071426	1.242849	0.000044
2	c	0.319463	1.210274	-0.000802
3	c	1.017747	-0.041959	-0.000447
4	c	0.243300	-1.246636	-0.000528
5	c	-1.146397	-1.195057	-0.000062

6	c	-1.812728	0.045803	0.000518
7	n	2.351546	-0.138704	0.000792
8	h	-2.888309	0.079541	0.001316
9	h	-1.583751	2.189570	0.000532
10	h	0.764363	-2.189008	-0.000593
11	h	-1.716566	-2.108100	0.000246
12	h	2.774180	0.781666	0.001302
13	h	0.889509	2.125607	-0.000681

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.227095	1.246323	-0.000009
2	c	0.944564	-0.000004	-0.000002
3	c	0.227076	-1.246323	-0.000006
4	c	-1.152507	-1.227050	0.000027
5	c	-1.852997	0.000014	-0.000001
6	c	-1.152467	1.227057	-0.000020
7	n	2.249847	-0.000013	0.000007
8	h	-2.928341	0.000021	0.000008
9	h	-1.696860	2.154485	-0.000073
10	h	0.783115	-2.168348	-0.000198
11	h	-1.696913	-2.154471	0.000090
12	h	2.781175	0.861106	-0.000050
13	h	2.781162	-0.861139	0.000057
14	h	0.783147	2.168341	0.000175

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.074424	1.214189	0.000136
2	c	0.308890	1.183552	0.000265
3	c	1.041178	-0.044033	-0.000481
4	c	0.233224	-1.222886	0.000223
5	c	-1.145917	-1.168320	0.000258
6	c	-1.835904	0.046855	-0.000271

7	n	2.379469	-0.134583	-0.000243
8	h	-2.912042	0.079484	-0.000865
9	h	-1.570847	2.172900	-0.000150
10	h	0.731676	-2.180271	0.000407
11	h	-1.701613	-2.093858	0.000097
12	h	2.774248	0.794838	0.000939
13	h	0.860023	2.112846	0.000487

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.932913	-0.000027	-0.011085
2	c	0.220653	-1.200764	-0.007032
3	c	-1.166099	-1.195363	0.004040
4	c	-1.873939	0.000089	0.009123
5	c	-1.165861	1.195409	0.004005
6	c	0.221070	1.200949	-0.006652
7	n	2.328438	-0.000565	-0.081675
8	h	-2.950012	0.000110	0.018039
9	h	-1.694711	2.133822	0.009138
10	h	0.756541	-2.135783	-0.013601
11	h	-1.694741	-2.133895	0.009184
12	h	2.757283	0.823821	0.300465
13	h	2.757369	-0.821933	0.306806
14	h	0.756777	2.136053	-0.012697

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.071514	1.243005	-0.000019
2	c	0.319302	1.209989	0.000066
3	c	1.017950	-0.042193	0.000000
4	c	0.243002	-1.246713	0.000000

5	c	-1.146732	-1.194810	0.000021
6	c	-1.812957	0.046075	-0.000022
7	n	2.351762	-0.138945	-0.000040
8	h	-2.888550	0.079969	-0.000056
9	h	-1.583564	2.189898	-0.000099
10	h	0.763103	-2.189686	0.000002
11	h	-1.716912	-2.107861	0.000069
12	h	2.779666	0.783111	0.000015
13	h	0.889618	2.125070	0.000067

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.227221	1.245744	0.000043
2	c	0.944906	-0.000001	-0.000010
3	c	0.227205	-1.245737	-0.000195
4	c	-1.153340	-1.226740	0.000207
5	c	-1.853649	0.000006	0.000069
6	c	-1.153325	1.226742	-0.000205
7	n	2.250473	-0.000010	0.000070
8	h	-2.929050	0.000013	0.000174
9	h	-1.697519	2.154350	-0.000714
10	h	0.783227	-2.167662	-0.000363
11	h	-1.697531	-2.154351	0.000693
12	h	2.785105	0.863930	0.002130
13	h	2.785093	-0.863956	-0.001880
14	h	0.783257	2.167663	0.000017

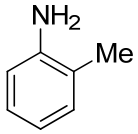
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.072292	1.215393	0.000222
2	c	0.310838	1.181632	-0.000063
3	c	1.039007	-0.046661	-0.000781
4	c	0.231450	-1.223897	-0.000067
5	c	-1.148109	-1.166890	0.000279

6	c	-1.835105	0.049313	-0.000173
7	n	2.380300	-0.135357	0.000290
8	h	-2.911048	0.084108	-0.000219
9	h	-1.566882	2.174845	0.000322
10	h	0.728154	-2.182146	0.000087
11	h	-1.705747	-2.091033	0.000423
12	h	2.774039	0.799334	0.000775
13	h	0.864661	2.109048	0.000081

No.6



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.826727	1.346989	-0.005133
2	c	1.985042	0.570546	-0.002173
3	c	1.894453	-0.823211	0.008469
4	c	0.630619	-1.420199	0.010809
5	c	-0.547020	-0.664599	0.001844
6	c	-0.442580	0.745611	-0.002076
7	c	-1.901851	-1.330485	-0.013491
8	n	-1.597917	1.539935	-0.072463
9	h	2.790634	-1.437411	0.013273
10	h	0.550608	-2.505707	0.015923
11	h	0.900450	2.433239	-0.014555
12	h	2.956640	1.058571	-0.004983
13	h	-2.428696	1.148691	0.354806
14	h	-1.465051	2.505987	0.203014
15	h	-2.499197	-1.012936	-0.879161
16	h	-1.801749	-2.419520	-0.058110
17	h	-2.490564	-1.098370	0.887542

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.407930	-1.459146	-0.000041
2	c	0.669767	-0.580676	-0.000051
3	c	0.406443	0.844295	-0.000028
4	c	-0.964640	1.281924	0.000004
5	c	-2.009811	0.378045	0.000033
6	c	-1.735836	-1.002127	0.000010
7	c	2.090659	-1.072185	0.000031
8	n	1.451652	1.677948	-0.000016
9	h	-2.553087	-1.718501	0.000033
10	h	-0.215925	-2.529946	-0.000075
11	h	-1.159625	2.352870	0.000004
12	h	-3.038593	0.729019	0.000056
13	h	1.115794	2.648247	0.000033
14	h	2.635208	-0.701681	0.876354
15	h	2.126802	-2.166463	-0.000962
16	h	2.635951	-0.699962	-0.875074

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.619126	-0.651104	-0.000067
2	c	0.379748	0.781167	-0.000097
3	c	-0.955742	1.309972	-0.000078
4	c	-2.025714	0.452172	0.000032
5	c	-1.801401	-0.948848	0.000061
6	c	-0.494911	-1.473862	-0.000000
7	n	1.412964	1.631590	0.000102
8	c	2.018791	-1.197761	-0.000019
9	h	-2.649456	-1.627255	0.000016
10	h	-0.357077	-2.550980	-0.000109
11	h	-1.098574	2.387297	-0.000051
12	h	-3.039486	0.839472	0.000129
13	h	2.375851	1.311845	0.000159

14	h	1.271216	2.637347	-0.000112
15	h	2.580590	-0.880984	0.889560
16	h	2.004919	-2.289871	-0.001501
17	h	2.581885	-0.878409	-0.887798

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.484177	0.840021	-0.000023
2	c	0.878704	1.322770	-0.000114
3	c	1.980757	0.473884	-0.000010
4	c	1.824863	-0.922277	0.000066
5	c	0.507187	-1.426840	0.000056
6	c	-0.616358	-0.609421	-0.000026
7	c	-2.007766	-1.183906	-0.000080
8	n	-1.586722	1.599913	0.000151
9	h	2.683449	-1.591324	0.000115
10	h	0.356087	-2.509753	0.000081
11	h	1.032035	2.404426	-0.000222
12	h	2.983952	0.906712	-0.000055
13	h	-1.299046	2.585780	0.000072
14	h	-2.581043	-0.838186	-0.873528
15	h	-1.986730	-2.283718	-0.000403
16	h	-2.580915	-0.838718	0.873677

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.438106	0.741381	-0.004115
2	c	0.822736	1.335615	-0.008091
3	c	1.973633	0.561768	-0.002521
4	c	1.881425	-0.821341	0.010839
5	c	0.623114	-1.411513	0.012908

6	c	-0.544522	-0.657953	0.000150
7	c	-1.898678	-1.328753	-0.016455
8	n	-1.587219	1.540230	-0.075765
9	h	2.767706	-1.432016	0.018257
10	h	0.545098	-2.486324	0.019415
11	h	0.897520	2.410967	-0.015711
12	h	2.936826	1.043610	-0.004935
13	h	-2.375321	1.186209	0.430994
14	h	-1.424427	2.493994	0.187997
15	h	-2.485363	-1.014354	-0.875765
16	h	-1.790935	-2.406394	-0.059941
17	h	-2.478184	-1.092525	0.873754

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.727176	-1.018997	0.000059
2	c	-0.391628	-1.463436	0.000045
3	c	0.679863	-0.570583	-0.000077
4	c	0.399314	0.844376	-0.000038
5	c	-0.969313	1.277012	-0.000050
6	c	-2.011195	0.358251	-0.000036
7	c	2.105099	-1.063230	-0.000045
8	n	1.418325	1.706934	0.000049
9	h	-2.529653	-1.736261	0.000172
10	h	-0.193074	-2.522071	0.000165
11	h	-1.173345	2.336057	-0.000136
12	h	-3.031800	0.700498	-0.000143
13	h	1.071613	2.658030	0.000498
14	h	2.643271	-0.709348	0.873569
15	h	2.131286	-2.147317	-0.000558
16	h	2.643641	-0.708480	-0.873060

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	0.478006	-1.472729	-0.000190
2	c	-0.630778	-0.641217	0.000098
3	c	-0.383957	0.785747	0.000123
4	c	0.962181	1.300962	0.000400
5	c	2.025602	0.428348	0.000099
6	c	1.793162	-0.964343	-0.000263
7	c	-2.036270	-1.181851	0.000283
8	n	-1.372301	1.637430	-0.000395
9	h	2.624909	-1.646099	-0.000628
10	h	0.329027	-2.538259	-0.000349
11	h	1.103357	2.368501	0.000674
12	h	3.031328	0.808895	0.000206
13	h	-2.341293	1.360991	-0.000936
14	h	-1.201903	2.634262	-0.000514
15	h	-2.585918	-0.858360	-0.880113
16	h	-2.015085	-2.263875	0.000801
17	h	-2.585987	-0.857566	0.880330

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.628918	-0.589659	-0.000014
2	c	-0.459307	0.838194	0.000016
3	c	0.891995	1.297971	0.000756
4	c	1.972341	0.432938	0.000588
5	c	1.790054	-0.944940	-0.000508
6	c	0.474348	-1.421290	-0.000870
7	n	-1.528196	1.649414	-0.001146
8	c	-2.023160	-1.165457	0.000929
9	h	2.625816	-1.623811	-0.000933
10	h	0.309523	-2.488555	-0.001388
11	h	1.067238	2.364238	0.001371
12	h	2.970614	0.843699	0.001194
13	h	-1.204770	2.606076	-0.001185
14	h	-2.590708	-0.841186	-0.868763
15	h	-1.995164	-2.251445	0.000704
16	h	-2.589299	-0.841467	0.871637

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.439414	0.741163	-0.003878
2	c	0.821457	1.335626	-0.009172
3	c	1.973072	0.562854	-0.003438
4	c	1.881969	-0.820210	0.011729
5	c	0.624017	-1.411057	0.014319
6	c	-0.544287	-0.658541	0.000537
7	c	-1.897022	-1.331486	-0.018508
8	n	-1.588757	1.539998	-0.074509
9	h	2.768647	-1.430295	0.019858
10	h	0.546706	-2.485914	0.021458
11	h	0.895329	2.410984	-0.017483
12	h	2.935874	1.045467	-0.006844
13	h	-2.373435	1.194283	0.446317
14	h	-1.421318	2.497873	0.179037
15	h	-2.482487	-1.018068	-0.879018
16	h	-1.787705	-2.409024	-0.061315
17	h	-2.479066	-1.095386	0.870033

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-2.011077	0.358349	-0.000029
2	c	-1.727320	-1.018863	0.000069
3	c	-0.391859	-1.463341	0.000062
4	c	0.679794	-0.570595	0.000002
5	c	0.399638	0.844535	-0.000033
6	c	-0.969042	1.276967	-0.000137
7	c	2.104629	-1.064485	-0.000095
8	n	1.418442	1.707571	0.000173
9	h	-2.529798	-1.736088	0.000132
10	h	-0.193324	-2.521934	0.000072

11	h	-1.172615	2.335980	-0.000113
12	h	-3.031587	0.700794	-0.000041
13	h	1.072745	2.662956	-0.000013
14	h	2.643371	-0.711324	0.873500
15	h	2.129875	-2.148497	-0.000709
16	h	2.643663	-0.710288	-0.873073

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.480477	-1.471896	-0.000641
2	c	-0.630210	-0.641675	0.000214
3	c	-0.386620	0.785554	0.000288
4	c	0.959047	1.301392	0.001575
5	c	2.024877	0.430248	0.000433
6	c	1.794801	-0.962317	-0.000987
7	c	-2.033318	-1.188258	0.001014
8	n	-1.373942	1.638979	-0.001369
9	h	2.627306	-1.643192	-0.002205
10	h	0.332623	-2.537617	-0.001113
11	h	1.098706	2.369039	0.002265
12	h	3.029883	0.812728	0.000429
13	h	-2.348063	1.370140	-0.003041
14	h	-1.200200	2.639465	-0.002058
15	h	-2.584907	-0.866217	-0.878605
16	h	-2.008096	-2.270197	0.001660
17	h	-2.583982	-0.865293	0.880880

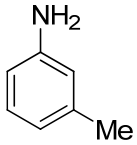
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.630196	-0.588949	-0.000152
2	c	-0.458351	0.837424	-0.000328
3	c	0.891873	1.296613	0.000735
4	c	1.972270	0.431062	0.000705
5	c	1.788329	-0.946474	-0.000565

6	c	0.472770	-1.421904	-0.000791
7	n	-1.525214	1.655870	-0.001125
8	c	-2.023896	-1.166503	0.001023
9	h	2.623277	-1.626414	-0.001062
10	h	0.307172	-2.489058	-0.001358
11	h	1.067308	2.362717	0.001575
12	h	2.970766	0.841294	0.001459
13	h	-1.192545	2.613337	-0.000564
14	h	-2.591837	-0.844081	-0.869132
15	h	-1.994220	-2.252479	0.000988
16	h	-2.590203	-0.844013	0.872206

No.7



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.272379	1.080676	-0.003335
2	c	-0.081175	1.808145	0.003870
3	c	1.155501	1.160975	0.006540
4	c	1.211693	-0.242296	0.001097
5	c	0.016216	-0.966574	-0.005583
6	c	-1.234321	-0.322323	-0.007772
7	c	2.545151	-0.956732	0.002475
8	n	-2.417222	-1.071863	-0.076385
9	h	2.075636	1.740872	0.013316
10	h	-2.230394	1.596682	-0.012077
11	h	-0.122512	2.894946	0.008638
12	h	-2.350212	-2.018464	0.278341
13	h	-3.245392	-0.603948	0.272223
14	h	0.050308	-2.055247	-0.016691
15	h	2.418980	-2.044626	0.003422
16	h	3.139636	-0.690315	-0.880788

17	h	3.140388	-0.688080	0.884555

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.030112	-1.000292	-0.000064
2	c	1.288462	-0.427498	0.000006
3	c	1.391303	1.002068	0.000053
4	c	0.249533	1.785953	0.000010
5	c	-1.022769	1.191740	-0.000059
6	c	-1.172811	-0.214872	-0.000065
7	n	2.424056	-1.139928	0.000010
8	c	-2.553981	-0.829962	0.000065
9	h	-1.910082	1.821242	-0.000125
10	h	2.386196	1.436857	0.000106
11	h	0.334649	2.869709	0.000014
12	h	2.199306	-2.142551	-0.000027
13	h	-0.118048	-2.085972	-0.000100
14	h	-2.504489	-1.923519	-0.001486
15	h	-3.126177	-0.520783	0.883885
16	h	-3.127497	-0.518313	-0.882014

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.220556	-0.362770	-0.000132
2	c	1.319372	1.072254	-0.000189
3	c	0.162975	1.818392	0.000008
4	c	-1.093413	1.176051	0.000197
5	c	-1.216692	-0.249598	-0.000125
6	c	-0.060983	-1.001048	-0.000338
7	c	-2.582453	-0.878900	0.000075
8	n	2.337803	-1.099827	0.000187
9	h	-1.997374	1.779629	0.000583
10	h	2.297856	1.544362	-0.000482
11	h	0.213673	2.902614	0.000002

12	h	2.307330	-2.115104	0.000689
13	h	3.259831	-0.674048	0.000933
14	h	-0.108194	-2.087079	-0.000667
15	h	-2.527001	-1.970241	-0.002176
16	h	-3.152439	-0.565648	0.883407
17	h	-3.154491	-0.561984	-0.880576

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.315414	-0.449704	-0.000165
2	c	1.359200	0.998202	-0.000110
3	c	0.204694	1.772803	0.000061
4	c	-1.078600	1.199542	0.000044
5	c	-1.173253	-0.213180	-0.000241
6	c	-0.026859	-0.994938	-0.000640
7	c	-2.540749	-0.870660	0.000285
8	n	2.368367	-1.272247	0.000445
9	h	-1.973700	1.820637	0.000244
10	h	2.337520	1.483544	-0.000223
11	h	0.301013	2.861437	0.000145
12	h	3.224450	-0.704654	0.000729
13	h	-0.109613	-2.082053	-0.000907
14	h	-2.456819	-1.964560	-0.005687
15	h	-3.127650	-0.585223	0.886741
16	h	-3.132856	-0.575785	-0.879560

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.226939	-0.319518	-0.011393
2	c	-1.266935	1.072469	-0.005121
3	c	-0.081480	1.795276	0.004785

4	c	1.147559	1.155206	0.007187
5	c	1.201589	-0.239787	0.000230
6	c	0.015612	-0.960869	-0.009705
7	c	2.536153	-0.951162	0.004076
8	n	-2.404522	-1.067945	-0.079868
9	h	2.057918	1.731173	0.015758
10	h	-2.215855	1.583022	-0.009155
11	h	-0.122901	2.871841	0.011614
12	h	-2.327042	-1.990408	0.305222
13	h	-3.207878	-0.602298	0.298289
14	h	0.045843	-2.038658	-0.017837
15	h	2.409449	-2.027926	0.003287
16	h	3.121845	-0.680143	-0.869652
17	h	3.116925	-0.680674	0.881205

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.170206	-0.215489	0.000152
2	c	-0.023322	-1.004171	0.000581
3	c	1.287665	-0.421394	0.000179
4	c	1.394931	1.005102	0.000063
5	c	0.247102	1.790162	0.000044
6	c	-1.025756	1.192591	-0.000073
7	n	2.409611	-1.147916	-0.000405
8	c	-2.549413	-0.832373	-0.000232
9	h	-1.904803	1.815412	-0.000463
10	h	2.376022	1.448797	-0.000041
11	h	0.330883	2.863491	-0.000075
12	h	2.191294	-2.136739	-0.000579
13	h	-0.104791	-2.080076	0.000752
14	h	-2.495147	-1.915308	-0.001129
15	h	-3.113336	-0.524094	0.875835
16	h	-3.113400	-0.522642	-0.875745

2.3 cation radical

Charge = 1 Multiplicity = 2

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	c	-0.065773	-1.002745	-0.000175
2	c	1.225328	-0.370972	-0.000077
3	c	1.331428	1.063162	-0.000007
4	c	0.172756	1.812228	0.000028
5	c	-1.087983	1.181314	-0.000047
6	c	-1.211175	-0.237562	-0.000097
7	n	2.306438	-1.101183	0.000106
8	c	-2.580298	-0.868326	0.000120
9	h	-1.978863	1.785442	-0.000117
10	h	2.307425	1.517485	0.000164
11	h	0.232080	2.886031	0.000129
12	h	2.264688	-2.111569	0.000078
13	h	3.228126	-0.685260	0.000148
14	h	-0.107691	-2.079123	-0.000275
15	h	-2.514349	-1.949750	-0.001621
16	h	-3.140274	-0.560178	0.877886
17	h	-3.141907	-0.557396	-0.875604

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.029714	-0.991220	-0.000790
2	c	1.294194	-0.446110	0.000062
3	c	1.358670	0.979843	0.000011
4	c	0.210951	1.753609	0.000077
5	c	-1.060796	1.190631	-0.000174
6	c	-1.168050	-0.209353	-0.000483
7	n	2.358527	-1.260206	0.000369
8	c	-2.538035	-0.854167	0.000456
9	h	-1.941781	1.811268	0.000027
10	h	2.327267	1.457987	0.000167
11	h	0.311514	2.828688	0.000266
12	h	3.200542	-0.703500	0.000455
13	h	-0.124341	-2.066765	-0.001083
14	h	-2.467287	-1.936603	-0.005387
15	h	-3.106495	-0.559159	0.878763
16	h	-3.112423	-0.549871	-0.870747

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.019334	-0.957951	-0.015876
2	c	-1.222168	-0.325288	-0.011040
3	c	-1.268137	1.071268	-0.001045
4	c	-0.090271	1.797743	0.006030
5	c	1.146060	1.161092	0.002000
6	c	1.205837	-0.229039	-0.006521
7	n	-2.400395	-1.073113	-0.079556
8	c	2.533756	-0.952411	0.010144
9	h	2.052326	1.742492	0.006261
10	h	-2.220262	1.575756	-0.002127
11	h	-0.135371	2.874118	0.013603
12	h	-2.319385	-2.000635	0.298024
13	h	-3.201378	-0.610745	0.312965
14	h	0.056955	-2.036017	-0.028713
15	h	2.562299	-1.736662	-0.739939
16	h	3.354130	-0.269877	-0.181581
17	h	2.706987	-1.419126	0.976248

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.170214	-0.215650	-0.000134
2	c	-0.023010	-1.003689	-0.000197
3	c	1.288046	-0.420957	-0.000030
4	c	1.394275	1.005835	-0.000013
5	c	0.246142	1.790449	0.000032
6	c	-1.026508	1.192481	-0.000023
7	n	2.410123	-1.147334	0.000150
8	c	-2.548896	-0.833577	0.000118

9	h	-1.905801	1.814918	-0.000036
10	h	2.375034	1.450355	0.000029
11	h	0.329542	2.863785	0.000076
12	h	2.195094	-2.140787	-0.000050
13	h	-0.103736	-2.079568	-0.000242
14	h	-2.493719	-1.916455	-0.001392
15	h	-3.112410	-0.526349	0.876798
16	h	-3.113874	-0.523915	-0.874750

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.065102	-1.001214	-0.000149
2	c	1.226012	-0.370177	-0.000084
3	c	1.331683	1.063396	0.000170
4	c	0.171716	1.812457	0.000010
5	c	-1.088990	1.181659	-0.000203
6	c	-1.211882	-0.236471	-0.000113
7	n	2.306471	-1.101558	-0.000138
8	c	-2.579952	-0.870209	0.000221
9	h	-1.979886	1.785856	-0.000473
10	h	2.307288	1.518271	0.000429
11	h	0.230565	2.886324	0.000049
12	h	2.264612	-2.116041	-0.000210
13	h	3.232236	-0.685305	0.001202
14	h	-0.106295	-2.077522	-0.000192
15	h	-2.510932	-1.951528	-0.001175
16	h	-3.141123	-0.563988	0.877909
17	h	-3.142678	-0.561799	-0.875686

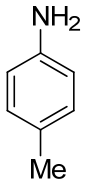
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.029745	-0.991112	-0.000258
2	c	1.292015	-0.445615	-0.000783
3	c	1.358120	0.978401	0.000075

4	c	0.210786	1.753187	0.000207
5	c	-1.060461	1.190030	-0.000320
6	c	-1.168758	-0.209159	-0.000250
7	n	2.361576	-1.259485	0.000333
8	c	-2.538653	-0.853991	0.000334
9	h	-1.941233	1.810928	-0.000286
10	h	2.326942	1.455713	0.000614
11	h	0.311559	2.828097	0.000654
12	h	3.204614	-0.696842	0.001021
13	h	-0.124840	-2.066631	-0.000174
14	h	-2.467809	-1.936382	-0.004751
15	h	-3.107675	-0.558506	0.878025
16	h	-3.112407	-0.550431	-0.871468

No.8



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.443978	0.000493	-0.004495
2	c	-0.723796	1.204899	-0.006755
3	c	0.672341	1.197574	-0.008225
4	c	1.403737	0.002711	-0.006392
5	c	0.673386	-1.195378	-0.008139
6	c	-0.720593	-1.204422	-0.007310
7	c	2.916061	-0.001194	0.018825
8	n	-2.846783	-0.002784	-0.068203
9	h	1.204480	-2.145824	-0.010976
10	h	-1.259207	2.152606	-0.016931
11	h	1.201872	2.148580	-0.010916
12	h	-3.289500	-0.837494	0.298071
13	h	-3.292759	0.833759	0.289859

14	h	-1.255488	-2.152453	-0.018545
15	h	3.320677	0.985070	-0.234478
16	h	3.304133	-0.269041	1.011395
17	h	3.330325	-0.723815	-0.695108

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.620361	-1.209736	-0.008531
2	c	-0.760542	-1.236123	-0.001899
3	c	-1.525962	-0.021327	0.002711
4	c	-0.786918	1.210655	-0.001949
5	c	0.596889	1.214006	-0.008695
6	c	1.334361	0.010743	-0.010141
7	n	-2.861730	-0.113742	0.008477
8	c	2.841633	0.019331	0.010976
9	h	1.175048	-2.146059	-0.013979
10	h	-1.337793	2.149440	-0.002655
11	h	1.131251	2.161904	-0.014278
12	h	-3.270230	0.828952	0.010379
13	h	-1.309020	-2.173617	-0.002258
14	h	3.243467	1.002262	-0.256211
15	h	3.223851	-0.232798	1.010363
16	h	3.256605	-0.719180	-0.685538

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.710875	-1.239463	-0.001681
2	c	-1.435902	-0.001546	0.001748
3	c	-0.717247	1.239463	-0.001468
4	c	0.655943	1.228823	-0.008041
5	c	1.387841	0.006973	-0.010530
6	c	0.660544	-1.221022	-0.008058
7	n	-2.775152	-0.004610	0.006580
8	c	2.881413	0.000406	0.007187

9	h	1.209396	-2.158522	-0.012329
10	h	-1.267219	2.176713	-0.000666
11	h	1.199125	2.169215	-0.012532
12	h	-3.307452	-0.869184	0.008543
13	h	-3.311420	0.857514	0.008894
14	h	-1.256285	-2.179360	-0.001072
15	h	3.302113	0.975890	-0.248792
16	h	3.242262	-0.266001	1.013197
17	h	3.285251	-0.755806	-0.676249

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.787374	1.194826	-0.004677
2	c	1.571275	-0.022501	0.005928
3	c	0.762917	-1.223109	-0.004068
4	c	-0.623434	-1.194468	-0.013951
5	c	-1.364234	0.009458	-0.019246
6	c	-0.605481	1.193797	-0.013896
7	n	2.905994	-0.108923	0.015842
8	c	-2.874827	0.018721	0.022865
9	h	-1.128210	2.154949	-0.020448
10	h	1.292393	-2.175182	-0.008024
11	h	-1.164758	-2.145054	-0.021037
12	h	3.293735	0.842345	0.018772
13	h	1.320796	2.148037	-0.010130
14	h	-3.316793	-0.715333	-0.670434
15	h	-3.288715	-0.212472	1.021834
16	h	-3.271956	1.004834	-0.259152

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	-0.717156	-1.195481	-0.010339
2	c	-1.435411	0.000828	-0.008759
3	c	-0.721712	1.195667	-0.009833
4	c	0.667661	1.189205	-0.007754
5	c	1.393987	0.003967	-0.004863
6	c	0.668387	-1.186008	-0.007938
7	n	-2.835276	-0.003612	-0.071942
8	c	2.906852	-0.001872	0.019951
9	h	1.192681	-2.128253	-0.009117
10	h	-1.252020	2.134124	-0.015635
11	h	1.188651	2.132835	-0.008600
12	h	-3.253918	-0.822366	0.328225
13	h	-3.258569	0.817218	0.318950
14	h	-1.246539	-2.134464	-0.016636
15	h	3.304584	0.975620	-0.231800
16	h	3.285839	-0.268037	1.003690
17	h	3.310581	-0.719233	-0.688270

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.334332	-0.014121	-0.009785
2	c	-0.626640	1.210515	-0.007680
3	c	0.761306	1.243301	-0.001187
4	c	1.521382	0.030220	0.002308
5	c	0.798288	-1.206290	-0.001355
6	c	-0.592838	-1.214137	-0.007796
7	n	2.855648	0.105172	0.007224
8	c	-2.843634	-0.026360	0.010398
9	h	-1.176671	2.137148	-0.012372
10	h	1.348431	-2.133854	-0.001185
11	h	-1.113155	-2.157385	-0.012497
12	h	3.262405	-0.822148	0.008537
13	h	1.291695	2.180643	-0.000791
14	h	-3.232154	-1.002825	-0.257480
15	h	-3.220928	0.221145	1.000048
16	h	-3.250356	0.702302	-0.684250

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.657659	-1.216298	-0.008382
2	c	-0.717598	-1.241678	-0.002045
3	c	-1.442887	-0.001385	0.001630
4	c	-0.723649	1.241692	-0.002035
5	c	0.653976	1.223663	-0.008195
6	c	1.378599	0.006658	-0.010138
7	n	-2.747902	-0.004397	0.007275
8	c	2.884035	-0.002183	0.010837
9	h	1.198230	-2.147124	-0.012847
10	h	-1.276994	2.165375	-0.001318
11	h	1.188545	2.157520	-0.012416
12	h	-3.276563	-0.866331	0.009611
13	h	-3.280584	0.855068	0.009726
14	h	-1.266754	-2.167857	-0.001071
15	h	3.286033	0.968106	-0.255809
16	h	3.246547	-0.256168	1.004096
17	h	3.276046	-0.740621	-0.680932

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.595546	1.182446	-0.002919
2	c	0.793431	1.177454	-0.001077
3	c	1.547534	-0.029032	0.000506
4	c	0.754807	-1.216383	-0.001265
5	c	-0.624349	-1.182801	-0.002605
6	c	-1.351102	0.014561	-0.002664
7	n	2.892024	-0.103327	0.003667
8	c	-2.865182	0.025348	0.004173
9	h	-1.101620	2.136840	-0.004067
10	h	1.264018	-2.168203	-0.001997
11	h	-1.159724	-2.121535	-0.003599

12	h	3.273179	0.831504	0.003237
13	h	1.321867	2.119927	-0.001693
14	h	-3.281245	-0.513655	-0.844759
15	h	-3.274047	-0.433508	0.902661
16	h	-3.244145	1.042354	-0.040344

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.717290	-1.195457	-0.009324
2	c	-1.435719	0.000913	-0.008562
3	c	-0.721465	1.195580	-0.009147
4	c	0.667870	1.189086	-0.007073
5	c	1.394130	0.003803	-0.004607
6	c	0.668360	-1.186105	-0.007175
7	n	-2.835511	-0.002996	-0.073987
8	c	2.907067	-0.001856	0.018791
9	h	1.192658	-2.128375	-0.008214
10	h	-1.251869	2.133954	-0.015121
11	h	1.188923	2.132704	-0.007979
12	h	-3.254547	-0.824626	0.325021
13	h	-3.259212	0.817065	0.323391
14	h	-1.246842	-2.134317	-0.015307
15	h	3.304275	0.975813	-0.233180
16	h	3.287273	-0.268160	1.002019
17	h	3.310192	-0.718866	-0.690140

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.591498	1.215584	-0.000660
2	c	-1.334245	0.017128	-0.000563
3	c	-0.627849	-1.209087	-0.000558

4	c	0.759477	-1.243834	-0.000233
5	c	1.521408	-0.031548	0.000325
6	c	0.800079	1.205816	-0.000112
7	c	-2.843651	0.026130	0.000785
8	n	2.855357	-0.107288	0.000604
9	h	-1.179390	-2.134869	-0.000829
10	h	1.352010	2.132103	-0.000233
11	h	-1.110347	2.159511	-0.000977
12	h	3.263483	0.823699	0.000311
13	h	1.288499	-2.181996	-0.000377
14	h	-3.230778	1.038893	-0.011229
15	h	-3.237593	-0.494614	-0.867909
16	h	-3.235719	-0.472838	0.883113

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.658242	-1.216070	-0.008268
2	c	-0.718088	-1.241214	-0.001657
3	c	-1.443270	-0.001374	0.001726
4	c	-0.724040	1.241156	-0.001761
5	c	0.654634	1.223267	-0.007814
6	c	1.378999	0.006566	-0.010045
7	n	-2.748371	-0.004280	0.006792
8	c	2.884775	-0.002137	0.010455
9	h	1.198752	-2.146965	-0.012988
10	h	-1.277370	2.164726	-0.000954
11	h	1.189197	2.157163	-0.011805
12	h	-3.280096	-0.869096	0.010586
13	h	-3.283981	0.858167	0.007337
14	h	-1.267298	-2.167240	-0.000754
15	h	3.286561	0.968390	-0.255873
16	h	3.248372	-0.256546	1.003190
17	h	3.276941	-0.739795	-0.682105

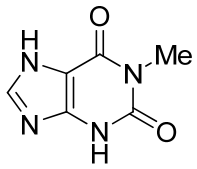
3.4 anion

Charge = -1 Multiplicity = 1

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	c	0.594869	-1.182067	-0.003835
2	c	-0.793805	-1.175434	0.001610
3	c	-1.545103	0.031032	0.001738
4	c	-0.754523	1.217563	-0.000027
5	c	0.625401	1.183322	-0.002280
6	c	1.350500	-0.014218	-0.004667
7	n	-2.893127	0.101216	0.001502
8	c	2.864537	-0.027533	0.004420
9	h	1.100328	-2.136713	-0.006992
10	h	-1.262922	2.169883	-0.001425
11	h	1.161512	2.121576	-0.004475
12	h	-3.270709	-0.839216	0.002193
13	h	-1.323816	-2.116922	0.000228
14	h	3.280706	0.572242	-0.802337
15	h	3.272862	0.363575	0.934802
16	h	3.242672	-1.038935	-0.114267

No.9



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.318100	1.222029	-0.000068
2	c	-0.935070	0.523687	0.000018
3	c	-1.050785	-0.849502	-0.000037
4	n	0.073974	-1.635453	-0.000160
5	c	1.348587	-1.083108	-0.000006
6	n	1.417816	0.322424	-0.000093
7	n	-2.239604	0.983260	0.000070
8	c	-3.037530	-0.116936	0.000044

9	n	-2.349701	-1.255267	-0.000042
10	o	2.352354	-1.781986	0.000175
11	c	2.774837	0.884942	-0.000020
12	o	0.458224	2.442641	0.000029
13	h	-4.116869	-0.050339	0.000097
14	h	0.016365	-2.646302	0.000149
15	h	3.316553	0.548294	0.887295
16	h	3.316747	0.547959	-0.887085
17	h	2.679127	1.969278	-0.000226
18	h	-2.522777	1.954455	0.000131

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.368198	1.200088	-0.000240
2	c	0.908126	0.516592	-0.000107
3	c	1.027832	-0.894730	-0.000047
4	n	0.002602	-1.725007	-0.000085
5	c	-1.266192	-1.136889	-0.000368
6	n	-1.420411	0.286394	-0.000149
7	n	2.171857	1.001670	0.000050
8	c	3.014715	-0.107383	0.000130
9	n	2.378802	-1.245127	0.000077
10	o	-2.275611	-1.827951	0.000255
11	c	-2.797868	0.797788	0.000163
12	o	-0.494846	2.423726	0.000062
13	h	4.090877	0.009870	0.000243
14	h	-3.325443	0.439526	-0.886817
15	h	-3.325199	0.439152	0.887135
16	h	-2.748567	1.885625	0.000391
17	h	2.431550	1.981321	0.000085

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.374476	1.224441	-0.000701

2	c	0.924940	0.550232	-0.000250
3	c	1.084706	-0.867586	-0.000107
4	n	-0.003131	-1.633471	-0.000111
5	c	-1.331274	-1.082255	0.000022
6	n	-1.442665	0.309734	-0.000169
7	n	2.178721	1.030816	0.000132
8	c	3.034585	-0.074022	0.000204
9	n	2.396275	-1.223539	0.000039
10	o	-2.270906	-1.839474	0.000157
11	c	-2.829518	0.840731	0.000210
12	o	-0.491195	2.434344	0.000216
13	h	4.111658	0.042742	0.000415
14	h	0.051006	-2.653452	-0.000009
15	h	-3.350779	0.487987	-0.891320
16	h	-3.350236	0.488134	0.892114
17	h	-2.764202	1.926744	0.000083
18	h	2.441175	2.014857	0.000229

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.318220	1.200600	-0.000173
2	c	0.913563	0.499120	-0.000097
3	c	0.991444	-0.898171	-0.000043
4	n	-0.058022	-1.734456	-0.000075
5	c	-1.282007	-1.154055	-0.000189
6	n	-1.392548	0.301413	-0.000091
7	n	2.221570	0.965271	0.000033
8	c	3.013362	-0.146537	0.000088
9	n	2.337205	-1.279145	0.000069
10	o	-2.361214	-1.773979	0.000159
11	c	-2.745079	0.843203	0.000096
12	o	-0.456004	2.446408	0.000059
13	h	4.094928	-0.073084	0.000167
14	h	-3.292396	0.495291	-0.882575
15	h	-3.292234	0.495088	0.882786
16	h	-2.669022	1.931467	0.000205
17	h	2.500664	1.935277	0.000034

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.323719	-1.232582	-0.000024
2	c	1.038735	-0.829240	0.000127
3	c	0.933621	0.522180	0.000272
4	n	2.237754	0.975371	0.000043
5	c	3.006152	-0.105568	-0.000015
6	n	-0.074815	-1.616584	0.000061
7	c	-1.319254	-1.066878	-0.000207
8	n	-1.406317	0.315598	0.000106
9	c	-0.324092	1.199326	-0.000454
10	o	-0.475204	2.398659	-0.000295
11	o	-2.312362	-1.755450	-0.000088
12	c	-2.767788	0.863719	0.000322
13	h	4.077674	-0.046195	0.000005
14	h	-0.009409	-2.622140	-0.000617
15	h	-3.296981	0.530452	-0.881506
16	h	-3.296741	0.529978	0.882123
17	h	-2.696743	1.936912	0.000611
18	h	2.556090	1.931459	0.000885

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.364234	-1.220991	0.000413
2	c	-1.028381	-0.877660	0.000320
3	c	-0.910286	0.519858	-0.000469
4	n	-2.175531	0.996018	-0.000134
5	c	-2.990422	-0.092784	0.000108
6	n	-0.011325	-1.695956	0.000658
7	c	1.259216	-1.108244	-0.000076
8	n	1.420019	0.276407	0.000053
9	c	0.377499	1.181673	-0.000424

10	o	0.521933	2.374760	-0.000214
11	o	2.227208	-1.817181	-0.001197
12	c	2.801080	0.773858	0.000926
13	h	-4.058649	0.019062	-0.000151
14	h	3.314906	0.420836	0.884070
15	h	3.316263	0.420414	-0.881238
16	h	2.771467	1.849678	0.000670
17	h	-2.471866	1.960839	-0.001302

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.352202	-1.213807	0.000035
2	c	-1.070978	-0.869430	0.000368
3	c	-0.927794	0.551988	0.000046
4	n	-2.184148	1.017081	-0.000782
5	c	-2.993587	-0.060357	-0.001041
6	n	0.010411	-1.617247	0.001520
7	c	1.299099	-1.070795	0.000093
8	n	1.423919	0.307870	-0.000582
9	c	0.379776	1.211452	0.000752
10	o	0.501401	2.398078	0.002046
11	o	2.241634	-1.795525	-0.000386
12	c	2.808020	0.819362	-0.001459
13	h	-4.064361	0.040732	-0.002040
14	h	-0.051207	-2.632486	0.002741
15	h	3.315915	0.477234	0.888557
16	h	3.320583	0.459735	-0.881669
17	h	2.765512	1.894507	-0.012275
18	h	-2.483802	1.989260	-0.002480

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.306182	-1.256105	0.000843
2	c	-0.992610	-0.867056	0.000548

3	c	-0.918504	0.501299	-0.000384
4	n	-2.229818	0.953588	-0.000265
5	c	-2.988067	-0.135807	0.000700
6	n	0.062106	-1.699094	0.000246
7	c	1.262767	-1.118438	-0.001031
8	n	1.388407	0.288197	0.000403
9	c	0.324233	1.174870	-0.000649
10	o	0.480331	2.389690	-0.001913
11	o	2.313933	-1.763325	-0.002024
12	c	2.747322	0.824801	0.002816
13	h	-4.060537	-0.078776	0.001100
14	h	3.280437	0.485531	0.880764
15	h	3.281340	0.492134	-0.877135
16	h	2.688862	1.899343	0.006819
17	h	-2.556637	1.906731	-0.000644

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.322174	-1.233454	0.000660
2	c	-1.037325	-0.830390	0.000156
3	c	-0.933893	0.521821	-0.000253
4	n	-2.237740	0.974570	-0.000494
5	c	-3.005038	-0.104920	0.000134
6	n	0.075885	-1.617160	0.000098
7	c	1.317545	-1.066416	-0.000351
8	n	1.405245	0.315957	-0.000165
9	c	0.322782	1.198198	-0.000208
10	o	0.474679	2.398963	0.000078
11	o	2.313485	-1.753780	-0.000516
12	c	2.766668	0.864624	0.000624
13	h	-4.076509	-0.046777	0.000194
14	h	0.009430	-2.629145	0.000356
15	h	3.295213	0.530907	0.882577
16	h	3.295954	0.531880	-0.881237
17	h	2.695680	1.937674	0.001215
18	h	-2.558025	1.937108	-0.000922

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.364198	-1.221376	-0.000004
2	c	1.028128	-0.879464	-0.000323
3	c	0.910836	0.519509	-0.000386
4	n	2.174827	0.995659	0.000236
5	c	2.989277	-0.090959	0.000597
6	n	0.011359	-1.695932	-0.000332
7	c	-1.258059	-1.107780	-0.000059
8	n	-1.419664	0.276323	-0.000145
9	c	-0.377417	1.180917	-0.000677
10	o	-0.522501	2.374522	-0.000132
11	o	-2.226670	-1.816970	0.000202
12	c	-2.801093	0.773925	0.000527
13	h	4.057543	0.020766	0.000889
14	h	-3.315650	0.420989	-0.882204
15	h	-3.314869	0.420816	0.883637
16	h	-2.771577	1.849807	0.000581
17	h	2.472840	1.967595	0.000177

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.350256	-1.213619	0.004752
2	c	1.068283	-0.869131	0.004301
3	c	0.928488	0.552268	-0.000362
4	n	2.183946	1.017068	-0.003206
5	c	2.992563	-0.059952	-0.001714
6	n	-0.010454	-1.619970	-0.000756
7	c	-1.296335	-1.071985	-0.001043
8	n	-1.422023	0.307369	-0.000692
9	c	-0.378670	1.211069	0.000455
10	o	-0.503517	2.397890	0.001485
11	o	-2.243003	-1.793216	-0.002948
12	c	-2.805406	0.820454	0.001613

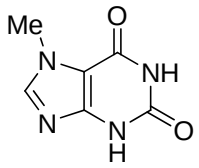
13	h	4.063287	0.039650	-0.004781
14	h	0.052176	-2.643657	-0.000918
15	h	-3.326987	0.444178	-0.866257
16	h	-3.305773	0.496870	0.902986
17	h	-2.761769	1.895283	-0.031062
18	h	2.485614	1.998010	-0.008450

3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.304765	-1.257632	0.000052
2	c	0.993072	-0.867677	-0.000701
3	c	0.919629	0.500702	-0.000908
4	n	2.230403	0.952632	0.000415
5	c	2.987532	-0.135347	0.001175
6	n	-0.063804	-1.698975	-0.000533
7	c	-1.262340	-1.115813	-0.000304
8	n	-1.388114	0.288414	-0.000374
9	c	-0.322848	1.173262	-0.000694
10	o	-0.479648	2.389187	-0.000612
11	o	-2.314495	-1.762451	0.000268
12	c	-2.747981	0.825280	0.001199
13	h	4.060018	-0.079399	0.002017
14	h	-3.282081	0.488340	-0.876982
15	h	-3.279352	0.489894	0.881672
16	h	-2.690601	1.899806	0.000171
17	h	2.560017	1.913946	0.000367

No.10



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.202819	1.355436	-0.000487
2	c	-0.555020	0.133438	-0.000232
3	c	0.038103	-1.117802	-0.000108
4	n	1.407676	-1.258771	-0.000061
5	c	2.250331	-0.157091	0.000216
6	n	1.586975	1.075911	-0.000099
7	n	-1.920040	-0.117688	0.000060
8	c	-2.044694	-1.468659	-0.000034
9	n	-0.879565	-2.115583	-0.000063
10	c	-2.992579	0.872601	0.000275
11	o	3.468274	-0.246504	0.000230
12	o	-0.218108	2.508273	0.000043
13	h	-3.013202	-1.951376	0.000020
14	h	2.200928	1.884157	0.000070
15	h	1.840203	-2.174315	0.000106
16	h	-3.947668	0.342985	0.000605
17	h	-2.920086	1.504981	0.888123
18	h	-2.920588	1.504797	-0.887748

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.884758	-2.141598	-0.000011
2	c	-0.099946	-1.156995	0.000001
3	c	0.522416	0.125276	0.000023
4	n	1.860189	-0.093554	0.000024
5	c	2.007703	-1.479840	-0.000021
6	n	-1.403045	-1.373165	0.000012
7	c	-2.211623	-0.236518	-0.000083
8	n	-1.605540	1.049200	-0.000032
9	c	-0.251568	1.352567	0.000011

10	o	0.195229	2.496967	-0.000007
11	o	-3.432305	-0.304870	0.000062
12	c	2.932256	0.900685	0.000012
13	h	2.996381	-1.922968	-0.000029
14	h	-2.252086	1.832633	-0.000044
15	h	3.887456	0.371796	-0.000201
16	h	2.857313	1.532389	-0.887941
17	h	2.857583	1.532146	0.888165

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.213136	1.380871	0.000404
2	c	0.562048	0.136329	0.000113
3	c	-0.053744	-1.156062	0.000052
4	n	-1.383561	-1.264607	0.000001
5	c	-2.245584	-0.119475	-0.000502
6	n	-1.589440	1.109498	-0.000049
7	n	1.883622	-0.100832	-0.000073
8	c	2.017507	-1.498089	-0.000025
9	n	0.874408	-2.146045	0.000136
10	c	2.983124	0.882043	-0.000141
11	o	-3.441299	-0.259058	0.000086
12	o	0.255793	2.499927	0.000019
13	h	2.996852	-1.962124	-0.000049
14	h	-2.208057	1.919923	-0.000006
15	h	-1.846738	-2.174716	0.000161
16	h	3.925479	0.333940	-0.000491
17	h	2.909787	1.508303	-0.891519
18	h	2.910241	1.507919	0.891548

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.236907	1.332815	-0.000680
2	c	-0.518916	0.126999	-0.000306

3	c	0.104519	-1.136209	-0.000174
4	n	1.428406	-1.370482	-0.000183
5	c	2.221869	-0.272344	-0.000016
6	n	1.592678	1.023429	-0.000089
7	n	-1.892965	-0.106611	0.000064
8	c	-2.022862	-1.463555	0.000160
9	n	-0.880263	-2.123902	-0.000044
10	c	-2.951232	0.882075	0.000233
11	o	3.467023	-0.270956	0.000464
12	o	-0.180258	2.513021	0.000158
13	h	-3.004695	-1.925861	0.000336
14	h	2.235135	1.807209	0.000316
15	h	-3.914078	0.359708	0.000588
16	h	-2.883318	1.523477	0.885071
17	h	-2.883860	1.523227	-0.884827

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.883783	-2.075221	-0.000261
2	c	-0.031779	-1.094558	-0.000249
3	c	0.549384	0.137554	0.000128
4	n	1.912423	-0.109373	-0.000057
5	c	2.034492	-1.427805	-0.000227
6	n	-1.391057	-1.251873	-0.000506
7	c	-2.214456	-0.171778	0.000056
8	n	-1.590300	1.053815	0.000036
9	c	-0.230972	1.336771	0.000216
10	o	0.161135	2.479477	-0.000776
11	o	-3.419350	-0.265521	0.000654
12	c	2.993412	0.868118	0.000702
13	h	2.994750	-1.908714	-0.000219
14	h	-2.210864	1.849481	-0.000770
15	h	-1.810134	-2.168767	0.001006
16	h	3.932094	0.330959	-0.000176
17	h	2.927464	1.488114	-0.882821
18	h	2.927981	1.486037	0.885721

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.284451	1.337959	-0.000630
2	c	0.520225	0.131474	-0.000324
3	c	-0.083130	-1.143992	-0.000614
4	n	-1.370657	-1.364690	-0.000491
5	c	-2.191248	-0.234111	0.000270
6	n	-1.623028	1.027979	-0.000395
7	n	1.856819	-0.082167	-0.000061
8	c	2.007006	-1.434604	-0.000289
9	n	0.903401	-2.103622	-0.000711
10	c	2.931142	0.907721	0.001777
11	o	-3.385035	-0.351977	0.001786
12	o	0.125599	2.466688	-0.001185
13	h	2.988503	-1.873142	-0.000259
14	h	-2.270956	1.802983	-0.000801
15	h	3.872065	0.375150	0.000636
16	h	2.861351	1.525867	-0.882438
17	h	2.861514	1.522281	0.888523

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.854951	-2.109477	-0.002337
2	c	-0.060260	-1.157865	-0.001208
3	c	0.560178	0.137142	0.000352
4	n	1.879644	-0.106623	0.000687
5	c	2.002372	-1.449217	-0.000573
6	n	-1.377464	-1.255888	-0.000282
7	c	-2.207337	-0.134256	0.001039
8	n	-1.581511	1.092885	0.000044
9	c	-0.235227	1.369727	-0.001199
10	o	0.222826	2.470166	-0.002903
11	o	-3.390343	-0.250251	0.002262
12	c	2.982481	0.870831	0.003047

13	h	2.969395	-1.921495	-0.000839
14	h	-2.208471	1.889861	-0.001589
15	h	-1.833446	-2.164839	0.001183
16	h	3.907772	0.313099	0.002222
17	h	2.911474	1.481669	-0.884914
18	h	2.910834	1.477948	0.893535

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.882165	-2.076349	-0.000834
2	c	0.080318	-1.109002	-0.000328
3	c	-0.518423	0.132846	0.000244
4	n	-1.890069	-0.099211	0.000121
5	c	-2.019033	-1.417908	-0.000382
6	n	1.406657	-1.351271	-0.000313
7	c	2.187234	-0.273683	0.001178
8	n	1.606980	0.996963	-0.000214
9	c	0.267948	1.311393	0.000045
10	o	-0.105964	2.476883	-0.001276
11	o	3.422257	-0.312700	0.000579
12	c	-2.961957	0.881258	0.001147
13	h	-2.986730	-1.885595	-0.000440
14	h	2.250460	1.772487	-0.000983
15	h	-3.905842	0.351997	0.000922
16	h	-2.897125	1.502910	0.884529
17	h	-2.897455	1.504392	-0.881199

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.883259	-2.074918	0.000371
2	c	0.033175	-1.094322	0.000142

3	c	-0.548786	0.137653	0.000167
4	n	-1.912031	-0.109332	-0.000295
5	c	-2.034056	-1.427259	0.000072
6	n	1.391190	-1.251759	-0.000175
7	c	2.211682	-0.171265	-0.000395
8	n	1.589929	1.054219	-0.000517
9	c	0.232196	1.335339	0.000274
10	o	-0.162239	2.479198	0.000740
11	o	3.418688	-0.265047	-0.000074
12	c	-2.993663	0.867411	-0.000432
13	h	-2.994266	-1.908098	-0.000029
14	h	2.214518	1.854524	-0.000417
15	h	1.813042	-2.174515	0.001916
16	h	-3.931710	0.329445	-0.001952
17	h	-2.929536	1.485440	0.884525
18	h	-2.927738	1.487177	-0.884033

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.287717	1.337879	-0.000439
2	c	-0.519902	0.131926	0.000010
3	c	0.082859	-1.144607	-0.000357
4	n	1.369371	-1.364006	-0.000283
5	c	2.189427	-0.233512	0.000440
6	n	1.624394	1.028570	-0.000332
7	n	-1.856420	-0.081218	0.000236
8	c	-2.007069	-1.433444	-0.000133
9	n	-0.904049	-2.103905	-0.000510
10	c	-2.932014	0.907667	0.000802
11	o	3.383833	-0.355256	0.000842
12	o	-0.125094	2.466667	-0.000573
13	h	-2.988947	-1.871406	-0.000169
14	h	2.278274	1.807447	-0.000538
15	h	-3.872245	0.373737	0.000402
16	h	-2.863141	1.523115	0.886988
17	h	-2.863027	1.524275	-0.884554

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.857448	-2.109171	0.000158
2	c	0.060557	-1.157206	0.001542
3	c	-0.559380	0.137665	0.001465
4	n	-1.879444	-0.105145	-0.000094
5	c	-2.002805	-1.448046	-0.001443
6	n	1.375650	-1.257302	0.001340
7	c	2.204148	-0.135671	-0.000373
8	n	1.582658	1.092037	-0.001407
9	c	0.238393	1.369240	0.000672
10	o	-0.220259	2.470425	0.000949
11	o	3.388757	-0.251398	-0.001145
12	c	-2.982135	0.871998	-0.000590
13	h	-2.970428	-1.919076	-0.003608
14	h	2.215482	1.893828	-0.001900
15	h	1.834557	-2.174461	0.001514
16	h	-3.907522	0.314355	-0.003081
17	h	-2.912898	1.479687	0.889703
18	h	-2.909751	1.482625	-0.888673

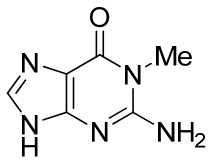
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.882275	-2.075540	-0.000367
2	c	-0.079402	-1.108150	-0.000673
3	c	0.518281	0.133595	-0.000355
4	n	1.890053	-0.098734	0.000139
5	c	2.019772	-1.416651	0.000264
6	n	-1.406062	-1.350259	-0.001110
7	c	-2.185315	-0.272036	0.000399
8	n	-1.608745	0.997382	0.000180
9	c	-0.270432	1.310305	-0.000577
10	o	0.104814	2.476802	-0.000920
11	o	-3.422058	-0.317221	0.001294

12	c	2.963611	0.880437	0.000973
13	h	2.987278	-1.884708	0.000870
14	h	-2.256771	1.778836	0.000501
15	h	3.906468	0.349475	0.001868
16	h	2.900396	1.502300	-0.882308
17	h	2.898845	1.502493	0.884001

No.11



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.242530	1.276925	0.017481
2	c	1.007288	0.572421	0.006532
3	c	1.001138	-0.819838	-0.002897
4	n	-0.062377	-1.654679	0.013491
5	c	-1.216803	-1.021447	0.010183
6	n	-1.364891	0.348203	0.001331
7	n	2.302489	1.061110	0.002114
8	c	3.057129	-0.007201	-0.010147
9	n	2.323355	-1.183390	-0.013056
10	n	-2.364607	-1.785351	-0.050481
11	c	-2.702280	0.944292	-0.053271
12	o	-0.450728	2.481672	0.030281
13	h	4.139082	-0.013513	-0.017972
14	h	-3.201331	-1.437889	0.398256
15	h	-2.184832	-2.768346	0.115293
16	h	2.676068	-2.130984	-0.021663
17	h	-3.268316	0.528983	-0.892372
18	h	-3.248372	0.779369	0.884254
19	h	-2.567914	2.016845	-0.189123

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.387578	-1.270734	0.005872
2	c	1.080825	-0.873998	0.002960
3	c	1.039735	0.579639	-0.002965
4	n	2.274193	1.060492	-0.003526
5	c	3.034682	-0.109020	0.002176
6	n	0.005839	-1.659760	0.000875
7	c	-1.167595	-1.019261	-0.002935
8	n	-1.344851	0.343767	-0.000073
9	c	-0.230661	1.273175	-0.005363
10	o	-0.440119	2.474199	-0.009200
11	n	-2.267822	-1.809618	0.012539
12	c	-2.692374	0.921042	0.017755
13	h	4.117205	-0.050744	0.003545
14	h	-3.204660	-1.465165	-0.123715
15	h	-2.101618	-2.805203	-0.052180
16	h	-3.241737	0.660601	-0.894483
17	h	-3.244091	0.585081	0.902247
18	h	-2.576389	2.003342	0.058603

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.364451	-1.154273	0.000145
2	c	-1.025399	-0.836576	-0.000089
3	c	-1.004287	0.596420	-0.000005
4	n	-2.243585	1.104493	-0.000023
5	c	-3.045540	0.032267	-0.000205
6	n	0.003338	-1.647104	0.000122
7	c	1.215186	-1.015855	0.000151
8	n	1.393386	0.335325	0.000158
9	c	0.286045	1.275618	0.000155
10	o	0.479604	2.468338	0.000005
11	n	2.269946	-1.832333	-0.000122

12	c	2.754279	0.908955	-0.000123
13	h	-4.127413	0.078483	-0.000222
14	h	3.229495	-1.513860	0.000023
15	h	2.093733	-2.831268	-0.000387
16	h	-2.761576	-2.088523	-0.000079
17	h	3.292865	0.604899	0.902653
18	h	3.293252	0.603043	-0.902028
19	h	2.650664	1.992788	-0.001266

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.341172	-1.312549	-0.015903
2	c	1.063415	-0.873801	-0.008524
3	c	1.046988	0.545889	0.005070
4	n	2.346175	1.005169	0.006712
5	c	3.039982	-0.139916	-0.008070
6	n	-0.065074	-1.665761	0.010583
7	c	-1.188035	-1.013825	0.005793
8	n	-1.322177	0.363615	-0.004727
9	c	-0.178432	1.266710	0.017518
10	o	-0.393048	2.488411	0.036410
11	n	-2.393135	-1.755060	-0.059338
12	c	-2.643950	0.974224	-0.063374
13	h	4.127492	-0.141743	-0.013397
14	h	-3.096397	-1.464453	0.615426
15	h	-2.158736	-2.734066	0.079473
16	h	-3.235591	0.532441	-0.871880
17	h	-3.191024	0.856980	0.884962
18	h	-2.489900	2.039974	-0.237636

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	n	-2.307655	-1.159596	0.017501
2	c	-1.002105	-0.807241	0.006317
3	c	-0.991636	0.559781	-0.007157
4	n	-2.285939	1.051946	-0.005549
5	c	-3.028121	0.002667	0.009555
6	n	0.059206	-1.631198	-0.005989
7	c	1.205250	-1.009843	-0.010114
8	n	1.352066	0.352629	0.001999
9	c	0.257568	1.240079	-0.019272
10	o	0.435168	2.439704	-0.038490
11	n	2.327606	-1.759870	0.028505
12	c	2.699118	0.932797	0.062143
13	h	-4.100946	-0.006557	0.016425
14	h	3.188496	-1.413420	-0.346817
15	h	2.176009	-2.740151	-0.129281
16	h	-2.680173	-2.095031	0.027913
17	h	3.244318	0.508820	0.894871
18	h	3.234255	0.748463	-0.862544
19	h	2.599262	1.993420	0.203254

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.249081	1.241713	-0.000431
2	c	1.035960	0.556085	-0.000470
3	c	1.079274	-0.890503	0.000842
4	n	-0.004839	-1.647861	0.001354
5	c	-1.165678	-1.008974	0.000283
6	n	-1.329616	0.357683	0.002942
7	n	2.265414	1.034837	-0.000642
8	c	3.009713	-0.083725	0.000521
9	n	2.350580	-1.261129	0.000835
10	n	-2.250254	-1.761007	-0.005605
11	c	-2.683901	0.929443	0.003026
12	o	-0.389525	2.431856	-0.003361
13	h	4.082700	-0.039053	0.000275
14	h	-3.189791	-1.417956	0.004295
15	h	-2.121708	-2.758024	-0.002378
16	h	-3.216503	0.623927	-0.889072

17	h	-3.220466	0.613560	0.889135
18	h	-2.594757	2.000798	0.009831

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.309355	1.248190	-0.000179
2	c	-0.987821	0.587250	0.000060
3	c	-1.028915	-0.846128	0.000692
4	n	-0.007358	-1.630313	0.000043
5	c	1.200108	-1.006938	-0.000250
6	n	1.380505	0.341622	0.001279
7	n	-2.222469	1.100480	-0.000480
8	c	-3.015711	0.055960	0.000122
9	n	-2.340837	-1.135185	0.000781
10	n	2.231748	-1.800753	-0.002079
11	c	2.748212	0.891291	0.002520
12	o	0.466438	2.431103	-0.002410
13	h	-4.088306	0.096174	0.000129
14	h	3.190449	-1.501327	-0.003218
15	h	2.060689	-2.795192	-0.003225
16	h	-2.757182	-2.057008	0.002223
17	h	3.272177	0.565198	0.892267
18	h	3.271951	0.570608	-0.889340
19	h	2.676231	1.964017	0.005845

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.194524	1.226911	0.020928
2	c	1.033707	0.526726	0.006337
3	c	1.051155	-0.855469	-0.007411
4	n	-0.064775	-1.642832	0.008034
5	c	-1.185945	-1.001470	0.009556
6	n	-1.309879	0.366435	-0.003203
7	n	2.334889	0.984869	0.004475

8	c	3.021648	-0.129871	-0.011792
9	n	2.320004	-1.285118	-0.019026
10	n	-2.347756	-1.723834	-0.041979
11	c	-2.643229	0.971004	-0.068578
12	o	-0.359061	2.438328	0.044215
13	h	4.097484	-0.136379	-0.019615
14	h	-3.145312	-1.376280	0.459556
15	h	-2.194368	-2.702839	0.132861
16	h	-3.204667	0.538877	-0.886017
17	h	-3.180719	0.820136	0.861625
18	h	-2.524183	2.026231	-0.234473

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.308553	-1.158907	0.017007
2	c	-1.003428	-0.807510	0.006479
3	c	-0.990576	0.559798	-0.006598
4	n	-2.284662	1.053262	-0.005641
5	c	-3.027010	0.003037	0.009302
6	n	0.058555	-1.631077	-0.005688
7	c	1.205380	-1.009694	-0.010045
8	n	1.352149	0.352752	0.001640
9	c	0.258084	1.238330	-0.018660
10	o	0.434357	2.439837	-0.037641
11	n	2.326781	-1.759648	0.028463
12	c	2.699823	0.932231	0.060728
13	h	-4.099862	-0.004812	0.015707
14	h	3.189863	-1.413402	-0.341924
15	h	2.176053	-2.740442	-0.127401
16	h	-2.684396	-2.099833	0.026385
17	h	3.243014	0.512102	0.896712
18	h	3.235769	0.742159	-0.862238
19	h	2.601174	1.993714	0.196179

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.249821	1.240308	0.002222
2	c	-1.034938	0.554906	0.000569
3	c	-1.079030	-0.891071	-0.001247
4	n	0.004103	-1.648889	-0.000289
5	c	1.166197	-1.009090	0.000741
6	n	1.329691	0.357759	-0.002782
7	n	-2.264575	1.034732	0.000521
8	c	-3.009962	-0.082563	-0.001322
9	n	-2.351225	-1.259960	-0.002419
10	n	2.250129	-1.760220	0.004358
11	c	2.684152	0.930261	-0.007792
12	o	0.388210	2.431334	0.006585
13	h	-4.082930	-0.037637	-0.002090
14	h	3.189791	-1.416892	0.014664
15	h	2.122380	-2.757576	0.009015
16	h	3.214764	0.637886	0.889936
17	h	3.221898	0.601702	-0.888343
18	h	2.594117	2.001380	-0.030605

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.310899	1.247669	-0.000431
2	c	-0.986855	0.587646	-0.000039
3	c	-1.030649	-0.846045	0.000288
4	n	-0.008286	-1.630607	0.000178
5	c	1.198417	-1.007611	-0.000378
6	n	1.380199	0.341368	0.000692
7	n	-2.220514	1.102272	-0.000377
8	c	-3.014140	0.057036	0.000170
9	n	-2.341855	-1.133871	0.000794
10	n	2.230579	-1.801039	-0.001579
11	c	2.748322	0.889695	0.002110

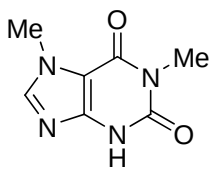
12	o	0.467741	2.431076	-0.001651
13	h	-4.086633	0.099149	0.000241
14	h	3.189119	-1.501471	-0.002515
15	h	2.059298	-2.795375	-0.001887
16	h	-2.761947	-2.062362	0.001495
17	h	3.271937	0.563197	0.891906
18	h	3.271939	0.568481	-0.889624
19	h	2.677525	1.962566	0.005313

3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.194772	1.224492	0.020384
2	c	1.032811	0.525759	0.007440
3	c	1.050530	-0.855366	-0.010975
4	n	-0.064598	-1.642502	0.004097
5	c	-1.187247	-1.000986	0.009543
6	n	-1.310020	0.366802	-0.003718
7	n	2.334494	0.984421	0.009639
8	c	3.021981	-0.129749	-0.009712
9	n	2.320127	-1.284856	-0.022566
10	n	-2.347290	-1.723167	-0.036307
11	c	-2.643808	0.971880	-0.069591
12	o	-0.356314	2.437980	0.042511
13	h	4.097664	-0.136110	-0.015569
14	h	-3.147441	-1.373200	0.459296
15	h	-2.195503	-2.702640	0.138606
16	h	-3.206242	0.534811	-0.883577
17	h	-3.178528	0.826123	0.862896
18	h	-2.525403	2.026117	-0.242293

No.12



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-1.627393	-1.995928	-0.000022
2	c	-0.495892	-1.248067	-0.000115
3	c	-0.764904	0.106753	-0.000240
4	n	-2.151326	0.195838	0.000082
5	c	-2.600127	-1.084985	0.000119
6	n	0.800577	-1.698594	-0.000136
7	c	1.877058	-0.823589	-0.000057
8	n	1.560609	0.546831	-0.000195
9	c	0.256977	1.115357	-0.000566
10	o	0.073658	2.331464	0.000039
11	o	3.033589	-1.223249	0.000323
12	c	2.714098	1.456348	0.000167
13	c	-2.954376	1.414583	0.000212
14	h	-3.657006	-1.317654	0.000268
15	h	1.016745	-2.687750	0.000135
16	h	3.326656	1.278998	0.887581
17	h	3.327383	1.278721	-0.886685
18	h	2.328392	2.474158	-0.000140
19	h	-4.008624	1.128989	0.000419
20	h	-2.732723	2.011724	0.887614
21	h	-2.733063	2.011668	-0.887312

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-1.658956	-2.003406	0.000062
2	c	-0.461551	-1.291005	-0.000120
3	c	-0.741912	0.100972	-0.000257
4	n	-2.092980	0.224055	0.000068
5	c	-2.581291	-1.082388	0.000153
6	n	0.750559	-1.809522	-0.000142

7	c	1.810719	-0.900319	-0.000314
8	n	1.567751	0.509582	-0.000263
9	c	0.305437	1.102137	-0.000605
10	o	0.107446	2.317924	0.000063
11	o	2.971380	-1.288136	0.000441
12	c	2.752934	1.377631	0.000243
13	c	-2.886491	1.451729	0.000198
14	h	-3.649305	-1.264692	0.000338
15	h	3.358014	1.176297	0.887303
16	h	3.358719	1.176276	-0.886326
17	h	2.409233	2.410792	0.000101
18	h	-3.942524	1.173901	0.000418
19	h	-2.658032	2.045831	0.887724
20	h	-2.658403	2.045780	-0.887457

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.667026	-2.002672	0.000012
2	c	0.514992	-1.284804	-0.000009
3	c	0.770457	0.119913	-0.000036
4	n	2.109476	0.235148	0.000014
5	c	2.601824	-1.078851	0.000021
6	n	-0.744553	-1.715667	-0.000007
7	c	-1.863134	-0.817933	-0.000011
8	n	-1.576215	0.548643	-0.000016
9	c	-0.293216	1.126395	-0.000117
10	o	-0.079426	2.324726	0.000002
11	o	-2.979369	-1.277823	0.000010
12	c	-2.757484	1.447235	0.000055
13	c	2.918281	1.467829	0.000021
14	h	3.668053	-1.272201	0.000043
15	h	-0.976100	-2.709951	0.000011
16	h	-3.356923	1.255036	-0.891422
17	h	-3.357000	1.254792	0.891426
18	h	-2.390568	2.471301	0.000212
19	h	3.969907	1.180289	0.000050
20	h	2.686287	2.054310	-0.890960
21	h	2.686243	2.054328	0.890978

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.617555	-2.008415	0.000063
2	c	0.429981	-1.275130	-0.000057
3	c	0.736119	0.094021	-0.000138
4	n	2.127633	0.191401	0.000027
5	c	2.572510	-1.097901	0.000102
6	n	-0.804614	-1.799264	-0.000089
7	c	-1.829681	-0.915796	-0.000253
8	n	-1.546474	0.514386	-0.000138
9	c	-0.270996	1.095955	-0.000262
10	o	-0.086456	2.336328	0.000029
11	o	-3.035061	-1.226387	0.000248
12	c	-2.705473	1.397302	0.000141
13	c	2.927584	1.398628	0.000076
14	h	3.635708	-1.315812	0.000201
15	h	-3.325695	1.207506	-0.882530
16	h	-3.325567	1.207114	0.882816
17	h	-2.342736	2.425923	0.000335
18	h	3.985116	1.112593	0.000197
19	h	2.713270	2.006933	-0.884544
20	h	2.713069	2.006993	0.884605

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.273973	1.097713	-0.000167
2	c	-0.759811	0.109414	0.000007
3	c	-0.491784	-1.221955	0.000117
4	n	0.792691	-1.680336	0.000107
5	c	1.843809	-0.817754	-0.000014
6	n	1.555160	0.535654	0.000004
7	n	-2.143674	0.196299	-0.000038

8	c	-2.576552	-1.055574	0.000046
9	n	-1.614048	-1.958969	0.000185
10	c	-2.964149	1.400406	-0.000114
11	o	2.985574	-1.214947	-0.000293
12	c	2.718981	1.429894	0.000263
13	o	0.107187	2.294849	-0.000032
14	h	-3.623895	-1.293014	0.000036
15	h	0.998823	-2.666651	-0.000642
16	h	3.318166	1.251159	0.882252
17	h	3.318787	1.250835	-0.881237
18	h	2.362300	2.444472	-0.000070
19	h	-4.002638	1.098217	-0.000007
20	h	-2.755571	1.987260	0.883634
21	h	-2.755761	1.987102	-0.884002

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.326071	1.087889	-0.000561
2	c	-0.740934	0.106565	-0.000142
3	c	-0.470575	-1.271757	0.000052
4	n	0.728756	-1.785253	-0.000007
5	c	1.794058	-0.879516	-0.000175
6	n	1.574709	0.495812	0.000019
7	n	-2.090634	0.227600	0.000137
8	c	-2.566054	-1.047477	0.000111
9	n	-1.659158	-1.965915	0.000173
10	c	-2.894535	1.446977	0.000131
11	o	2.917708	-1.301427	-0.000346
12	c	2.770355	1.347327	0.000777
13	o	0.152053	2.277291	-0.000516
14	h	-3.624820	-1.233246	0.000250
15	h	3.360763	1.145501	0.883578
16	h	3.361602	1.145923	-0.881552
17	h	2.452475	2.375393	0.000848
18	h	-3.935898	1.155896	0.000313
19	h	-2.678985	2.029044	0.885119
20	h	-2.679246	2.028821	-0.885068

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.305428	1.117944	-0.000456
2	c	-0.769541	0.120708	-0.000692
3	c	-0.501846	-1.284634	-0.000760
4	n	0.749049	-1.697221	-0.000404
5	c	1.830541	-0.813016	-0.000290
6	n	1.561961	0.544817	-0.000479
7	n	-2.108507	0.222473	0.000202
8	c	-2.568535	-1.045554	0.000500
9	n	-1.628228	-1.976140	-0.000343
10	c	-2.929711	1.445581	0.000475
11	o	2.940041	-1.242299	0.001552
12	c	2.745600	1.425748	-0.000252
13	o	0.093629	2.292521	0.000234
14	h	-3.623926	-1.255728	0.001050
15	h	0.974523	-2.688392	-0.000236
16	h	3.333353	1.233914	0.885607
17	h	3.335087	1.231681	-0.884468
18	h	2.402296	2.445463	-0.001931
19	h	-3.965448	1.137864	0.001583
20	h	-2.707548	2.017930	0.888924
21	h	-2.709237	2.017330	-0.888803

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.289743	1.074863	-0.000355
2	c	0.736379	0.098996	-0.000177
3	c	0.441498	-1.242198	-0.000073
4	n	-0.795277	-1.767024	-0.000105
5	c	-1.800208	-0.891385	-0.000126
6	n	-1.550467	0.497030	-0.000050
7	n	2.126293	0.189657	0.000092
8	c	2.554295	-1.064937	0.000242

9	n	1.599390	-1.966871	0.000143
10	c	2.948932	1.386647	-0.000048
11	o	-2.984613	-1.236203	-0.000101
12	c	-2.721427	1.371333	0.000421
13	o	-0.131386	2.288827	-0.000113
14	h	3.603559	-1.297823	0.000416
15	h	-3.324663	1.186904	-0.878409
16	h	-3.324431	1.186176	0.879255
17	h	-2.384496	2.393165	0.000802
18	h	3.987796	1.083294	0.000089
19	h	2.746212	1.978783	-0.882563
20	h	2.746081	1.979057	0.882253

---

3. Aqueous solution(UAKS)

3.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.273653	1.097040	-0.000726
2	c	-0.759412	0.109610	-0.000354
3	c	-0.490026	-1.221699	-0.000180
4	n	0.793362	-1.680078	-0.000232
5	c	1.841867	-0.817442	-0.000114
6	n	1.554404	0.536108	-0.000112
7	n	-2.143432	0.195833	0.000044
8	c	-2.575475	-1.055584	0.000324
9	n	-1.612510	-1.958978	0.000023
10	c	-2.965051	1.399281	0.000260
11	o	2.985618	-1.213186	0.000291
12	c	2.718864	1.429925	0.000433
13	o	0.105855	2.295211	-0.000178
14	h	-3.622584	-1.293791	0.000612
15	h	0.999876	-2.673006	-0.000113
16	h	3.317593	1.250251	0.882422
17	h	3.318141	1.250728	-0.881273
18	h	2.363410	2.444763	0.000575
19	h	-4.003066	1.095840	0.000637
20	h	-2.756911	1.986061	0.884089
21	h	-2.757535	1.985976	-0.883777

3.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.326289	1.087508	0.000197
2	c	-0.740963	0.106743	0.000067
3	c	-0.470083	-1.272047	0.000155
4	n	0.728584	-1.784562	0.000055
5	c	1.793317	-0.878694	-0.000371
6	n	1.574783	0.495819	0.000490
7	n	-2.090569	0.227480	-0.000121
8	c	-2.565861	-1.046993	0.000137
9	n	-1.658830	-1.965850	0.000367
10	c	-2.895187	1.446826	-0.000036
11	o	2.917152	-1.301880	-0.000956
12	c	2.771151	1.347130	0.001007
13	o	0.152158	2.277228	-0.001067
14	h	-3.624605	-1.233123	0.000193
15	h	3.361630	1.143878	0.883361
16	h	3.361126	1.146027	-0.882178
17	h	2.453668	2.375302	0.002331
18	h	-3.936311	1.155084	-0.000373
19	h	-2.680101	2.028256	0.885458
20	h	-2.679633	2.028749	-0.885088

3.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.305975	1.117653	0.000021
2	c	-0.769110	0.121171	-0.000297
3	c	-0.500194	-1.283605	-0.000866
4	n	0.748492	-1.697463	-0.000392
5	c	1.828597	-0.813345	0.000714
6	n	1.561943	0.544933	-0.000252
7	n	-2.108606	0.222851	0.000129
8	c	-2.568250	-1.045450	-0.000453
9	n	-1.628828	-1.975475	-0.001001

10	c	-2.930582	1.445250	0.001220
11	o	2.939493	-1.241870	0.002330
12	c	2.746166	1.425054	-0.001673
13	o	0.094857	2.292881	0.000269
14	h	-3.623681	-1.255504	-0.000294
15	h	0.975573	-2.697367	-0.000112
16	h	3.334185	1.233858	0.884149
17	h	3.334959	1.229563	-0.886025
18	h	2.403679	2.445086	-0.004314
19	h	-3.966124	1.136836	0.001110
20	h	-2.709877	2.016848	0.890552
21	h	-2.710137	2.018304	-0.887245

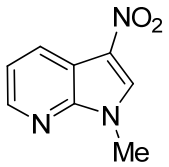
3.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.290011	1.073622	-0.000826
2	c	0.736505	0.098901	-0.000282
3	c	0.442233	-1.241930	-0.000775
4	n	-0.795609	-1.765976	-0.000597
5	c	-1.799302	-0.889399	0.000287
6	n	-1.551058	0.496898	-0.000496
7	n	2.126227	0.189516	0.000094
8	c	2.554794	-1.063966	-0.000146
9	n	1.599193	-1.966578	-0.001056
10	c	2.949329	1.386714	0.002048
11	o	-2.984003	-1.238201	0.002035
12	c	-2.722588	1.371606	0.000108
13	o	-0.131736	2.288219	-0.001616
14	h	3.603928	-1.297254	0.000154
15	h	-3.325906	1.186163	-0.878342
16	h	-3.324037	1.187432	0.880130
17	h	-2.385970	2.393493	-0.000970
18	h	3.987971	1.082810	0.001245
19	h	2.746250	1.980035	-0.879509
20	h	2.746653	1.976865	0.885851

The Cartesian Coordinates of the 70 test set compounds.

No.1



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.452433	0.138986	-0.000196
2	c	1.143241	0.368280	-0.000186
3	c	0.104522	-0.600370	0.000016
4	c	0.489708	-1.946789	0.000118
5	c	1.857797	-2.212573	0.000078
6	c	2.789772	-1.156760	-0.000081
7	c	-1.113503	0.157610	0.000007
8	c	-0.785057	1.502794	-0.000214
9	n	0.569435	1.637414	-0.000457
10	c	1.323413	2.884486	0.000518
11	n	-2.446469	-0.336445	0.000031
12	o	-2.598529	-1.566687	0.000237
13	o	-3.376516	0.483159	-0.000134
14	h	-0.251145	-2.738424	0.000240
15	h	2.217994	-3.236953	0.000169
16	h	3.856296	-1.369527	-0.000112
17	h	-1.446155	2.357296	-0.000307
18	h	0.619512	3.718736	-0.006917
19	h	1.952638	2.941807	0.893010
20	h	1.964065	2.935542	-0.884090

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.469184	0.095204	-0.000025
2	c	1.160089	0.375696	-0.000030
3	c	0.088285	-0.575710	-0.000006
4	c	0.435313	-1.925787	0.000003
5	c	1.806171	-2.242743	0.000010
6	c	2.761837	-1.219263	0.000008
7	c	-1.135165	0.187824	0.000002
8	c	-0.779388	1.543909	-0.000017
9	n	0.620770	1.638955	-0.000036
10	c	1.373642	2.867768	0.000044
11	n	-2.418703	-0.313237	0.000005
12	o	-2.588042	-1.593346	0.000020
13	o	-3.398792	0.522407	-0.000007
14	h	-0.343570	-2.680405	0.000005
15	h	2.134177	-3.279861	0.000018
16	h	3.824470	-1.463568	0.000013
17	h	-1.410399	2.417850	-0.000033
18	h	1.144750	3.469667	-0.891604
19	h	1.144867	3.469502	0.891838
20	h	2.436916	2.617712	-0.000035

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.534521	1.623607	-0.000415
2	c	1.122469	0.373867	-0.000222
3	c	0.119164	-0.602926	0.000031
4	c	-1.110345	0.143219	0.000075
5	c	-0.795418	1.476069	-0.000304
6	c	0.523254	-1.934035	0.000295
7	c	1.884408	-2.178947	0.000198

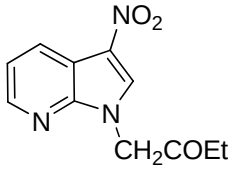
8	c	2.785203	-1.110017	-0.000152
9	n	2.421431	0.160286	-0.000310
10	n	-2.419000	-0.355826	-0.000048
11	o	-3.340386	0.423139	0.000143
12	c	1.259035	2.887551	0.000549
13	o	-2.565548	-1.550898	-0.000100
14	h	-0.187636	-2.738934	0.000594
15	h	2.261443	-3.186841	0.000422
16	h	3.844891	-1.302654	-0.000238
17	h	-1.453724	2.322768	-0.000593
18	h	0.538381	3.693542	-0.004424
19	h	1.875428	2.956323	0.887173
20	h	1.883404	2.952713	-0.880695

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.438786	0.112062	-0.001438
2	c	-1.147582	0.378401	-0.000987
3	c	-0.100658	-0.583249	0.000541
4	c	-0.462799	-1.931393	0.000849
5	c	-1.827834	-2.225827	-0.000502
6	c	-2.763999	-1.188372	-0.001297
7	c	1.123954	0.171610	-0.000421
8	c	0.774509	1.515655	-0.000433
9	n	-0.603220	1.628490	0.000494
10	c	-1.349305	2.868618	0.002340
11	n	2.402059	-0.316272	-0.000582
12	o	2.599953	-1.586343	0.004368
13	o	3.388227	0.512363	-0.003978
14	h	0.280385	-2.704809	0.001209
15	h	-2.170654	-3.246502	-0.000894
16	h	-3.817800	-1.411058	-0.001949
17	h	1.403530	2.380126	-0.000283
18	h	-0.647056	3.691684	0.006670
19	h	-1.973955	2.942699	-0.880909
20	h	-1.977966	2.937078	0.883181

No.2



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.380807	-0.073513	0.741606
2	c	0.416622	1.001544	0.345361
3	c	1.690034	0.503490	-0.033267
4	c	1.604353	-0.918348	0.144621
5	c	0.335958	-1.224498	0.601206
6	c	2.640531	1.442244	-0.452225
7	c	2.247796	2.779876	-0.462062
8	c	0.948947	3.144174	-0.061158
9	n	0.020231	2.268871	0.346460
10	n	2.621610	-1.884486	-0.090731
11	o	2.365891	-3.074989	0.137205
12	c	-1.774248	0.041514	1.111784
13	c	-2.742640	-0.345066	-0.023658
14	c	-4.187832	0.068483	0.189845
15	c	-5.164143	-0.539630	-0.817172
16	o	3.711917	-1.470785	-0.511392
17	o	-2.353109	-0.948777	-1.001704
18	h	3.633882	1.131412	-0.755716
19	h	2.940780	3.553183	-0.779539
20	h	0.646230	4.188601	-0.069440
21	h	-0.083409	-2.194055	0.825014
22	h	-1.981503	-0.602058	1.976783
23	h	-1.951800	1.075742	1.421056
24	h	-4.212573	1.168602	0.143459
25	h	-4.471544	-0.180373	1.223701
26	h	-6.181718	-0.186190	-0.619814
27	h	-4.893453	-0.264238	-1.840658

28	h	-5.161971	-1.633024	-0.758709

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.411021	-0.091043	-0.486472
2	c	-0.429385	0.970138	-0.234508
3	c	-1.739738	0.459914	0.023958
4	c	-1.651684	-0.974446	-0.102078
5	c	-0.327531	-1.288009	-0.437420
6	c	-2.739040	1.391683	0.302292
7	c	-2.376765	2.751222	0.294171
8	c	-1.060038	3.125639	0.003681
9	n	-0.066451	2.255517	-0.266289
10	n	-2.678697	-1.876960	0.070485
11	o	-2.423167	-3.127268	-0.086776
12	c	1.759964	0.042640	-0.940234
13	c	2.852554	-0.267951	0.089963
14	c	4.273967	-0.273467	-0.475693
15	c	5.361463	-0.413981	0.589032
16	o	-3.851711	-1.433444	0.371642
17	o	2.625773	-0.482189	1.263967
18	h	-3.748401	1.052874	0.507639
19	h	-3.115620	3.520752	0.506234
20	h	-0.780602	4.179013	-0.014250
21	h	0.144326	-2.252956	-0.525535
22	h	1.926865	-0.592561	-1.827123
23	h	1.905214	1.083758	-1.260270
24	h	4.414287	0.644557	-1.065514
25	h	4.334314	-1.096915	-1.204365
26	h	6.355952	-0.426717	0.126635
27	h	5.321546	0.416613	1.301861
28	h	5.231236	-1.338101	1.160965

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.191558	2.101000	0.428281
2	c	0.327263	0.892691	0.382520
3	c	1.629162	0.563308	-0.013022
4	c	2.466025	1.607301	-0.392846
5	c	1.938874	2.885224	-0.349569
6	c	0.618051	3.079504	0.063532
7	c	1.693184	-0.868847	0.109580
8	c	0.478620	-1.310093	0.555579
9	n	-0.342738	-0.265293	0.730855
10	c	-1.730368	-0.345329	1.133922
11	c	-2.685226	-0.383673	-0.049162
12	o	-2.285846	-0.471735	-1.174574
13	n	2.784498	-1.706936	-0.159430
14	o	3.803158	-1.196071	-0.546534
15	o	2.661281	-2.895389	0.004933
16	c	-4.150985	-0.316293	0.311554
17	c	-5.093383	-0.538172	-0.865320
18	h	3.477761	1.432169	-0.707184
19	h	2.534495	3.735860	-0.631597
20	h	0.208009	4.074888	0.096539
21	h	0.159434	-2.312815	0.762089
22	h	-1.873446	-1.259295	1.723902
23	h	-1.969549	0.504652	1.779558
24	h	-4.320700	0.660342	0.763702
25	h	-4.334483	-1.043205	1.100623
26	h	-6.123314	-0.473959	-0.529384
27	h	-4.942011	0.207959	-1.637152
28	h	-4.943648	-1.516162	-1.310244

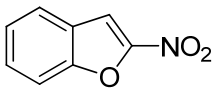
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.115836	2.156606	-0.430964
2	c	-0.335627	0.919518	-0.395768
3	c	-1.641268	0.524970	0.002629
4	c	-2.531218	1.529348	0.387327

5	c	-2.064216	2.844765	0.351257
6	c	-0.754327	3.105932	-0.058188
7	c	-1.672755	-0.908895	-0.114275
8	c	-0.423813	-1.309994	-0.567065
9	n	0.374387	-0.193844	-0.751229
10	c	1.762267	-0.228723	-1.119691
11	c	2.716041	-0.355026	0.057624
12	o	2.330809	-0.370174	1.192908
13	n	-2.724338	-1.740897	0.155470
14	o	-3.838118	-1.247764	0.564663
15	o	-2.576120	-3.009977	-0.007248
16	c	4.177753	-0.470848	-0.316051
17	c	5.133879	-0.419817	0.869668
18	h	-3.530599	1.293866	0.697438
19	h	-2.702062	3.663649	0.637169
20	h	-0.388370	4.118483	-0.086977
21	h	-0.063215	-2.292789	-0.784175
22	h	1.933379	-1.072907	-1.800109
23	h	2.020242	0.684322	-1.669391
24	h	4.404839	0.316520	-1.032364
25	h	4.290894	-1.407693	-0.860992
26	h	6.158380	-0.511827	0.522953
27	h	5.042967	0.517691	1.408391
28	h	4.939489	-1.226427	1.567730

No.3



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.922651	-1.443919	0.000033
2	c	-0.806439	-0.614708	-0.000204
3	c	-0.875533	0.795549	-0.000165
4	c	-2.138788	1.416959	0.000128

5	c	-3.267157	0.605788	0.000368
6	c	-3.160585	-0.803371	0.000321
7	c	0.486099	1.249716	-0.000487
8	c	1.237125	0.112882	-0.000663
9	o	0.499030	-1.030965	-0.000488
10	n	2.662530	-0.036006	-0.000980
11	o	3.126867	-1.175823	0.000802
12	o	3.318686	1.012631	0.000958
13	h	-2.227124	2.499533	0.000165
14	h	-4.253909	1.059959	0.000596
15	h	-4.066459	-1.402976	0.000514
16	h	-1.827287	-2.524618	-0.000006
17	h	0.867985	2.260021	-0.000564

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.807661	-0.613137	0.000023
2	c	0.867470	0.807781	-0.000025
3	c	2.144293	1.411852	-0.000045
4	c	3.281924	0.597091	-0.000012
5	c	3.184097	-0.804799	0.000040
6	c	-1.273433	0.110107	-0.000090
7	c	-0.483899	1.256371	0.000031
8	h	2.242142	2.495531	-0.000051
9	h	4.267321	1.060779	-0.000013
10	h	4.086191	-1.412403	0.000064
11	n	-2.633192	-0.037526	-0.000146
12	o	-0.493624	-1.038088	-0.000037
13	c	1.922317	-1.432700	0.000060
14	h	1.818943	-2.514510	0.000082
15	o	-3.333288	1.047139	0.000146
16	o	-3.150209	-1.212395	0.000013
17	h	-0.867863	2.264644	0.000073

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	-0.496401	-1.012602	-0.000011
2	c	0.793220	-0.607446	-0.000005
3	c	0.868002	0.779630	0.000118
4	c	-0.498864	1.240642	0.000264
5	c	-1.222723	0.117219	0.000057
6	c	2.119708	1.406300	0.000145
7	c	3.239829	0.605582	0.000025
8	c	3.130652	-0.798234	-0.000182
9	c	1.905935	-1.434693	-0.000193
10	n	-2.635580	-0.035467	-0.000058
11	o	-3.290394	0.969669	-0.000649
12	o	-3.083296	-1.143209	0.000527
13	h	2.200731	2.479350	0.000335
14	h	4.217935	1.053724	0.000123
15	h	4.028936	-1.391016	-0.000373
16	h	1.814631	-2.507204	-0.000381
17	h	-0.867005	2.248546	0.000400

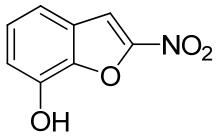
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	0.497890	-1.025000	-0.000167
2	c	-0.800762	-0.615889	-0.000027
3	c	-0.868283	0.789235	-0.000933
4	c	0.482462	1.248992	-0.001232
5	c	1.261552	0.103979	-0.000728
6	c	-2.131246	1.414469	-0.000968
7	c	-3.267734	0.603516	0.000120
8	c	-3.164095	-0.800676	0.001122
9	c	-1.912376	-1.439060	0.001000
10	n	2.603757	-0.033702	0.000215

11	o	3.322661	1.035864	0.003407
12	o	3.138729	-1.196316	-0.002263
13	h	-2.216902	2.487466	-0.001698
14	h	-4.243716	1.057833	0.000215
15	h	-4.059767	-1.397364	0.002019
16	h	-1.823268	-2.512425	0.001804
17	h	0.846004	2.256624	-0.001794

No.4



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.887350	0.993153	-0.000012
2	c	-0.689298	0.278027	-0.000053
3	c	-0.613249	-1.127200	-0.000041
4	c	-1.801936	-1.881731	0.000037
5	c	-3.003394	-1.180745	0.000098
6	c	-3.053246	0.229356	0.000085
7	c	0.793456	-1.423364	-0.000119
8	c	1.420244	-0.213249	-0.000146
9	o	0.560101	0.845318	-0.000094
10	n	2.818306	0.095664	-0.000182
11	o	3.148313	1.282474	0.000215
12	o	-1.950535	2.353299	-0.000024
13	o	3.589944	-0.870164	0.000159
14	h	-1.780994	-2.966724	0.000048
15	h	-3.941219	-1.728848	0.000159
16	h	-4.007689	0.746956	0.000134
17	h	-1.055429	2.732230	-0.000080
18	h	1.283236	-2.386158	-0.000136

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.880724	0.983248	0.000059
2	c	-0.693765	0.270399	-0.000016
3	c	-0.611709	-1.140152	-0.000055
4	c	-1.824360	-1.867903	-0.000036
5	c	-3.028156	-1.157435	0.000020
6	c	-3.076265	0.249538	0.000079
7	c	0.784594	-1.437981	-0.000011
8	c	1.451164	-0.215083	-0.000205
9	o	0.551355	0.846485	-0.000144
10	n	2.783941	0.085939	-0.000290
11	o	3.159937	1.315329	0.000070
12	o	-1.901758	2.361477	0.000074
13	o	3.603968	-0.910946	0.000347
14	h	-1.822684	-2.955152	-0.000032
15	h	-3.967626	-1.707678	0.000052
16	h	-4.023449	0.781392	0.000138
17	h	-0.980357	2.672805	0.000040
18	h	1.273840	-2.399494	0.000052

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	-0.560134	0.833120	-0.000241
2	c	0.675950	0.281587	-0.000161
3	c	0.604408	-1.103347	-0.000039
4	c	-0.808724	-1.405416	-0.000265
5	c	-1.403861	-0.209711	-0.000129
6	c	1.773440	-1.870501	0.000143
7	c	2.969435	-1.187269	0.000192
8	c	3.022296	0.216749	0.000066
9	c	1.875318	0.983602	-0.000093

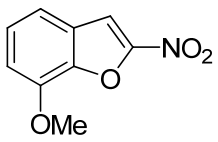
10	o	1.962268	2.325403	-0.000093
11	n	-2.793261	0.098951	-0.000052
12	o	-3.553661	-0.827826	0.000125
13	o	-3.114059	1.249172	0.000291
14	h	1.737202	-2.945257	0.000240
15	h	3.896530	-1.733416	0.000281
16	h	3.975306	0.718787	0.000140
17	h	1.105106	2.760467	0.001026
18	h	-1.286198	-2.366350	-0.000258

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	0.560609	0.844415	-0.001957
2	c	-0.681700	0.288560	-0.001102
3	c	-0.601081	-1.113277	-0.001374
4	c	0.794501	-1.417552	-0.001873
5	c	1.443860	-0.194668	-0.001098
6	c	-1.784241	-1.877599	-0.000466
7	c	-2.997804	-1.189809	0.001518
8	c	-3.051767	0.216510	0.001693
9	c	-1.880342	0.983756	-0.000006
10	o	-1.975869	2.333315	0.000231
11	n	2.762263	0.092223	0.000399
12	o	3.596225	-0.889817	0.002160
13	o	3.161864	1.307577	0.001084
14	h	-1.752763	-2.953091	-0.000183
15	h	-3.922204	-1.741289	0.003076
16	h	-4.002050	0.724075	0.003207
17	h	-1.116547	2.764440	-0.003359
18	h	1.266528	-2.379146	-0.001431

No.5



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	0.675606	-0.755173	-0.000112
2	c	-0.421311	0.060716	-0.000191
3	c	-0.044534	1.416578	-0.000039
4	c	1.391301	1.408235	-0.000146
5	c	1.739684	0.090688	-0.000094
6	c	-1.037002	2.418757	0.000124
7	c	-2.359647	2.004695	0.000084
8	c	-2.722378	0.636641	-0.000154
9	c	-1.756399	-0.372149	-0.000279
10	o	-1.978180	-1.708613	-0.000486
11	c	-3.327585	-2.168326	0.000605
12	n	3.043063	-0.506236	0.000037
13	o	3.999469	0.278751	0.000523
14	o	3.120277	-1.734181	-0.000221
15	h	-0.773461	3.471618	0.000260
16	h	-3.154431	2.745401	0.000189
17	h	-3.775065	0.377004	-0.000240
18	h	2.074639	2.244540	-0.000203
19	h	-3.264524	-3.257087	0.001185
20	h	-3.858828	-1.829021	0.898659
21	h	-3.859925	-1.830070	-0.897203

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.749663	-0.362801	-0.000124
2	c	-0.421486	0.053726	-0.000057
3	c	-0.033688	1.416806	0.000025
4	c	-1.044515	2.407308	0.000039
5	c	-2.375506	1.997694	-0.000028
6	c	-2.742814	0.636592	-0.000109

7	c	1.390014	1.412826	0.000075
8	c	1.775561	0.075126	0.000045
9	o	0.673019	-0.766516	-0.000044
10	n	3.020133	-0.492718	0.000076
11	o	3.143100	-1.770514	-0.000092
12	o	-1.990506	-1.717056	-0.000226
13	c	-3.335129	-2.147935	0.000272
14	o	4.024733	0.320409	0.000038
15	h	-0.787259	3.463804	0.000101
16	h	-3.166246	2.746274	-0.000019
17	h	-3.793936	0.369312	-0.000176
18	h	2.071839	2.248792	0.000141
19	h	-3.298604	-3.240413	0.000387
20	h	-3.872764	-1.802566	0.895791
21	h	-3.873367	-1.802813	-0.894983

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.742458	-0.364575	-0.000269
2	c	-0.414707	0.069047	-0.000388
3	c	-0.047244	1.401857	-0.000179
4	c	-1.028629	2.404848	-0.000146
5	c	-2.337579	1.994342	-0.000220
6	c	-2.698247	0.629054	-0.000201
7	c	1.396452	1.395361	0.000156
8	c	1.719071	0.098534	-0.000093
9	o	0.670272	-0.735514	-0.000439
10	n	3.008947	-0.502693	0.000000
11	o	3.074657	-1.695108	-0.001426
12	o	-1.955017	-1.687657	-0.000179
13	c	-3.281310	-2.174513	0.001040
14	o	3.951584	0.238269	0.001748
15	h	-0.762961	3.446888	-0.000033
16	h	-3.127541	2.724928	-0.000247
17	h	-3.743281	0.378199	-0.000048
18	h	2.068992	2.231359	0.000418
19	h	-3.201049	-3.250687	0.001253

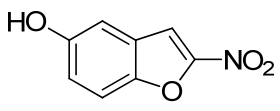
20	h	-3.809666	-1.847520	0.888951
21	h	-3.811189	-1.847965	-0.886124

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	-0.671770	-0.748027	-0.000850
2	c	0.421418	0.060372	-0.000764
3	c	0.042097	1.409084	-0.000084
4	c	-1.386459	1.409346	0.000217
5	c	-1.756307	0.076126	-0.000159
6	c	1.034081	2.410653	0.000367
7	c	2.362609	1.998984	0.000301
8	c	2.724052	0.634113	-0.000362
9	c	1.746189	-0.366907	-0.001048
10	o	1.973318	-1.697218	-0.002087
11	c	3.301821	-2.169973	0.002102
12	n	-2.984024	-0.485875	0.000160
13	o	-4.007732	0.296597	0.000616
14	o	-3.116591	-1.758376	0.000318
15	h	0.773141	3.454474	0.000908
16	h	3.148674	2.734300	0.000783
17	h	3.767866	0.378297	-0.000385
18	h	-2.052921	2.247821	0.000745
19	h	3.234448	-3.247667	0.001719
20	h	3.833949	-1.840273	-0.883042
21	h	3.828195	-1.840430	0.890757

No.6



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	-0.989225	1.064468	0.000124
2	c	0.346913	0.750446	0.000042
3	c	0.530398	-0.648880	-0.000038
4	c	-0.792017	-1.208367	0.000000
5	c	-1.630795	-0.133514	0.000096
6	c	1.830987	-1.179766	-0.000087
7	c	2.895843	-0.284432	-0.000054
8	c	2.683127	1.114779	0.000047
9	c	1.399683	1.656103	0.000097
10	o	4.159442	-0.816555	-0.000081
11	n	-3.064181	-0.099815	-0.000005
12	o	-3.633817	-1.197687	0.000218
13	o	-3.618852	0.998903	-0.000358
14	h	2.020167	-2.248162	-0.000132
15	h	3.541704	1.783193	0.000087
16	h	-1.092757	-2.245631	-0.000066
17	h	1.231759	2.727816	0.000191
18	h	4.823185	-0.109760	0.000104

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.397078	1.645422	-0.000010
2	c	0.347016	0.750262	0.000078
3	c	0.519377	-0.662057	0.000096
4	c	1.835257	-1.176314	0.000022
5	c	2.900210	-0.275943	-0.000067
6	c	2.705748	1.114938	-0.000084
7	c	-0.790530	-1.213768	0.000193
8	c	-1.668917	-0.132142	0.000251
9	o	-0.986935	1.073357	0.000173
10	n	-3.036881	-0.096298	0.000313
11	o	-3.646374	1.032347	-0.000304
12	o	4.183938	-0.816258	-0.000139
13	o	-3.645645	-1.233546	-0.000360
14	h	2.034201	-2.244204	0.000031
15	h	3.563692	1.786251	-0.000154

16	h	-1.093906	-2.249222	0.000235
17	h	1.222496	2.717509	-0.000008
18	h	4.820385	-0.085835	-0.000131

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.390832	1.641612	0.000036
2	c	0.338629	0.741843	0.000025
3	c	0.524563	-0.631972	0.000030
4	c	1.814587	-1.170577	0.000003
5	c	2.872531	-0.288984	-0.000027
6	c	2.660612	1.103441	0.000032
7	c	-0.803271	-1.198853	0.000064
8	c	-1.612596	-0.134948	0.000054
9	o	-0.983646	1.047372	0.000038
10	n	-3.035384	-0.098727	-0.000019
11	o	-3.572202	0.968213	-0.000126
12	o	4.122803	-0.806360	-0.000074
13	o	-3.605064	-1.153942	0.000013
14	h	1.985614	-2.233503	-0.000010
15	h	3.515929	1.760216	0.000039
16	h	-1.091105	-2.232315	0.000063
17	h	1.230128	2.706017	0.000087
18	h	4.796679	-0.120962	-0.000154

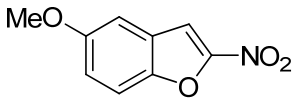
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.392651	1.649832	-0.001360
2	c	0.343250	0.751814	-0.001576
3	c	0.521991	-0.642679	-0.000923
4	c	1.824685	-1.176044	0.000380

5	c	2.894420	-0.282097	0.000715
6	c	2.689511	1.110133	-0.000246
7	c	-0.788050	-1.206627	-0.001097
8	c	-1.655112	-0.126157	-0.001261
9	o	-0.985360	1.059631	-0.001930
10	n	-3.004193	-0.097669	0.000230
11	o	-3.631219	1.017835	0.004752
12	o	4.145984	-0.813511	0.001999
13	o	-3.634419	-1.221743	-0.001200
14	h	2.002910	-2.238305	0.001218
15	h	3.542816	1.769572	0.000044
16	h	-1.071227	-2.239624	-0.000405
17	h	1.232714	2.714770	-0.001901
18	h	4.822173	-0.129477	0.002683

No.7



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	1.425659	1.065313	-0.000027
2	c	0.088807	0.749765	0.000000
3	c	-0.092788	-0.650720	0.000005
4	c	1.231110	-1.208572	0.000051
5	c	2.067951	-0.132638	0.000000
6	c	-1.390726	-1.180079	0.000032
7	c	-2.466050	-0.289605	0.000031
8	c	-2.253447	1.111022	-0.000059
9	c	-0.965640	1.649747	-0.000047
10	o	-3.706494	-0.863714	-0.000007
11	c	-4.858412	-0.028972	0.000033
12	n	3.501191	-0.098189	0.000015
13	o	4.072098	-1.195644	-0.000150
14	o	4.055556	1.000834	0.000149

15	h	-1.579834	-2.248624	0.000037
16	h	-3.097935	1.789865	-0.000206
17	h	1.533645	-2.245318	0.000040
18	h	-0.800201	2.721989	-0.000130
19	h	-5.712178	-0.708329	0.000028
20	h	-4.895600	0.601842	0.897773
21	h	-4.895618	0.601896	-0.897655

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.962167	1.639266	-0.000007
2	c	0.089331	0.748519	0.000002
3	c	-0.082015	-0.664376	0.000005
4	c	-1.395441	-1.174699	-0.000002
5	c	-2.470180	-0.277458	-0.000011
6	c	-2.275577	1.114142	-0.000014
7	c	1.229803	-1.215103	0.000015
8	c	2.106282	-0.132652	0.000017
9	o	1.422306	1.072865	0.000010
10	n	3.473853	-0.094396	0.000026
11	o	4.082346	1.035052	-0.000012
12	o	-3.727848	-0.869441	-0.000017
13	c	-4.860736	-0.029045	0.000017
14	o	4.084861	-1.230808	-0.000028
15	h	-1.596523	-2.242303	0.000000
16	h	-3.114903	1.800014	-0.000021
17	h	1.534573	-2.250070	0.000019
18	h	-0.789233	2.711779	-0.000008
19	h	-5.729979	-0.692967	0.000023
20	h	-4.894988	0.610704	0.894786
21	h	-4.895031	0.610718	-0.894741

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.955944	1.638189	0.000113
2	c	-0.095136	0.743823	-0.000040
3	c	0.091039	-0.631973	-0.000205
4	c	1.377588	-1.166602	-0.000286
5	c	2.444760	-0.287941	-0.000176
6	c	2.232087	1.103424	0.000055
7	c	-1.237875	-1.199338	-0.000205
8	c	-2.045906	-0.135473	0.000068
9	o	-1.418287	1.048220	0.000055
10	n	-3.469466	-0.099750	0.000096
11	o	-4.006126	0.967069	-0.000519
12	o	3.674717	-0.849696	-0.000217
13	c	4.827915	-0.039620	0.000354
14	o	-4.038534	-1.155146	0.000687
15	h	1.549937	-2.229247	-0.000414
16	h	3.065152	1.781151	0.000205
17	h	-1.526056	-2.232705	-0.000323
18	h	0.797603	2.702949	0.000313
19	h	5.666824	-0.719233	0.000081
20	h	4.868172	0.582861	-0.886473
21	h	4.867975	0.581952	0.887827

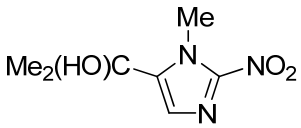
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	o	1.422117	1.059593	-0.001537
2	c	0.093616	0.752977	-0.002092
3	c	-0.086326	-0.641692	-0.001629
4	c	1.223885	-1.207172	-0.001048
5	c	2.091038	-0.127098	-0.000570
6	c	-1.387523	-1.170298	-0.001164
7	c	-2.465405	-0.277843	-0.001201
8	c	-2.258105	1.113260	-0.002132
9	c	-0.955358	1.647641	-0.002633
10	o	-3.696265	-0.852934	-0.000223
11	c	-4.850213	-0.047428	0.004978
12	n	3.440195	-0.099538	0.001259

13	o	4.069593	-1.224033	-0.000732
14	o	4.067922	1.015332	0.005405
15	h	-1.568401	-2.231959	-0.000369
16	h	-3.088425	1.794462	-0.002409
17	h	1.506535	-2.240278	-0.000250
18	h	-0.796472	2.712722	-0.003205
19	h	-5.689336	-0.727604	0.006702
20	h	-4.889868	0.574360	0.892735
21	h	-4.895986	0.577313	-0.880387

No.8



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.111905	1.690560	0.058576
2	c	-0.244753	1.703066	0.041443
3	c	-0.760765	0.414973	-0.028435
4	n	0.338246	-0.423498	-0.051707
5	c	1.428720	0.415673	0.002845
6	c	-2.209251	-0.029302	-0.005116
7	o	-2.374973	-0.946193	-1.110618
8	n	2.797381	-0.043807	0.023947
9	o	3.682960	0.795242	-0.098781
10	c	0.326805	-1.889948	-0.184297
11	o	2.986358	-1.261683	0.176010
12	c	-3.135649	1.178971	-0.214034
13	c	-2.552815	-0.734068	1.323792
14	h	-0.791198	2.634535	0.083511
15	h	-0.678730	-2.189168	-0.466910
16	h	1.029267	-2.190622	-0.961054
17	h	0.632345	-2.353599	0.755962
18	h	-2.917066	1.675984	-1.163579

19	h	-4.177561	0.836544	-0.235200
20	h	-3.047064	1.905714	0.600232
21	h	-1.928581	-1.617732	1.482628
22	h	-2.411168	-0.054445	2.170987
23	h	-3.602818	-1.053808	1.317764
24	h	-3.308657	-1.211302	-1.150133

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.460564	0.426607	-0.015398
2	n	1.107066	1.719833	-0.019307
3	c	-0.253082	1.709134	-0.070801
4	c	-0.773037	0.430026	-0.104885
5	n	0.350018	-0.416735	-0.058651
6	c	-2.196682	-0.022982	0.027718
7	c	-2.414336	-0.876035	1.297358
8	c	0.356691	-1.836372	-0.411979
9	n	2.758733	-0.043422	0.071394
10	o	2.933159	-1.305255	0.357482
11	o	-2.536715	-0.836300	-1.144460
12	c	-3.151214	1.183567	0.050129
13	o	3.736592	0.774376	-0.091418
14	h	-0.807499	2.640407	-0.050101
15	h	-0.636313	-2.097608	-0.780031
16	h	1.094580	-2.020363	-1.196016
17	h	0.635344	-2.453645	0.445986
18	h	-3.024514	1.786334	-0.853860
19	h	-4.190780	0.829890	0.085163
20	h	-2.979794	1.816622	0.927501
21	h	-1.769115	-1.758492	1.298153
22	h	-2.186145	-0.287605	2.193015
23	h	-3.460699	-1.212079	1.367298
24	h	-3.423501	-1.207435	-0.996836

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.408408	-0.402291	0.003858
2	n	-1.110059	-1.653162	0.064749
3	c	0.241857	-1.679207	0.053764
4	c	0.745303	-0.408856	-0.019696
5	n	-0.342367	0.423487	-0.049578
6	c	2.198055	0.031552	-0.015180
7	c	2.545632	0.755419	1.293057
8	c	-0.337183	1.890127	-0.174162
9	n	-2.776528	0.040280	0.021649
10	o	-2.986222	1.209309	0.174970
11	o	2.359549	0.896933	-1.123016
12	c	3.114562	-1.181640	-0.190958
13	o	-3.626510	-0.787093	-0.106269
14	h	0.777160	-2.605012	0.103756
15	h	0.666084	2.197583	-0.394551
16	h	-0.984918	2.183608	-0.985366
17	h	-0.680956	2.337064	0.746676
18	h	2.874507	-1.721721	-1.099553
19	h	4.140473	-0.834189	-0.263930
20	h	3.052205	-1.860090	0.652549
21	h	1.912786	1.617926	1.461105
22	h	2.441853	0.083860	2.138296
23	h	3.576588	1.096494	1.254484
24	h	3.253451	1.246420	-1.140779

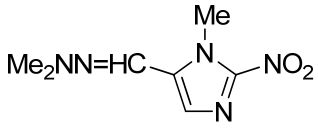
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.348968	-0.411434	-0.064065
2	c	1.430256	0.407797	0.005397
3	n	1.106017	1.667857	0.075044

4	c	-0.258456	1.682885	0.059839
5	c	-0.759330	0.423635	-0.024514
6	n	2.744737	-0.045220	0.014208
7	o	3.689683	0.787823	-0.220099
8	c	-2.203109	-0.031321	-0.004186
9	c	-3.140475	1.178697	-0.024310
10	c	0.349822	-1.852972	-0.316204
11	c	-2.502764	-0.886895	1.234224
12	o	-2.417638	-0.790474	-1.185460
13	o	2.988312	-1.243347	0.396490
14	h	-0.796017	2.607470	0.124841
15	h	-0.622403	-2.127773	-0.681673
16	h	1.089864	-2.088698	-1.064558
17	h	0.580350	-2.399275	0.586774
18	h	-2.962502	1.791831	-0.900417
19	h	-4.167526	0.827684	-0.060070
20	h	-3.027438	1.790423	0.863904
21	h	-1.877454	-1.769572	1.276156
22	h	-2.345455	-0.311092	2.140187
23	h	-3.540413	-1.210289	1.213835
24	h	-3.307585	-1.152111	-1.184216

No.9



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-1.251104	-1.490628	-0.546339
2	c	0.046451	-1.160672	-0.744525
3	c	0.275194	0.186835	-0.453051
4	n	-0.956906	0.690384	-0.070358
5	c	-1.825911	-0.374077	-0.145797
6	c	1.442356	1.038883	-0.673221

7	n	2.713310	0.803418	-0.553251
8	n	3.245687	-0.276072	0.048694
9	c	4.704202	-0.179194	0.141304
10	n	-3.229329	-0.281016	0.156333
11	o	-3.884403	-1.318275	0.173969
12	c	-1.201237	2.064596	0.381636
13	o	-3.685260	0.854889	0.376772
14	c	2.587310	-0.915863	1.190232
15	h	0.759956	-1.877631	-1.126941
16	h	-0.233010	2.542566	0.534044
17	h	-1.780908	2.615342	-0.362175
18	h	-1.757991	2.056121	1.318292
19	h	1.239867	1.995101	-1.154188
20	h	3.352761	-1.403877	1.797763
21	h	2.074095	-0.162559	1.806723
22	h	1.854535	-1.668532	0.888219
23	h	5.125272	-1.183064	0.249089
24	h	5.080204	0.269564	-0.778560
25	h	5.020712	0.438410	0.996785

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.848747	-0.395583	-0.073436
2	n	-1.095820	-1.508327	-0.201271
3	c	0.176849	-1.093749	-0.195500
4	c	0.285032	0.303438	-0.070019
5	n	-1.055216	0.743039	0.013882
6	c	1.382084	1.217547	-0.073032
7	n	2.682618	1.048565	-0.127817
8	n	3.124893	-0.318397	-0.137244
9	c	3.190752	-0.832814	1.233289
10	c	-1.433857	2.142701	0.117228
11	n	-3.232045	-0.422365	-0.019342
12	o	-3.873135	0.690598	0.144976
13	c	4.444965	-0.341100	-0.754574
14	o	-3.833523	-1.538970	-0.130838
15	h	0.998046	-1.788701	-0.296880
16	h	-0.982617	2.590054	1.013696
17	h	-1.081621	2.698335	-0.763604

18	h	-2.518959	2.188585	0.179509
19	h	1.116610	2.274107	-0.037472
20	h	3.539652	-1.872456	1.211112
21	h	3.878760	-0.235857	1.862490
22	h	2.196095	-0.813812	1.685863
23	h	4.808236	-1.375497	-0.786402
24	h	4.369706	0.037866	-1.777801
25	h	5.175875	0.284117	-0.204800

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

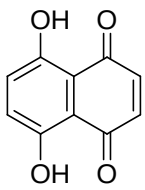
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.768987	-0.401110	-0.082126
2	n	-1.097026	-1.487607	-0.269950
3	c	0.187671	-1.086483	-0.350634
4	c	0.266481	0.276307	-0.210715
5	n	-1.025716	0.713125	-0.030191
6	c	1.392218	1.218819	-0.335509
7	n	2.629018	0.992637	-0.277361
8	n	3.040850	-0.331391	-0.012566
9	c	3.186607	-0.509709	1.429063
10	c	-1.453485	2.089314	0.267044
11	n	-3.205766	-0.418004	0.028874
12	o	-3.780910	0.629429	-0.037860
13	c	4.308328	-0.540919	-0.693461
14	o	-3.734571	-1.477002	0.165659
15	h	0.986221	-1.776505	-0.511488
16	h	-0.584511	2.667079	0.533220
17	h	-1.936854	2.521397	-0.596675
18	h	-2.132294	2.081095	1.104206
19	h	1.133787	2.244888	-0.537568
20	h	3.537963	-1.517126	1.617006
21	h	3.898998	0.198828	1.853764
22	h	2.230270	-0.381851	1.919947
23	h	4.637411	-1.556970	-0.509556
24	h	4.172331	-0.409944	-1.760010
25	h	5.078015	0.151064	-0.348858

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.819206	-0.383399	-0.060564
2	n	-1.090366	-1.476982	-0.167204
3	c	0.190129	-1.074339	-0.175000
4	c	0.271834	0.307866	-0.075337
5	n	-1.047796	0.741534	0.001326
6	c	1.374796	1.236689	-0.085445
7	n	2.646282	1.021224	-0.115825
8	n	3.067787	-0.325138	-0.093715
9	c	3.285698	-0.736051	1.289712
10	c	-1.420648	2.150954	0.093931
11	n	-3.194416	-0.429991	-0.011744
12	o	-3.870673	0.647041	0.130646
13	c	4.299241	-0.416834	-0.860473
14	o	-3.780379	-1.562542	-0.106156
15	h	0.995966	-1.770351	-0.255182
16	h	-0.956135	2.590536	0.968839
17	h	-1.083057	2.677045	-0.791908
18	h	-2.485833	2.225991	0.174322
19	h	1.121050	2.282381	-0.078630
20	h	3.621575	-1.766260	1.295681
21	h	4.037161	-0.117017	1.782053
22	h	2.361148	-0.672276	1.848850
23	h	4.636232	-1.446939	-0.857401
24	h	4.111586	-0.118714	-1.884831
25	h	5.087224	0.215771	-0.448511

No.10



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.673673	2.507235	0.000007
2	c	-1.450680	1.252592	0.000005
3	c	-0.714790	-0.010535	0.000002
4	c	0.714778	-0.010589	0.000000
5	c	1.450763	1.252481	0.000003
6	c	0.673850	2.507184	0.000006
7	c	1.413503	-1.230935	-0.000002
8	c	0.687696	-2.450658	-0.000026
9	c	-0.687841	-2.450630	-0.000025
10	c	-1.413599	-1.230879	0.000000
11	o	-2.751883	-1.304877	0.000019
12	o	2.751789	-1.304988	0.000036
13	o	-2.699191	1.295038	-0.000013
14	o	2.699275	1.294833	-0.000035
15	h	-1.250514	-3.379195	-0.000026
16	h	1.250331	-3.379246	-0.000028
17	h	1.254708	3.425544	-0.000009
18	h	-1.254461	3.425638	-0.000008
19	h	3.099188	-0.372264	0.000114
20	h	-3.099213	-0.372123	0.000068

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.691070	2.468491	0.000008
2	6	-1.457835	1.258822	0.000047
3	6	-0.715595	-0.001157	0.000032
4	6	0.715525	-0.000960	0.000023
5	6	1.457403	1.259196	0.000007
6	6	0.690327	2.468666	-0.000022
7	6	1.414179	-1.238402	0.000009

8	6	0.700210	-2.439044	-0.000018
9	6	-0.699459	-2.439261	-0.000030
10	6	-1.413798	-1.238846	-0.000017
11	8	-2.773062	-1.278283	-0.000009
12	8	2.773500	-1.277442	0.000040
13	8	-2.744857	1.276189	-0.000002
14	8	2.744420	1.276761	-0.000059
15	1	-1.256150	-3.373225	-0.000068
16	1	1.257189	-3.372833	-0.000012
17	1	1.251394	3.401106	-0.000051
18	1	-1.252378	3.400787	-0.000015
19	1	3.060113	-0.308928	0.000140
20	1	-3.059497	-0.309735	0.000018

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

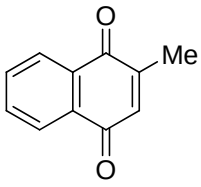
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.403616	-1.219793	-0.000236
2	c	0.715687	-0.024078	-0.000252
3	c	-0.715676	-0.024104	-0.000191
4	c	-1.403562	-1.219845	-0.000011
5	c	-0.679440	-2.432882	0.000197
6	c	0.679536	-2.432857	0.000037
7	c	-1.445348	1.258521	-0.000298
8	c	-0.662077	2.516608	0.000077
9	c	0.661973	2.516632	0.000208
10	c	1.445290	1.258576	-0.000013
11	o	2.655633	1.315804	0.000397
12	o	-2.655696	1.315704	-0.000342
13	o	-2.734531	-1.338586	0.000367
14	o	2.734592	-1.338484	-0.000300
15	h	1.231758	-3.357307	0.000308
16	h	-1.231644	-3.357344	0.000600
17	h	-1.236370	3.428038	0.000300
18	h	1.236232	3.428085	0.000531
19	h	-3.155829	-0.478879	0.000280
20	h	3.155874	-0.478767	-0.000109

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.399011	-1.230899	0.000274
2	c	0.710471	-0.003311	-0.000159
3	c	-0.710466	-0.003326	-0.000201
4	c	-1.399003	-1.230916	-0.000195
5	c	-0.694284	-2.417960	0.000269
6	c	0.694271	-2.417970	0.000608
7	c	-1.446130	1.267775	-0.000318
8	c	-0.684359	2.464464	0.000363
9	c	0.684365	2.464455	0.000160
10	c	1.446116	1.267758	-0.000580
11	o	2.706247	1.290691	-0.000511
12	o	-2.706242	1.290725	0.000867
13	o	-2.747272	-1.305248	-0.000910
14	o	2.747272	-1.305226	0.000245
15	h	1.238349	-3.347833	0.000937
16	h	-1.238358	-3.347824	0.000282
17	h	-1.230674	3.393567	0.001013
18	h	1.230691	3.393549	0.000516
19	h	-3.099987	-0.409718	-0.001096
20	h	3.100001	-0.409698	-0.000505

No.11



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	1.653576	1.304231	0.000014
2	c	0.236458	1.726526	0.000014
3	c	-0.803924	0.657082	0.000000
4	c	-0.419859	-0.698356	-0.000014
5	c	1.023087	-1.079999	-0.000014
6	c	2.049538	0.012608	0.000024
7	c	-1.399717	-1.698576	-0.000006
8	c	-2.750969	-1.351387	0.000014
9	c	-3.131407	-0.003548	0.000027
10	c	-2.160604	0.998669	0.000020
11	o	-0.057157	2.920187	-0.000065
12	o	1.376906	-2.255449	-0.000062
13	c	3.488568	-0.412282	0.000047
14	h	-4.184778	0.263893	0.000060
15	h	-2.433867	2.049384	0.000030
16	h	-1.085662	-2.737717	-0.000017
17	h	-3.508919	-2.130210	0.000020
18	h	2.375147	2.118248	0.000025
19	h	3.708407	-1.033204	0.876439
20	h	3.708454	-1.033072	-0.876426
21	h	4.154741	0.454956	0.000127

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.162667	0.961506	-0.000010
2	c	0.784488	0.658982	-0.000165
3	c	0.373290	-0.705179	-0.000160
4	c	1.359954	-1.715664	0.000002
5	c	2.710774	-1.398542	0.000153
6	c	3.117162	-0.045900	0.000147
7	c	-1.052829	-1.077576	-0.000296
8	c	-2.006006	0.012778	-0.000028
9	c	-1.588025	1.333514	-0.000035
10	c	-0.210565	1.748256	-0.000342
11	o	0.134590	2.968466	0.000165
12	o	-1.423382	-2.291695	-0.000027
13	c	-3.469747	-0.348638	0.000259
14	h	4.177235	0.204762	0.000265

15	h	2.445449	2.010974	-0.000010
16	h	1.020509	-2.748072	0.000003
17	h	3.457628	-2.191593	0.000276
18	h	-2.325228	2.136491	0.000195
19	h	-3.727218	-0.959261	-0.875902
20	h	-3.726866	-0.959295	0.876501
21	h	-4.098149	0.550594	0.000411

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

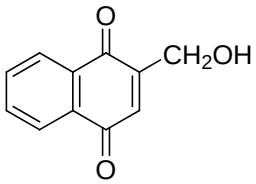
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-2.145409	1.004587	-0.000132
2	c	-0.802844	0.653393	0.000136
3	c	-0.431945	-0.691701	0.000256
4	c	-1.408634	-1.678320	0.000233
5	c	-2.749753	-1.323675	0.000111
6	c	-3.117830	0.015381	-0.000092
7	c	1.009576	-1.079715	0.000253
8	c	2.043425	0.006380	0.000164
9	c	1.664669	1.280727	0.000191
10	c	0.247603	1.710379	0.000199
11	o	-0.029325	2.881616	-0.000358
12	o	1.348229	-2.231637	-0.000735
13	c	3.481368	-0.427302	0.000091
14	h	-4.158927	0.287852	-0.000268
15	h	-2.423087	2.042507	-0.000262
16	h	-1.119447	-2.712971	0.000326
17	h	-3.505500	-2.089829	0.000175
18	h	2.386110	2.081540	0.000033
19	h	3.696007	-1.032605	0.874578
20	h	3.696081	-1.032370	-0.874543
21	h	4.136176	0.435243	0.000241

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.231287	1.721920	-0.000471
2	c	-0.776020	0.653241	-0.000484
3	c	-0.382373	-0.694116	-0.000652
4	c	1.038668	-1.068714	-0.000665
5	c	1.996984	-0.004161	0.000346
6	c	1.591331	1.310324	0.000521
7	c	-1.373174	-1.695848	-0.000230
8	c	-2.706284	-1.368931	0.000523
9	c	-3.099176	-0.019781	0.000821
10	c	-2.148184	0.969978	0.000232
11	o	1.386106	-2.270446	-0.000871
12	c	3.461236	-0.363780	0.001026
13	o	-0.104543	2.930563	-0.000783
14	h	-4.145609	0.234938	0.001625
15	h	-2.438694	2.004328	0.000503
16	h	-1.066558	-2.725398	-0.000394
17	h	-3.452805	-2.145260	0.001018
18	h	2.331603	2.095149	0.001125
19	h	3.717763	-0.958206	0.873197
20	h	3.719123	-0.956217	-0.872120
21	h	4.076892	0.528943	0.002474

No.12



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.118346	1.602015	-0.101497
2	c	0.345241	1.811750	-0.005136

3	c	1.215804	0.599965	0.011634
4	c	0.640705	-0.684936	-0.066509
5	c	-0.835802	-0.845809	-0.161797
6	c	-1.687238	0.382188	-0.183114
7	c	1.462821	-1.818319	-0.050129
8	c	2.847294	-1.673446	0.041714
9	c	3.417642	-0.396830	0.119282
10	c	2.604537	0.737383	0.104476
11	o	0.806476	2.948007	0.055346
12	o	-1.362584	-1.958365	-0.221816
13	c	-3.180348	0.171524	-0.315875
14	o	-3.713417	-0.647244	0.716256
15	h	4.496421	-0.287464	0.191190
16	h	3.027500	1.735438	0.164183
17	h	1.002620	-2.799621	-0.109775
18	h	3.483288	-2.554445	0.053593
19	h	-1.716145	2.511062	-0.107628
20	h	-3.696333	1.132914	-0.247928
21	h	-3.396226	-0.259948	-1.305827
22	h	-3.318783	-1.530034	0.605610

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-2.613581	0.664033	-0.073495
2	c	-1.206792	0.591545	-0.010336
3	c	-0.580072	-0.685939	0.047672
4	c	-1.385970	-1.845898	0.040314
5	c	-2.768723	-1.753494	-0.020195
6	c	-3.389460	-0.486854	-0.077897
7	c	0.881027	-0.810778	0.116611
8	c	1.643640	0.414692	0.127910
9	c	1.023643	1.649833	0.059513
10	c	-0.402971	1.830950	-0.007047
11	o	-0.942123	2.974212	-0.060759
12	o	1.450638	-1.955812	0.160980
13	c	3.146869	0.299951	0.278513
14	o	3.733782	-0.693300	-0.561846
15	h	-4.475007	-0.414075	-0.125933
16	h	-3.064130	1.651937	-0.118359

17	h	-0.884327	-2.808614	0.083914
18	h	-3.375957	-2.657593	-0.024306
19	h	1.620928	2.561607	0.059588
20	h	3.625622	1.254500	0.030548
21	h	3.387567	0.073887	1.334287
22	h	3.141270	-1.470699	-0.436118

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

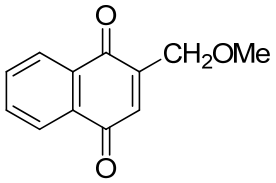
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.575961	0.782539	0.123566
2	c	1.204346	0.605419	0.009059
3	c	0.670100	-0.681622	-0.072322
4	c	1.513114	-1.783919	-0.038559
5	c	2.883616	-1.602867	0.077179
6	c	3.414307	-0.322146	0.157921
7	c	-0.802911	-0.882226	-0.200001
8	c	-1.688339	0.324058	-0.207696
9	c	-1.160710	1.540282	-0.133670
10	c	0.298691	1.787863	-0.028848
11	o	0.716098	2.914156	0.026945
12	o	-1.281629	-1.979416	-0.303441
13	c	-3.177454	0.090448	-0.316430
14	o	-3.689367	-0.558988	0.821309
15	h	4.477862	-0.184515	0.247277
16	h	2.980294	1.776124	0.185042
17	h	1.098211	-2.772833	-0.102176
18	h	3.535641	-2.458596	0.103784
19	h	-1.778007	2.424089	-0.145253
20	h	-3.678498	1.049250	-0.388871
21	h	-3.395697	-0.480789	-1.215615
22	h	-3.584954	-1.505718	0.736125

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.327543	1.796761	-0.016790
2	c	1.182334	0.601830	0.008589
3	c	0.616107	-0.680435	-0.065820
4	c	-0.838413	-0.858001	-0.174735
5	c	-1.641698	0.323101	-0.197087
6	c	-1.073856	1.572157	-0.118863
7	c	1.461722	-1.805999	-0.039186
8	c	2.823435	-1.660924	0.058040
9	c	3.389774	-0.377573	0.132380
10	c	2.580705	0.731179	0.108072
11	o	-1.348369	-1.999816	-0.243451
12	c	-3.136151	0.156661	-0.332895
13	o	-3.718588	-0.536508	0.753662
14	o	0.815935	2.947738	0.050132
15	h	4.458232	-0.266099	0.208405
16	h	3.005144	1.716574	0.164504
17	h	1.021264	-2.784135	-0.096646
18	h	3.459332	-2.529899	0.077361
19	h	-1.703805	2.447972	-0.136573
20	h	-3.614698	1.129809	-0.361435
21	h	-3.370580	-0.362863	-1.261104
22	h	-3.395740	-1.435208	0.752512

No.13



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.684216	1.606061	-0.285554

2	c	0.769945	1.798147	-0.073390
3	c	1.617027	0.576053	0.028750
4	c	1.035178	-0.700078	-0.110224
5	c	-0.427559	-0.848514	-0.371931
6	c	-1.261887	0.394604	-0.408422
7	c	1.838181	-1.843119	-0.016210
8	c	3.207277	-1.716965	0.219780
9	c	3.784471	-0.448158	0.357035
10	c	2.992213	0.695759	0.259925
11	o	1.237120	2.930083	0.021827
12	o	-0.935237	-1.946720	-0.573452
13	c	-2.750495	0.225387	-0.564495
14	o	-3.290071	-0.069769	0.717397
15	c	-4.644041	-0.488207	0.659733
16	h	4.851595	-0.353350	0.539500
17	h	3.419840	1.688517	0.361147
18	h	1.373698	-2.817742	-0.128986
19	h	3.826653	-2.606662	0.296361
20	h	-1.270739	2.521481	-0.321565
21	h	-3.198565	1.148981	-0.963698
22	h	-2.958763	-0.598940	-1.261023
23	h	-4.956887	-0.683249	1.688154
24	h	-5.287502	0.294826	0.228068
25	h	-4.750381	-1.408435	0.065885

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.965662	0.796664	0.209152
2	c	1.580064	0.613906	0.015665
3	c	1.061825	-0.708194	-0.078786
4	c	1.949955	-1.799967	0.023787
5	c	3.310210	-1.601346	0.215496
6	c	3.823192	-0.289897	0.309095
7	c	-0.380355	-0.961280	-0.283279
8	c	-1.225630	0.212263	-0.371742
9	c	-0.702388	1.493976	-0.284879
10	c	0.689959	1.787526	-0.091185
11	o	1.136622	2.971887	-0.019804
12	o	-0.829176	-2.140263	-0.386016

13	c	-2.697553	0.004807	-0.573812
14	o	-3.398210	0.047485	0.686392
15	c	-4.754575	-0.294901	0.548377
16	h	4.890339	-0.131750	0.459717
17	h	3.332474	1.817437	0.276300
18	h	1.528228	-2.798567	-0.051523
19	h	3.981173	-2.455753	0.294284
20	h	-1.365967	2.354957	-0.361898
21	h	-3.118103	0.792169	-1.223627
22	h	-2.867469	-0.976157	-1.038014
23	h	-5.209163	-0.238983	1.543534
24	h	-5.288388	0.401138	-0.125433
25	h	-4.879197	-1.318706	0.154747

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.993277	0.677338	0.247261
2	c	1.626382	0.566992	0.032184
3	c	1.038785	-0.691124	-0.105524
4	c	1.825006	-1.832627	-0.026002
5	c	3.190167	-1.718934	0.193263
6	c	3.773964	-0.466117	0.329243
7	c	-0.429516	-0.823451	-0.351251
8	c	-1.258286	0.424669	-0.364086
9	c	-0.678404	1.612978	-0.246957
10	c	0.783172	1.791431	-0.054969
11	o	1.247832	2.896990	0.029203
12	o	-0.935101	-1.893545	-0.547315
13	c	-2.748015	0.276076	-0.530423
14	o	-3.281412	-0.208431	0.672565
15	c	-4.656752	-0.473956	0.607205
16	h	4.833461	-0.380719	0.498113
17	h	3.438364	1.650012	0.350105
18	h	1.370519	-2.800109	-0.134435
19	h	3.797205	-2.605452	0.256708
20	h	-1.252696	2.525019	-0.275315
21	h	-3.183538	1.245203	-0.771086

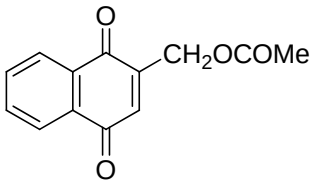
22	h	-2.964557	-0.413150	-1.345073
23	h	-4.964250	-0.827464	1.581868
24	h	-5.215156	0.425636	0.359640
25	h	-4.868587	-1.238720	-0.135814

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.697805	1.774731	-0.078231
2	c	1.578816	0.601459	0.018813
3	c	1.049967	-0.693308	-0.087311
4	c	-0.392816	-0.915816	-0.295539
5	c	-1.220856	0.247447	-0.375801
6	c	-0.683645	1.511454	-0.275889
7	c	1.919719	-1.796142	0.007300
8	c	3.267534	-1.616813	0.201464
9	c	3.795067	-0.320060	0.307185
10	c	2.961877	0.767896	0.216693
11	o	-0.844203	-2.075573	-0.399267
12	c	-2.704508	0.083570	-0.574097
13	o	-3.339902	-0.124944	0.670233
14	c	-4.726330	-0.284271	0.563658
15	o	1.152425	2.938084	0.009959
16	h	4.852063	-0.180623	0.459258
17	h	3.356087	1.764198	0.296011
18	h	1.509637	-2.785450	-0.074574
19	h	3.921181	-2.469725	0.272823
20	h	-1.332303	2.370472	-0.349593
21	h	-3.114918	0.982957	-1.033844
22	h	-2.912032	-0.760285	-1.227969
23	h	-5.117588	-0.431873	1.561696
24	h	-5.189426	0.597972	0.126876
25	h	-4.975034	-1.149067	-0.047540

No.14



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.098104	1.767302	-0.238228
2	c	1.549667	1.802777	0.063855
3	c	2.277142	0.502798	0.098998
4	c	1.590915	-0.698357	-0.172362
5	c	0.136785	-0.688428	-0.507133
6	c	-0.577189	0.628311	-0.490429
7	c	2.281869	-1.915576	-0.139952
8	c	3.643213	-1.937183	0.163748
9	c	4.324225	-0.743139	0.432654
10	c	3.643913	0.474206	0.399156
11	o	2.107281	2.874698	0.282221
12	o	-0.464668	-1.714852	-0.805008
13	c	-2.050647	0.616260	-0.784743
14	o	-2.716612	0.103105	0.393056
15	c	-4.037185	-0.177772	0.248672
16	c	-4.606765	-0.765748	1.515755
17	o	-4.648881	0.024032	-0.778919
18	h	5.385014	-0.763643	0.667606
19	h	4.153392	1.411128	0.602204
20	h	1.738338	-2.830429	-0.354302
21	h	4.175811	-2.884039	0.190389
22	h	-0.397646	2.735673	-0.235290
23	h	-2.420361	1.623897	-0.995282
24	h	-2.282215	-0.032624	-1.632892
25	h	-4.146682	-1.741887	1.706232
26	h	-4.380976	-0.122722	2.372483
27	h	-5.685918	-0.883923	1.408103

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.413436	1.802559	-0.048708
2	c	2.230023	0.576623	0.068931
3	c	1.653735	-0.709191	-0.125941
4	c	0.220381	-0.871926	-0.450670
5	c	-0.549999	0.349838	-0.555973
6	c	0.028082	1.597746	-0.365851
7	c	2.471817	-1.852376	-0.006624
8	c	3.821372	-1.737211	0.296764
9	c	4.392462	-0.461623	0.489693
10	c	3.603475	0.674462	0.375849
11	o	-0.288135	-2.015432	-0.630628
12	c	-2.001138	0.231144	-0.893016
13	8	-2.772732	0.058457	0.355609
14	c	-4.092785	-0.098958	0.243540
15	c	-4.725660	-0.348108	1.599342
16	o	1.912872	2.954793	0.118743
17	o	-4.717693	-0.059174	-0.804746
18	h	5.451132	-0.369620	0.728300
19	h	4.016708	1.669244	0.518931
20	h	2.006097	-2.821911	-0.160627
21	h	4.439069	-2.629700	0.385968
22	h	-0.579468	2.497880	-0.456712
23	h	-2.387152	1.128884	-1.384180
24	h	-2.198798	-0.646539	-1.510709
25	h	-4.419017	-1.334377	1.966805
26	h	-4.380755	0.393555	2.327063
27	h	-5.813509	-0.314458	1.509311

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Atomic Coordinates (Angstroms)

Number	Number	X	Y	Z
1	c	3.616454	0.497785	0.419397
2	c	2.264736	0.507706	0.104499
3	c	1.603987	-0.688247	-0.181272
4	c	2.301774	-1.887802	-0.149402
5	c	3.651891	-1.894142	0.169134
6	c	4.308551	-0.703699	0.452402
7	c	0.152890	-0.689944	-0.531887
8	c	-0.582663	0.613363	-0.494509
9	c	0.062372	1.742784	-0.231980
10	c	1.516275	1.793971	0.071179
11	o	2.045233	2.850876	0.287986
12	o	-0.416044	-1.697418	-0.849497
13	c	-2.054992	0.591826	-0.797159
14	o	-2.705383	-0.001802	0.326267
15	c	-4.011470	-0.186190	0.261009
16	o	-4.665934	0.115934	-0.694567
17	c	-4.555244	-0.806197	1.515801
18	h	5.356187	-0.711634	0.698223
19	h	4.118456	1.422675	0.636481
20	h	1.790684	-2.806330	-0.371209
21	h	4.190419	-2.825480	0.195573
22	h	-0.445140	2.693865	-0.219898
23	h	-2.427319	1.600596	-0.933924
24	h	-2.261181	0.005828	-1.684672
25	h	-4.063789	-1.756174	1.695533
26	h	-4.347246	-0.157277	2.359821
27	h	-5.621407	-0.954073	1.419288

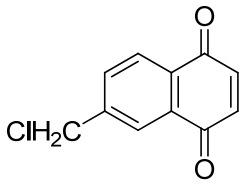
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.391618	1.783975	-0.030172
2	c	2.214907	0.569129	0.076546
3	c	1.644338	-0.695707	-0.128102
4	c	0.211640	-0.846900	-0.448185
5	c	-0.553064	0.355085	-0.551825
6	c	0.021569	1.591431	-0.352231
7	c	2.459690	-1.837643	-0.025873

8	c	3.796622	-1.724980	0.269895
9	c	4.365415	-0.458819	0.476356
10	c	3.584478	0.667233	0.380792
11	o	-0.282836	-1.979874	-0.622413
12	c	-2.012153	0.262875	-0.892318
13	o	-2.749934	0.012575	0.321689
14	c	-4.055441	-0.112294	0.246610
15	c	-4.677585	-0.396811	1.585449
16	o	1.882899	2.920024	0.148054
17	o	-4.672547	-0.015168	-0.778276
18	h	5.413315	-0.371818	0.708770
19	h	4.011400	1.640794	0.536182
20	h	2.018119	-2.803697	-0.184932
21	h	4.409485	-2.607383	0.343670
22	h	-0.583179	2.480371	-0.441848
23	h	-2.371876	1.193467	-1.316041
24	h	-2.212095	-0.547530	-1.580141
25	h	-4.375923	-1.387362	1.911974
26	h	-4.327155	0.318174	2.320727
27	h	-5.754960	-0.354913	1.507564

No.15



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	3.053168	1.302344	-0.219662
2	c	1.635466	1.663361	0.031483
3	c	0.655166	0.544459	0.167159
4	c	1.082581	-0.795266	0.073396
5	c	2.519982	-1.116528	-0.169883
6	c	3.460291	0.023480	-0.311447

7	c	0.149229	-1.829587	0.209575
8	c	-1.192157	-1.533293	0.436628
9	c	-1.628535	-0.200685	0.529407
10	c	-0.694161	0.831022	0.393736
11	c	-3.076484	0.113286	0.772587
12	cl	-4.038577	0.141534	-0.786687
13	o	1.300365	2.840319	0.122554
14	o	2.926457	-2.271549	-0.253143
15	h	-0.999148	1.871857	0.458524
16	h	0.492395	-2.856944	0.137367
17	h	-1.912706	-2.341441	0.537701
18	h	3.739452	2.139067	-0.321342
19	h	4.498073	-0.243987	-0.492861
20	h	-3.207281	1.098632	1.221078
21	h	-3.556826	-0.638965	1.400048

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.654898	0.864635	0.345712
2	c	0.706745	0.576627	0.135064
3	c	1.123316	-0.785246	0.063351
4	c	0.153099	-1.802387	0.210821
5	c	-1.178681	-1.497443	0.425974
6	c	-1.601589	-0.144892	0.497931
7	c	2.536028	-1.142589	-0.154709
8	c	3.443826	-0.030007	-0.288361
9	c	3.043202	1.288321	-0.216605
10	c	1.674105	1.685022	0.000335
11	o	1.316761	2.896228	0.074265
12	o	2.920002	-2.348211	-0.218809
13	c	-3.023314	0.194679	0.771253
14	cl	-4.145929	0.060816	-0.734186
15	h	-0.941828	1.912853	0.392758
16	h	0.494158	-2.832524	0.155296
17	h	-1.912306	-2.295016	0.536621
18	h	3.766798	2.095414	-0.321320
19	h	4.490495	-0.282839	-0.452025
20	h	-3.147053	1.227330	1.097120
21	h	-3.494606	-0.483557	1.484473

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.593848	1.656896	0.051230
2	c	0.630973	0.522765	0.173923
3	c	1.077991	-0.795148	0.062954
4	c	2.522234	-1.082547	-0.180192
5	c	3.445903	0.075416	-0.298966
6	c	3.021792	1.326342	-0.193405
7	c	0.174051	-1.840227	0.183144
8	c	-1.166366	-1.572815	0.411174
9	c	-1.619957	-0.262279	0.519873
10	c	-0.711449	0.782434	0.402606
11	c	-3.073367	0.022452	0.774669
12	cl	-3.992386	0.205159	-0.783002
13	o	2.940776	-2.204074	-0.278952
14	o	1.244718	2.802500	0.143408
15	h	-1.043556	1.801470	0.489246
16	h	0.517972	-2.854816	0.101794
17	h	-1.861916	-2.389504	0.506380
18	h	3.691557	2.165915	-0.279306
19	h	4.481444	-0.163806	-0.475859
20	h	-3.216352	0.951128	1.306820
21	h	-3.556458	-0.785225	1.304250

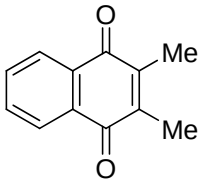
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.660617	1.659976	0.006547
2	c	0.689965	0.563378	0.149866
3	c	1.099175	-0.775773	0.070627
4	c	2.510229	-1.122533	-0.158215

5	c	3.413467	-0.031466	-0.292519
6	c	3.013866	1.278669	-0.214961
7	c	0.135529	-1.792796	0.218128
8	c	-1.182189	-1.487947	0.435033
9	c	-1.600566	-0.144959	0.511644
10	c	-0.669272	0.854709	0.371623
11	c	-3.041546	0.185613	0.766252
12	cl	-4.043500	0.074797	-0.758866
13	o	2.881405	-2.315819	-0.228769
14	o	1.302933	2.856366	0.077264
15	h	-0.968428	1.885472	0.431571
16	h	0.452487	-2.817654	0.162446
17	h	-1.905512	-2.278536	0.549286
18	h	3.736909	2.071393	-0.322925
19	h	4.451518	-0.269923	-0.461461
20	h	-3.171066	1.198622	1.116597
21	h	-3.506764	-0.506515	1.453107

No.16



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.694932	0.680235	0.000035
2	c	-0.414812	1.454037	0.000006
3	c	0.872638	0.702856	0.000000
4	c	0.872637	-0.702860	0.000022
5	c	-0.414813	-1.454038	0.000006
6	c	-1.694933	-0.680234	-0.000034
7	c	2.086168	-1.400870	0.000038
8	c	3.292500	-0.700291	0.000011
9	c	3.292501	0.700289	-0.000031

10	c	2.086169	1.400871	-0.000026
11	o	-0.425988	2.683141	-0.000031
12	o	-0.425991	-2.683142	0.000024
13	c	-2.970467	-1.479660	-0.000073
14	c	-2.970465	1.479663	0.000063
15	h	4.233592	1.243891	-0.000052
16	h	2.064329	2.486060	-0.000059
17	h	2.064326	-2.486059	0.000055
18	h	4.233591	-1.243894	0.000024
19	h	-3.581882	-1.245603	0.881139
20	h	-3.581804	-1.245642	-0.881350
21	h	-2.752896	-2.548871	-0.000066
22	h	-3.581897	1.245568	-0.881126
23	h	-3.581785	1.245685	0.881363
24	h	-2.752892	2.548875	0.000005

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.650377	0.697244	-0.000069
2	c	0.424120	1.471065	-0.000530
3	c	-0.836634	0.710821	-0.000251
4	c	-0.836626	-0.710836	0.000034
5	c	0.424137	-1.471067	-0.000028
6	c	1.650383	-0.697234	-0.000076
7	c	-2.070513	-1.397251	0.000274
8	c	-3.273765	-0.706142	0.000277
9	c	-3.273772	0.706124	-0.000027
10	c	-2.070527	1.397248	-0.000244
11	o	0.417486	2.740916	0.000205
12	o	0.417517	-2.740919	-0.000134
13	c	2.948670	-1.469594	-0.000187
14	c	2.948654	1.469617	0.000471
15	h	-4.217040	1.251087	-0.000123
16	h	-2.040327	2.483390	-0.000480
17	h	-2.040301	-2.483393	0.000473
18	h	-4.217026	-1.251114	0.000530
19	h	3.566996	-1.232066	-0.879312
20	h	3.562754	-1.239069	0.883884
21	h	2.734105	-2.541482	-0.004551

22	h	3.566706	1.232076	0.879786
23	h	3.563020	1.239120	-0.883411
24	h	2.734076	2.541502	0.004774

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.419931	-1.434819	0.000015
2	c	-0.872242	-0.695023	0.000101
3	c	-0.872240	0.695004	-0.000116
4	c	0.419922	1.434821	-0.000072
5	c	1.710127	0.669116	0.000093
6	c	1.710126	-0.669107	-0.000121
7	c	-2.074043	1.391415	-0.000309
8	c	-3.272680	0.694913	-0.000160
9	c	-3.272682	-0.694914	0.000225
10	c	-2.074047	-1.391418	0.000314
11	o	0.438663	2.637031	-0.000077
12	c	2.932383	1.551379	0.000457
13	c	2.932380	-1.551372	-0.000375
14	o	0.438689	-2.637030	-0.000016
15	h	-4.204673	-1.233062	0.000455
16	h	-2.067214	-2.465565	0.000595
17	h	-2.067198	2.465560	-0.000574
18	h	-4.204670	1.233064	-0.000375
19	h	3.851233	0.987268	0.000433
20	h	2.925339	2.195958	-0.872024
21	h	2.925110	2.195494	0.873281
22	h	3.851220	-0.987248	-0.000282
23	h	2.925253	-2.195954	0.872106
24	h	2.925176	-2.195498	-0.873190

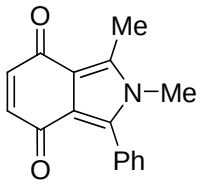
2.2 anion radical

Charge = -1 Multiplicity = 2

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	c	-0.432269	-1.438748	-0.000120
2	c	0.833076	-0.701092	-0.000086
3	c	0.836819	0.698815	-0.000031
4	c	-0.421611	1.452094	0.000060
5	c	-1.647398	0.703406	-0.000066
6	c	-1.647546	-0.680064	-0.000328
7	c	2.070273	1.381851	0.000066
8	c	3.256386	0.692260	0.000065
9	c	3.251670	-0.713895	-0.000055
10	c	2.060350	-1.394289	-0.000128
11	o	-0.397449	2.705726	-0.000234
12	c	-2.942313	1.489772	0.000428
13	c	-2.923861	-1.490721	-0.000420
14	o	-0.437543	-2.691733	0.000623
15	h	4.183533	-1.253950	-0.000104
16	h	2.046666	-2.468373	-0.000203
17	h	2.065796	2.455813	0.000173
18	h	4.192047	1.225732	0.000172
19	h	-3.545850	1.264919	0.875752
20	h	-2.735272	2.549361	0.000643
21	h	-3.546432	1.265451	-0.874603
22	h	-3.808035	-0.870047	-0.002264
23	h	-2.965951	-2.139885	-0.870481
24	h	-2.968021	-2.137313	0.871498

No.17



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	2.433392	-0.774520	-0.944920
2	c	1.831186	0.097783	-0.023087
3	c	2.639374	0.720113	0.945747
4	c	4.014753	0.484647	0.984812
5	c	4.603881	-0.376849	0.055260
6	c	3.808335	-1.006354	-0.906683
7	c	0.375899	0.338964	-0.061118
8	n	-0.166655	1.619599	-0.121608
9	c	-1.547073	1.564877	-0.099249
10	c	-1.902984	0.226762	-0.026122
11	c	-0.695665	-0.548682	-0.010141
12	c	-3.228681	-0.384598	0.060717
13	c	-3.227277	-1.869892	0.189580
14	c	-2.095998	-2.600797	0.217581
15	c	-0.728406	-2.008732	0.108708
16	c	0.584392	2.861872	-0.278218
17	c	-2.401688	2.788436	-0.158224
18	o	-4.294882	0.237569	0.041636
19	o	0.259463	-2.745242	0.113585
20	h	-4.209481	-2.331199	0.260484
21	h	-2.118181	-3.683994	0.311457
22	h	-2.130623	3.512613	0.620987
23	h	-2.315360	3.300433	-1.127059
24	h	-3.444772	2.497936	-0.022765
25	h	0.077451	3.506004	-1.000579
26	h	0.668870	3.397377	0.674129
27	h	1.584585	2.635916	-0.646852
28	h	2.184566	1.371279	1.688216
29	h	4.622608	0.966083	1.746600
30	h	5.674327	-0.563042	0.085806
31	h	4.257754	-1.685917	-1.625947
32	h	1.817537	-1.277471	-1.682835

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-2.431116	-0.952263	0.752703
2	c	-1.829816	0.089306	0.012088
3	c	-2.677124	0.891447	-0.785109
4	c	-4.058646	0.687119	-0.817435

5	c	-4.637201	-0.337954	-0.063452
6	c	-3.808563	-1.159217	0.712466
7	c	-0.381022	0.314134	0.064607
8	n	0.165458	1.605363	0.107815
9	c	1.543957	1.545428	0.079243
10	c	1.909977	0.205996	0.008696
11	c	0.701882	-0.579808	0.011273
12	c	3.252241	-0.383397	-0.080285
13	c	3.249348	-1.817608	-0.174106
14	c	2.088060	-2.580893	-0.181138
15	c	0.753216	-2.044320	-0.095251
16	c	-0.558857	2.839383	0.362265
17	c	2.409197	2.763748	0.146788
18	o	4.314072	0.315793	-0.079525
19	o	-0.278194	-2.785612	-0.101369
20	h	4.224050	-2.299269	-0.242730
21	h	2.150302	-3.666203	-0.253098
22	h	2.159003	3.499893	-0.632266
23	h	2.337213	3.281389	1.117287
24	h	3.443840	2.437130	0.013092
25	h	0.006301	3.458547	1.065634
26	h	-0.716481	3.421383	-0.556394
27	h	-1.532005	2.613087	0.799636
28	h	-2.243059	1.662739	-1.416160
29	h	-4.679960	1.320064	-1.449089
30	h	-5.712315	-0.504008	-0.090209
31	h	-4.239579	-1.974928	1.289797
32	h	-1.795733	-1.615423	1.326817

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.724805	-1.994938	-0.100298
2	c	0.693039	-0.537536	-0.002731
3	c	1.896735	0.241414	0.016935
4	c	3.215116	-0.378220	-0.020150
5	c	3.208819	-1.870696	-0.101013
6	c	2.094925	-2.593279	-0.135577

7	c	-0.357591	0.336218	0.032965
8	n	0.165827	1.602593	0.080783
9	c	1.529378	1.559148	0.063826
10	c	-1.822327	0.085254	0.017066
11	c	-2.454439	-0.456069	1.131531
12	c	-3.823005	-0.686176	1.117630
13	c	-4.569596	-0.379844	-0.012386
14	c	-3.943444	0.159532	-1.128334
15	c	-2.575657	0.393789	-1.112209
16	c	-0.604772	2.840542	0.154154
17	c	2.358881	2.804187	0.095508
18	o	4.269362	0.214010	0.010306
19	o	-0.242150	-2.714970	-0.157480
20	h	4.179015	-2.339175	-0.129898
21	h	2.129692	-3.668910	-0.194518
22	h	2.045048	3.498794	-0.677324
23	h	2.266315	3.307744	1.054046
24	h	3.396880	2.555054	-0.060404
25	h	-0.132642	3.518846	0.850558
26	h	-0.666316	3.309355	-0.821028
27	h	-1.599271	2.621836	0.507996
28	h	-2.094085	0.810439	-1.980914
29	h	-4.516042	0.397388	-2.008327
30	h	-5.630981	-0.559886	-0.023361
31	h	-4.303217	-1.103534	1.986025
32	h	-1.878077	-0.698386	2.007549

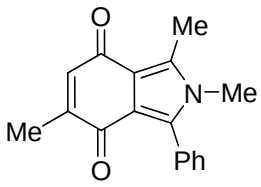
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.741057	-2.030290	-0.083369
2	c	-0.703484	-0.565667	-0.009082
3	c	-1.910801	0.216516	0.007382
4	c	-3.236480	-0.407647	-0.019904
5	c	-3.216625	-1.826658	-0.075175
6	c	-2.052279	-2.583109	-0.106300
7	c	-1.536906	1.538558	0.044101
8	n	-0.173386	1.582070	0.049264
9	c	0.351157	0.314033	0.017325
10	c	1.819891	0.076183	0.005013

11	c	2.567411	0.320606	-1.144284
12	c	3.941016	0.117274	-1.153812
13	c	4.585742	-0.331666	-0.009027
14	c	3.848602	-0.576742	1.142305
15	c	2.475461	-0.373271	1.147561
16	c	-2.355618	2.793377	0.078061
17	c	0.581340	2.821849	0.162195
18	o	-4.301500	0.256169	0.005644
19	o	0.288877	-2.737905	-0.121018
20	h	-4.171896	-2.327705	-0.095660
21	h	-2.123070	-3.658680	-0.153841
22	h	-2.146825	3.381089	0.968464
23	h	-2.150231	3.423551	-0.783881
24	h	-3.402998	2.535448	0.074210
25	h	1.635863	2.602395	0.180423
26	h	0.373114	3.468018	-0.682189
27	h	0.317663	3.338187	1.077697
28	h	1.909289	-0.567181	2.042239
29	h	4.340923	-0.924347	2.034814
30	h	5.650997	-0.489073	-0.013757
31	h	4.503562	0.308735	-2.051900
32	h	2.074071	0.668881	-2.036409

No.18



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-4.645216	-0.873325	0.049126
2	c	-4.190312	0.042696	1.001422
3	c	-2.869069	0.491971	0.964076
4	c	-1.981099	0.032779	-0.025676

5	c	-2.447473	-0.896150	-0.970616
6	c	-3.768632	-1.341961	-0.934206
7	c	-0.582618	0.502655	-0.063173
8	c	0.618204	-0.203760	-0.038045
9	c	1.683951	0.753394	-0.042666
10	c	1.121332	2.018598	-0.082071
11	n	-0.251507	1.853947	-0.095877
12	c	0.877712	-1.642115	0.045865
13	c	2.330639	-2.044605	0.129234
14	c	3.315219	-1.117059	0.108816
15	c	3.087375	0.347496	0.020427
16	o	0.004266	-2.511186	0.044071
17	c	2.602931	-3.518733	0.223836
18	o	4.043774	1.130082	0.010979
19	c	1.771217	3.362799	-0.116340
20	c	-1.188710	2.966207	-0.219980
21	h	4.361708	-1.411207	0.160165
22	h	-1.317435	3.483994	0.737235
23	h	-0.814282	3.679638	-0.958368
24	h	-2.156007	2.589687	-0.551167
25	h	2.848198	3.236644	0.006712
26	h	1.596692	3.877256	-1.072082
27	h	1.396815	4.017610	0.681394
28	h	2.106923	-3.948304	1.102195
29	h	2.191730	-4.046097	-0.645102
30	h	3.676821	-3.717633	0.286765
31	h	-2.516049	1.185111	1.723806
32	h	-1.766743	-1.274458	-1.725799
33	h	-4.859601	0.401159	1.779377
34	h	-4.112140	-2.061913	-1.672368
35	h	-5.673096	-1.225600	0.077799

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	3.104802	0.362133	0.046911
2	c	1.688864	0.736219	-0.023214
3	c	0.626309	-0.235026	-0.035172
4	c	0.911208	-1.670470	0.043774
5	c	2.318778	-2.014383	0.112710

6	c	3.328476	-1.055502	0.111432
7	c	1.111870	1.999999	-0.065949
8	n	-0.258101	1.836948	-0.087248
9	c	-0.588574	0.472694	-0.067178
10	c	-1.981677	0.017999	-0.013919
11	c	-2.942233	0.661887	0.798753
12	c	-4.273434	0.239826	0.831234
13	c	-4.686058	-0.851454	0.061208
14	c	-3.741209	-1.517178	-0.731182
15	c	-2.414481	-1.093396	-0.771186
16	c	1.770218	3.342118	-0.114329
17	c	-1.173006	2.941329	-0.322678
18	o	0.007093	-2.564461	0.043220
19	c	2.652000	-3.484154	0.186035
20	o	4.044847	1.217769	0.055126
21	h	4.370949	-1.369840	0.164715
22	h	-1.421718	3.475905	0.604607
23	h	-0.716406	3.654817	-1.015593
24	h	-2.097531	2.567894	-0.764828
25	h	2.843988	3.184782	0.017547
26	h	1.617446	3.854898	-1.078152
27	h	1.404371	4.017865	0.673601
28	h	2.182475	-3.955053	1.060638
29	h	2.263619	-4.025604	-0.687882
30	h	3.736660	-3.639663	0.242179
31	h	-2.633517	1.482683	1.441037
32	h	-1.685052	-1.637340	-1.358565
33	h	-4.984007	0.755442	1.475384
34	h	-4.040233	-2.381029	-1.321901
35	h	-5.720972	-1.186709	0.087680

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-3.071382	0.347962	0.000623
2	c	-1.676128	0.764304	0.022115
3	c	-0.614057	-0.194751	0.010744
4	c	-0.869877	-1.632350	-0.048920

5	c	-2.323865	-2.037481	-0.068374
6	c	-3.293875	-1.123873	-0.045793
7	c	-1.106230	2.007896	0.048437
8	n	0.247194	1.834841	0.060342
9	c	0.562706	0.500710	0.031104
10	c	1.970114	0.022167	0.016196
11	c	2.735829	0.130719	-1.140923
12	c	4.051235	-0.311594	-1.155447
13	c	4.612237	-0.861835	-0.010678
14	c	3.853187	-0.969698	1.147019
15	c	2.536806	-0.530384	1.159795
16	c	-1.727682	3.369018	0.066206
17	c	1.203399	2.936980	0.093321
18	o	-0.014212	-2.480765	-0.085386
19	c	-2.604937	-3.513443	-0.117077
20	o	-4.023421	1.096663	0.016751
21	h	-4.329646	-1.422730	-0.061142
22	h	1.293870	3.391024	-0.886630
23	h	0.874233	3.680653	0.805483
24	h	2.166468	2.565525	0.403638
25	h	-2.796181	3.283227	-0.055839
26	h	-1.527892	3.874529	1.007177
27	h	-1.332114	3.987057	-0.733850
28	h	-2.165735	-3.956175	-1.005065
29	h	-2.168864	-4.013636	0.741486
30	h	-3.672194	-3.697760	-0.125048
31	h	2.303949	0.555281	-2.031634
32	h	1.949863	-0.618875	2.057665
33	h	4.633896	-0.226591	-2.056632
34	h	4.283125	-1.394891	2.037678
35	h	5.633053	-1.203783	-0.020694

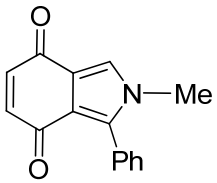
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.539197	-0.567847	1.141322
2	c	1.968296	0.015607	0.013710
3	c	2.753489	0.180070	-1.124895
4	c	4.078519	-0.235340	-1.139948
5	c	4.637767	-0.817813	-0.010572

6	c	3.864005	-0.981715	1.131261
7	c	0.554585	0.478463	0.031314
8	c	-0.627859	-0.222830	0.005980
9	c	-1.693573	0.740135	0.021266
10	c	-1.115496	1.987386	0.054876
11	n	0.238841	1.812626	0.066882
12	c	-0.891642	-1.662892	-0.056200
13	c	-2.277149	-2.030463	-0.073292
14	c	-3.293425	-1.077490	-0.046134
15	c	-3.095827	0.323320	-0.001615
16	o	-4.050889	1.148025	0.015802
17	o	0.018962	-2.513811	-0.094758
18	c	-2.616381	-3.500313	-0.128128
19	c	-1.730335	3.354207	0.080373
20	c	1.191852	2.912041	0.106902
21	h	-4.318637	-1.414285	-0.062851
22	h	1.316447	3.351391	-0.877024
23	h	0.842847	3.672320	0.791755
24	h	2.146825	2.551460	0.454424
25	h	-2.800482	3.261786	-0.018822
26	h	-1.516454	3.872276	1.012470
27	h	-1.356724	3.973828	-0.730620
28	h	-2.209963	-3.968771	-1.020759
29	h	-2.202131	-4.035717	0.722104
30	h	-3.691009	-3.647829	-0.129215
31	h	2.327155	0.629690	-2.006013
32	h	1.944162	-0.701173	2.027931
33	h	4.669777	-0.104184	-2.030359
34	h	4.290090	-1.430967	2.012362
35	h	5.665478	-1.139089	-0.019241

No.19



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.104535	-1.710099	0.145899
2	c	-0.891267	-0.266857	0.000423
3	c	-2.001230	0.637114	-0.051401
4	c	-3.395861	0.197130	0.019051
5	c	-3.576502	-1.274448	0.172424
6	c	-2.537816	-2.130746	0.236841
7	c	0.277787	0.494920	-0.060373
8	n	-0.117604	1.823978	-0.158859
9	c	-1.486913	1.911615	-0.153663
10	c	1.697301	0.094822	-0.022403
11	c	2.184394	-0.877291	-0.912313
12	c	3.525893	-1.257555	-0.880660
13	c	4.401844	-0.679397	0.042973
14	c	3.926344	0.279888	0.941103
15	c	2.584600	0.663825	0.908723
16	c	0.757131	2.984056	-0.313254
17	o	-4.364489	0.955443	-0.033332
18	o	-0.214663	-2.560290	0.186405
19	h	-4.606607	-1.617732	0.231472
20	h	-2.688869	-3.201711	0.349991
21	h	0.222711	3.750262	-0.879383
22	h	1.046295	3.395978	0.659088
23	h	1.657010	2.698204	-0.859868
24	h	2.217399	1.389187	1.630174
25	h	4.595874	0.722825	1.673938
26	h	5.445859	-0.980696	0.068453
27	h	3.885849	-2.011937	-1.575211
28	h	1.505026	-1.339846	-1.620246
29	h	-1.991120	2.864536	-0.231203

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.127689	-1.746443	0.136020
2	c	-0.901022	-0.300395	0.008289
3	c	-2.014081	0.611994	-0.030694

4	c	-3.417899	0.194919	0.030575
5	c	-3.586703	-1.228591	0.146827
6	c	-2.520102	-2.119271	0.195895
7	c	0.276996	0.470729	-0.048382
8	n	-0.124276	1.809779	-0.131801
9	c	-1.494065	1.889544	-0.127149
10	c	1.693025	0.088236	-0.006364
11	c	2.158884	-1.037764	-0.720707
12	c	3.505897	-1.393721	-0.699738
13	c	4.436912	-0.643630	0.030846
14	c	3.991431	0.462244	0.760075
15	c	2.640059	0.816509	0.747167
16	c	0.718334	2.971033	-0.362933
17	o	-4.373719	1.026824	-0.012590
18	o	-0.192010	-2.604523	0.180976
19	h	-4.611047	-1.595983	0.197744
20	h	-2.709771	-3.188449	0.284464
21	h	0.143149	3.711536	-0.927104
22	h	1.053924	3.433052	0.574834
23	h	1.599131	2.690761	-0.945355
24	h	2.309131	1.649953	1.360426
25	h	4.692389	1.042887	1.357580
26	h	5.487732	-0.926041	0.042572
27	h	3.831579	-2.270597	-1.255983
28	h	1.441255	-1.646592	-1.256869
29	h	-2.001549	2.840250	-0.215160

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-2.473043	0.307032	-1.117377
2	c	-1.691071	0.085443	0.012429
3	c	-2.262738	-0.509585	1.132568
4	c	-3.600490	-0.877992	1.123551
5	c	-4.376127	-0.656680	-0.006852
6	c	-3.810213	-0.064823	-1.128022
7	c	-0.260979	0.489289	0.027952
8	c	0.885861	-0.262260	-0.012109

9	c	1.989233	0.644560	0.033580
10	c	1.467893	1.900517	0.100932
11	n	0.116017	1.802025	0.097878
12	c	3.377279	0.199870	0.003592
13	c	3.558271	-1.279652	-0.086632
14	c	2.537364	-2.128483	-0.141208
15	c	1.100350	-1.704992	-0.117103
16	o	0.232251	-2.538744	-0.186995
17	o	4.335168	0.934343	0.044773
18	c	-0.781704	2.950806	0.177499
19	h	4.577479	-1.629505	-0.107780
20	h	2.701846	-3.191545	-0.208728
21	h	-0.193608	3.819420	0.439164
22	h	-1.267330	3.122598	-0.774138
23	h	-1.528349	2.784666	0.941493
24	h	-2.037597	0.761331	-1.991390
25	h	-4.405406	0.106548	-2.008454
26	h	-5.413687	-0.943882	-0.014014
27	h	-4.034256	-1.336322	1.995691
28	h	-1.663085	-0.685457	2.008899
29	h	1.953225	2.854890	0.155086

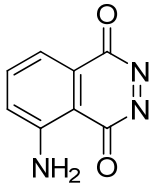
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-2.482773	0.345112	-1.103171
2	c	-1.687207	0.081081	0.008766
3	c	-2.264620	-0.532239	1.117336
4	c	-3.609210	-0.875474	1.115050
5	c	-4.395107	-0.609516	0.000940
6	c	-3.828206	0.001025	-1.109365
7	c	-0.251504	0.469684	0.023557
8	c	0.898898	-0.291509	-0.021405
9	c	2.008025	0.615007	0.031354
10	c	1.483282	1.876396	0.106661
11	n	0.126596	1.778389	0.101931
12	c	3.399270	0.167743	0.005094
13	c	3.556604	-1.235655	-0.084836
14	c	2.492274	-2.126574	-0.149758
15	c	1.115659	-1.736772	-0.130267

16	o	0.189429	-2.564679	-0.205699
17	o	4.361230	0.981380	0.058537
18	c	-0.761962	2.928672	0.186102
19	h	4.564383	-1.620763	-0.107469
20	h	2.690947	-3.184160	-0.224081
21	h	-0.175115	3.789142	0.477517
22	h	-1.230218	3.128298	-0.769890
23	h	-1.528343	2.757312	0.929931
24	h	-2.049787	0.814079	-1.970730
25	h	-4.428918	0.208400	-1.978687
26	h	-5.438473	-0.875871	-0.001448
27	h	-4.041582	-1.348377	1.980548
28	h	-1.659734	-0.743580	1.981952
29	h	1.964855	2.831300	0.169791

No.20



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.458825	-0.798599	-0.016292
2	c	1.946876	0.591193	0.003537
3	c	0.491579	0.832724	-0.001670
4	c	-0.374217	-0.286891	-0.000287
5	c	0.210579	-1.611215	0.001226
6	n	1.682768	-1.775695	-0.016459
7	c	-1.787369	-0.086481	0.000537
8	c	-2.265552	1.249948	-0.003982
9	c	-1.392391	2.324655	-0.006379
10	c	-0.000536	2.131784	-0.004173
11	n	-2.651380	-1.130602	0.004849
12	o	2.790180	1.462870	0.021423

13	o	-0.418680	-2.664223	0.011649
14	h	-1.794587	3.334171	-0.009440
15	h	0.689681	2.968149	-0.004447
16	h	-3.339626	1.420688	-0.004784
17	h	-3.648422	-0.975616	0.005265
18	h	-2.284343	-2.076600	0.011294

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.379819	-0.904366	-0.020102
2	c	-1.998478	0.431761	-0.010587
3	c	-0.561220	0.778435	-0.008439
4	c	0.381410	-0.270524	-0.023981
5	c	-0.129341	-1.648346	0.014263
6	n	-1.496914	-1.880821	-0.000261
7	c	1.776908	0.041455	-0.027987
8	c	2.163815	1.390470	0.009563
9	c	1.208591	2.414393	0.034728
10	c	-0.150839	2.122048	0.018078
11	n	2.723504	-0.966960	-0.117627
12	o	-2.879030	1.321228	-0.007165
13	o	0.642111	-2.647531	0.069613
14	h	1.543131	3.450629	0.061770
15	h	-0.909528	2.897624	0.030108
16	h	3.226104	1.633712	0.004023
17	h	3.631458	-0.767933	0.281447
18	h	2.331721	-1.896736	0.055164

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.034419	-2.111823	-0.002968

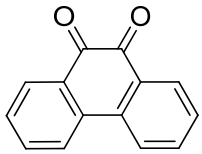
2	c	-0.463152	-0.840071	-0.000956
3	c	0.374825	0.294909	0.000065
4	c	1.773189	0.132120	0.000515
5	c	2.272502	-1.197197	-0.002943
6	c	1.432881	-2.273446	-0.004724
7	c	-0.250164	1.598961	0.000659
8	n	-1.711631	1.706378	-0.012300
9	n	-2.445396	0.738493	-0.012158
10	c	-1.922957	-0.621364	0.002435
11	o	-2.740936	-1.480506	0.015926
12	o	0.311246	2.654712	0.008635
13	n	2.642578	1.155847	0.003293
14	h	1.850131	-3.265606	-0.007259
15	h	-0.620698	-2.962353	-0.003393
16	h	3.339420	-1.342796	-0.003835
17	h	3.626253	0.977486	0.004449
18	h	2.334310	2.102071	0.009196

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.094115	2.103610	0.014503
2	c	-0.524198	0.788664	0.000334
3	c	0.377768	-0.280260	-0.010627
4	c	1.765989	-0.021617	-0.016838
5	c	2.183402	1.314715	0.003156
6	c	1.272161	2.352066	0.020237
7	c	-0.193016	-1.639158	0.008606
8	n	-1.550895	-1.817683	-0.003694
9	n	-2.394137	-0.816574	-0.013838
10	c	-1.977505	0.475715	-0.005418
11	o	-2.808747	1.374573	-0.006106
12	o	0.512024	-2.641526	0.041699
13	n	2.716051	-1.012963	-0.099363
14	h	1.632723	3.366843	0.035250
15	h	-0.806429	2.906217	0.023003
16	h	3.239717	1.526879	-0.000429
17	h	3.627387	-0.766129	0.235629
18	h	2.420345	-1.930059	0.156345

No.21



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.485734	-1.978611	0.000252
2	c	-0.743301	-0.784339	0.000047
3	c	-1.467824	0.433457	-0.000129
4	c	-2.871357	0.434476	-0.000098
5	c	-3.583223	-0.759755	0.000107
6	c	-2.880001	-1.968964	0.000303
7	c	-0.774310	1.745569	-0.000351
8	c	0.774315	1.745552	0.000307
9	c	1.467825	0.433438	0.000088
10	c	0.743297	-0.784355	-0.000063
11	c	1.485725	-1.978630	-0.000244
12	c	2.880017	-1.968960	-0.000274
13	c	3.583222	-0.759742	-0.000103
14	c	2.871341	0.434479	0.000077
15	o	1.367732	2.810068	0.000707
16	o	-1.367722	2.810086	-0.000652
17	h	-3.380250	1.393446	-0.000254
18	h	4.669561	-0.753060	-0.000127
19	h	3.380221	1.393456	0.000230
20	h	0.982253	-2.938555	-0.000381
21	h	3.418353	-2.913285	-0.000433
22	h	-4.669562	-0.753089	0.000130
23	h	-3.418325	-2.913297	0.000481
24	h	-0.982267	-2.938537	0.000401

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.495431	-1.994539	-0.000081
2	c	0.732059	-0.804781	-0.000011
3	c	1.428480	0.440708	0.000041
4	c	2.842965	0.436931	0.000042
5	c	3.567555	-0.744009	-0.000027
6	c	2.884912	-1.976445	-0.000100
7	c	0.740461	1.749299	0.000095
8	c	-0.740468	1.749298	-0.000089
9	c	-1.428484	0.440705	-0.000017
10	c	-0.732061	-0.804781	0.000011
11	c	-1.495433	-1.994541	0.000059
12	c	-2.884901	-1.976450	0.000079
13	c	-3.567547	-0.744014	0.000051
14	c	-2.842959	0.436927	0.000004
15	o	-1.401186	2.818089	-0.000262
16	o	1.401178	2.818091	0.000216
17	h	3.335590	1.404935	0.000100
18	h	-4.656306	-0.720600	0.000083
19	h	-3.335603	1.404922	-0.000034
20	h	-0.993542	-2.958046	0.000081
21	h	-3.438444	-2.913934	0.000116
22	h	4.656314	-0.720594	-0.000024
23	h	3.438455	-2.913928	-0.000154
24	h	0.993542	-2.958045	-0.000155

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-2.861182	0.432628	-0.000105
2	c	-1.467312	0.429398	-0.000111
3	c	-0.747415	-0.774260	-0.000046
4	c	-1.478212	-1.962628	0.000240
5	c	-2.863676	-1.952163	0.000286
6	c	-3.566418	-0.754381	0.000069

7	c	0.747442	-0.774280	-0.000119
8	c	1.467284	0.429405	0.000019
9	c	0.770508	1.731875	0.000019
10	c	-0.770540	1.731869	-0.000231
11	c	2.861158	0.432670	0.000201
12	c	3.566431	-0.754331	0.000105
13	c	2.863719	-1.952133	-0.000219
14	c	1.478255	-1.962634	-0.000318
15	o	1.336274	2.784563	0.000341
16	o	-1.336316	2.784554	-0.000250
17	h	3.379437	1.373751	0.000451
18	h	-4.642068	-0.750386	0.000057
19	h	-3.379484	1.373695	-0.000238
20	h	-0.984615	-2.914579	0.000384
21	h	-3.394868	-2.888380	0.000526
22	h	4.642081	-0.750309	0.000263
23	h	3.394934	-2.888336	-0.000395
24	h	0.984672	-2.914593	-0.000511

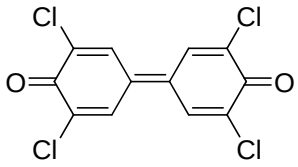
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.841093	0.440651	-0.001565
2	c	1.429240	0.435834	-0.000987
3	c	0.742785	-0.792859	0.000537
4	c	1.490203	-1.981599	0.001998
5	c	2.879755	-1.961432	0.001753
6	c	3.561738	-0.740493	-0.000166
7	c	-0.742809	-0.792846	0.000324
8	c	-1.429243	0.435862	0.000470
9	c	-0.721895	1.728155	0.001677
10	c	0.721956	1.728147	-0.001282
11	c	-2.841103	0.440705	-0.000719
12	c	-3.561771	-0.740426	-0.001713
13	c	-2.879809	-1.961380	-0.001433
14	c	-1.490257	-1.981572	-0.000479
15	o	-1.366945	2.798626	0.005218
16	o	1.367056	2.798590	-0.003655
17	h	-3.349478	1.386025	-0.000853
18	h	4.638314	-0.719606	-0.000413

19	h	3.349468	1.385971	-0.002841
20	h	0.998563	-2.935950	0.003499
21	h	3.425403	-2.889627	0.003014
22	h	-4.638345	-0.719519	-0.002728
23	h	-3.425473	-2.889567	-0.002067
24	h	-0.998640	-2.935935	-0.000595

No.22



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.463296	1.233233	0.000374
2	c	0.704205	-0.000267	0.000000
3	c	1.463583	-1.233605	-0.000375
4	c	2.819721	-1.243570	-0.000339
5	c	3.633908	0.000070	-0.000004
6	c	2.819438	1.243526	0.000335
7	c	-0.704205	-0.000267	0.000003
8	c	-1.463582	-1.233605	0.000383
9	c	-2.819720	-1.243570	0.000348
10	c	-3.633907	0.000070	0.000007
11	c	-2.819437	1.243525	-0.000336
12	c	-1.463302	1.233229	-0.000375
13	cl	-3.696181	-2.738358	0.000732
14	o	-4.855382	0.000197	0.000009
15	cl	-3.695559	2.738511	-0.000746
16	cl	3.696182	-2.738358	-0.000744
17	o	4.855383	0.000199	0.000012
18	cl	3.695559	2.738512	0.000738
19	h	-0.953150	-2.187155	0.000741
20	h	-0.952600	2.186655	-0.000734
21	h	0.953151	-2.187156	-0.000728

22	h	0.952573	2.186646	0.000729

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.476320	1.200846	0.161950
2	c	-0.723904	-0.000010	0.000002
3	c	-1.476321	-1.200868	-0.161943
4	c	-2.848177	-1.199420	-0.163902
5	c	-3.668327	0.000005	0.000007
6	c	-2.848165	1.199424	0.163912
7	c	0.723906	-0.000010	0.000000
8	c	1.476322	-1.200868	0.161944
9	c	2.848178	-1.199420	0.163902
10	c	3.668329	0.000005	-0.000006
11	c	2.848166	1.199424	-0.163910
12	c	1.476310	1.200857	-0.161963
13	cl	3.706953	-2.716635	0.393479
14	o	4.913683	0.000002	0.000010
15	cl	3.706938	2.716641	-0.393478
16	cl	-3.706952	-2.716635	-0.393479
17	o	-4.913681	0.000002	-0.000008
18	cl	-3.706937	2.716642	0.393481
19	h	0.966722	-2.144092	0.321688
20	h	0.966698	2.144076	-0.321696
21	h	-0.966721	-2.144092	-0.321678
22	h	-0.966718	2.144071	0.321683

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.458000	-1.243827	0.000486
2	c	-0.681413	-0.000170	0.000028

3	c	-1.457809	1.243591	-0.000406
4	c	-2.786370	1.243897	-0.000465
5	c	-3.592756	0.000045	-0.000144
6	c	-2.786577	-1.243938	0.000414
7	c	0.681425	-0.000175	0.000008
8	c	1.458004	-1.243841	-0.000318
9	c	2.786563	-1.243939	-0.000633
10	c	3.592755	0.000043	-0.000661
11	c	2.786378	1.243904	0.000449
12	c	1.457821	1.243585	0.000472
13	cl	3.672703	2.729297	0.001367
14	o	4.788316	0.000120	-0.000069
15	cl	3.673110	-2.729204	-0.001116
16	cl	-3.672683	2.729299	-0.001240
17	o	-4.788320	0.000154	0.000014
18	cl	-3.673135	-2.729192	0.001242
19	h	-0.954245	2.190489	-0.000850
20	h	-0.954613	-2.190809	0.001028
21	h	0.954257	2.190483	0.001052
22	h	0.954610	-2.190818	-0.000453

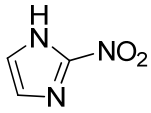
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.472510	-1.201148	-0.130868
2	c	-0.716313	-0.000014	0.000136
3	c	-1.472523	1.201110	0.131146
4	c	-2.827439	1.201291	0.132595
5	c	-3.629827	0.000011	-0.000244
6	c	-2.827425	-1.201309	-0.132596
7	c	0.716391	-0.000002	0.000169
8	c	1.472601	1.201107	-0.130517
9	c	2.827514	1.201330	-0.132292
10	c	3.630009	0.000018	-0.000025
11	c	2.827544	-1.201296	0.132418
12	c	1.472632	-1.201099	0.130772
13	cl	3.684166	2.709552	-0.316239
14	o	4.855603	-0.000021	-0.000453
15	cl	3.684240	-2.709507	0.316255
16	cl	-3.684385	2.709416	0.316186

17	o	-4.855396	0.000014	-0.000422
18	cl	-3.684360	-2.709454	-0.316080
19	h	0.973913	2.144412	-0.254220
20	h	0.973975	-2.144423	0.254442
21	h	-0.973860	2.144380	0.255248
22	h	-0.973839	-2.144445	-0.254720

No.23



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.021067	-0.101769	0.000563
2	n	0.755669	-1.189903	0.000083
3	c	2.043174	-0.731586	-0.000269
4	c	2.070336	0.654524	-0.000149
5	n	0.759218	1.044330	0.000058
6	n	-1.417229	-0.029470	0.000072
7	o	-2.058004	-1.072151	0.000005
8	o	-1.895686	1.117840	-0.000387
9	h	0.373161	1.980398	0.001099
10	h	2.883215	1.365854	0.000282
11	h	2.882078	-1.413481	-0.000685

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.003452	-0.132362	0.000715
2	n	-0.785093	-1.215313	0.000465
3	c	-2.062805	-0.710256	-0.000301

4	c	-2.072051	0.669505	-0.000905
5	n	-0.734133	1.030002	0.000399
6	n	1.380668	-0.040888	-0.000224
7	o	2.111880	-1.097366	-0.000126
8	o	1.867115	1.180381	-0.000246
9	h	-0.281675	1.933460	0.000662
10	h	-2.871002	1.397702	0.001790
11	h	-2.920959	-1.373201	-0.000998

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.764645	1.040626	0.001289
2	c	-0.026961	-0.075174	-0.000084
3	n	-0.721373	-1.159355	-0.001547
4	c	-2.014498	-0.735215	-0.001255
5	c	-2.055360	0.630567	0.001320
6	n	1.405178	-0.021517	-0.000027
7	o	1.901702	1.069700	-0.002575
8	o	2.008858	-1.048419	0.002563
9	h	-0.430397	1.992515	0.001988
10	h	-2.873262	1.323640	0.002673
11	h	-2.834023	-1.425750	-0.002462

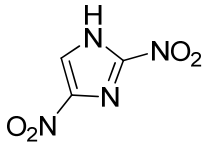
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.758697	1.032716	0.000459
2	c	-0.009916	-0.088470	-0.000081
3	n	-0.740566	-1.172066	-0.000381
4	c	-2.037111	-0.724487	-0.000615
5	c	-2.069549	0.633950	0.000550
6	n	1.368321	-0.025911	-0.000075

7	o	1.908427	1.139236	-0.000884
8	o	2.062280	-1.097956	0.000887
9	h	-0.404640	1.974414	0.000720
10	h	-2.881038	1.334485	0.001213
11	h	-2.863925	-1.408265	-0.001094

No.24



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.023397	0.067298	0.000093
2	n	0.018362	-0.722856	-0.000009
3	c	1.065095	0.137534	0.000023
4	c	0.661744	1.463919	0.000146
5	n	-0.697174	1.396591	0.000236
6	n	2.445594	-0.309436	-0.000021
7	o	2.667181	-1.512343	-0.000015
8	n	-2.414676	-0.333101	-0.000052
9	o	-3.229223	0.602068	-0.000342
10	o	3.296155	0.588228	-0.000178
11	o	-2.676256	-1.524956	0.000174
12	h	-1.367620	2.157748	-0.000023
13	h	1.219373	2.387377	0.000258

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.700403	1.346226	0.000086

2	6	-1.046216	0.004553	0.000162
3	7	0.029436	-0.784530	0.000216
4	6	1.074680	0.101109	0.000171
5	6	0.652642	1.423628	0.000091
6	7	-2.391638	-0.312567	0.000134
7	8	-2.764528	-1.526906	-0.000107
8	7	2.440805	-0.281021	0.000183
9	8	3.299827	0.644457	-0.000294
10	8	2.732563	-1.489984	-0.000161
11	8	-3.209348	0.700879	-0.000309
12	1	-1.408484	2.070868	0.000023
13	1	1.206340	2.349072	0.000054

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.682639	1.404383	-0.003207
2	c	1.005229	0.098010	-0.001162
3	n	-0.003632	-0.688268	0.000336
4	c	-1.053068	0.157556	-0.000687
5	c	-0.657431	1.464907	-0.003222
6	n	2.378457	-0.332097	0.000551
7	o	2.595651	-1.500025	-0.004945
8	n	-2.400913	-0.310489	0.000939
9	o	-3.262045	0.524565	0.002227
10	o	-2.594561	-1.487334	0.001185
11	o	3.201168	0.535584	0.007723
12	h	1.318607	2.192599	-0.004682
13	h	-1.204550	2.387537	-0.004730

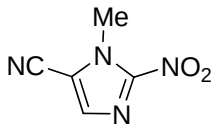
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	c	1.062832	0.152903	-0.000077
2	c	0.663240	1.450902	0.001246
3	n	-0.682586	1.383782	0.001408
4	c	-1.025707	0.068583	0.000104
5	n	0.011942	-0.712430	-0.000780
6	n	-2.347462	-0.315800	-0.000397
7	o	-2.647371	-1.552272	-0.000889
8	n	2.408934	-0.297650	-0.000176
9	o	3.274257	0.540058	-0.003410
10	o	-3.226989	0.615604	-0.000299
11	o	2.622732	-1.475364	0.002992
12	h	-1.325976	2.161146	0.002536
13	h	1.206954	2.375018	0.002282

No.25



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.473296	-1.667762	0.000184
2	c	0.877363	-1.722616	0.000149
3	c	1.409153	-0.435629	0.000018
4	n	0.334092	0.436046	-0.000051
5	c	-0.763001	-0.381205	0.000135
6	c	2.757882	-0.003007	-0.000080
7	n	3.869832	0.343015	-0.000156
8	n	-2.125560	0.116415	-0.000031
9	o	-3.028507	-0.707810	-0.000424
10	c	0.437641	1.903740	-0.000004
11	o	-2.268147	1.347184	0.000281
12	h	1.418537	-2.658736	0.000246
13	h	-0.046562	2.311433	-0.887661
14	h	-0.046306	2.311332	0.887811

15	h	1.497860	2.159281	-0.000179

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.330263	0.454539	-0.000249
2	c	-0.802398	-0.354318	0.000119
3	n	-0.472033	-1.665732	0.000340
4	c	0.867167	-1.708135	0.000184
5	c	1.424540	-0.427460	-0.000185
6	n	-2.106069	0.104306	-0.000033
7	o	-3.059821	-0.744008	0.000328
8	c	2.765455	-0.017900	-0.000372
9	n	3.895294	0.302759	-0.000512
10	c	0.487484	1.902588	0.001239
11	o	-2.313143	1.385733	-0.001316
12	h	1.409247	-2.646765	0.000240
13	h	-0.507451	2.342136	-0.003952
14	h	1.043033	2.215589	0.894941
15	h	1.053209	2.215486	-0.886054

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.741192	-0.369147	-0.000133
2	n	0.463161	-1.631986	-0.000239
3	c	-0.881866	-1.688845	-0.000033
4	c	-1.383797	-0.418888	0.000018
5	n	-0.320849	0.442720	-0.000002
6	c	-2.747616	0.003189	0.000004
7	n	-3.839889	0.318176	-0.000010
8	c	-0.410052	1.913538	0.000309
9	n	2.107244	0.103748	-0.000035

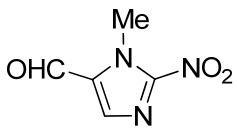
10	o	2.278850	1.286373	-0.000588
11	o	2.968243	-0.716181	0.000571
12	h	-1.423501	-2.615023	-0.000058
13	h	0.064611	2.305089	0.886200
14	h	0.063814	2.305470	-0.885841
15	h	-1.456498	2.175229	0.000857

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.888303	-1.686366	-0.000712
2	c	-1.398025	-0.413589	-0.000065
3	n	-0.318647	0.447946	0.000304
4	c	0.770054	-0.360385	-0.000191
5	n	0.454027	-1.640368	-0.000617
6	c	-2.755192	-0.003399	-0.000409
7	n	-3.854073	0.305564	-0.000839
8	c	-0.420598	1.909576	0.003613
9	n	2.070042	0.090668	-0.000387
10	o	3.023713	-0.758773	0.003889
11	o	2.289108	1.347783	-0.005759
12	h	-1.434482	-2.611012	-0.001316
13	h	0.044050	2.318927	-0.878909
14	h	-1.470620	2.162974	0.008657
15	h	0.051425	2.315328	0.883885

No.26



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Atomic Coordinates (Angstroms)

Number	Number	X	Y	Z
1	n	-0.319095	-0.368727	0.000023
2	c	0.823184	0.380109	0.000035
3	n	0.619286	1.686144	0.000011
4	c	-0.724760	1.813232	-0.000019
5	c	-1.344724	0.563096	-0.000013
6	n	2.161491	-0.189337	0.000072
7	o	2.245112	-1.424384	-0.000081
8	c	-2.785305	0.317801	-0.000019
9	o	-3.345395	-0.767557	0.000004
10	c	-0.486169	-1.835429	0.000022
11	o	3.104175	0.589893	-0.000015
12	h	-1.203618	2.784285	-0.000044
13	h	-0.011909	-2.257659	-0.886589
14	h	-0.011929	-2.257658	0.886645
15	h	-1.554454	-2.038508	0.000010
16	h	-3.374346	1.256509	-0.000065

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.310729	0.380149	-0.000040
2	c	-0.862368	-0.364578	-0.000001
3	n	-0.613814	-1.695811	0.000016
4	c	0.715321	-1.803079	0.000010
5	c	1.359000	-0.550456	-0.000011
6	n	-2.135516	0.174086	-0.000042
7	o	-2.248159	1.456469	-0.000352
8	c	2.767552	-0.332302	-0.000042
9	o	3.399454	0.746861	-0.000129
10	c	0.492618	1.832780	0.000325
11	o	-3.140809	-0.604265	0.000167
12	h	1.205398	-2.771589	-0.000012
13	h	0.024484	2.274769	-0.881844
14	h	0.024803	2.274290	0.882919
15	h	1.566889	2.017970	0.000205
16	h	3.331995	-1.291112	0.000024

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.342475	-0.554989	-0.000164
2	n	-0.318628	0.373939	0.000263
3	c	0.821262	-0.372518	0.000067
4	n	0.615105	-1.682903	-0.000146
5	c	-0.728582	-1.810255	-0.000203
6	c	-0.478280	1.840654	0.000306
7	n	2.150882	0.185207	-0.000019
8	o	3.098365	-0.601235	0.000830
9	c	-2.784752	-0.322068	-0.000164
10	o	-3.349514	0.766996	0.000328
11	o	2.262189	1.416882	-0.001034
12	h	-1.218611	-2.780607	-0.000531
13	h	-0.005520	2.258251	0.890638
14	h	-0.005668	2.258248	-0.890092
15	h	-1.544880	2.049019	0.000411
16	h	-3.368177	-1.264696	-0.001157

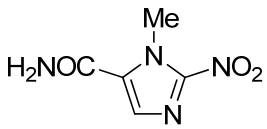
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.339589	-0.533402	0.000275
2	n	-0.302109	0.383244	0.001015
3	c	0.832208	-0.358477	-0.000207
4	n	0.595332	-1.658903	-0.001242
5	c	-0.738232	-1.774651	-0.000998
6	c	-0.460061	1.841948	0.009496
7	n	2.107243	0.159303	-0.001052
8	o	3.103284	-0.640798	0.007888
9	c	-2.767038	-0.323190	-0.001243
10	o	-3.359174	0.731141	-0.003019
11	o	2.268497	1.424317	-0.013203

12	h	-1.227613	-2.731668	-0.002379
13	h	0.005932	2.259368	0.888025
14	h	-0.006826	2.268760	-0.871172
15	h	-1.514502	2.049184	0.018222
16	h	-3.324838	-1.261795	-0.001013

No.27



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.767707	-1.665542	-0.109008
2	c	-0.584572	-1.643443	-0.106679
3	c	-1.061151	-0.337408	-0.027581
4	n	0.057952	0.472475	0.016986
5	c	1.117028	-0.396657	-0.028240
6	c	-2.466978	0.150222	-0.052512
7	n	-3.389448	-0.780206	0.341408
8	n	2.506169	0.017600	0.021439
9	o	3.358878	-0.851630	-0.106422
10	c	0.069988	1.944608	0.123576
11	o	-2.791850	1.270317	-0.439115
12	o	2.730836	1.223701	0.193116
13	h	-1.158611	-2.556022	-0.200400
14	h	-3.133018	-1.596636	0.877984
15	h	-4.357208	-0.484975	0.364592
16	h	0.652204	2.362429	-0.697872
17	h	-0.960641	2.283518	0.060915
18	h	0.531809	2.238359	1.066989

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.151796	-0.374706	-0.018828
2	n	0.753370	-1.666026	-0.051659
3	c	-0.584697	-1.621315	-0.052844
4	c	-1.077577	-0.310783	-0.025379
5	n	0.071418	0.502697	-0.028365
6	c	-2.444595	0.150704	-0.074195
7	o	-2.821750	1.316674	-0.290072
8	c	0.061557	1.917256	0.345962
9	n	2.484238	0.003106	-0.036882
10	o	2.775275	1.248526	-0.221740
11	n	-3.421324	-0.856811	0.093553
12	o	3.379526	-0.891384	0.124897
13	h	-1.167297	-2.533526	-0.129307
14	h	-3.184915	-1.615445	0.722349
15	h	-4.333833	-0.455027	0.276042
16	h	1.004680	2.356767	0.031039
17	h	-0.797273	2.391842	-0.127520
18	h	-0.038585	2.017180	1.437898

1.3 cation radical

Charge = 1 Multiplicity = 2

1.4 anion

Charge = -1 Multiplicity = 1

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.092115	-0.392966	-0.029383
2	n	0.769351	-1.632482	-0.184557
3	c	-0.581740	-1.627751	-0.186822

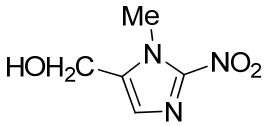
4	c	-1.043661	-0.352521	-0.026370
5	n	0.059256	0.453532	0.072348
6	c	-2.447646	0.145630	-0.069223
7	o	-2.712710	1.237853	-0.524045
8	c	0.072182	1.896101	0.374072
9	n	2.475029	0.024735	-0.009520
10	o	2.706718	1.177683	-0.225733
11	n	-3.369187	-0.710181	0.374371
12	o	3.296719	-0.810023	0.203775
13	h	-1.148667	-2.527559	-0.328081
14	h	-3.139580	-1.548338	0.874367
15	h	-4.336333	-0.440453	0.330822
16	h	0.277087	2.455660	-0.526281
17	h	-0.895405	2.161527	0.759280
18	h	0.828452	2.094882	1.115779

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.115035	-0.392783	-0.022507
2	7	0.754638	-1.647869	-0.143589
3	6	-0.597710	-1.629075	-0.133117
4	6	-1.059657	-0.351403	-0.001282
5	7	0.064649	0.452504	0.071233
6	6	-2.445546	0.152921	-0.079795
7	8	-2.698615	1.278371	-0.469291
8	6	0.083542	1.865763	0.458670
9	7	2.437990	0.021110	-0.014283
10	8	2.710782	1.224475	-0.352512
11	7	-3.403608	-0.719578	0.259135
12	8	3.355492	-0.840585	0.211494
13	1	-1.170152	-2.529260	-0.256223
14	1	-3.210890	-1.584709	0.729682
15	1	-4.363488	-0.425651	0.195255
16	1	0.920719	2.042495	1.112020
17	1	0.168585	2.498364	-0.412846
18	1	-0.835712	2.084974	0.975292

No.28



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.088916	0.587206	-0.000562
2	c	0.882011	-0.394965	-0.000211
3	n	0.386994	-1.613139	0.000512
4	c	-0.961543	-1.444193	0.000811
5	c	-1.283175	-0.095078	0.000165
6	n	2.292277	-0.113111	0.000116
7	o	2.627416	1.085211	0.002968
8	c	-2.625013	0.573203	-0.000634
9	o	-3.601386	-0.458853	0.000574
10	c	0.058130	2.046796	-0.001057
11	o	3.070377	-1.060309	-0.002295
12	h	-1.646091	-2.279243	0.001531
13	h	0.599779	2.374602	0.887259
14	h	0.609424	2.372847	-0.883931
15	h	-0.938334	2.490243	-0.007047
16	h	-2.733733	1.216541	0.887931
17	h	-2.733609	1.214316	-0.890851
18	h	-4.483640	-0.058963	0.000238

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.216637	0.395998	0.147574
2	c	-0.942383	-0.368330	0.006568

3	n	-0.659446	-1.682846	-0.022452
4	c	0.687941	-1.761875	0.105579
5	c	1.275078	-0.516085	0.218849
6	n	-2.224006	0.148879	-0.097669
7	o	-2.378823	1.444492	-0.128092
8	c	2.688227	-0.138996	0.402961
9	o	3.264631	0.401223	-0.824707
10	c	0.393845	1.831247	0.310668
11	o	-3.216453	-0.659088	-0.163775
12	h	1.196194	-2.721054	0.110680
13	h	1.182372	2.178563	-0.367920
14	h	-0.559007	2.308342	0.087550
15	h	0.687299	2.068098	1.345176
16	h	2.810416	0.617232	1.196351
17	h	3.247877	-1.037244	0.700866
18	h	4.131464	0.783060	-0.600034

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

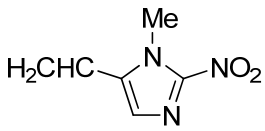
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.264487	-0.101990	0.000262
2	n	0.087912	0.580699	0.000073
3	c	-0.867543	-0.377402	-0.000014
4	n	-0.403326	-1.579375	0.000000
5	c	0.941824	-1.431767	-0.000470
6	c	-0.047707	2.042301	0.000522
7	n	-2.274082	-0.106347	-0.000174
8	o	-3.021815	-1.036909	0.001622
9	c	2.610873	0.558565	0.001395
10	o	3.573588	-0.459394	-0.001871
11	o	-2.621724	1.041028	-0.002124
12	h	1.605217	-2.271401	-0.000684
13	h	-0.574458	2.364901	-0.884412
14	h	-0.579764	2.363793	0.882609
15	h	0.942603	2.468391	0.003866
16	h	2.716506	1.191452	-0.879622
17	h	2.717324	1.185913	0.886340
18	h	4.447047	-0.063934	0.001430

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.262585	-0.545154	0.198570
2	n	0.221339	0.363757	0.174576
3	c	-0.908362	-0.375998	0.011716
4	n	-0.662582	-1.658173	-0.058602
5	c	0.692256	-1.767779	0.053626
6	c	0.366809	1.802693	0.379406
7	n	-2.183064	0.160371	-0.082003
8	o	-3.194595	-0.626110	-0.077903
9	c	2.702242	-0.189169	0.361426
10	o	3.150275	0.518085	-0.777413
11	o	-2.320322	1.423957	-0.231867
12	h	1.184371	-2.721435	0.021902
13	h	1.390675	1.994117	0.658041
14	h	0.136011	2.344295	-0.525245
15	h	-0.287622	2.136163	1.169175
16	h	2.859439	0.411519	1.256921
17	h	3.260291	-1.116576	0.477423
18	h	4.050940	0.815212	-0.627011

No.29



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.356244	-0.159239	-0.095360

2	n	-0.175861	0.559438	-0.028749
3	c	0.824253	-0.386682	-0.013786
4	n	0.374270	-1.624578	-0.067976
5	c	-0.971206	-1.500775	-0.122119
6	c	-0.066805	2.018467	0.085761
7	n	2.226515	-0.065263	0.025809
8	o	3.024213	-0.988370	0.150798
9	c	-2.682596	0.440806	-0.159034
10	c	-3.808596	-0.180537	0.226970
11	o	2.534206	1.135491	-0.074046
12	h	-1.614706	-2.365693	-0.209377
13	h	0.596501	2.278491	0.910049
14	h	0.337803	2.444874	-0.834213
15	h	-1.060532	2.420113	0.281620
16	h	-2.757085	1.442355	-0.577943
17	h	-4.776603	0.295794	0.106151
18	h	-3.800041	-1.172323	0.671511

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.369553	-0.168939	0.000341
2	n	-0.170495	0.567484	-0.000052
3	c	0.866667	-0.365532	0.000077
4	n	0.386825	-1.624348	0.000456
5	c	-0.952087	-1.503014	0.000571
6	c	-0.128309	2.019547	0.000107
7	n	2.217820	-0.065447	-0.000051
8	o	3.066533	-1.018794	-0.000881
9	c	-2.672928	0.426887	-0.000168
10	c	-3.880332	-0.208464	-0.000560
11	o	2.582624	1.181349	0.000283
12	h	-1.589606	-2.380286	0.001031
13	h	0.917853	2.319606	-0.000286
14	h	-0.637077	2.414124	-0.891326
15	h	-0.635942	2.414053	0.892265
16	h	-2.693017	1.516828	-0.000095
17	h	-4.805406	0.360780	-0.000752
18	h	-3.969859	-1.292280	-0.000727

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.942695	-1.502725	-0.173433
2	c	-1.329817	-0.187176	-0.143302
3	n	-0.179960	0.543506	-0.047979
4	c	0.810100	-0.372946	-0.020210
5	n	0.401647	-1.594531	-0.090303
6	c	-2.676041	0.397202	-0.224471
7	c	-3.739701	-0.156668	0.338436
8	c	-0.104588	2.003583	0.085538
9	n	2.204890	-0.044857	0.044181
10	o	2.512455	1.107508	-0.072053
11	o	2.979765	-0.938589	0.201880
12	h	-1.564958	-2.370048	-0.272756
13	h	0.504677	2.261206	0.937381
14	h	0.313102	2.438082	-0.810481
15	h	-1.104616	2.373557	0.242046
16	h	-2.786187	1.301056	-0.801837
17	h	-4.715725	0.276880	0.213173
18	h	-3.673631	-1.048525	0.937211

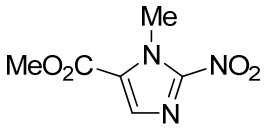
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.384703	-1.587670	-0.006496
2	c	-0.961101	-1.481634	-0.032056
3	c	-1.350362	-0.155332	-0.029983
4	n	-0.166232	0.569219	-0.003109
5	c	0.842871	-0.354269	0.007305
6	c	-2.661804	0.448131	-0.056064
7	c	-3.833769	-0.234998	-0.015209
8	c	-0.122741	2.011455	0.208152
9	n	2.190185	-0.065416	-0.018200

10	o	3.036288	-1.005502	0.190614
11	o	2.582267	1.121262	-0.302726
12	h	-1.587516	-2.352619	-0.064027
13	h	0.893162	2.316197	0.365613
14	h	-0.518732	2.527011	-0.659767
15	h	-0.721891	2.265334	1.075267
16	h	-2.705319	1.522518	-0.119296
17	h	-4.770739	0.290513	-0.051842
18	h	-3.876562	-1.308075	0.052710

No.30



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-1.089299	-1.668470	-0.000083
2	c	0.258704	-1.582363	0.000061
3	c	0.669115	-0.251529	0.000172
4	n	-0.489462	0.508213	0.000021
5	c	-1.500944	-0.414004	0.000018
6	c	2.044342	0.280339	-0.000123
7	o	2.930813	-0.734842	0.000694
8	c	4.322833	-0.356641	-0.000029
9	n	-2.910427	-0.067800	-0.000098
10	o	-3.716605	-0.988883	-0.000448
11	c	-0.579150	1.981373	0.000555
12	o	-3.197228	1.137469	0.000243
13	o	2.366809	1.455933	-0.001024
14	h	0.888554	-2.460316	0.000172
15	h	0.435598	2.369638	0.000388
16	h	-1.121147	2.313327	-0.885556
17	h	-1.120908	2.312635	0.887035
18	h	4.871942	-1.297913	0.000190

19	h	4.554925	0.228893	-0.893079
20	h	4.555640	0.229672	0.892324

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.492994	0.527075	-0.019593
2	c	1.540250	-0.388116	0.000387
3	n	1.092104	-1.665343	0.009373
4	c	-0.241398	-1.575717	0.012867
5	c	-0.683566	-0.246266	0.004107
6	n	2.886932	-0.066999	-0.045002
7	o	3.745916	-0.998544	0.094282
8	c	-2.020055	0.266552	-0.035895
9	o	-2.950328	-0.762976	0.047491
10	c	-4.311509	-0.352448	-0.020594
11	c	0.529394	1.963074	0.254446
12	o	-2.390686	1.440559	-0.131821
13	o	3.229798	1.165270	-0.232839
14	h	-0.869120	-2.458154	0.003424
15	h	0.243449	2.152855	1.298959
16	h	1.545279	2.306676	0.075738
17	h	-0.189773	2.469442	-0.390491
18	h	-4.898169	-1.271823	0.057532
19	h	-4.564077	0.327302	0.801072
20	h	-4.528096	0.153617	-0.968487

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.491783	0.495579	0.053327
2	c	1.472694	-0.408255	-0.004048
3	n	1.086241	-1.638862	-0.082536

4	c	-0.260678	-1.564353	-0.083854
5	c	-0.655226	-0.259161	-0.000399
6	n	2.878293	-0.065574	-0.028629
7	o	3.651679	-0.910553	0.293907
8	c	-2.031623	0.277051	-0.019341
9	o	-2.910241	-0.692928	0.059474
10	c	-4.294715	-0.347059	0.007802
11	c	0.592779	1.954192	0.246935
12	o	-2.313391	1.434992	-0.112163
13	o	3.171131	1.034950	-0.391460
14	h	-0.877907	-2.437276	-0.155191
15	h	-0.320356	2.291709	0.699696
16	h	1.424669	2.165287	0.897850
17	h	0.736083	2.437518	-0.708677
18	h	-4.825025	-1.282762	0.081567
19	h	-4.545740	0.297789	0.837165
20	h	-4.518740	0.143556	-0.928176

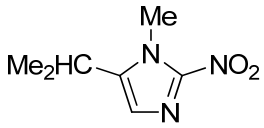
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.062838	-1.637196	-0.001245
2	c	0.276278	-1.539842	-0.001739
3	c	0.668203	-0.225793	-0.001549
4	n	-0.503237	0.518964	-0.001105
5	c	-1.503227	-0.394991	-0.000678
6	c	2.040355	0.282741	-0.000843
7	o	2.910009	-0.710658	0.000042
8	c	4.295950	-0.383615	0.002892
9	n	-2.849427	-0.090739	0.000805
10	o	-3.699893	-1.045434	0.001249
11	c	-0.602704	1.984067	-0.001661
12	o	-3.219141	1.130716	0.002706
13	o	2.373080	1.436655	-0.000373
14	h	0.905488	-2.408017	-0.002042
15	h	0.395932	2.376704	-0.002637
16	h	-1.131952	2.316047	-0.880551
17	h	-1.130566	2.316871	0.877733
18	h	4.813610	-1.329995	0.002849
19	h	4.548858	0.183714	-0.881315

20	h	4.545575	0.181842	0.889250

No.31



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.799813	-1.644625	0.194084
2	c	0.553840	-1.583459	0.112294
3	c	0.989090	-0.281989	-0.113285
4	n	-0.160699	0.482938	-0.171803
5	c	-1.200190	-0.404091	0.022144
6	c	2.386654	0.269374	-0.232344
7	c	2.829624	0.977970	1.068065
8	n	-2.586924	-0.018690	0.045070
9	o	-3.427652	-0.901798	0.176030
10	c	-0.223125	1.925898	-0.428426
11	o	-2.840360	1.193813	-0.066660
12	c	3.386738	-0.835956	-0.613415
13	h	1.158903	-2.473293	0.215587
14	h	0.785439	2.279544	-0.638987
15	h	-0.868644	2.128605	-1.283279
16	h	-0.624286	2.450552	0.440391
17	h	2.400395	1.010426	-1.044503
18	h	3.099199	-1.336569	-1.544131
19	h	4.383965	-0.404175	-0.751501
20	h	3.462170	-1.594436	0.174571
21	h	2.145918	1.784873	1.353943
22	h	2.868197	0.263593	1.898624
23	h	3.829102	1.410921	0.942670

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.233868	-0.396996	0.026143
2	n	-0.810233	-1.658585	0.166284
3	c	0.552640	-1.591026	0.078955
4	c	1.000165	-0.302689	-0.112932
5	n	-0.158734	0.488052	-0.132058
6	c	2.384614	0.279482	-0.187002
7	c	3.417554	-0.776379	-0.616304
8	c	-0.186208	1.855627	-0.629443
9	n	-2.563575	-0.006087	0.074829
10	o	-2.845055	1.271999	0.128627
11	c	2.818556	0.932632	1.147381
12	o	-3.477489	-0.908060	0.088164
13	h	1.153540	-2.488826	0.172830
14	h	0.525640	2.477133	-0.071707
15	h	0.084708	1.888956	-1.697056
16	h	-1.201653	2.228123	-0.490933
17	h	2.394613	1.073212	-0.951843
18	h	3.161679	-1.208523	-1.590263
19	h	4.419366	-0.331779	-0.684388
20	h	3.467113	-1.596131	0.111694
21	h	2.093971	1.683852	1.479946
22	h	2.889508	0.172306	1.935679
23	h	3.798937	1.422591	1.047544

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.180455	-0.391551	0.017449
2	n	-0.804612	-1.609244	0.203406
3	c	0.544930	-1.566061	0.127243
4	c	0.971226	-0.285083	-0.111299

5	n	-0.162430	0.475598	-0.182827
6	c	2.372330	0.260243	-0.239145
7	c	3.370337	-0.855062	-0.567890
8	c	-0.223723	1.911544	-0.478967
9	n	-2.563988	-0.016282	0.052610
10	o	-2.828203	1.152763	0.033042
11	c	2.795281	1.003872	1.038818
12	o	-3.376471	-0.889254	0.108353
13	h	1.137085	-2.450319	0.248046
14	h	0.760524	2.237236	-0.769410
15	h	-0.907967	2.087840	-1.293731
16	h	-0.546525	2.458492	0.394518
17	h	2.390829	0.962275	-1.068993
18	h	3.098023	-1.377443	-1.479174
19	h	4.357402	-0.426456	-0.707469
20	h	3.437347	-1.581698	0.236227
21	h	2.114545	1.811079	1.287915
22	h	2.829002	0.321763	1.883333
23	h	3.784780	1.431241	0.907989

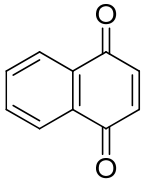
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-0.162665	0.448563	-0.200558
2	6	-1.197845	-0.403404	0.023885
3	7	-0.804428	-1.626656	0.231386
4	6	0.561493	-1.579650	0.149315
5	6	0.988820	-0.317984	-0.113009
6	7	-2.529910	-0.003457	0.045396
7	8	-3.449128	-0.890315	-0.058632
8	6	2.382980	0.240558	-0.249555
9	6	2.758204	1.121100	0.953714
10	6	-0.231840	1.839818	-0.636216
11	6	3.413042	-0.878761	-0.431761
12	8	-2.804644	1.219308	0.315967
13	1	1.151884	-2.462688	0.293545
14	1	-0.404145	2.501167	0.200764
15	1	0.701758	2.095451	-1.113139
16	1	-1.031788	1.961171	-1.348989
17	1	2.420661	0.858591	-1.144788

18	1	3.188164	-1.490191	-1.299818
19	1	4.400134	-0.448518	-0.570298
20	1	3.454999	-1.526848	0.438939
21	1	2.055369	1.934453	1.099372
22	1	2.779646	0.530725	1.865728
23	1	3.743389	1.555525	0.808202

No.32



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.283746	0.672362	0.000055
2	c	1.026241	1.461772	-0.000091
3	c	-0.261233	0.705384	-0.000017
4	c	-0.261206	-0.705382	-0.000008
5	c	1.026266	-1.461761	-0.000004
6	c	2.283767	-0.672348	0.000059
7	c	-1.475356	-1.401552	-0.000002
8	c	-2.681540	-0.700215	0.000015
9	c	-2.681543	0.700190	0.000027
10	c	-1.475358	1.401533	0.000021
11	o	1.065398	2.688741	-0.000029
12	o	1.065428	-2.688730	-0.000050
13	h	-3.622763	1.243448	0.000041
14	h	-1.454347	2.487005	0.000014
15	h	-1.454360	-2.487023	-0.000011
16	h	-3.622767	-1.243460	0.000020
17	h	3.202473	-1.253351	0.000095
18	h	3.202439	1.253385	0.000133

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.238704	0.691348	0.000013
2	c	1.034892	1.479834	-0.000050
3	c	-0.228544	0.712784	-0.000013
4	c	-0.228530	-0.712782	-0.000007
5	c	1.034902	-1.479827	-0.000014
6	c	2.238712	-0.691338	0.000017
7	c	-1.462726	-1.397290	0.000007
8	c	-2.666131	-0.705876	0.000014
9	c	-2.666145	0.705860	0.000008
10	c	-1.462736	1.397280	-0.000006
11	o	1.046055	2.747802	0.000019
12	o	1.046068	-2.747795	-0.000009
13	h	-3.609334	1.250903	-0.000003
14	h	-1.432912	2.483733	-0.000027
15	h	-1.432899	-2.483744	0.000012
16	h	-3.609320	-1.250921	0.000025
17	h	3.176549	-1.245520	0.000046
18	h	3.176539	1.245531	0.000055

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.469796	-1.391132	-0.001731
2	c	0.267154	-0.698779	-0.000920
3	c	0.267147	0.698766	0.000452
4	c	1.469784	1.391129	0.001673
5	c	2.669487	0.694210	0.001172
6	c	2.669493	-0.694196	-0.000800
7	c	-1.021670	1.450526	0.000026
8	c	-2.281847	0.662462	0.000616
9	c	-2.281843	-0.662468	-0.000115

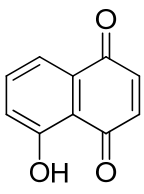
10	c	-1.021661	-1.450523	-0.000850
11	o	-1.060950	-2.651538	0.001797
12	o	-1.060950	2.651543	-0.001707
13	h	3.601139	-1.232856	-0.001560
14	h	1.464119	-2.465576	-0.003118
15	h	1.464097	2.465574	0.003084
16	h	3.601126	1.232877	0.002283
17	h	-3.195166	1.234095	0.001293
18	h	-3.195148	-1.234123	0.000171

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.459503	-1.388217	-0.004217
2	c	0.230714	-0.702167	0.000219
3	c	0.230775	0.702147	0.003725
4	c	1.459628	1.388097	0.005759
5	c	2.649204	0.701938	-0.000416
6	c	2.649134	-0.702164	-0.002517
7	c	-1.034008	1.457361	0.001658
8	c	-2.229022	0.686748	-0.001841
9	c	-2.229096	-0.686545	-0.000232
10	c	-1.034165	-1.457277	0.004782
11	o	-1.041284	-2.708871	0.000698
12	o	-1.040979	2.708946	-0.004268
13	h	3.582940	-1.238708	-0.004901
14	h	1.451171	-2.462536	-0.005982
15	h	1.451387	2.462416	0.007419
16	h	3.583056	1.238405	-0.000648
17	h	-3.163164	1.225728	-0.005817
18	h	-3.163295	-1.225433	-0.003023

No.33



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.623439	1.825796	0.000008
2	c	-0.155156	1.648872	-0.000047
3	c	0.381641	0.284819	-0.000002
4	c	-0.491670	-0.834826	0.000006
5	c	-1.970716	-0.625147	0.000037
6	c	-2.463448	0.775434	0.000058
7	c	0.017645	-2.128120	-0.000035
8	c	1.408591	-2.325309	-0.000085
9	c	2.282675	-1.247976	-0.000053
10	c	1.781652	0.068612	0.000010
11	o	2.667141	1.076797	0.000184
12	o	0.582952	2.652404	-0.000204
13	o	-2.767608	-1.559117	0.000046
14	h	3.359326	-1.387538	-0.000025
15	h	-0.670816	-2.966540	-0.000044
16	h	1.807226	-3.336261	-0.000117
17	h	-3.543553	0.895343	0.000080
18	h	-1.973895	2.854541	-0.000045
19	h	2.155183	1.926849	0.000553

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.407064	1.950644	-0.000040
2	c	0.004395	1.670660	-0.000040
3	c	-0.390375	0.262039	0.000023
4	c	0.586662	-0.776281	0.000019
5	c	2.030235	-0.450446	0.000083
6	c	2.361553	0.951600	0.000058
7	c	0.174984	-2.123432	-0.000047
8	c	-1.178102	-2.441576	-0.000129

9	c	-2.156878	-1.433823	-0.000084
10	c	-1.773443	-0.092004	0.000044
11	o	-2.729523	0.867912	0.000231
12	o	-0.878323	2.611143	-0.000251
13	o	2.916616	-1.353716	0.000062
14	h	-3.217714	-1.672218	-0.000081
15	h	0.942304	-2.891494	-0.000049
16	h	-1.490183	-3.485323	-0.000196
17	h	3.422337	1.196526	0.000054
18	h	1.694538	3.000701	-0.000121
19	h	-2.218016	1.744809	0.000739

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

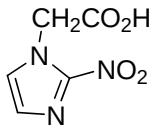
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.766689	0.129730	0.000016
2	c	0.381165	0.298521	0.000075
3	c	-0.445996	-0.845468	0.000236
4	c	0.092546	-2.109211	0.000395
5	c	1.483586	-2.258774	0.000482
6	c	2.308826	-1.161407	0.000329
7	c	-1.933969	-0.689028	-0.000016
8	c	-2.487769	0.688094	0.001470
9	c	-1.703077	1.754653	0.001209
10	c	-0.222940	1.644926	-0.000272
11	o	0.445258	2.654550	-0.001314
12	o	-2.672687	-1.635979	-0.002060
13	o	2.638858	1.139120	-0.000174
14	h	3.380275	-1.267763	0.000379
15	h	-0.549759	-2.969461	0.000532
16	h	1.913042	-3.245598	0.000607
17	h	-3.562235	0.767200	0.002210
18	h	-2.097097	2.757330	0.001738
19	h	2.189981	1.984538	-0.000622

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.763302	-0.029182	-0.000022
2	c	0.381044	0.278357	0.000237
3	c	-0.544484	-0.786436	0.000565
4	c	-0.090473	-2.112831	0.000798
5	c	1.260237	-2.379090	0.000936
6	c	2.192246	-1.341094	0.000596
7	c	-1.992454	-0.513665	-0.000223
8	c	-2.386800	0.852611	0.002063
9	c	-1.485965	1.886046	0.002329
10	c	-0.083782	1.671576	0.000167
11	o	0.735067	2.630218	-0.002145
12	o	-2.825909	-1.446768	-0.003516
13	o	2.701414	0.933835	-0.000820
14	h	3.250232	-1.544111	0.000460
15	h	-0.808178	-2.911001	0.000981
16	h	1.608343	-3.398348	0.001246
17	h	-3.445337	1.058280	0.002553
18	h	-1.826890	2.908658	0.003098
19	h	2.260026	1.790491	-0.001156

No.34



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.307081	-0.467845	0.325877

2	c	2.090436	-1.808214	0.222719
3	c	0.810516	-2.053590	-0.236213
4	n	0.221968	-0.828878	-0.429608
5	c	1.181353	0.088540	-0.059952
6	n	0.973350	1.514600	-0.105119
7	o	-0.138445	1.906074	-0.501075
8	c	-1.151296	-0.633731	-0.869031
9	c	-2.063065	-0.203042	0.275636
10	o	-3.273857	0.141801	-0.210535
11	o	1.894247	2.241696	0.241067
12	o	-1.770682	-0.200865	1.446489
13	h	0.276984	-2.971753	-0.436952
14	h	2.857121	-2.525921	0.479545
15	h	-1.200441	0.105021	-1.668704
16	h	-1.514332	-1.588472	-1.262640
17	h	-3.833908	0.406554	0.544176

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.160629	0.277280	-0.049794
2	n	2.419731	-0.039943	0.269180
3	c	2.476192	-1.405860	0.187604
4	c	1.265303	-1.941598	-0.179053
5	n	0.405973	-0.858465	-0.337583
6	c	-0.966114	-0.952920	-0.781337
7	c	-1.959340	-0.436919	0.246693
8	o	-1.864284	-0.538786	1.452131
9	n	0.616484	1.545053	-0.091557
10	o	1.337440	2.570205	0.170179
11	o	-0.657398	1.631184	-0.411909
12	o	-3.103057	-0.007462	-0.360274
13	h	0.924220	-2.957534	-0.321478
14	h	3.394732	-1.939153	0.404351
15	h	-1.120616	-0.417002	-1.718628
16	h	-1.181629	-2.018773	-0.946257
17	h	-3.673650	0.324927	0.356053

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.208447	-0.816603	-0.405512
2	c	1.170854	0.064309	-0.060731
3	n	2.271743	-0.486040	0.319184
4	c	2.042798	-1.819680	0.234302
5	c	0.772407	-2.036307	-0.210150
6	n	1.001246	1.489145	-0.099377
7	o	-0.085262	1.908653	-0.383271
8	c	-1.154898	-0.615258	-0.869289
9	c	-2.070680	-0.170079	0.247692
10	o	-3.252330	0.157129	-0.225861
11	o	-1.782013	-0.146090	1.404934
12	o	1.945467	2.169221	0.155022
13	h	0.230168	-2.940288	-0.408079
14	h	2.792455	-2.541567	0.489987
15	h	-1.185908	0.095522	-1.694827
16	h	-1.525880	-1.578437	-1.238255
17	h	-3.850666	0.410044	0.493567

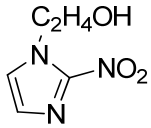
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.257685	-0.831600	-0.401490
2	c	1.164025	0.129769	-0.065766
3	n	2.309992	-0.380175	0.304418
4	c	2.153307	-1.734844	0.213977
5	c	0.901867	-2.032064	-0.212543
6	n	0.901083	1.485100	-0.110194
7	o	-0.250339	1.877521	-0.511236
8	c	-1.117374	-0.721367	-0.832782
9	c	-2.038588	-0.245459	0.262992
10	o	-3.203102	0.127630	-0.229531

11	o	-1.794028	-0.257276	1.432888
12	o	1.804896	2.315969	0.249372
13	h	0.411862	-2.966308	-0.403773
14	h	2.950068	-2.410011	0.459395
15	h	-1.214462	-0.075588	-1.701614
16	h	-1.460190	-1.726108	-1.116758
17	h	-3.807459	0.377775	0.486398

No.35



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.124336	0.805851	-0.279937
2	c	-1.649945	2.077605	-0.197880
3	c	-0.312169	2.067489	0.153882
4	n	0.052837	0.752593	0.291095
5	c	-1.093443	0.040047	0.011003
6	n	-1.171863	-1.400559	0.035929
7	o	-2.270959	-1.917592	-0.121162
8	c	1.411409	0.319443	0.653889
9	c	2.249262	-0.046986	-0.572484
10	o	3.577276	-0.231879	-0.089968
11	o	-0.110052	-2.021247	0.213692
12	h	0.396614	2.865231	0.325658
13	h	-2.284814	2.931618	-0.389802
14	h	1.351738	-0.526726	1.336397
15	h	1.881801	1.158596	1.173496
16	h	1.854723	-0.960677	-1.031015
17	h	2.208944	0.769686	-1.309183
18	h	4.093732	-0.722773	-0.746114

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.946155	0.123364	0.040032
2	n	2.110500	-0.392466	-0.368668
3	c	1.933777	-1.748025	-0.337498
4	c	0.669840	-2.077463	0.089332
5	n	0.022042	-0.874241	0.345679
6	c	-1.350180	-0.802363	0.845311
7	c	-2.423207	-0.664690	-0.246271
8	o	-2.391088	0.550527	-0.954206
9	n	0.675515	1.478368	0.143155
10	o	-0.556529	1.841732	0.472290
11	o	1.595123	2.334773	-0.083866
12	h	0.172008	-3.025123	0.242740
13	h	2.732429	-2.421720	-0.626160
14	h	-1.419149	0.032269	1.543511
15	h	-1.535251	-1.737782	1.391219
16	h	-2.318395	-1.498797	-0.959975
17	h	-3.401900	-0.787859	0.256737
18	h	-1.724495	1.156195	-0.508407

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.077477	0.041168	0.010522
2	n	-2.101246	0.773998	-0.272580
3	c	-1.647252	2.048282	-0.199736
4	c	-0.326890	2.041652	0.141914
5	n	0.044717	0.742255	0.276010
6	c	1.402822	0.330304	0.664295
7	c	2.267393	0.034220	-0.551991
8	o	3.529212	-0.331765	-0.053345
9	n	-1.158534	-1.393523	0.026233

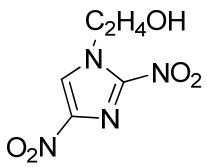
10	o	-0.135327	-2.008427	0.121063
11	o	-2.239720	-1.889012	-0.062291
12	h	0.369095	2.840740	0.308422
13	h	-2.283353	2.889586	-0.390598
14	h	1.346155	-0.525160	1.320504
15	h	1.822501	1.162182	1.220251
16	h	1.838835	-0.768306	-1.141758
17	h	2.343387	0.920919	-1.176683
18	h	4.123925	-0.519194	-0.781227

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.133371	0.824123	0.358483
2	6	-0.926436	0.029615	0.043030
3	7	-1.955261	0.718125	-0.381420
4	6	-1.556625	2.022847	-0.352294
5	6	-0.280286	2.108073	0.096828
6	7	-0.934409	-1.353654	0.144424
7	8	-2.023337	-1.988588	-0.027479
8	6	1.458090	0.521296	0.905536
9	6	2.517386	0.294619	-0.165282
10	8	2.231731	-0.775675	-1.029640
11	8	0.174354	-1.980420	0.351419
12	1	0.364172	2.948492	0.265461
13	1	-2.211264	2.817561	-0.653998
14	1	1.381948	-0.329155	1.565163
15	1	1.754156	1.383285	1.499243
16	1	2.627614	1.188334	-0.772053
17	1	3.462615	0.119970	0.346340
18	1	1.580102	-1.349884	-0.621884

No.36



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.311836	0.982993	-0.000791
2	c	1.541469	-0.344095	0.000235
3	c	0.367318	-1.075962	0.001599
4	n	-0.638620	-0.154156	0.001726
5	c	0.004208	1.073579	0.000073
6	n	2.874181	-0.913591	-0.000018
7	o	3.833565	-0.154175	-0.001656
8	n	-0.691048	2.347659	0.000052
9	o	-0.010081	3.361889	-0.003939
10	c	-2.088996	-0.450978	0.001913
11	c	-2.380086	-1.950585	-0.001591
12	o	-3.797924	-2.036106	-0.002993
13	o	-1.928737	2.303210	0.004290
14	o	2.926886	-2.150452	0.001503
15	h	0.207369	-2.141113	0.002605
16	h	-2.540037	0.013454	-0.876594
17	h	-2.539104	0.009487	0.882970
18	h	-1.954273	-2.428713	-0.896315
19	h	-1.955768	-2.432594	0.891736
20	h	-4.065773	-2.967553	-0.002198

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.018061	1.132828	-0.000088
2	n	1.313597	1.049192	-0.000694
3	c	1.566420	-0.290346	0.000113
4	c	0.400427	-1.035146	0.001169
5	n	-0.623997	-0.139064	0.000981
6	n	2.856357	-0.867978	-0.000149
7	o	2.923779	-2.134907	0.000959

8	c	-2.055771	-0.479216	0.001529
9	c	-2.288399	-1.987669	-0.001269
10	o	-3.708840	-2.166687	-0.001491
11	n	-0.752462	2.310941	-0.000246
12	o	-2.041852	2.218400	0.001992
13	o	3.859008	-0.124885	-0.000939
14	o	-0.132817	3.416818	-0.001667
15	h	0.268291	-2.103779	0.001924
16	h	-2.529371	-0.027655	-0.871573
17	h	-2.528150	-0.030976	0.877059
18	h	-1.844646	-2.450907	-0.894762
19	h	-1.844615	-2.454403	0.890380
20	h	-3.897877	-3.116532	-0.001839

1.3 cation radical

Charge = 1 Multiplicity = 2

1.4 anion

Charge = -1 Multiplicity = 1

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.023834	1.043290	0.000465
2	n	-1.301855	0.941164	-0.000209
3	c	-1.509333	-0.381756	0.000563
4	c	-0.335682	-1.077352	0.001847
5	n	0.635284	-0.146108	0.001462
6	n	-2.819095	-0.946337	-0.000512
7	o	-2.891432	-2.144030	0.000450
8	c	2.096138	-0.405727	0.003022
9	c	2.412472	-1.893206	0.000408
10	o	3.814051	-1.960060	-0.003451
11	n	0.622351	2.333844	-0.000202
12	o	1.816444	2.352326	-0.001710

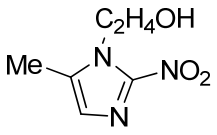
13	o	-3.756835	-0.208906	-0.002374
14	o	-0.080225	3.294014	0.000520
15	h	-0.154823	-2.132458	0.002843
16	h	2.515594	0.054495	0.888461
17	h	2.517891	0.057722	-0.879423
18	h	2.011008	-2.380207	0.885469
19	h	2.006528	-2.378000	-0.883834
20	h	4.092419	-2.877750	-0.002592

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.437022	-0.595139	-0.491236
2	c	0.298417	0.736432	-0.181687
3	n	-0.933190	1.058253	0.084085
4	c	-1.613967	-0.104178	-0.051557
5	c	-0.800855	-1.129580	-0.402299
6	n	1.339581	1.649060	-0.151719
7	o	1.075679	2.874402	0.034193
8	c	1.612210	-1.396058	-0.876826
9	c	2.332197	-2.007025	0.318386
10	o	2.770592	-1.064695	1.260812
11	o	2.551383	1.226679	-0.257510
12	h	2.269814	-0.777865	-1.466194
13	h	1.241288	-2.200467	-1.507532
14	h	1.673623	-2.699059	0.833708
15	h	3.174104	-2.575116	-0.073864
16	h	2.896562	-0.216540	0.832286
17	h	-0.998273	-2.165105	-0.600066
18	n	-3.016331	-0.188722	0.151942
19	o	-3.616683	0.802896	0.450490
20	o	-3.532809	-1.267725	0.011272

No.37



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-1.950220	1.114802	-0.321953
2	c	-1.120744	2.189786	-0.302288
3	c	0.172504	1.817757	0.036853
4	n	0.130390	0.451865	0.229071
5	c	-1.183795	0.093927	-0.006082
6	c	1.401052	2.650114	0.209340
7	n	-1.681585	-1.255062	0.076918
8	o	-2.890398	-1.428712	-0.029712
9	c	1.289982	-0.366472	0.611310
10	c	1.973490	-1.007021	-0.598953
11	o	3.194168	-1.557770	-0.109969
12	o	-0.846393	-2.160975	0.248413
13	h	0.971771	-1.136388	1.312007
14	h	2.001072	0.291555	1.115919
15	h	1.322447	-1.778798	-1.023878
16	h	2.169827	-0.244464	-1.368066
17	h	3.512588	-2.234596	-0.725233
18	h	-1.479728	3.184965	-0.529945
19	h	1.759943	2.647207	1.246714
20	h	2.227075	2.314905	-0.429282
21	h	1.170954	3.685491	-0.057427

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.453025	-0.941134	0.026373
2	n	-0.030925	-2.107754	-0.403003
3	c	-1.389401	-1.945276	-0.417837
4	c	-1.763845	-0.689791	-0.001154
5	n	-0.569229	-0.028486	0.300536
6	c	-3.117951	-0.078602	0.156358

7	c	-0.501183	1.337469	0.817893
8	c	-0.350131	2.425872	-0.258829
9	o	0.852276	2.370585	-0.985728
10	n	1.801972	-0.656910	0.175624
11	o	2.150799	0.585153	0.487071
12	o	2.671458	-1.577032	0.004315
13	h	0.332910	1.393004	1.517384
14	h	-1.432860	1.527387	1.365976
15	h	-1.192946	2.358713	-0.966071
16	h	-0.443076	3.398300	0.263828
17	h	1.466989	1.724293	-0.521087
18	h	-2.045365	-2.748797	-0.736188
19	h	-3.354305	0.185742	1.199294
20	h	-3.250404	0.834050	-0.443832
21	h	-3.873030	-0.801506	-0.173497

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.164582	0.070318	-0.004753
2	n	-1.953205	1.041246	-0.308827
3	c	-1.165361	2.142215	-0.297070
4	c	0.117377	1.802239	0.030212
5	n	0.117076	0.449065	0.216776
6	c	1.319061	2.676842	0.192897
7	c	1.291948	-0.335335	0.624258
8	c	2.041500	-0.894520	-0.576311
9	o	3.149144	-1.586256	-0.057409
10	n	-1.638782	-1.283403	0.062549
11	o	-0.826048	-2.160957	0.131987
12	o	-2.818911	-1.459020	0.036616
13	h	0.977849	-1.128959	1.284833
14	h	1.938013	0.324990	1.187622
15	h	1.403591	-1.560420	-1.146432
16	h	2.365740	-0.087797	-1.228580
17	h	3.658072	-1.968494	-0.773966
18	h	-1.550558	3.117853	-0.520325
19	h	1.684389	2.663539	1.214962

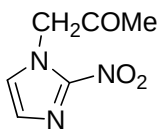
20	h	2.129646	2.375366	-0.461926
21	h	1.044504	3.694870	-0.054632

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.527160	-0.102422	0.299398
2	c	0.589669	-0.836796	0.019738
3	n	0.302939	-2.029084	-0.423834
4	c	-1.061976	-2.086605	-0.445546
5	c	-1.598593	-0.920972	-0.007332
6	n	1.895042	-0.386535	0.175928
7	o	2.854054	-1.221667	0.113751
8	c	-3.032059	-0.531217	0.166900
9	c	-0.652100	1.232558	0.887197
10	c	-0.781634	2.349398	-0.143509
11	o	0.290648	2.412119	-1.047700
12	o	2.126802	0.878190	0.291846
13	h	0.195949	1.405141	1.530993
14	h	-1.538923	1.238411	1.512329
15	h	-1.688782	2.226848	-0.725256
16	h	-0.865801	3.285461	0.406764
17	h	1.054506	1.976891	-0.662704
18	h	-1.581950	-2.965325	-0.776756
19	h	-3.270181	-0.320254	1.205467
20	h	-3.292516	0.344027	-0.419790
21	h	-3.659920	-1.352237	-0.159362

No.38



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.353087	-0.332732	0.310018
2	c	-2.230833	-1.681786	0.185212
3	c	-0.968427	-2.009165	-0.275807
4	n	-0.295368	-0.828228	-0.449357
5	c	-1.187288	0.148200	-0.063605
6	n	-0.876267	1.553662	-0.079640
7	o	-1.748403	2.342819	0.257535
8	c	1.095073	-0.713507	-0.866299
9	c	2.035521	-0.347913	0.298648
10	c	3.380247	0.206139	-0.106091
11	o	0.272108	1.871818	-0.441464
12	o	1.697133	-0.521715	1.450092
13	h	1.187963	0.015260	-1.672766
14	h	1.400656	-1.691622	-1.256982
15	h	-3.046134	-2.348425	0.429838
16	h	-0.500142	-2.959573	-0.488341
17	h	3.811503	-0.353701	-0.945576
18	h	3.243508	1.242963	-0.440704
19	h	4.063239	0.191012	0.745736

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.170516	0.301707	-0.048046
2	n	-2.438646	0.012886	0.259538
3	c	-2.531233	-1.348812	0.145443
4	c	-1.332455	-1.905478	-0.231432
5	n	-0.446037	-0.843569	-0.364399
6	c	0.932308	-0.959523	-0.794045
7	c	1.952509	-0.524312	0.268813
8	o	1.820530	-0.845482	1.439796
9	n	-0.595260	1.558370	-0.055870
10	o	0.689658	1.617627	-0.341306
11	o	-1.290605	2.595812	0.222050
12	c	3.206835	0.145670	-0.256866
13	h	1.093286	-0.396993	-1.716641

14	h	1.112279	-2.025531	-1.002906
15	h	-3.463305	-1.863131	0.349592
16	h	-1.016159	-2.926275	-0.393992
17	h	3.689653	-0.495135	-1.011523
18	h	2.937997	1.093191	-0.733452
19	h	3.904502	0.320883	0.566528

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.186978	0.094414	-0.066917
2	n	-2.318181	-0.408266	0.292805
3	c	-2.145755	-1.749480	0.205188
4	c	-0.877878	-2.018578	-0.219470
5	n	-0.259543	-0.824611	-0.400315
6	c	1.123638	-0.681010	-0.831459
7	c	2.046267	-0.244143	0.290747
8	o	1.688537	-0.230464	1.432255
9	n	-0.956443	1.509798	-0.103022
10	o	0.142462	1.882919	-0.397283
11	o	-1.867291	2.229356	0.163027
12	c	3.435226	0.148313	-0.135521
13	h	1.193757	-0.005726	-1.684197
14	h	1.458573	-1.670557	-1.168871
15	h	-2.928997	-2.439742	0.447231
16	h	-0.371364	-2.944167	-0.410983
17	h	3.830783	-0.553250	-0.863198
18	h	3.391691	1.124994	-0.611167
19	h	4.087936	0.198411	0.725508

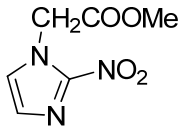
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	n	-0.322222	-0.839503	-0.409475
2	c	-1.168549	0.173620	-0.074456
3	n	-2.349407	-0.264711	0.279826
4	c	-2.275569	-1.625764	0.184881
5	c	-1.040191	-1.997541	-0.230714
6	n	-0.821893	1.510872	-0.110259
7	o	-1.670881	2.393381	0.261104
8	c	1.072062	-0.810101	-0.798763
9	c	1.997600	-0.350020	0.309159
10	c	3.355696	0.118998	-0.139967
11	o	1.684985	-0.401594	1.466663
12	o	0.349085	1.836256	-0.515204
13	h	1.216801	-0.205638	-1.691597
14	h	1.364155	-1.842257	-1.044803
15	h	-3.115196	-2.251436	0.418246
16	h	-0.606840	-2.959445	-0.420974
17	h	3.764620	-0.550136	-0.891461
18	h	3.249203	1.099363	-0.595321
19	h	4.030114	0.183449	0.703926

No.39



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.684254	-0.259458	0.442108
2	c	2.613199	-1.615998	0.353131
3	c	1.398038	-1.998713	-0.183112
4	n	0.702215	-0.845318	-0.441033
5	c	1.535195	0.171383	-0.028648
6	n	1.185062	1.566698	-0.116745
7	o	0.072256	1.836137	-0.602377
8	c	-0.652640	-0.798222	-0.973295

9	c	-1.674865	-0.414481	0.096658
10	o	-2.854028	-0.151205	-0.484910
11	c	-3.929343	0.227113	0.403813
12	o	1.996325	2.390818	0.283668
13	o	-1.458890	-0.388954	1.286094
14	h	-0.894462	-1.798213	-1.346816
15	h	-0.714475	-0.097963	-1.805672
16	h	3.429978	-2.247149	0.674783
17	h	0.975551	-2.969827	-0.398247
18	h	-4.788264	0.398078	-0.244429
19	h	-4.130947	-0.577309	1.115375
20	h	-3.660900	1.138063	0.943616

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.474189	0.355920	-0.035968
2	n	2.741329	0.171538	0.349004
3	c	2.940460	-1.181959	0.288888
4	c	1.809807	-1.840954	-0.129655
5	n	0.854532	-0.853171	-0.346752
6	c	-0.482646	-1.096751	-0.842619
7	c	-1.562681	-0.658214	0.136158
8	o	-1.499662	-0.743629	1.345415
9	n	0.810156	1.563825	-0.119687
10	o	1.411538	2.656305	0.171586
11	o	-0.446107	1.523551	-0.509617
12	o	-2.692337	-0.313235	-0.534444
13	c	-3.730102	0.247154	0.276045
14	h	-0.578776	-2.181951	-0.990757
15	h	-0.649862	-0.596820	-1.797438
16	h	3.896297	-1.616894	0.557879
17	h	1.581342	-2.887532	-0.275571
18	h	-4.543577	0.486116	-0.412689
19	h	-4.066346	-0.467491	1.034809
20	h	-3.362823	1.154110	0.765195

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.672117	-0.831602	-0.413866
2	c	1.534495	0.132893	-0.030167
3	n	2.653964	-0.316036	0.423505
4	c	2.544537	-1.665536	0.347583
5	c	1.325692	-1.996010	-0.166482
6	n	1.247248	1.537353	-0.105334
7	o	0.152571	1.859187	-0.472906
8	c	-0.671720	-0.754408	-0.965583
9	c	-1.688019	-0.357189	0.080727
10	o	-2.849245	-0.115713	-0.478311
11	c	-3.946990	0.223640	0.368563
12	o	-1.476464	-0.300947	1.253567
13	o	2.109331	2.300013	0.202930
14	h	-0.934191	-1.756038	-1.325405
15	h	-0.707164	-0.069284	-1.811202
16	h	3.335792	-2.317368	0.660165
17	h	0.874559	-2.945266	-0.380292
18	h	-4.785081	0.373693	-0.292907
19	h	-4.147411	-0.584903	1.056458
20	h	-3.727316	1.130505	0.912967

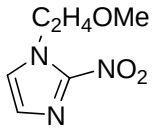
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.514192	0.214828	-0.036495
2	n	2.693197	-0.160007	0.388035
3	c	2.689377	-1.524819	0.316695
4	c	1.496391	-1.964046	-0.153007
5	n	0.732383	-0.844861	-0.387310
6	c	-0.616485	-0.889010	-0.907994
7	c	-1.647035	-0.453873	0.105879

8	o	-1.496188	-0.459397	1.291578
9	n	1.104879	1.531708	-0.116611
10	o	1.902843	2.464370	0.244365
11	o	-0.074245	1.785610	-0.548134
12	o	-2.780733	-0.144887	-0.485984
13	c	-3.890789	0.208245	0.332907
14	h	-0.841412	-1.936286	-1.153797
15	h	-0.714588	-0.300060	-1.816053
16	h	3.543794	-2.104810	0.607405
17	h	1.119266	-2.949395	-0.343452
18	h	-4.695913	0.431277	-0.349554
19	h	-4.159726	-0.619012	0.974484
20	h	-3.651970	1.076888	0.929657

No.40



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-2.383426	1.257892	-0.000036
2	c	-1.517069	2.304175	0.000046
3	c	-0.211145	1.847438	0.000128
4	n	-0.269261	0.475625	0.000096
5	c	-1.618165	0.186811	0.000065
6	n	-2.150328	-1.154551	-0.000017
7	o	-3.368373	-1.287070	-0.000567
8	c	0.882097	-0.449094	0.000323
9	c	2.222997	0.282174	-0.000172
10	o	3.207579	-0.729159	-0.000478
11	c	4.531879	-0.220195	0.000042
12	o	-1.329774	-2.086496	0.000517
13	h	0.816940	-1.093682	-0.878073
14	h	0.817170	-1.092939	0.879291

15	h	2.328609	0.920453	-0.893471
16	h	2.329190	0.920520	0.893005
17	h	-1.864551	3.328225	0.000073
18	h	0.724682	2.383958	-0.000008
19	h	4.724441	0.388588	0.896798
20	h	5.200772	-1.083362	-0.000217
21	h	4.724842	0.389428	-0.896061

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.505691	0.076825	-0.014855
2	n	-2.575235	-0.590119	-0.472466
3	c	-2.245353	-1.913349	-0.376697
4	c	-0.981859	-2.082022	0.136024
5	n	-0.493773	-0.801222	0.387489
6	c	0.858260	-0.552569	0.872255
7	c	1.818274	-0.191881	-0.261304
8	n	-1.398469	1.454121	0.061776
9	o	-2.364198	2.187433	-0.361094
10	o	-0.292567	1.955591	0.552923
11	o	3.149721	-0.217188	0.260960
12	c	4.096623	0.299607	-0.645465
13	h	1.202859	-1.475390	1.355342
14	h	0.841243	0.258273	1.598450
15	h	-2.944146	-2.685466	-0.679182
16	h	-0.393025	-2.960126	0.363820
17	h	5.075848	0.250942	-0.157319
18	h	4.132348	-0.291821	-1.577344
19	h	3.875085	1.346790	-0.907087
20	h	1.565426	0.810076	-0.629810
21	h	1.731528	-0.919104	-1.086520

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.591852	0.188394	-0.000191
2	n	-2.353224	1.231133	0.000102
3	c	-1.500919	2.280366	-0.000864
4	c	-0.214312	1.824972	-0.001645
5	n	-0.270178	0.467343	-0.001312
6	c	0.880286	-0.458560	-0.001256
7	c	2.210197	0.278943	0.001180
8	o	3.190226	-0.718425	0.000955
9	c	4.503404	-0.224033	0.001799
10	n	-2.138268	-1.139850	0.000211
11	o	-1.372171	-2.060461	-0.007173
12	o	-3.326238	-1.250579	0.007540
13	h	0.817171	-1.082186	-0.883739
14	h	0.814945	-1.084914	0.879233
15	h	2.317153	0.905882	-0.882335
16	h	2.315256	0.903793	0.886410
17	h	-1.846098	3.295158	-0.001014
18	h	0.708290	2.367247	-0.002236
19	h	4.690036	0.377461	0.887435
20	h	5.168848	-1.076050	0.001555
21	h	4.690731	0.378444	-0.883028

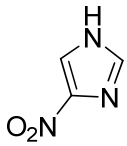
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.481217	0.031171	-0.016051
2	n	-2.506755	-0.650356	-0.461330
3	c	-2.151145	-1.963364	-0.348128
4	c	-0.902896	-2.062753	0.169811
5	n	-0.462832	-0.778751	0.392821
6	c	0.886227	-0.490976	0.877791
7	c	1.841639	-0.199790	-0.268965
8	n	-1.458688	1.414142	0.038592
9	o	-2.440844	2.075814	-0.449604
10	o	-0.464658	2.004253	0.586460
11	o	3.108379	0.024718	0.289025
12	c	4.115104	0.253147	-0.658551

13	h	1.217678	-1.380121	1.407078
14	h	0.860538	0.334930	1.568174
15	h	-2.815824	-2.753067	-0.640878
16	h	-0.290946	-2.911393	0.404573
17	h	5.038703	0.418281	-0.120338
18	h	4.232132	-0.605435	-1.315204
19	h	3.890475	1.130122	-1.260724
20	h	1.515421	0.676157	-0.823133
21	h	1.880469	-1.047611	-0.952616

No.41



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.975659	-0.762491	-0.000315
2	n	0.728089	-1.168135	-0.000482
3	c	-0.004783	-0.017924	0.000028
4	c	0.787669	1.108985	0.000515
5	n	2.062684	0.610974	0.000147
6	n	-1.449960	-0.013202	-0.000085
7	o	-1.991732	1.101058	-0.000742
8	o	-2.039549	-1.088448	0.000784
9	h	2.913273	1.159304	0.001099
10	h	0.550897	2.160839	0.000797
11	h	2.849110	-1.399895	-0.000663

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	n	2.080936	0.606549	-0.000130
2	c	1.987246	-0.758742	0.000031
3	n	0.741876	-1.177817	0.000009
4	c	-0.035914	-0.026317	0.000033
5	c	0.778899	1.110056	0.000048
6	n	-1.418132	-0.019668	0.000021
7	o	-2.086166	-1.124830	-0.000034
8	o	-1.982603	1.158771	0.000006
9	h	2.930054	1.151619	0.000320
10	h	0.542129	2.159970	-0.000102
11	h	2.863823	-1.396539	0.000038

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.034307	0.600961	-0.000118
2	c	1.948582	-0.750071	-0.000017
3	n	0.721681	-1.154532	-0.000065
4	c	-0.007544	-0.007155	-0.000457
5	c	0.781267	1.098528	0.000166
6	n	-1.429084	-0.009942	-0.000069
7	o	-2.002015	-1.059390	0.000297
8	o	-1.983549	1.057751	-0.000076
9	h	2.885901	1.142220	0.001162
10	h	0.559394	2.146734	0.000437
11	h	2.817049	-1.379052	0.000242

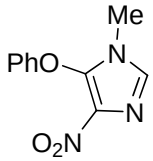
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.789648	1.101133	0.000248
2	n	2.065614	0.589785	-0.000177

3	c	1.966201	-0.747469	0.000035
4	n	0.731718	-1.154383	-0.000065
5	c	-0.020954	-0.007215	0.000055
6	n	-1.401618	-0.012936	0.000001
7	o	-2.007859	1.125206	-0.000193
8	o	-2.055696	-1.114984	0.000102
9	h	2.923261	1.120998	0.000007
10	h	0.578276	2.149099	0.000537
11	h	2.827534	-1.387841	-0.000151

No.42



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	3.898496	0.160100	0.717707
2	c	3.740137	-0.068616	-0.653243
3	c	2.482312	-0.362874	-1.180701
4	c	1.389033	-0.425630	-0.320460
5	c	1.521312	-0.207484	1.048501
6	c	2.787713	0.090820	1.561222
7	o	0.170890	-0.786706	-0.916200
8	c	-0.998075	-0.513029	-0.313041
9	c	-1.713490	0.638047	-0.004123
10	n	-2.932472	0.329930	0.526830
11	c	-2.978357	-0.979256	0.533017
12	n	-1.826803	-1.550093	0.037833
13	n	-1.289621	1.993662	-0.214017
14	o	-0.172129	2.145089	-0.731191
15	c	-1.536055	-2.969222	-0.134679
16	o	-2.044670	2.904219	0.118321
17	h	-3.808670	-1.580320	0.879638
18	h	2.334721	-0.529720	-2.243062

19	h	0.657956	-0.254554	1.705654
20	h	4.596779	-0.010028	-1.319228
21	h	2.898474	0.271342	2.627091
22	h	4.878348	0.395236	1.123317
23	h	-1.476830	-3.220978	-1.197246
24	h	-0.588249	-3.221567	0.346973
25	h	-2.341148	-3.541850	0.329698

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.473501	1.767734	0.097168
2	c	0.871106	0.508021	-0.098383
3	c	1.947761	-0.413126	-0.039080
4	n	3.111933	0.251000	0.313967
5	c	2.784751	1.518271	0.389935
6	o	-0.275546	0.520132	-0.879936
7	c	-1.487707	0.155458	-0.350405
8	c	-2.615826	0.567111	-1.071953
9	c	-3.894122	0.243954	-0.612390
10	c	-4.056372	-0.491730	0.566932
11	c	-2.920438	-0.907304	1.270882
12	c	-1.635373	-0.595509	0.820939
13	n	1.885710	-1.778725	-0.206274
14	o	2.945636	-2.496066	-0.126997
15	c	0.762172	3.008920	0.298554
16	o	0.709610	-2.281904	-0.425317
17	h	3.460056	2.317633	0.677524
18	h	-2.471472	1.134174	-1.988009
19	h	-0.751572	-0.962647	1.327171
20	h	-4.764637	0.569589	-1.179008
21	h	-3.030568	-1.503836	2.174460
22	h	-5.051343	-0.748032	0.924471
23	h	0.039719	3.161613	-0.509104
24	h	0.217868	3.014571	1.255962
25	h	1.480642	3.835177	0.290343

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.603039	1.619109	-0.051473
2	c	0.948437	0.482882	-0.366443
3	c	1.773987	-0.528744	0.033456
4	n	2.912397	-0.031871	0.587961
5	c	2.778664	1.247233	0.518479
6	o	-0.208569	0.525018	-1.011164
7	c	-1.406771	0.261117	-0.367032
8	c	-2.476608	-0.024676	-1.197747
9	c	-3.719200	-0.262181	-0.633706
10	c	-3.887922	-0.215107	0.746205
11	c	-2.802214	0.075221	1.556539
12	c	-1.548331	0.321228	1.005552
13	n	1.545280	-1.918813	-0.097576
14	o	2.393578	-2.678137	0.273541
15	c	1.146254	2.980457	-0.319226
16	o	0.500737	-2.264385	-0.583084
17	h	3.492668	1.971543	0.860658
18	h	-2.327843	-0.061443	-2.263353
19	h	-0.714841	0.550032	1.647606
20	h	-4.555331	-0.486812	-1.273146
21	h	-2.920821	0.117583	2.625464
22	h	-4.854089	-0.402343	1.181149
23	h	1.014601	3.119178	-1.383661
24	h	0.214342	3.167549	0.196539
25	h	1.902551	3.661198	0.045548

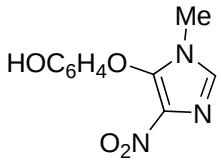
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.521222	-0.158799	0.985487
2	c	-1.445851	-0.005473	-0.388193

3	c	-2.583957	-0.096309	-1.178469
4	c	-3.809126	-0.346901	-0.583298
5	c	-3.906027	-0.502921	0.795600
6	c	-2.760106	-0.406798	1.568856
7	o	-0.279987	0.256835	-1.062369
8	c	0.861827	0.485379	-0.393237
9	n	1.201270	1.771177	-0.036980
10	c	2.400568	1.689196	0.559768
11	n	2.859551	0.477509	0.613492
12	c	1.908246	-0.306156	0.011451
13	c	0.420512	2.972141	-0.281882
14	n	2.058884	-1.672919	-0.127648
15	o	1.136024	-2.330676	-0.734138
16	o	3.103003	-2.258807	0.336740
17	h	2.906231	2.557993	0.937184
18	h	-2.497790	0.029449	-2.244774
19	h	-0.641375	-0.092447	1.600424
20	h	-4.690072	-0.417754	-1.198392
21	h	-2.818666	-0.525560	2.637474
22	h	-4.859499	-0.695299	1.256155
23	h	0.134574	3.019595	-1.324527
24	h	-0.467824	2.985094	0.337614
25	h	1.034988	3.829589	-0.041569

No.43



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-3.584798	-0.022838	-0.370623
2	c	-3.315124	-0.321685	0.970238
3	c	-2.010836	-0.592314	1.374004
4	c	-0.981254	-0.566923	0.436011

5	c	-1.233746	-0.282459	-0.900638
6	c	-2.543975	-0.003748	-1.302506
7	o	0.295127	-0.912894	0.914670
8	c	1.402074	-0.502325	0.276360
9	c	1.992385	0.720487	-0.026779
10	n	3.204315	0.543200	-0.630532
11	c	3.370328	-0.754500	-0.684120
12	n	2.303026	-1.445491	-0.153379
13	n	1.464419	2.024286	0.255325
14	o	0.390042	2.059264	0.875353
15	c	2.154669	-2.889906	-0.014721
16	o	-4.889502	0.239745	-0.704617
17	o	2.096330	3.009474	-0.120052
18	h	4.233740	-1.264667	-1.090458
19	h	-1.781350	-0.809310	2.412425
20	h	-0.428471	-0.260086	-1.628804
21	h	-4.131537	-0.327177	1.685516
22	h	-2.744952	0.229632	-2.346263
23	h	2.204942	-3.181291	1.038285
24	h	1.196513	-3.211570	-0.429642
25	h	2.966355	-3.371238	-0.563661
26	h	-4.951867	0.474292	-1.643484

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-1.769366	1.750940	-0.219649
2	c	-1.249528	0.514102	0.194255
3	c	-2.286517	-0.415470	-0.030092
4	n	-3.358495	0.230336	-0.626716
5	c	-3.012277	1.492553	-0.719204
6	o	-0.158450	0.559244	1.033671
7	c	1.100547	0.244347	0.540670
8	c	2.162181	1.057525	0.943542
9	c	3.465660	0.779764	0.518947
10	c	3.698275	-0.319395	-0.308812
11	c	2.634672	-1.141021	-0.694463
12	c	1.331984	-0.869829	-0.268576
13	o	5.003127	-0.558190	-0.714882
14	n	-2.284059	-1.776421	0.208678

15	o	-3.340168	-2.478094	-0.002560
16	c	-1.052975	3.004628	-0.249693
17	o	-1.158252	-2.298135	0.618152
18	h	-3.617970	2.275481	-1.163213
19	h	1.962570	1.906380	1.592573
20	h	0.497775	-1.535550	-0.481818
21	h	4.299234	1.407957	0.821495
22	h	2.821080	-2.018625	-1.314491
23	h	-0.644315	3.237104	0.739487
24	h	-0.222422	2.976458	-0.969039
25	h	-1.748876	3.797901	-0.540385
26	h	5.014180	-1.362900	-1.255294

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.162221	-1.491534	-0.037096
2	c	1.370793	-0.467291	0.340769
3	c	2.012950	0.659072	-0.094242
4	n	3.171681	0.337122	-0.732778
5	c	3.232115	-0.947025	-0.674959
6	o	0.273651	-0.702390	1.042760
7	c	-0.988050	-0.444262	0.514484
8	c	-1.979250	-0.123934	1.424771
9	c	-3.270941	0.088386	0.980717
10	c	-3.568874	-0.015638	-0.374674
11	c	-2.567729	-0.337506	-1.275661
12	c	-1.269163	-0.561949	-0.828704
13	o	-4.849457	0.204874	-0.751382
14	n	1.606482	2.000347	0.085528
15	o	2.281311	2.873433	-0.381982
16	c	1.927064	-2.907683	0.231706
17	o	0.596754	2.194679	0.709339
18	h	4.020236	-1.556753	-1.073213
19	h	-1.736971	-0.039127	2.470347
20	h	-0.504401	-0.821457	-1.541751
21	h	-4.052657	0.339445	1.677444
22	h	-2.792118	-0.424614	-2.326718

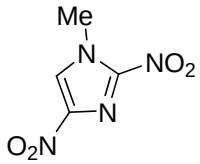
23	h	2.022158	-3.102672	1.291593
24	h	0.939474	-3.187706	-0.107108
25	h	2.668733	-3.475950	-0.311851
26	h	-4.958701	0.129490	-1.703444

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.248670	-0.194875	-0.763801
2	c	1.062751	0.145229	0.560801
3	c	2.154369	0.265635	1.408989
4	c	3.432973	0.043250	0.931103
5	c	3.629381	-0.295812	-0.403468
6	c	2.537344	-0.411429	-1.245176
7	o	-0.170775	0.376952	1.132449
8	c	-1.263145	0.497549	0.362380
9	n	-1.639301	1.736052	-0.108007
10	c	-2.785294	1.548415	-0.780590
11	n	-3.175933	0.311904	-0.784351
12	c	-2.233118	-0.376396	-0.063980
13	c	-0.951314	2.994504	0.123430
14	n	-2.319017	-1.738903	0.152011
15	o	-1.415328	-2.301502	0.872475
16	o	4.903856	-0.498930	-0.820717
17	o	-3.280281	-2.417036	-0.363659
18	h	-3.304197	2.360802	-1.253615
19	h	1.996652	0.531255	2.441052
20	h	0.413351	-0.298974	-1.433237
21	h	4.282860	0.134653	1.586740
22	h	2.679943	-0.675467	-2.281369
23	h	-0.838463	3.166662	1.186197
24	h	0.023794	2.988650	-0.347011
25	h	-1.547771	3.788780	-0.305457
26	h	4.938111	-0.732033	-1.753369

No.44



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.669869	1.312581	0.000000
2	c	-1.212745	0.038989	-0.000058
3	n	-0.262173	-0.916720	-0.000692
4	c	0.860888	-0.239791	-0.000335
5	n	0.680259	1.130816	0.000204
6	n	-2.630528	-0.262774	0.000065
7	o	-3.385338	0.717911	-0.000047
8	n	2.166318	-0.870872	-0.000047
9	o	2.206589	-2.091506	0.000176
10	c	1.663266	2.225419	-0.000023
11	o	3.145157	-0.110605	0.000221
12	o	-2.977109	-1.436314	0.000340
13	h	-1.131692	2.287784	0.000426
14	h	1.104130	3.162350	-0.000292
15	h	2.293325	2.164153	0.887550
16	h	2.293473	2.163495	-0.887412

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.680716	1.273241	-0.000165
2	c	1.226095	0.000596	-0.000022
3	n	0.261949	-0.964934	0.000088

4	c	-0.885950	-0.282984	0.000082
5	n	-0.667077	1.104265	-0.000237
6	n	2.617065	-0.254014	0.000004
7	o	3.389763	0.750337	-0.000386
8	n	-2.160791	-0.830333	-0.000141
9	o	-2.288001	-2.092564	0.000607
10	c	-1.622127	2.211870	0.000831
11	o	-3.165375	-0.013233	-0.001112
12	o	3.021937	-1.433857	0.000212
13	h	1.149266	2.245082	-0.000290
14	h	-1.042183	3.140481	0.001297
15	h	-2.262379	2.164499	-0.880533
16	h	-2.261723	2.163244	0.882599

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

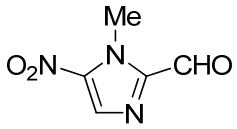
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.674485	1.123044	0.000240
2	c	-0.655450	1.310393	0.000161
3	c	-1.197472	0.057585	0.000170
4	n	-0.250897	-0.891919	0.000295
5	c	0.843300	-0.223088	0.000252
6	n	-2.588589	-0.256822	-0.000179
7	o	-2.913104	-1.404818	-0.000232
8	n	2.131350	-0.870249	-0.000416
9	o	3.095424	-0.164304	-0.002483
10	c	1.657108	2.221257	0.000945
11	o	-3.351502	0.669176	-0.000548
12	o	2.147157	-2.059368	0.001703
13	h	-1.104131	2.284976	0.000259
14	h	1.091886	3.141650	0.002289
15	h	2.269966	2.160352	0.886518
16	h	2.269121	2.162288	-0.885332

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.206106	0.050898	0.000020
2	c	-0.671443	1.296686	0.000009
3	n	0.666140	1.114271	0.000095
4	c	0.866671	-0.243539	0.000108
5	n	-0.250945	-0.910039	0.000120
6	c	1.622405	2.226822	0.000135
7	n	2.113290	-0.837448	0.000128
8	o	2.190650	-2.112092	0.000626
9	n	-2.590884	-0.256205	-0.000072
10	o	-3.365382	0.667685	0.000316
11	o	3.149268	-0.092332	-0.000860
12	o	-2.928505	-1.405648	-0.000563
13	h	-1.123106	2.269260	-0.000084
14	h	2.241083	2.186698	0.881899
15	h	2.241804	2.186111	-0.881077
16	h	1.039604	3.137768	-0.000405

No.45



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.321154	-0.564805	-0.000020
2	n	0.842149	-1.816703	-0.000023
3	c	-0.499524	-1.700171	0.000021
4	c	-0.842917	-0.354063	0.000028
5	n	0.324997	0.376325	0.000033
6	n	-2.161367	0.202384	0.000010
7	o	-2.282061	1.433095	-0.000132

8	c	0.494580	1.841095	0.000081
9	c	2.777612	-0.336366	-0.000041
10	o	3.337894	0.746236	-0.000007
11	o	-3.095684	-0.602390	0.000044
12	h	-1.169961	-2.547387	0.000015
13	h	0.020282	2.263192	-0.886868
14	h	0.020191	2.263144	0.887002
15	h	1.562493	2.045022	0.000141
16	h	3.339925	-1.287679	-0.000075

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.343561	-0.565968	0.000010
2	n	0.826889	-1.823616	0.000027
3	c	-0.499722	-1.690687	0.000025
4	c	-0.869156	-0.328876	0.000029
5	n	0.322936	0.385027	0.000011
6	n	-2.139861	0.195417	0.000029
7	o	-2.301461	1.468008	-0.000064
8	c	0.512763	1.835314	0.000087
9	c	2.757750	-0.351916	-0.000015
10	o	3.379798	0.733845	-0.000083
11	o	-3.121590	-0.628760	-0.000056
12	h	-1.181469	-2.529247	0.000036
13	h	0.045047	2.277555	-0.882761
14	h	0.045272	2.277435	0.883121
15	h	1.587076	2.017116	-0.000030
16	h	3.309167	-1.312606	-0.000017

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

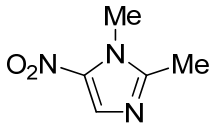
1	n	-0.324149	0.379372	0.000035
2	c	-1.293249	-0.545502	-0.000130
3	n	-0.832631	-1.775820	-0.000307
4	c	0.503921	-1.672173	0.000303
5	c	0.833632	-0.349742	-0.000143
6	c	-2.767641	-0.340161	-0.000110
7	o	-3.323511	0.713992	0.000007
8	n	2.143550	0.192772	-0.000067
9	o	3.051215	-0.590668	0.000422
10	c	-0.481957	1.844325	0.000479
11	o	2.277509	1.382046	-0.000687
12	h	1.159983	-2.519723	0.000405
13	h	-0.016106	2.251711	0.884498
14	h	-0.016294	2.252263	-0.883384
15	h	-1.532919	2.062001	0.000657
16	h	-3.311998	-1.283977	-0.000129

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.320479	0.389989	0.000121
2	c	1.317406	-0.537972	-0.000127
3	n	0.842600	-1.774752	0.000026
4	c	-0.491710	-1.671707	0.000135
5	c	-0.850778	-0.329303	-0.000182
6	c	2.762707	-0.347541	-0.000183
7	o	3.355150	0.701433	-0.000149
8	n	-2.116290	0.180380	-0.000282
9	o	-3.094337	-0.655718	0.000435
10	c	0.488211	1.845652	0.000602
11	o	-2.315363	1.441699	-0.000620
12	h	-1.144105	-2.520174	0.000128
13	h	0.027704	2.268544	-0.878791
14	h	0.028071	2.267886	0.880509
15	h	1.541983	2.056063	0.000459
16	h	3.300213	-1.295727	-0.000158

No.46



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.649366	-0.311825	-0.000039
2	n	1.320623	-1.605480	-0.000077
3	c	-0.034439	-1.650570	-0.000020
4	c	-0.542126	-0.365405	0.000054
5	n	0.549283	0.498235	0.000041
6	n	-1.900777	0.041362	-0.000027
7	o	-2.154059	1.257271	-0.000376
8	c	0.554451	1.962865	0.000220
9	c	3.058720	0.183984	-0.000058
10	o	-2.755516	-0.851473	0.000240
11	h	-0.592280	-2.575818	-0.000049
12	h	0.045319	2.344827	-0.886111
13	h	0.044487	2.344575	0.886171
14	h	1.592698	2.295267	0.000763
15	h	3.718573	-0.685944	-0.000143
16	h	3.283999	0.788870	-0.887039
17	h	3.284071	0.788734	0.886998

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.555180	0.490566	-0.000218
2	c	1.662860	-0.339221	-0.000173
3	n	1.324707	-1.616851	0.000135

4	c	-0.050359	-1.647104	-0.000067
5	c	-0.568624	-0.351832	0.000013
6	c	3.064438	0.178971	-0.000232
7	n	-1.887911	0.050625	-0.000035
8	o	-2.789512	-0.880027	0.000511
9	c	0.612482	1.944082	0.000682
10	o	-2.190935	1.324328	-0.000850
11	h	-0.616443	-2.565333	-0.000084
12	h	1.143561	2.308576	-0.889733
13	h	-0.417691	2.304495	-0.000918
14	h	1.139930	2.307762	0.893659
15	h	3.741719	-0.680084	0.000131
16	h	3.292052	0.794895	-0.884444
17	h	3.291836	0.795521	0.883587

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

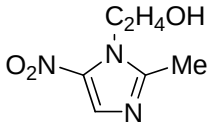
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	0.555488	0.491881	-0.000073
2	c	1.618915	-0.317125	-0.000013
3	n	1.281384	-1.592991	-0.000005
4	c	-0.062046	-1.627345	-0.000016
5	c	-0.538874	-0.354098	0.000125
6	c	3.037039	0.155167	0.000038
7	n	-1.882526	0.050555	0.000066
8	o	-2.720174	-0.813795	-0.000131
9	c	0.581893	1.956030	-0.000098
10	o	-2.137067	1.224398	0.000121
11	h	-0.622242	-2.541603	-0.000013
12	h	0.089260	2.333419	-0.883557
13	h	0.089042	2.333416	0.883235
14	h	1.611903	2.273627	0.000012
15	h	3.683889	-0.711107	-0.000707
16	h	3.251912	0.753460	-0.879364
17	h	3.252186	0.752070	0.880337

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.056767	-1.631243	-0.000103
2	c	-0.551165	-0.352016	0.000024
3	n	0.554385	0.486066	-0.000250
4	c	1.639978	-0.329714	-0.000296
5	n	1.313005	-1.589455	-0.000581
6	n	-1.863606	0.048095	0.000004
7	o	-2.770519	-0.869601	0.001981
8	c	0.590924	1.944195	0.001913
9	c	3.052360	0.165798	-0.000329
10	o	-2.172409	1.292494	-0.002954
11	h	-0.606598	-2.549312	-0.000145
12	h	1.623749	2.256328	0.002820
13	h	0.102277	2.336363	-0.876996
14	h	0.101553	2.333844	0.881668
15	h	3.714187	-0.690116	-0.002353
16	h	3.264325	0.768996	-0.877852
17	h	3.265472	0.765692	0.879188

No.47



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-1.072645	2.271093	-0.292183
2	c	-1.891677	1.191243	-0.312099
3	c	-1.174300	0.053904	0.007481

4	n	0.139891	0.459481	0.236084
5	c	0.136186	1.812673	0.038254
6	n	-1.653981	-1.278382	0.088652
7	o	-2.861872	-1.452988	-0.107500
8	c	1.339454	2.684123	0.194561
9	c	1.316082	-0.338949	0.604433
10	c	1.967257	-1.010792	-0.606568
11	o	3.201288	-1.546660	-0.135844
12	o	-0.847148	-2.188067	0.344440
13	h	1.024541	-1.090185	1.337067
14	h	2.036829	0.338041	1.068047
15	h	1.307348	-1.795798	-0.993027
16	h	2.140109	-0.268452	-1.400834
17	h	3.518145	-2.220782	-0.754967
18	h	-2.943334	1.255488	-0.551302
19	h	1.693429	2.709007	1.233062
20	h	2.174847	2.357233	-0.435304
21	h	1.059073	3.698600	-0.095755

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.766812	-0.662319	-0.005760
2	n	-1.555659	-1.901830	-0.412077
3	c	-0.193793	-2.086209	-0.388600
4	c	0.443202	-0.925940	0.040748
5	n	-0.584145	-0.007188	0.295627
6	n	1.791981	-0.680588	0.187850
7	o	2.202889	0.534415	0.516588
8	c	-0.488293	1.360066	0.803873
9	c	-0.278844	2.436341	-0.274495
10	o	0.939709	2.345360	-0.970011
11	c	-3.119155	-0.040718	0.139872
12	o	2.613875	-1.647890	-0.026200
13	h	0.333062	1.394572	1.520868
14	h	-1.424529	1.580106	1.331104
15	h	-1.104230	2.386823	-1.002995
16	h	-0.359331	3.413830	0.240451
17	h	1.535172	1.696596	-0.484904
18	h	0.278452	-3.011053	-0.681143

19	h	-3.361933	0.217269	1.182617
20	h	-3.234447	0.876303	-0.455711
21	h	-3.857062	-0.769616	-0.206930

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.072919	1.795401	0.037173
2	n	-1.137194	2.205331	-0.284392
3	c	-1.913472	1.107574	-0.302568
4	c	-1.158901	0.021230	0.008806
5	n	0.133392	0.471479	0.229674
6	n	-1.599197	-1.310517	0.082820
7	o	-0.804332	-2.178608	0.319473
8	c	1.338562	-0.276416	0.610244
9	c	2.030132	-0.885604	-0.600697
10	o	3.144366	-1.584117	-0.105906
11	c	1.238660	2.719350	0.181876
12	o	-2.771281	-1.513029	-0.101876
13	h	1.067739	-1.041097	1.322168
14	h	2.006558	0.414031	1.107538
15	h	1.358259	-1.555046	-1.126382
16	h	2.342445	-0.103280	-1.288266
17	h	3.631030	-1.976293	-0.832459
18	h	-2.959215	1.137541	-0.536924
19	h	1.592476	2.739567	1.207815
20	h	2.063455	2.422760	-0.456608
21	h	0.920823	3.714586	-0.096134

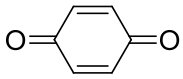
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	-0.570476	-0.058376	0.299835

2	c	-1.646358	-0.833585	-0.003363
3	n	-1.305072	-2.019456	-0.415166
4	c	0.062833	-2.056602	-0.390472
5	c	0.545080	-0.848733	0.048071
6	c	-3.063624	-0.376386	0.141167
7	n	1.859295	-0.482160	0.198725
8	o	2.761186	-1.366136	-0.026237
9	c	-0.644496	1.303738	0.830697
10	c	-0.594712	2.388818	-0.239127
11	o	0.568544	2.357166	-1.024792
12	o	2.182196	0.733756	0.490805
13	h	0.155480	1.435070	1.543203
14	h	-1.577917	1.401620	1.373693
15	h	-1.441938	2.297034	-0.911017
16	h	-0.678208	3.347530	0.270974
17	h	1.267335	1.906165	-0.544570
18	h	0.623584	-2.919182	-0.684723
19	h	-3.307667	-0.164410	1.177947
20	h	-3.259536	0.519552	-0.438589
21	h	-3.715099	-1.165214	-0.210724

No.48



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.672421	-1.270973	0.000000
2	c	-1.443455	-0.000001	0.000017
3	c	-0.672421	1.270975	0.000003
4	c	0.672418	1.270976	0.000017
5	c	1.443455	-0.000001	-0.000064
6	c	0.672425	-1.270972	0.000023
7	o	-2.670648	-0.000002	-0.000015
8	o	2.670649	0.000000	0.000004
9	h	-1.260003	2.185243	-0.000002

10	h	1.259999	2.185246	0.000056
11	h	1.259991	-2.185251	0.000047
12	h	-1.260001	-2.185242	-0.000006

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.687478	-1.224770	0.000003
2	c	-1.467438	-0.000006	-0.000003
3	c	-0.687489	1.224787	0.000006
4	c	0.687491	1.224786	0.000000
5	c	1.467439	-0.000006	-0.000061
6	c	0.687477	-1.224772	0.000002
7	o	-2.740134	-0.000006	0.000003
8	o	2.740133	-0.000007	0.000027
9	h	-1.248900	2.158910	0.000019
10	h	1.248903	2.158910	0.000023
11	h	1.248855	-2.158915	0.000028
12	h	-1.248857	-2.158914	0.000013

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.662491	1.274044	0.000035
2	c	0.662547	1.274063	-0.000053
3	c	1.430865	-0.000004	-0.000089
4	c	0.662491	-1.274044	0.000023
5	c	-0.662548	-1.274062	-0.000007
6	c	-1.430865	0.000004	0.000067
7	o	2.631831	-0.000029	0.000047
8	o	-2.631831	0.000029	-0.000033
9	h	1.241175	-2.182927	0.000012
10	h	-1.241221	-2.182951	-0.000055

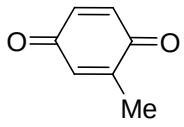
11	h	-1.241174	2.182927	0.000110
12	h	1.241221	2.182951	-0.000035

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.441199	0.000003	-0.000573
2	c	-0.678234	-1.219935	-0.000001
3	c	0.681259	-1.224364	0.000020
4	c	1.443995	-0.000007	-0.000490
5	c	0.681287	1.224365	0.000018
6	c	-0.678207	1.219967	0.000017
7	o	2.695404	-0.000020	0.000269
8	o	-2.703265	-0.000005	0.000306
9	h	1.230280	2.152860	0.000352
10	h	-1.225494	2.149879	0.000354
11	h	-1.225542	-2.149835	0.000371
12	h	1.230233	-2.152872	0.000390

No.49



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.151982	1.669641	0.000192
2	c	1.404638	1.184192	-0.000040
3	c	1.650923	-0.281589	-0.000080
4	c	0.472254	-1.177152	-0.000269
5	c	-0.796351	-0.714261	0.000073
6	c	-1.028947	0.768374	0.000004

7	o	2.794747	-0.730082	0.000113
8	c	-2.010692	-1.594943	0.000176
9	o	-2.166342	1.229669	-0.000208
10	h	0.694167	-2.241905	-0.000516
11	h	-0.067370	2.734101	0.000340
12	h	2.285393	1.820860	-0.000053
13	h	-2.636795	-1.391472	-0.876478
14	h	-1.729390	-2.651793	-0.000345
15	h	-2.636086	-1.392060	0.877471

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.049349	1.635536	0.000059
2	c	-1.351280	1.193862	0.000042
3	c	-1.682199	-0.218045	-0.000057
4	c	-0.544355	-1.119299	0.000024
5	c	0.765404	-0.693751	0.000084
6	c	1.083897	0.733007	0.000024
7	o	-2.883239	-0.639190	-0.000056
8	c	1.920582	-1.662708	0.000012
9	o	2.286644	1.151619	-0.000112
10	h	-0.777304	-2.184951	0.000019
11	h	0.183190	2.700201	0.000102
12	h	-2.185851	1.894491	0.000069
13	h	2.565251	-1.510024	0.876291
14	h	1.565724	-2.701132	-0.000287
15	h	2.565550	-1.509623	-0.875981

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.006581	0.781868	-0.000430

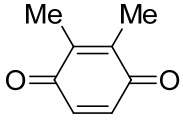
2	c	0.189343	1.666954	0.001119
3	c	1.415204	1.167429	0.000940
4	c	1.632154	-0.303054	-0.000315
5	c	0.439632	-1.183661	0.000158
6	c	-0.800315	-0.704477	0.000238
7	o	2.743715	-0.762599	-0.001078
8	c	-2.029667	-1.566484	0.000777
9	o	-2.110926	1.251896	-0.001616
10	h	0.640775	-2.242641	0.000298
11	h	-0.005779	2.726585	0.001904
12	h	2.296348	1.787412	0.001614
13	h	-2.638344	-1.361321	-0.873760
14	h	-1.756408	-2.614516	0.000675
15	h	-2.637520	-1.361344	0.875898

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.056616	0.741280	-0.000140
2	c	0.075390	1.631647	0.000077
3	c	1.355883	1.173326	-0.000021
4	c	1.652731	-0.230770	-0.000177
5	c	0.519215	-1.117339	0.000003
6	c	-0.772918	-0.684030	-0.000054
7	o	2.839286	-0.666245	0.000087
8	c	-1.933304	-1.645639	0.000050
9	o	-2.229167	1.176010	0.000028
10	h	0.730216	-2.175944	0.000106
11	h	-0.131988	2.690282	0.000243
12	h	2.185037	1.863624	0.000099
13	h	-2.562297	-1.497704	-0.872911
14	h	-1.582020	-2.671513	0.000028
15	h	-2.562183	-1.497708	0.873093

No.50



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.426533	-0.606392	-0.000024
2	c	-0.661373	-1.877342	-0.000100
3	c	0.679568	-1.869863	-0.000119
4	c	1.438092	-0.593605	-0.000021
5	c	0.681175	0.700534	-0.000036
6	c	-0.678330	0.688704	-0.000036
7	o	2.666606	-0.618426	0.000200
8	c	1.509905	1.961124	-0.000052
9	c	-1.535673	1.923660	-0.000028
10	o	-2.655270	-0.626521	0.000179
11	h	-1.250986	-2.790300	-0.000153
12	h	1.278571	-2.776594	-0.000190
13	h	-2.196014	1.932023	-0.875404
14	h	-2.195776	1.932179	0.875529
15	h	-0.940108	2.837936	-0.000182
16	h	1.299971	2.575860	-0.883606
17	h	1.300139	2.575753	0.883625
18	h	2.572527	1.711801	-0.000157

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	C	-0.692588	0.644036	0.000033
2	C	0.692614	0.643936	0.000027
3	C	1.459270	-0.603080	0.000064
4	C	0.686044	-1.826197	0.000015
5	C	-0.686179	-1.826170	0.000020
6	C	-1.459350	-0.602988	-0.000054
7	C	1.476519	1.935562	0.000053
8	O	2.733058	-0.620580	-0.000110

9	O	-2.733180	-0.620483	0.000047
10	C	-1.476279	1.935830	-0.000072
11	H	1.251933	-2.757254	-0.000026
12	H	-1.252094	-2.757189	-0.000017
13	H	2.546659	1.709773	-0.000875
14	H	1.248048	2.554798	-0.881093
15	H	1.249440	2.553662	0.882400
16	H	-1.247737	2.554941	0.881173
17	H	-1.249162	2.553979	-0.882374
18	H	-2.546414	1.710222	0.000798

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

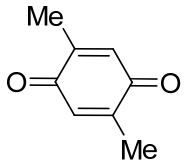
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.665803	0.689319	0.000031
2	c	1.412119	-0.608636	-0.000027
3	c	0.649354	-1.881540	0.000243
4	c	-0.671784	-1.872331	0.000173
5	c	-1.427271	-0.592765	-0.000131
6	c	-0.670695	0.702875	0.000005
7	o	2.614155	-0.628156	-0.000306
8	o	-2.628946	-0.616901	-0.000224
9	c	-1.494704	1.969673	0.000082
10	c	1.531614	1.920588	0.000099
11	h	1.229304	-2.789406	0.000425
12	h	-1.263115	-2.772739	0.000330
13	h	2.175175	1.927753	0.873905
14	h	2.175637	1.927524	-0.873363
15	h	0.942377	2.825593	-0.000193
16	h	-1.279142	2.570525	0.877505
17	h	-1.279478	2.570413	-0.877500
18	h	-2.549048	1.737693	0.000289

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.665406	-1.821754	-0.000021
2	c	-1.423339	-0.607938	-0.000026
3	c	-0.681860	0.639196	0.000312
4	c	0.688780	0.657726	-0.000416
5	c	1.442567	-0.590680	-0.000352
6	c	0.693119	-1.818260	0.000027
7	o	-2.688342	-0.622544	-0.001031
8	c	-1.513837	1.900260	0.001530
9	c	1.477985	1.950680	-0.001463
10	o	2.693084	-0.611121	0.001255
11	h	1.254304	-2.739126	0.000240
12	h	-1.212741	-2.751484	0.000012
13	h	2.537858	1.743001	-0.005011
14	h	1.251320	2.554560	-0.875606
15	h	1.256942	2.552753	0.875419
16	h	-2.162925	1.928020	0.872085
17	h	-0.908780	2.795625	0.003178
18	h	-2.161969	1.930589	-0.869655

No.51



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.320925	1.390333	-0.000060
2	c	1.366381	0.537925	0.000005
3	c	1.087322	-0.936417	0.000040
4	c	-0.320943	-1.390353	0.000048
5	c	-1.366374	-0.537903	0.000024

6	c	-1.087325	0.936388	-0.000080
7	c	2.803079	0.967699	0.000091
8	o	2.008597	-1.749515	-0.000140
9	c	-2.803105	-0.967742	0.000052
10	o	-2.008555	1.749561	-0.000032
11	h	-0.458377	-2.469318	0.000039
12	h	0.458322	2.469311	-0.000105
13	h	-3.326859	-0.568592	-0.876509
14	h	-2.886825	-2.058274	-0.000280
15	h	-3.326635	-0.569174	0.877022
16	h	2.886819	2.058244	-0.000710
17	h	3.326441	0.569635	0.877394
18	h	3.327023	0.568208	-0.876194

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.228047	-1.375379	-0.000099
2	c	-1.323922	-0.542006	-0.000093
3	c	-1.142508	0.906502	-0.000311
4	c	0.228021	1.375507	-0.000092
5	c	1.323930	0.542048	-0.000062
6	c	1.142551	-0.906394	-0.000323
7	c	-2.735164	-1.072607	0.000226
8	o	-2.132685	1.707206	0.000066
9	c	2.735146	1.072583	0.000236
10	o	2.132613	-1.707262	0.000074
11	h	0.359599	2.458423	0.000053
12	h	-0.359515	-2.458335	0.000047
13	h	3.293851	0.714908	-0.875675
14	h	2.744831	2.170004	0.000128
15	h	3.293430	0.715050	0.876418
16	h	-2.744563	-2.170106	-0.000579
17	h	-3.293116	-0.716209	0.877056
18	h	-3.293974	-0.714807	-0.875461

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.061569	0.946959	-0.000530
2	c	-0.356441	1.380040	0.000319
3	c	-1.368554	0.520381	0.000385
4	c	-1.061568	-0.946958	-0.000664
5	c	0.356441	-1.380040	0.000197
6	c	1.368554	-0.520382	0.000340
7	c	-2.814132	0.925257	0.001190
8	o	-1.946951	-1.759901	-0.001490
9	c	2.814131	-0.925259	0.001246
10	o	1.946953	1.759903	-0.001608
11	h	0.513176	-2.446531	0.000583
12	h	-0.513196	2.446528	0.000708
13	h	3.319516	-0.529258	0.876011
14	h	2.904571	-2.004643	0.001932
15	h	3.320364	-0.530330	-0.873505
16	h	-2.904572	2.004641	0.002019
17	h	-3.320250	0.530456	-0.873687
18	h	-3.319630	0.529126	0.875829

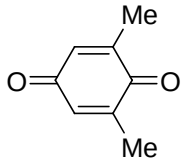
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.107733	0.912453	-0.001000
2	6	-0.258347	1.362127	-0.000355
3	6	-1.327385	0.519610	-0.000273
4	6	-1.107697	-0.912393	-0.000902
5	6	0.258362	-1.362087	-0.000381
6	6	1.327384	-0.519583	-0.000356
7	6	-2.743992	1.033339	0.000525
8	8	-2.065440	-1.726429	0.000494
9	6	2.743912	-1.033508	0.000557

10	8	2.065502	1.726538	0.000520
11	1	0.412161	-2.430443	0.000173
12	1	-0.412165	2.430481	0.000192
13	1	3.286077	-0.681297	0.873362
14	1	2.760625	-2.118006	0.001027
15	1	3.286958	-0.682021	-0.871989
16	1	-2.760857	2.117833	0.000813
17	1	-3.286992	0.681625	-0.871960
18	1	-3.286123	0.681212	0.873388

No.52



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.027094	-1.268266	-0.000003
2	c	1.791238	-0.000763	0.000072
3	c	1.028333	1.267402	0.000003
4	c	-0.320198	1.295147	0.000015
5	c	-1.078036	0.000476	0.000102
6	c	-0.321400	-1.294852	0.000058
7	o	3.021221	-0.001335	-0.000033
8	c	-1.132232	2.557142	-0.000052
9	o	-2.305618	0.000982	0.000004
10	c	-1.134537	-2.556176	-0.000062
11	h	1.624609	2.176990	-0.000041
12	h	-0.488061	-3.438330	-0.000637
13	h	-1.791055	-2.595416	0.877148
14	h	-1.791719	-2.594814	-0.876717
15	h	1.622580	-2.178355	-0.000103
16	h	-1.789003	2.596646	-0.876978
17	h	-1.788933	2.596786	0.876920
18	h	-0.484825	3.438652	-0.000148

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.340258	-1.242446	0.000096
2	6	1.036473	-1.224481	0.000005
3	6	1.812178	-0.000010	0.000195
4	6	1.036489	1.224470	0.000013
5	6	-0.340243	1.242453	0.000105
6	6	-1.104524	0.000003	0.000485
7	8	3.084997	-0.000018	-0.000156
8	6	-1.120135	2.533428	-0.000111
9	8	-2.378652	0.000011	-0.000183
10	6	-1.120167	-2.533411	-0.000107
11	1	1.602465	2.156899	-0.000205
12	1	-0.447671	-3.400680	-0.000649
13	1	-1.779520	-2.598755	0.876239
14	1	-1.780135	-2.598104	-0.876031
15	1	1.602436	-2.156917	-0.000238
16	1	-1.779895	2.598247	-0.876186
17	1	-1.779695	2.598662	0.876084
18	1	-0.447628	3.400687	-0.000394

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.313032	1.295893	-0.000077
2	c	-1.014603	1.271343	-0.000067
3	c	-1.774445	-0.000042	-0.000318
4	c	-1.014542	-1.271390	0.000029
5	c	0.313095	-1.295876	-0.000019
6	c	1.070861	0.000021	-0.000344
7	o	-2.979103	-0.000071	0.000182

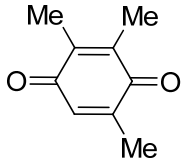
8	c	1.125393	-2.559104	0.000128
9	o	2.270265	0.000050	0.000006
10	c	1.125269	2.559161	0.000171
11	h	-1.603868	-2.174014	0.000169
12	h	0.475065	3.425580	-0.000052
13	h	1.765605	2.600153	0.875235
14	h	1.766224	2.600139	-0.874430
15	h	-1.603989	2.173930	0.000089
16	h	1.765784	-2.600325	-0.874884
17	h	1.766297	-2.599791	0.874782
18	h	0.475231	-3.425553	0.000575

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.089532	0.000081	-0.000038
2	c	-0.339816	-1.242114	-0.000022
3	c	1.023549	-1.218489	-0.000046
4	c	1.781299	-0.000128	-0.000108
5	c	1.023730	1.218344	-0.000032
6	c	-0.339631	1.242171	-0.000068
7	c	-1.109743	-2.538085	0.000088
8	o	3.048009	-0.000222	0.000078
9	c	-1.109344	2.538272	0.000080
10	o	-2.339082	0.000130	-0.000054
11	h	1.579586	2.143581	0.000123
12	h	-0.433541	-3.385885	-0.000230
13	h	-1.751662	-2.611246	0.873107
14	h	-1.752143	-2.611005	-0.872594
15	h	1.579268	-2.143808	-0.000034
16	h	-1.751294	2.611606	-0.872901
17	h	-1.751701	2.611225	0.872789
18	h	-0.433000	3.385962	0.000423

No.53



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.796042	-1.404146	-0.000011
2	c	0.667137	-1.612851	0.000090
3	c	1.543710	-0.590705	-0.000028
4	c	1.015612	0.812031	-0.000041
5	c	-0.462854	1.044209	-0.000037
6	c	-1.325471	-0.004584	-0.000144
7	c	3.034235	-0.761552	-0.000062
8	o	1.802544	1.756107	0.000077
9	c	-0.930721	2.475293	0.000114
10	c	-2.819635	0.169798	-0.000124
11	o	-1.554024	-2.373069	0.000067
12	h	0.988998	-2.651706	0.000153
13	h	-1.546688	2.687791	-0.883363
14	h	-1.553463	2.685429	0.879337
15	h	-0.080366	3.159296	0.004015
16	h	3.480781	-0.278177	-0.876858
17	h	3.480846	-0.278107	0.876659
18	h	3.306361	-1.821016	-0.000033
19	h	-3.151176	0.730384	0.883707
20	h	-3.150565	0.737847	-0.879288
21	h	-3.318728	-0.801001	-0.004024

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	C	-1.297999	0.057587	-0.000150
2	C	-0.917848	-1.353380	-0.000236
3	C	0.501134	-1.634399	0.000010
4	C	1.466498	-0.656078	-0.000069
5	C	1.090034	0.751564	-0.000394
6	C	-0.338670	1.056680	-0.000058
7	O	-1.779141	-2.292557	0.000210
8	C	2.937949	-0.984906	0.000127
9	O	1.979635	1.664859	0.000027
10	C	-0.731511	2.515859	0.000287
11	C	-2.773337	0.381126	-0.000098
12	H	0.779611	-2.688622	0.000253
13	H	-1.333685	2.778050	-0.883308
14	H	-1.340184	2.775825	0.880005
15	H	0.169428	3.135613	0.004021
16	H	3.441524	-0.554182	-0.876104
17	H	3.441414	-0.553706	0.876184
18	H	3.097543	-2.070668	0.000421
19	H	-3.065492	0.969303	0.883661
20	H	-3.064179	0.975474	-0.880083
21	H	-3.347431	-0.549823	-0.003469

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.332545	0.044354	0.000160
2	c	-0.819481	-1.364007	-0.000129
3	c	0.638085	-1.614762	0.000362
4	c	1.519840	-0.625604	0.000292
5	c	1.013570	0.783345	-0.000188
6	c	-0.462593	1.058466	0.000099
7	o	-1.585329	-2.292810	-0.000739
8	c	3.007871	-0.824214	0.000406
9	o	1.795277	1.695267	-0.000915
10	c	-0.807879	2.525240	0.000270
11	c	-2.834850	0.155214	0.000297
12	h	0.933243	-2.651294	0.000592

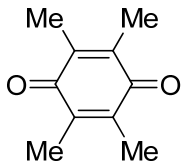
13	h	-0.381138	3.009010	-0.871944
14	h	-1.872736	2.697317	-0.001005
15	h	-0.383284	3.008327	0.873935
16	h	3.454432	-0.363327	-0.874422
17	h	3.454444	-0.362514	0.874805
18	h	3.246245	-1.880797	0.000853
19	h	-3.244542	-0.342584	0.872882
20	h	-3.173707	1.179308	0.001096
21	h	-3.244643	-0.341297	-0.872976

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.065288	0.758508	-0.000212
2	c	-0.360481	1.057212	0.000831
3	c	-1.286974	0.046815	0.003088
4	c	-0.876706	-1.340081	0.000534
5	c	0.528595	-1.611162	0.003412
6	c	1.474185	-0.631336	0.002488
7	c	-0.765821	2.517181	-0.002763
8	c	-2.776251	0.300997	0.005227
9	o	-1.725091	-2.280833	-0.009047
10	c	2.948121	-0.946631	0.001584
11	o	1.924855	1.665995	-0.003325
12	h	0.824409	-2.649224	0.003859
13	h	-1.358469	2.762866	-0.879674
14	h	-1.361319	2.767123	0.870910
15	h	0.108773	3.150482	-0.003026
16	h	3.437941	-0.530401	-0.873938
17	h	3.441145	-0.522424	0.871383
18	h	3.109334	-2.019192	0.006022
19	h	-3.016784	1.354725	0.004178
20	h	-3.243190	-0.153654	-0.863795
21	h	-3.239671	-0.150610	0.877925

No.54



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.012697	1.421761	0.000056
2	c	1.294745	0.692762	0.000056
3	c	1.299853	-0.662349	0.000037
4	c	0.012710	-1.421745	-0.000096
5	c	-1.294762	-0.692759	-0.000007
6	c	-1.299871	0.662346	0.000051
7	c	2.542237	1.541162	0.000077
8	c	2.544991	-1.505338	0.000165
9	o	0.038927	-2.651773	-0.000298
10	c	-2.542238	-1.541179	0.000107
11	c	-2.545007	1.505336	0.000121
12	o	-0.038892	2.651789	-0.000317
13	h	-2.563070	2.165262	0.875541
14	h	-2.563228	2.165204	-0.875339
15	h	-3.450831	0.896532	0.000243
16	h	-3.160052	-1.340515	0.883810
17	h	-3.160531	-1.340013	-0.883141
18	h	-2.276646	-2.599638	-0.000234
19	h	2.562755	-2.165738	0.875229
20	h	2.563502	-2.164747	-0.875642
21	h	3.450825	-0.896551	0.000876
22	h	3.160539	1.339855	0.883280
23	h	3.160028	1.340629	-0.883680
24	h	2.276664	2.599624	0.000572

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.001376	1.451994	-0.000043
2	c	-1.244640	0.692209	-0.000031
3	c	-1.245878	-0.690158	-0.000152
4	c	-0.001375	-1.451994	-0.000429
5	c	1.244640	-0.692210	-0.000142
6	c	1.245878	0.690158	-0.000040
7	c	-2.535913	1.476956	0.000234
8	c	-2.538417	-1.472875	0.000019
9	o	-0.002851	-2.727105	0.000218
10	c	2.535913	-1.476957	0.000041
11	c	2.538417	1.472874	0.000213
12	0	0.002852	2.727106	-0.000234
13	h	-2.315552	-2.543246	0.000369
14	h	-3.156896	-1.243095	0.881513
15	h	-3.156703	-1.243703	-0.881781
16	h	-3.154296	1.248785	0.882238
17	h	-2.311215	2.546895	-0.000209
18	h	-3.155059	1.248126	-0.881065
19	h	2.315553	2.543245	0.000707
20	h	3.156889	1.242979	0.881681
21	h	3.156689	1.243818	-0.881628
22	h	3.154297	-1.248876	0.882068
23	h	2.311215	-2.546897	-0.000547
24	h	3.155066	-1.248023	-0.881226

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.304965	0.666999	-0.000135
2	c	-1.305316	-0.666319	-0.000163
3	c	-0.000470	-1.401175	-0.000329
4	c	1.304942	-0.666997	-0.000329
5	c	1.305316	0.666321	0.000043
6	c	0.000482	1.401200	0.000364

7	c	-2.518067	-1.560041	0.000270
8	o	-0.000975	-2.603985	0.000305
9	c	2.517290	-1.561376	-0.000339
10	c	2.518083	1.560022	0.000568
11	o	0.001008	2.604011	-0.000489
12	c	-2.517328	1.561356	-0.000040
13	h	-2.507419	-2.204506	-0.872317
14	h	-2.507311	-2.203842	0.873354
15	h	-3.440464	-1.000689	0.000119
16	h	-3.439899	1.002365	0.000389
17	h	-2.506201	2.205837	0.872566
18	h	-2.506631	2.205223	-0.873089
19	h	2.507290	2.204816	-0.871772
20	h	2.507510	2.203501	0.873894
21	h	3.440470	1.000654	0.000045
22	h	3.439871	-1.002401	0.000340
23	h	2.506054	-2.206120	0.872070
24	h	2.506679	-2.204979	-0.873585

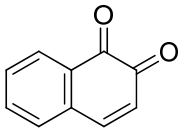
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.258215	-0.651485	-0.000087
2	c	1.232721	0.714526	-0.000496
3	c	-0.031832	1.422443	0.000054
4	c	-1.256399	0.650898	-0.000002
5	c	-1.234481	-0.715180	-0.000580
6	c	0.031907	-1.423109	0.000139
7	c	2.502649	1.541251	-0.001598
8	o	-0.080143	2.681614	0.001024
9	c	-2.539820	1.448757	0.000873
10	c	-2.503818	-1.542593	-0.001366
11	o	0.079679	-2.677399	0.000660
12	c	2.541260	-1.449948	0.001106
13	h	-2.263822	-2.595353	-0.005324
14	h	-3.112933	-1.340400	0.875581
15	h	-3.115844	-1.334279	-0.874743
16	h	-2.589733	2.095151	0.872402
17	h	-2.590008	2.096870	-0.869326
18	h	-3.416471	0.816539	0.000490

19	h	2.262084	2.593789	-0.003731
20	h	3.113048	1.337709	0.874193
21	h	3.113606	1.334138	-0.876113
22	h	2.592550	-2.094287	0.874135
23	h	2.591329	-2.099612	-0.867958
24	h	3.417507	-0.817327	-0.001349

No.55



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.723614	1.564410	0.000005
2	c	-0.412340	1.891567	0.000006
3	c	0.666364	0.903985	0.000002
4	c	0.368609	-0.480329	-0.000004
5	c	-1.049537	-0.935019	-0.000005
6	c	-2.160173	0.162166	0.000000
7	c	1.403006	-1.421094	-0.000008
8	c	2.735963	-1.003292	-0.000007
9	c	3.036662	0.362214	-0.000001
10	c	2.008643	1.308882	0.000003
11	o	-1.367766	-2.110192	0.000026
12	o	-3.334567	-0.168142	-0.000020
13	h	-0.118280	2.939829	0.000010
14	h	4.072133	0.692019	0.000000
15	h	2.247443	2.369820	0.000007
16	h	1.145606	-2.476036	-0.000012
17	h	3.535875	-1.738435	-0.000010
18	h	-2.505627	2.318535	0.000009

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.050265	1.288854	0.000014
2	c	0.680600	0.931019	-0.000015
3	c	0.329301	-0.457475	-0.000031
4	c	1.365578	-1.417592	-0.000018
5	c	2.702194	-1.043806	0.000010
6	c	3.050062	0.326300	0.000027
7	c	-1.077790	-0.902580	-0.000062
8	c	-2.137230	0.159760	-0.000075
9	c	-1.686312	1.540626	-0.000012
10	c	-0.364950	1.912460	-0.000001
11	o	-1.370415	-2.122736	0.000037
12	o	-3.363973	-0.126203	0.000069
13	h	-0.087619	2.967235	0.000031
14	h	4.097096	0.625815	0.000049
15	h	2.312763	2.347161	0.000031
16	h	1.073629	-2.464416	-0.000031
17	h	3.482867	-1.803091	0.000020
18	h	-2.473957	2.293402	0.000032

1.3 cation radical

Charge = 1 Multiplicity = 2

1.4 anion

Charge = -1 Multiplicity = 1

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

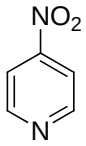
1	c	-1.985082	1.303254	0.000037
2	c	-0.661320	0.888411	0.000068
3	c	-0.373217	-0.483246	-0.000036
4	c	-1.401025	-1.414616	-0.000189
5	c	-2.723807	-0.990782	-0.000135
6	c	-3.012061	0.365349	-0.000033
7	c	1.039870	-0.931912	-0.000117
8	c	2.143500	0.157820	-0.000368
9	c	1.719403	1.561083	0.000146
10	c	0.426422	1.881160	0.000207
11	o	1.369770	-2.079386	0.000643
12	o	3.289471	-0.185596	-0.000358
13	h	0.134185	2.918189	0.000392
14	h	-4.035704	0.697873	-0.000088
15	h	-2.216755	2.354687	0.000083
16	h	-1.166604	-2.463704	-0.000284
17	h	-3.520257	-1.714073	-0.000189
18	h	2.495121	2.307754	0.000330

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.375958	1.899492	-0.000306
2	c	0.676035	0.906909	-0.000173
3	c	0.333761	-0.454876	-0.000005
4	c	-1.076289	-0.879505	-0.000205
5	c	-2.106415	0.152191	0.000248
6	c	-1.677706	1.534937	-0.000004
7	c	1.362587	-1.414461	0.000337
8	c	2.684524	-1.033418	0.000404
9	c	3.023512	0.327746	0.000022
10	c	2.031468	1.280966	-0.000169
11	o	-1.372410	-2.089047	-0.000859
12	o	-3.328199	-0.143534	0.000631
13	h	-0.099163	2.940889	-0.000286
14	h	4.058509	0.625042	-0.000024
15	h	2.286413	2.327974	-0.000364
16	h	1.099815	-2.456165	0.000630
17	h	3.461111	-1.779456	0.000700
18	h	-2.454927	2.282472	0.000272

No.56



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.537502	0.000034	-0.000027
2	c	1.844914	-1.146436	0.000002
3	c	0.448702	-1.210683	0.000016
4	c	-0.235501	-0.000107	0.000021
5	c	0.448652	1.210639	0.000012
6	c	1.844620	1.146605	-0.000002
7	n	-1.716874	-0.000019	0.000036
8	o	-2.284437	-1.090884	-0.000032
9	o	-2.284426	1.090859	-0.000017
10	h	-0.083080	2.154404	0.000015
11	h	2.431838	2.061873	-0.000010
12	h	-0.082643	-2.154616	0.000039
13	h	2.432070	-2.061672	-0.000002

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	2.567432	-0.000053	-0.000526
2	c	1.840297	1.141531	-0.000214
3	c	0.455179	1.209971	0.000427
4	c	-0.286224	0.000053	0.000776
5	c	0.455137	-1.209869	0.000416
6	c	1.840194	-1.141614	-0.000182

7	n	-1.676450	-0.000001	0.001295
8	o	-2.297817	1.126704	-0.000821
9	o	-2.297834	-1.126712	-0.000825
10	h	-0.070251	-2.157546	0.000646
11	h	2.420518	-2.065682	-0.000446
12	h	-0.069983	2.157692	0.000682
13	h	2.420559	2.065554	-0.000436

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.826554	1.138070	-0.000466
2	n	2.500852	-0.000013	-0.000025
3	c	1.826547	-1.138074	0.000448
4	c	0.440614	-1.203364	0.000406
5	c	-0.232370	0.000005	0.000029
6	c	0.440636	1.203376	-0.000372
7	n	-1.698860	0.000001	0.000098
8	o	-2.256020	1.055938	0.001000
9	o	-2.256015	-1.055938	-0.001101
10	h	-0.069973	2.147525	-0.000652
11	h	2.405235	2.045723	-0.000743
12	h	-0.070007	-2.147507	0.000705
13	h	2.405201	-2.045744	0.000715

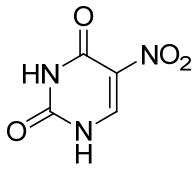
2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.838809	-1.144816	-0.000196
2	n	2.534186	0.000003	-0.000330
3	c	1.838809	1.144821	-0.000112
4	c	0.447816	1.207693	0.000323
5	c	-0.278760	-0.000003	0.000592

6	c	0.447838	-1.207689	0.000232
7	n	-1.655040	-0.000003	0.000778
8	o	-2.290256	-1.112482	-0.000376
9	o	-2.290257	1.112477	-0.000674
10	h	-0.055093	-2.154961	0.000270
11	h	2.416616	-2.053927	-0.000493
12	h	-0.055132	2.154957	0.000561
13	h	2.416617	2.053932	-0.000107

No.57



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.443170	0.985833	-0.015817
2	c	0.030740	1.127063	-0.041382
3	c	-0.646814	-0.181344	-0.001415
4	c	0.076074	-1.335291	0.019486
5	n	1.431280	-1.331947	0.031023
6	c	2.209136	-0.160877	0.016419
7	o	-0.459558	2.233828	-0.106965
8	n	-2.099240	-0.303210	0.014432
9	o	-2.568054	-1.436642	-0.164737
10	o	3.423747	-0.192011	0.029804
11	o	-2.763146	0.705562	0.215713
12	h	-0.420334	-2.298677	0.030954
13	h	1.960414	1.860064	-0.043323
14	h	1.954724	-2.199329	0.055739

1.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	n	1.427478	0.970833	-0.001301
2	c	0.002403	1.102607	-0.000174
3	c	-0.682585	-0.182204	0.000008
4	c	0.073616	-1.371308	-0.000952
5	n	1.473742	-1.320140	-0.000281
6	c	2.209947	-0.171489	0.000000
7	o	-0.444439	2.244983	0.000017
8	n	-2.074897	-0.289581	0.000203
9	o	-2.556847	-1.477970	-0.000170
10	o	3.449535	-0.143359	0.001260
11	o	-2.816983	0.735720	0.000871
12	h	-0.392475	-2.342595	0.000165
13	h	1.928742	1.850569	-0.001209
14	h	2.009053	-2.176385	0.001560

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

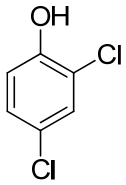
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.164712	-0.165526	0.002440
2	n	1.424160	0.976753	-0.006774
3	c	0.044315	1.111560	-0.007751
4	c	-0.641499	-0.181879	0.001513
5	c	0.080464	-1.329522	0.008123
6	n	1.414887	-1.322596	0.010300
7	o	-0.441911	2.204992	-0.016972
8	n	-2.067480	-0.295433	0.001662
9	o	-2.727264	0.696697	0.042657
10	o	3.361937	-0.181683	0.002243
11	o	-2.539370	-1.403509	-0.038006
12	h	-0.388727	-2.294896	0.015081
13	h	1.948649	1.840989	-0.013457
14	h	1.924018	-2.196935	0.016737

2.2 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.175215	-0.182577	-0.000356
2	n	1.427903	0.963455	-0.000055
3	c	0.051562	1.100667	0.001800
4	c	-0.671424	-0.189142	0.001353
5	c	0.071402	-1.341661	0.001489
6	n	1.450790	-1.318120	0.000040
7	o	-0.414862	2.206416	0.001712
8	n	-2.048450	-0.277750	-0.000079
9	o	-2.795029	0.753582	-0.003338
10	o	3.386095	-0.156582	-0.001976
11	o	-2.563705	-1.456938	0.000305
12	h	-0.383379	-2.308241	0.001662
13	h	1.951099	1.829019	-0.001013
14	h	1.960071	-2.189413	0.000688

No.58



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.632117	-1.405906	0.000000
2	c	-0.724481	-1.750818	0.000000
3	c	-1.710830	-0.768013	0.000000
4	c	-1.342340	0.579248	0.000000
5	c	0.000000	0.952246	0.000000

6	c	0.973900	-0.045464	0.000000
7	cl	-2.580852	1.825693	0.000000
8	cl	2.678302	0.398185	0.000000
9	o	1.548111	-2.410557	0.000000
10	h	0.289426	1.997023	0.000000
11	h	-0.988326	-2.803881	0.000000
12	h	-2.759447	-1.046050	0.000000
13	h	2.446602	-2.036311	0.000000

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.000000	0.927754	0.000000
2	c	1.026269	0.001770	-0.000000
3	c	0.762644	-1.443790	-0.000000
4	c	-0.641549	-1.828002	-0.000000
5	c	-1.654590	-0.901041	0.000000
6	c	-1.330536	0.475664	0.000000
7	cl	2.672138	0.531868	-0.000000
8	o	1.676400	-2.294016	-0.000000
9	cl	-2.616526	1.648511	0.000000
10	h	0.214524	1.990869	0.000000
11	h	-0.848227	-2.893912	-0.000000
12	h	-2.696324	-1.205401	0.000000

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.995656	0.026824	0.000000
2	c	0.651351	-1.377863	0.000000
3	c	-0.717393	-1.778752	0.000000
4	c	-1.704031	-0.829842	0.000000
5	c	-1.351024	0.556242	0.000000
6	c	0.000000	0.977651	0.000000
7	o	1.552125	-2.330583	0.000000
8	cl	-2.585948	1.725331	0.000000

9	cl	2.663066	0.457259	0.000000
10	h	0.243223	2.034923	0.000000
11	h	-0.938814	-2.841382	0.000000
12	h	-2.751696	-1.111968	0.000000
13	h	2.471927	-1.986506	0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.006084	-0.056450	0.000000
2	c	0.773317	-1.490408	0.000000
3	c	-0.640165	-1.812501	0.000000
4	c	-1.656408	-0.865069	0.000000
5	c	-1.335663	0.496223	0.000000
6	c	0.000000	0.903427	0.000000
7	o	1.684913	-2.365548	0.000000
8	cl	-2.633077	1.724676	0.000000
9	cl	2.689976	0.508505	0.000000
10	h	0.255715	1.958966	0.000000
11	h	-0.886337	-2.872786	0.000000
12	h	-2.698948	-1.177209	0.000000

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.975138	-0.050832	0.000000
2	c	0.637303	-1.397343	-0.000000
3	c	-0.711926	-1.741418	-0.000000
4	c	-1.693186	-0.770530	-0.000000
5	c	-1.328030	0.567412	0.000000
6	c	-0.000000	0.936341	0.000000
7	o	1.521542	-2.406320	-0.000000
8	cl	-2.561442	1.804170	0.000000

9	cl	2.651866	0.430070	0.000000
10	h	0.286779	1.973272	0.000000
11	h	-0.976535	-2.785028	-0.000000
12	h	-2.731318	-1.054228	-0.000000
13	h	2.435741	-2.127303	-0.000000

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.331718	0.469067	-0.000000
2	c	0.000000	0.925455	-0.000000
3	c	1.027401	-0.002809	0.000000
4	c	0.754847	-1.430900	0.000000
5	c	-0.632111	-1.836053	0.000000
6	c	-1.653259	-0.902633	0.000000
7	cl	2.669427	0.534171	-0.000000
8	o	1.667276	-2.270541	0.000000
9	cl	-2.611820	1.639891	-0.000000
10	h	0.214253	1.979665	-0.000000
11	h	-0.839757	-2.892381	0.000000
12	h	-2.682984	-1.214760	0.000000

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.000000	0.954609	-0.000000
2	c	1.008768	0.027562	0.000000
3	c	0.677127	-1.382894	0.000000
4	c	-0.702538	-1.789092	0.000000
5	c	-1.691915	-0.848808	-0.000000
6	c	-1.346186	0.525197	-0.000000
7	cl	2.650925	0.514408	0.000000
8	o	1.526355	-2.320273	0.000000
9	cl	-2.589511	1.705054	-0.000000
10	h	0.232190	2.006325	-0.000000
11	h	-0.906109	-2.846752	0.000000

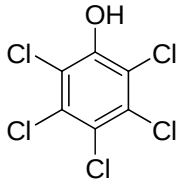
12	h	-2.727141	-1.143999	-0.000000
13	h	2.474634	-2.103692	0.000000

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.000000	0.894860	-0.000000
2	c	0.999403	-0.062919	0.000000
3	c	0.743961	-1.455446	0.000000
4	c	-0.635666	-1.794529	0.000000
5	c	-1.641662	-0.852322	0.000000
6	c	-1.322110	0.498674	-0.000000
7	cl	2.663431	0.498231	-0.000000
8	o	1.660031	-2.349577	0.000000
9	cl	-2.595297	1.707417	-0.000000
10	h	0.258884	1.939425	-0.000000
11	h	-0.888994	-2.842009	0.000000
12	h	-2.671966	-1.166715	0.000000

No.59



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.215765	-0.879106	0.000000
2	c	1.204069	0.521806	0.000000
3	c	-0.021442	1.206598	0.000000
4	c	-1.225512	0.477492	0.000000

5	c	-1.204417	-0.923932	0.000000
6	c	0.019731	-1.612625	0.000000
7	cl	2.703215	1.396376	0.000000
8	cl	-0.048734	2.943164	0.000000
9	cl	-2.746216	1.312457	0.000000
10	cl	-2.665978	-1.857001	0.000000
11	o	-0.011604	-2.962657	0.000000
12	cl	2.714498	-1.779087	0.000000
13	h	0.898346	-3.310599	0.000015

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.248440	-0.927829	0.000043
2	c	-0.000617	-1.704469	0.000068
3	c	1.247876	-0.928619	0.000045
4	c	1.238524	0.455819	0.000063
5	c	0.000442	1.158033	0.000083
6	c	-1.238167	0.456577	0.000065
7	o	-0.001092	-2.942325	-0.000003
8	cl	2.708884	-1.832400	-0.000033
9	cl	2.728853	1.346068	-0.000018
10	cl	0.001343	2.880126	-0.000025
11	cl	-2.728233	1.347408	-0.000014
12	cl	-2.710198	-1.830525	-0.000037

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.013083	-1.598976	0.000000
2	c	-1.235345	-0.905222	0.000000
3	c	-1.252462	0.478075	-0.000000
4	c	0.000000	1.203137	-0.000000
5	c	1.249769	0.513454	-0.000000
6	c	1.261714	-0.877662	0.000000
7	cl	-2.675324	-1.854422	0.000000

8	cl	-2.732836	1.328917	-0.000000
9	cl	-0.026908	2.895417	-0.000000
10	cl	2.721100	1.392736	-0.000000
11	cl	2.705183	-1.780239	0.000000
12	o	0.090575	-2.906043	0.000000
13	h	-0.795805	-3.329413	0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.000196	-1.741226	0.000000
2	c	1.212852	-0.936781	0.000000
3	c	1.208449	0.454677	0.000000
4	c	0.000000	1.177710	0.000000
5	c	-1.208570	0.454588	0.000000
6	c	-1.213176	-0.936683	0.000000
7	cl	2.718784	-1.834131	0.000000
8	cl	2.730598	1.340208	0.000000
9	cl	-0.000254	2.935118	0.000000
10	cl	-2.730745	1.340612	0.000000
11	cl	-2.718421	-1.834462	0.000000
12	o	0.000268	-2.992323	0.000000

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.010885	-1.605522	0.000299
2	c	1.201728	-0.889342	0.000131
3	c	1.193921	0.500083	0.000151
4	c	-0.009522	1.191285	0.000214
5	c	-1.206707	0.478868	0.000216
6	c	-1.194840	-0.905952	0.000217
7	cl	2.690690	-1.773109	-0.000234

8	cl	2.688545	1.361056	-0.000166
9	cl	-0.022887	2.920013	0.000135
10	cl	-2.711550	1.322278	-0.000149
11	cl	-2.662261	-1.817599	-0.000270
12	o	-0.058193	-2.931980	0.000446
13	h	0.789602	-3.375555	0.000685

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.233992	0.460477	-0.000021
2	c	1.242856	-0.929610	0.000087
3	c	0.000288	-1.680843	0.000203
4	c	-1.242494	-0.929946	-0.000000
5	c	-1.234156	0.460153	-0.000003
6	c	-0.000214	1.162622	0.000000
7	cl	2.702320	-1.831756	-0.000016
8	o	0.000445	-2.913613	0.000079
9	cl	-2.701648	-1.832627	-0.000073
10	cl	-2.718951	1.333671	-0.000038
11	cl	-0.000614	2.881757	0.000101
12	cl	2.718588	1.334354	-0.000105

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.250421	-0.899008	0.000407
2	c	-0.008909	-1.615674	-0.001169
3	c	-1.258590	-0.887921	-0.000564
4	c	-1.235053	0.487499	0.000555
5	c	0.009492	1.188037	0.000273
6	c	1.245669	0.478971	-0.000098
7	o	0.075764	-2.867475	0.000133
8	cl	-2.709815	-1.781824	-0.000987
9	cl	-2.704120	1.362871	0.001102
10	cl	0.014112	2.891679	-0.000083

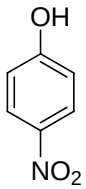
11	cl	2.724921	1.339177	-0.001103
12	cl	2.681229	-1.821046	0.001187
13	h	-0.731852	-3.416178	0.000559

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.198253	-0.927216	0.000000
2	c	0.000006	-1.698218	0.000000
3	c	1.198259	-0.927229	0.000000
4	c	1.196587	0.453958	0.000000
5	c	0.000000	1.167682	-0.000000
6	c	-1.196585	0.453939	-0.000000
7	o	-0.000008	-2.955163	0.000000
8	cl	2.693189	-1.815370	0.000000
9	cl	2.699195	1.319021	-0.000000
10	cl	-0.000072	2.904631	-0.000000
11	cl	-2.699138	1.319085	-0.000000
12	cl	-2.693175	-1.815378	0.000000

No.60



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.385731	-1.205852	0.000011
2	c	-0.005218	-1.214249	0.000078
3	c	-0.692682	0.000696	0.000118

4	c	-0.012780	1.223288	0.000071
5	c	1.375465	1.229149	0.000004
6	c	2.077964	0.014583	-0.000016
7	n	-2.155971	-0.006682	0.000189
8	o	-2.738454	1.081062	-0.000139
9	o	3.437081	0.087450	-0.000083
10	o	-2.728038	-1.100429	-0.000151
11	h	-0.575845	2.149044	0.000104
12	h	1.932324	2.160585	-0.000034
13	h	1.933324	-2.145961	-0.000021
14	h	-0.559411	-2.145354	0.000116
15	h	3.825808	-0.801892	-0.000107

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.423488	1.245450	-0.000054
2	c	2.179597	0.000184	-0.000049
3	c	1.423611	-1.245326	0.000064
4	c	0.047297	-1.238781	0.000100
5	c	-0.625705	-0.000171	0.000069
6	c	0.047234	1.238536	0.000002
7	o	3.434795	-0.000023	-0.000045
8	n	-2.097559	-0.000005	0.000130
9	o	-2.667668	1.092483	0.000044
10	o	-2.667847	-1.092376	-0.000232
11	h	-0.531404	2.154858	-0.000002
12	h	1.988621	2.172252	-0.000104
13	h	1.989335	-2.171820	0.000101
14	h	-0.531000	-2.155274	0.000167

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.356782	-1.242092	0.200837
2	c	2.063154	-0.006455	0.000888

3	c	1.367447	1.230028	-0.201804
4	c	-0.004242	1.226814	-0.200134
5	c	-0.681003	-0.006746	-0.004965
6	c	-0.016014	-1.238552	0.193603
7	o	3.372690	-0.094745	0.017332
8	n	-2.144295	0.005294	-0.001149
9	o	-2.703352	-0.898056	-0.608897
10	o	-2.673413	0.922347	0.617299
11	h	-0.590503	-2.149349	0.327732
12	h	1.933766	-2.149685	0.348625
13	h	1.924284	2.151499	-0.351424
14	h	-0.576899	2.138496	-0.336828
15	h	3.835281	0.757627	-0.116485

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	2.210561	0.000074	-0.000007
2	c	1.424282	1.227429	0.000007
3	c	0.050144	1.223669	0.000044
4	c	-0.667259	0.000017	0.000071
5	c	0.050177	-1.223714	0.000038
6	c	1.424265	-1.227413	0.000000
7	n	-2.077023	-0.000002	0.000110
8	o	-2.693951	1.096130	-0.000091
9	o	3.470201	-0.000041	-0.000060
10	o	-2.693921	-1.096152	-0.000077
11	h	-0.512798	-2.151606	0.000060
12	h	1.976620	-2.164947	-0.000008
13	h	1.976430	2.165082	0.000002
14	h	-0.512745	2.151617	0.000069

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Atomic Coordinates (Angstroms)

Number	Number	X	Y	Z
1	c	2.061378	0.016176	0.000011
2	c	1.375601	-1.197620	0.000299
3	c	-0.004314	-1.205428	0.000595
4	c	-0.690539	0.000331	0.000349
5	c	-0.016275	1.216698	0.000265
6	c	1.360538	1.223599	-0.000031
7	n	-2.133892	-0.008289	-0.000110
8	o	-2.698983	-1.066709	-0.000707
9	o	3.394699	0.084517	-0.000460
10	o	-2.710867	1.043606	0.000142
11	h	-0.560799	2.141257	0.000009
12	h	1.905950	2.151271	-0.000375
13	h	1.923183	-2.125852	0.000192
14	h	-0.536955	-2.136912	0.000607
15	h	3.808729	-0.785577	-0.000400

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.039728	1.238305	-0.000328
2	c	-1.425433	1.242357	-0.000304
3	c	-2.160240	-0.000007	-0.000039
4	c	-1.425392	-1.242348	0.000376
5	c	-0.039686	-1.238250	0.000412
6	c	0.630721	0.000011	0.000015
7	o	-3.411451	-0.000039	-0.000054
8	n	2.087522	-0.000003	0.000032
9	o	2.647795	-1.056504	-0.000980
10	o	2.647815	1.056486	0.000891
11	h	0.514753	2.156081	-0.000588
12	h	-1.978515	2.165815	-0.000564
13	h	-1.978443	-2.165824	0.000589
14	h	0.514825	-2.156008	0.000687

2.3 cation radical

Charge = 1 Multiplicity = 2

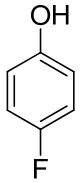
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.359184	1.267925	-0.005993
2	c	-2.079029	0.015568	0.000074
3	c	-1.374221	-1.245823	0.004941
4	c	-0.000277	-1.239265	0.006193
5	c	0.677839	0.001947	-0.001256
6	c	0.015912	1.249926	-0.007687
7	o	-3.337792	0.087922	0.000392
8	n	2.138975	-0.008445	0.000143
9	o	2.694968	1.046323	0.017392
10	o	2.680543	-1.070870	-0.016033
11	h	0.575904	2.164749	-0.011984
12	h	-1.927408	2.182796	-0.008314
13	h	-1.944378	-2.161461	0.010751
14	h	0.549659	-2.160268	0.011939
15	h	-3.814591	-0.775370	0.004969

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.413001	-1.218563	0.000504
2	c	2.167470	-0.000004	0.000169
3	c	1.412983	1.218550	-0.000222
4	c	0.047149	1.215013	-0.000333
5	c	-0.656593	0.000048	0.000256
6	c	0.047159	-1.214899	0.001025
7	o	3.431419	-0.000018	-0.000534
8	n	-2.065202	-0.000010	-0.000115
9	o	-2.656380	-1.056818	-0.001571
10	o	-2.656503	1.056724	0.001121
11	h	-0.492582	-2.143063	0.001247
12	h	1.953132	-2.150400	0.000653
13	h	1.953136	2.150376	-0.000729
14	h	-0.492571	2.143188	-0.000888

No.61



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.694155	-1.201280	-0.000001
2	c	0.704468	-1.216304	0.000000
3	c	1.385301	-0.007304	0.000000
4	c	0.720336	1.214126	0.000000
5	c	-0.674390	1.223509	0.000000
6	c	-1.382813	0.016296	-0.000001
7	f	2.748678	-0.016786	0.000000
8	o	-2.753888	0.095747	-0.000002
9	h	1.289012	2.138624	0.000001
10	h	-1.225136	2.158992	0.000000
11	h	-1.241770	-2.141820	-0.000002
12	h	1.256832	-2.150541	0.000000
13	h	-3.138424	-0.794421	0.000029

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.727294	-1.241830	0.000011
2	c	1.485053	-0.000118	-0.000117
3	c	0.727316	1.241730	0.000006
4	c	-0.651146	1.236552	0.000007
5	c	-1.316397	0.000102	-0.000027
6	c	-0.651097	-1.236413	-0.000000

7	o	2.743873	0.000063	0.000051
8	f	-2.665755	-0.000069	0.000016
9	h	-1.234229	-2.152356	0.000036
10	h	1.291451	-2.169441	0.000055
11	h	1.291640	2.169234	0.000046
12	h	-1.234187	2.152545	0.000034

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.000000	1.372270	0.000000
2	c	1.250337	0.671877	0.000000
3	c	1.245791	-0.699138	0.000000
4	c	-0.005985	-1.372363	-0.000000
5	c	-1.254142	-0.701425	-0.000000
6	c	-1.252301	0.669101	-0.000000
7	f	-0.000548	-2.686629	-0.000000
8	o	-0.085269	2.685501	0.000000
9	h	-2.171453	-1.281460	-0.000000
10	h	-2.170094	1.248632	-0.000000
11	h	2.185346	1.226141	0.000000
12	h	2.161439	-1.282065	0.000000
13	h	0.779640	3.142462	0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.000492	-1.527687	0.000000
2	c	1.214048	-0.738322	0.000000
3	c	1.211703	0.657820	0.000000
4	c	0.000000	1.341074	0.000000
5	c	-1.211973	0.657459	0.000000
6	c	-1.213794	-0.738237	0.000000
7	f	-0.000518	2.737919	0.000000
8	o	0.000119	-2.804461	0.000000
9	h	-2.144622	1.220929	0.000000

10	h	-2.158258	-1.280654	0.000000
11	h	2.159216	-1.279509	0.000000
12	h	2.144512	1.220999	0.000000

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.373633	0.019259	0.000029
2	c	-0.692133	-1.189660	0.000027
3	c	0.697598	-1.206296	0.000016
4	c	1.374900	-0.009308	0.000008
5	c	0.719968	1.204385	0.000031
6	c	-0.665941	1.215992	0.000042
7	f	2.720898	-0.021168	-0.000044
8	o	-2.725223	0.093259	-0.000139
9	h	1.282373	2.122763	0.000040
10	h	-1.202861	2.149342	0.000060
11	h	-1.240016	-2.118378	-0.000016
12	h	1.239307	-2.137003	-0.000019
13	h	-3.129644	-0.778515	0.000538

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.651453	-1.234518	0.000015
2	c	0.734090	-1.242849	-0.000008
3	c	1.472025	0.000001	-0.000255
4	c	0.734068	1.242838	-0.000011
5	c	-0.651483	1.234531	0.000012
6	c	-1.312975	-0.000001	-0.000034
7	o	2.720359	0.000013	0.000134
8	f	-2.648841	-0.000013	0.000030
9	h	-1.223683	-2.146361	0.000085

10	h	1.289234	-2.164884	0.000073
11	h	1.289211	2.164873	0.000084
12	h	-1.223698	2.146383	0.000096

2.3 cation radical

Charge = 1 Multiplicity = 2

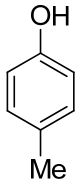
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.361310	-0.007112	0.000056
2	c	-0.708808	1.239907	0.000101
3	c	0.658509	1.262968	-0.000012
4	c	1.379582	0.017460	-0.000086
5	c	0.684065	-1.241855	0.000066
6	c	-0.682249	-1.241264	0.000032
7	o	2.649127	0.096604	-0.000032
8	f	-2.675884	-0.022743	-0.000097
9	h	-1.289824	2.146595	0.000144
10	h	1.224229	2.179097	-0.000034
11	h	1.258030	-2.154842	0.000054
12	h	-1.245974	-2.158993	0.000013
13	h	3.124754	-0.760630	0.000009

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.199290	-0.732163	0.000000
2	c	0.000022	-1.479284	0.000000
3	c	1.199315	-0.732184	-0.000000
4	c	1.201231	0.655347	-0.000000
5	c	0.000000	1.329533	-0.000000
6	c	-1.201247	0.655319	0.000000
7	o	-0.000004	-2.780840	0.000000
8	f	-0.000020	2.686869	-0.000000
9	h	-2.127890	1.206004	0.000000
10	h	-2.137351	-1.263278	0.000000
11	h	2.137391	-1.263271	-0.000000
12	h	2.127879	1.206028	-0.000000

No.62



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.751645	1.196770	-0.000002
2	c	-0.647460	1.200712	-0.000001
3	c	-1.383255	0.010493	0.000000
4	c	-0.664489	-1.196945	0.000000
5	c	0.728508	-1.220857	0.000000
6	c	1.441847	-0.017181	-0.000002
7	c	-2.895657	0.015361	0.000001
8	o	2.814160	-0.095718	-0.000003
9	h	-1.206212	-2.141073	0.000002
10	h	1.275449	-2.159180	0.000000
11	h	1.298660	2.138547	-0.000003
12	h	-1.170359	2.154875	-0.000001
13	h	3.193648	0.796723	0.000044
14	h	-3.289633	1.037404	0.000000
15	h	-3.300834	-0.495831	-0.882958
16	h	-3.300833	-0.495830	0.882962

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.589641	1.223947	-0.000004
2	c	-0.789591	1.236547	-0.000000

3	c	-1.547807	-0.001748	0.000013
4	c	-0.781298	-1.237104	0.000000
5	c	0.594425	-1.216102	-0.000004
6	c	1.314980	0.008018	0.000005
7	o	-2.807082	-0.005959	-0.000003
8	c	2.820366	-0.000610	0.000001
9	h	1.139410	2.162831	-0.000015
10	h	-1.353016	2.165274	-0.000008
11	h	-1.340289	-2.168547	-0.000007
12	h	1.150678	-2.151726	-0.000014
13	h	3.212135	-0.525664	-0.881460
14	h	3.231301	1.013412	-0.000026
15	h	3.212140	-0.525603	0.881496

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.727028	1.251512	-0.000017
2	c	1.435518	0.006332	-0.000006
3	c	0.734674	-1.239462	-0.000007
4	c	-0.635249	-1.225792	-0.000019
5	c	-1.369712	0.009353	-0.000009
6	c	-0.644404	1.239714	-0.000008
7	o	2.750945	0.091887	0.000024
8	c	-2.857907	-0.013487	0.000023
9	h	-1.194662	2.175687	-0.000016
10	h	1.301380	2.172608	-0.000016
11	h	1.288150	-2.175215	-0.000015
12	h	-1.185256	-2.162781	-0.000020
13	h	3.201201	-0.775881	0.000045
14	h	-3.232640	-0.563159	0.876712
15	h	-3.292784	0.987699	0.000081
16	h	-3.232640	-0.563077	-0.876706

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	c	0.790615	-1.209928	-0.004387
2	c	1.583992	0.000105	0.007353
3	c	0.790817	1.210046	-0.004371
4	c	-0.601751	1.195510	-0.016738
5	c	-1.345836	0.000103	-0.022287
6	c	-0.601762	-1.195477	-0.016700
7	o	2.860701	-0.000230	0.018408
8	c	-2.857945	-0.000132	0.026267
9	h	-1.138354	-2.149004	-0.025423
10	h	1.330726	-2.156781	-0.009266
11	h	1.330621	2.157065	-0.009242
12	h	-1.138225	2.149090	-0.025421
13	h	-3.278320	0.889964	-0.465061
14	h	-3.279508	-0.879923	-0.482463
15	h	-3.261324	-0.009929	1.054788

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.436000	-0.018527	0.000177
2	c	-0.753167	1.185807	0.000392
3	c	0.639198	1.191363	-0.000421
4	c	1.372884	0.013227	-0.000216
5	c	0.660909	-1.187817	-0.000001
6	c	-0.722830	-1.213000	-0.000012
7	c	2.885728	0.018181	0.000136
8	o	-2.789422	-0.094044	-0.000182
9	h	1.197123	-2.123090	0.000129
10	h	-1.257200	-2.148470	-0.000070
11	h	-1.299342	2.116197	0.000455
12	h	1.151182	2.139430	-0.000534
13	h	-3.191706	0.778272	0.000329
14	h	3.271365	1.031971	0.000055
15	h	3.281546	-0.488468	0.876007
16	h	3.282077	-0.488905	-0.875236

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.589230	-1.219032	-0.011169
2	c	-1.311584	0.000417	-0.013908
3	c	-0.589445	1.219068	-0.011148
4	c	0.794352	1.237695	-0.001736
5	c	1.538900	0.000005	0.003610
6	c	0.794083	-1.237858	-0.001757
7	c	-2.819270	-0.000152	0.014216
8	o	2.785810	-0.000079	0.010454
9	h	-1.130262	2.150499	-0.017891
10	h	1.346101	2.162666	-0.000833
11	h	1.346127	-2.162658	-0.000827
12	h	-1.130932	-2.149894	-0.017885
13	h	-3.183420	-0.007211	1.039378
14	h	-3.220611	0.882986	-0.471244
15	h	-3.220319	-0.876617	-0.482970

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.641887	1.233917	0.000100
2	c	0.724986	1.258314	0.000004
3	c	1.442154	0.014615	-0.000095
4	c	0.739014	-1.236092	0.000035
5	c	-0.622728	-1.218683	0.000066
6	c	-1.356267	0.006266	0.000016
7	o	2.716130	0.085541	-0.000102
8	c	-2.857564	-0.025406	-0.000083
9	h	-1.187797	2.160891	0.000207
10	h	1.293097	2.173033	0.000083
11	h	1.307002	-2.152680	-0.000045
12	h	-1.162711	-2.149997	0.000130
13	h	3.173801	-0.779524	0.000512
14	h	-3.222615	-0.553630	0.876504

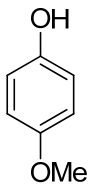
15	h	-3.273600	0.974129	-0.000411
16	h	-3.222468	-0.554136	-0.876415

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.601764	-1.195476	-0.016695
2	c	0.790613	-1.209931	-0.004390
3	c	1.583992	0.000102	0.007353
4	c	0.790819	1.210043	-0.004369
5	c	-0.601749	1.195509	-0.016737
6	c	-1.345836	0.000103	-0.022288
7	o	2.860701	-0.000226	0.018407
8	c	-2.857945	-0.000129	0.026264
9	h	-1.138356	-2.149003	-0.025413
10	h	1.330722	-2.156785	-0.009270
11	h	1.330624	2.157061	-0.009238
12	h	-1.138222	2.149090	-0.025419
13	h	-3.278319	0.889968	-0.465063
14	h	-3.279509	-0.879919	-0.482467
15	h	-3.261325	-0.009928	1.054785

No.63



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.327276	1.170074	-0.000002

2	c	-0.050829	1.374005	-0.000001
3	c	-0.929038	0.282456	0.000000
4	c	-0.407744	-1.017418	0.000000
5	c	0.976863	-1.218362	0.000000
6	c	1.847691	-0.130009	-0.000002
7	o	-2.266916	0.589547	0.000000
8	c	-3.203011	-0.476945	0.000001
9	o	3.199703	-0.393120	-0.000003
10	h	-1.060875	-1.882909	0.000000
11	h	1.386778	-2.224007	0.000000
12	h	1.997271	2.028539	-0.000003
13	h	-0.463323	2.378495	-0.000001
14	h	3.695541	0.439929	0.000045
15	h	-4.188752	-0.007921	0.000002
16	h	-3.098089	-1.103180	-0.896616
17	h	-3.098087	-1.103180	0.896620

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.013940	-1.247656	-0.000020
2	c	1.953402	-0.141166	0.000042
3	c	1.378806	1.195589	0.000004
4	c	0.021252	1.388285	-0.000005
5	c	-0.861898	0.275339	0.000003
6	c	-0.351341	-1.043740	-0.000002
7	o	3.197964	-0.330385	-0.000006
8	o	-2.178317	0.586135	-0.000028
9	c	-3.151171	-0.459505	0.000020
10	h	-1.022940	-1.895542	-0.000013
11	h	1.430018	-2.250911	-0.000043
12	h	2.069222	2.033940	-0.000001
13	h	-0.414562	2.383447	-0.000017
14	h	-4.118851	0.043268	0.000037
15	h	-3.059019	-1.081562	-0.897980
16	h	-3.058980	-1.081516	0.898046

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.842736	-0.121462	-0.000000
2	c	-1.326170	1.206030	-0.000000
3	c	0.029437	1.395716	0.000000
4	c	0.916769	0.267166	0.000000
5	c	0.394331	-1.062012	-0.000000
6	c	-0.964184	-1.248263	-0.000000
7	o	2.196297	0.570117	0.000000
8	c	3.233481	-0.445977	0.000000
9	o	-3.138108	-0.398799	-0.000000
10	h	1.059185	-1.917856	-0.000000
11	h	-1.402648	-2.241244	-0.000000
12	h	-2.004487	2.055454	-0.000000
13	h	0.467648	2.388688	0.000000
14	h	-3.704011	0.396371	-0.000000
15	h	4.167065	0.112949	0.000000
16	h	3.153092	-1.056039	0.903447
17	h	3.153081	-1.056050	-0.903439

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.000000	1.997201	0.000000
2	c	-1.266688	1.295854	0.000000
3	c	-1.365630	-0.092503	0.000000
4	c	-0.219394	-0.898848	0.000000
5	c	1.036309	-0.279913	0.000000
6	c	1.141907	1.116559	0.000000
7	o	-0.434281	-2.291057	0.000000
8	c	0.703054	-3.111791	0.000000
9	o	0.091214	3.273033	0.000000
10	h	1.949708	-0.872499	0.000000
11	h	2.128113	1.579995	0.000000
12	h	-2.170985	1.903868	0.000000
13	h	-2.341720	-0.578752	0.000000
14	h	0.341453	-4.146078	0.000000
15	h	1.330306	-2.950849	-0.893208

16	h	1.330306	-2.950849	0.893208

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.839309	-0.132258	-0.000273
2	c	-1.321808	1.158608	-0.000317
3	c	0.046943	1.358614	-0.000330
4	c	0.922849	0.277399	-0.000320
5	c	0.406452	-1.009995	-0.000529
6	c	-0.972057	-1.208479	-0.000578
7	o	2.246772	0.578148	0.000112
8	c	3.192757	-0.462374	0.000578
9	o	-3.174313	-0.384784	0.000861
10	h	1.048349	-1.871719	-0.000353
11	h	-1.369041	-2.209838	-0.000349
12	h	-1.988067	2.006995	0.000262
13	h	0.447726	2.358335	0.000123
14	h	-3.686029	0.427731	0.000988
15	h	4.162611	0.012803	0.001497
16	h	3.094182	-1.080386	0.886582
17	h	3.095645	-1.079920	-0.885908

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.351165	-1.040590	-0.000365
2	c	1.019381	-1.249802	-0.000036
3	c	1.940370	-0.139918	0.000296
4	c	1.385704	1.194033	0.000139
5	c	0.021339	1.381294	-0.000044
6	c	-0.860295	0.272655	-0.000166
7	o	3.173008	-0.326735	0.000053

8	o	-2.170716	0.577747	-0.000490
9	c	-3.139048	-0.449207	0.000511
10	h	-1.008341	-1.890658	-0.000706
11	h	1.425578	-2.247002	-0.000203
12	h	2.065416	2.029194	0.000153
13	h	-0.399831	2.372359	-0.000065
14	h	-4.097404	0.047497	0.000546
15	h	-3.051087	-1.065720	-0.886486
16	h	-3.050381	-1.064563	0.888253

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.943520	-1.243083	-0.000379
2	c	-1.831833	-0.126122	-0.000105
3	c	-1.320794	1.197444	-0.000112
4	c	0.018515	1.385220	-0.000320
5	c	0.913801	0.264799	-0.000143
6	c	0.399921	-1.058628	-0.000303
7	o	-3.104735	-0.395642	0.000449
8	o	2.173458	0.566589	0.000182
9	c	3.200294	-0.431197	0.000312
10	h	1.057306	-1.908663	-0.000271
11	h	-1.371399	-2.231712	-0.000314
12	h	-2.004943	2.030517	0.000016
13	h	0.449632	2.372149	-0.000365
14	h	-3.669856	0.395107	0.001121
15	h	4.125999	0.119606	0.000460
16	h	3.122459	-1.037589	0.892001
17	h	3.122715	-1.037584	-0.891404

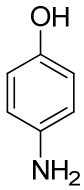
2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.836335	-1.345137	0.000000
2	c	-0.454426	-1.895854	-0.000000

3	c	-1.516131	-0.962271	-0.000000
4	c	-1.293196	0.402097	-0.000000
5	c	0.000000	0.917795	0.000000
6	c	1.063538	0.031595	0.000000
7	o	-0.669852	-3.186509	-0.000000
8	o	0.114631	2.282905	0.000000
9	c	1.393598	2.857294	0.000000
10	h	2.080648	0.381755	0.000000
11	h	1.683222	-2.013128	0.000000
12	h	-2.528981	-1.333183	-0.000000
13	h	-2.126994	1.086011	-0.000000
14	h	1.247767	3.928138	0.000000
15	h	1.953896	2.573066	0.885251
16	h	1.953896	2.573066	-0.885251

No.64



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.724892	-1.193852	-0.000072
2	c	-0.672674	-1.204803	-0.005195
3	c	-1.402420	-0.007642	-0.006592
4	c	-0.688344	1.202639	-0.005615
5	c	0.705224	1.217333	-0.000159
6	c	1.420549	0.017028	0.002380
7	n	-2.810030	-0.015839	-0.079200
8	o	2.797552	0.094500	0.009214
9	h	-1.230541	2.146075	-0.015796
10	h	1.249322	2.157288	0.002156
11	h	1.267822	-2.137934	0.002765
12	h	-1.197657	-2.157848	-0.015100

13	h	3.174408	-0.798601	0.002564
14	h	-3.243859	-0.851831	0.295797
15	h	-3.253061	0.813505	0.299827

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.616529	-1.226748	-0.003903
2	c	0.756795	-1.233419	-0.000786
3	c	1.526693	0.000007	0.001865
4	c	0.756796	1.233417	-0.000786
5	c	-0.616540	1.226738	-0.003903
6	c	-1.336218	0.000005	-0.003256
7	o	2.784708	0.000000	0.006569
8	n	-2.709567	-0.000003	-0.041483
9	h	-1.171683	-2.163332	-0.009193
10	h	1.314608	-2.165437	0.001169
11	h	1.314571	2.165457	0.001169
12	h	-1.171666	2.163338	-0.009177
13	h	-3.211259	0.854161	0.159212
14	h	-3.211251	-0.854163	0.159255

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.408018	-0.009461	0.000055
2	c	0.710436	1.229864	-0.000327
3	c	-0.661230	1.238604	-0.000521
4	c	-1.390340	0.004421	-0.000102
5	c	-0.674581	-1.237665	-0.000525
6	c	0.694034	-1.242014	-0.000310
7	n	-2.732516	0.013278	0.000619
8	o	2.733796	-0.100007	0.000649
9	h	-1.226462	-2.173413	-0.001034
10	h	1.259728	-2.168119	-0.000444
11	h	1.263660	2.165536	-0.000529

12	h	-1.202624	2.180498	-0.001058
13	h	3.178092	0.767961	0.000984
14	h	-3.261988	0.878588	0.001457
15	h	-3.271187	-0.846436	0.001485

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.787202	1.210358	-0.000152
2	c	1.563715	-0.010311	0.000036
3	c	0.755840	-1.212509	-0.000038
4	c	-0.636272	-1.181281	-0.000084
5	c	-1.354083	0.029386	-0.000084
6	c	-0.606035	1.217586	-0.000012
7	o	2.840028	-0.030296	0.000153
8	n	-2.810197	0.093981	0.000167
9	h	-1.148738	2.163974	0.000141
10	h	1.340794	2.149194	-0.000328
11	h	1.284873	-2.165500	-0.000039
12	h	-1.192385	-2.123716	-0.000473
13	h	-3.198029	-0.379221	-0.815871
14	h	-3.197559	-0.379602	0.816181

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.414056	0.019306	0.002912
2	c	0.724636	-1.181991	-0.000631
3	c	-0.665187	-1.193401	-0.008570
4	c	-1.392503	-0.008724	-0.011018
5	c	-0.686242	1.193077	-0.008879
6	c	0.699598	1.208862	-0.000675
7	n	-2.798306	-0.019780	-0.081672

8	o	2.773289	0.091335	0.011134
9	h	-1.224112	2.127010	-0.014801
10	h	1.230858	2.146228	0.003412
11	h	1.266649	-2.114922	0.003559
12	h	-1.182839	-2.138649	-0.013958
13	h	3.170756	-0.782601	0.010401
14	h	-3.206124	-0.842715	0.321910
15	h	-3.219511	0.790668	0.333281

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.329615	0.000010	-0.004701
2	c	-0.612725	-1.221062	-0.006883
3	c	0.765261	-1.235175	-0.000306
4	c	1.515086	-0.000009	0.003545
5	c	0.765295	1.235176	-0.000257
6	c	-0.612691	1.221101	-0.006897
7	o	2.759540	-0.000026	0.009264
8	n	-2.716057	-0.000007	-0.075052
9	h	-1.159024	-2.149682	-0.012549
10	h	1.314121	-2.161733	0.002272
11	h	1.314179	2.161721	0.002330
12	h	-1.158965	2.149735	-0.012736
13	h	-3.158955	0.825557	0.282479
14	h	-3.158949	-0.825585	0.282451

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.686191	1.236895	-0.000083
2	c	1.399336	0.016170	-0.000053
3	c	0.710494	-1.215274	0.000014
4	c	-0.662471	-1.240207	-0.000074
5	c	-1.396154	-0.006964	0.000071
6	c	-0.684033	1.239562	0.000132

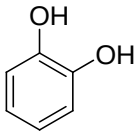
7	o	2.731153	0.095116	-0.000071
8	n	-2.702818	-0.019470	-0.000010
9	h	-1.241931	2.160240	-0.000072
10	h	1.236163	2.162430	-0.000051
11	h	1.267519	-2.138360	0.000003
12	h	-1.203285	-2.171037	0.000007
13	h	3.157068	-0.770064	0.000819
14	h	-3.224504	-0.884597	-0.000145
15	h	-3.240703	0.835659	0.000043

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.606035	1.217581	-0.000014
2	c	0.787202	1.210358	-0.000152
3	c	1.563715	-0.010311	0.000036
4	c	0.755840	-1.212508	-0.000038
5	c	-0.636273	-1.181279	-0.000084
6	c	-1.354083	0.029386	-0.000083
7	o	2.840028	-0.030296	0.000154
8	n	-2.810197	0.093982	0.000167
9	h	-1.148737	2.163970	0.000148
10	h	1.340794	2.149194	-0.000328
11	h	1.284874	-2.165499	-0.000040
12	h	-1.192386	-2.123715	-0.000473
13	h	-3.198029	-0.379219	-0.815870
14	h	-3.197559	-0.379602	0.816181

No.65



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.656111	1.404742	-0.000005
2	c	-1.884701	0.733553	-0.000003
3	c	-1.913026	-0.663121	0.000003
4	c	-0.720258	-1.392985	0.000006
5	c	0.504945	-0.727999	0.000005
6	c	0.530051	0.675484	-0.000001
7	o	1.668130	-1.446223	-0.000012
8	o	1.793684	1.235533	-0.000003
9	h	-2.808982	1.303973	-0.000006
10	h	-2.863191	-1.189766	0.000004
11	h	-0.720824	-2.479053	0.000011
12	h	-0.620642	2.492985	-0.000010
13	h	2.415903	-0.823706	0.000037
14	h	1.737828	2.203038	0.000057

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.601826	-0.673658	0.000002
2	c	-0.538702	0.793347	0.000029
3	c	0.771779	1.397935	0.000023
4	c	1.895927	0.606673	0.000014
5	c	1.789404	-0.813731	-0.000011
6	c	0.551336	-1.454255	-0.000027
7	o	-1.629110	1.424845	-0.000053
8	o	-1.825443	-1.210869	0.000029
9	h	2.883142	1.060765	0.000009
10	h	2.696482	-1.411903	-0.000034
11	h	0.470759	-2.537054	-0.000047
12	h	0.825085	2.482463	0.000026
13	h	-2.446551	-0.443950	0.000063

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.000000	0.895709	0.000000
2	c	1.390439	0.760574	-0.000000
3	c	1.928361	-0.517909	-0.000000
4	c	1.092811	-1.686498	-0.000000
5	c	-0.277256	-1.578068	0.000000
6	c	-0.852478	-0.287428	0.000000
7	o	-2.160987	-0.163413	0.000000
8	o	-0.686292	2.036360	0.000000
9	h	3.007049	-0.642566	-0.000000
10	h	1.560381	-2.666078	-0.000000
11	h	-0.933758	-2.441942	0.000000
12	h	2.030028	1.638794	-0.000000
13	h	-2.449594	0.773731	0.000000
14	h	-0.127127	2.836206	0.000000

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.578970	0.763884	0.000005
2	c	0.688292	1.404874	0.000005
3	c	1.883979	0.664690	0.000000
4	c	1.873090	-0.732877	-0.000003
5	c	0.630499	-1.410742	-0.000002
6	c	-0.544541	-0.682544	0.000001
7	o	-1.791026	-1.262164	0.000002
8	o	-1.745246	1.325937	-0.000009
9	h	2.837403	1.195721	0.000000
10	h	2.803554	-1.298594	-0.000006
11	h	0.586461	-2.499905	-0.000005
12	h	0.710302	2.494324	0.000007
13	h	-2.361626	-0.445433	0.000022

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.535283	0.674037	-0.000095
2	c	0.647720	1.390793	-0.000036
3	c	1.868928	0.724436	0.000178
4	c	1.898775	-0.660337	-0.000086
5	c	0.708641	-1.380051	-0.000144
6	c	-0.506126	-0.719326	0.000019
7	o	-1.647622	-1.447961	0.000164
8	o	-1.764865	1.246494	-0.000202
9	h	2.783694	1.291188	0.000467
10	h	2.838185	-1.185360	-0.000151
11	h	0.712773	-2.457415	-0.000188
12	h	0.610658	2.468959	0.000166
13	h	-2.425041	-0.889632	0.000472
14	h	-1.716304	2.206678	0.000515

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.467740	-1.451018	0.000017
2	c	-0.653003	-0.632243	0.000068
3	c	-0.508445	0.809292	-0.000011
4	c	0.829991	1.357774	0.000012
5	c	1.927693	0.521715	0.000004
6	c	1.752560	-0.881640	-0.000007
7	o	-1.876882	-1.179544	-0.000053
8	o	-1.515446	1.535177	-0.000040
9	h	2.920933	0.935232	0.000054
10	h	2.613981	-1.525913	-0.000144
11	h	0.340331	-2.520375	-0.000054
12	h	0.927336	2.430219	0.000036
13	h	-2.563156	-0.507507	0.000359

2.3 cation radical

Charge = 1 Multiplicity = 2

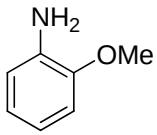
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.481892	-0.749750	0.000178
2	c	-0.587094	0.689684	0.000009
3	c	0.571143	1.456975	0.000702
4	c	1.805517	0.817576	0.000080
5	c	1.907794	-0.609584	-0.000403
6	c	0.797984	-1.383370	-0.000044
7	o	-1.820344	1.142306	-0.000947
8	o	-1.522304	-1.495493	0.000341
9	h	2.705915	1.405706	0.000006
10	h	2.883149	-1.062762	-0.001125
11	h	0.829881	-2.459310	-0.000211
12	h	0.499358	2.532060	0.000891
13	h	-2.375027	-1.030014	0.001076
14	h	-1.882812	2.110617	0.001073

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.571575	-0.649689	-0.001153
2	c	-0.555644	0.767869	-0.001603
3	c	0.707282	1.372558	-0.000190
4	c	1.883069	0.621886	0.001086
5	c	1.833769	-0.760278	-0.000195
6	c	0.586370	-1.393042	-0.000782
7	o	-1.682097	1.424974	0.000337
8	o	-1.776934	-1.287249	0.000781
9	h	2.833509	1.129931	0.002151
10	h	2.736157	-1.347168	0.001145
11	h	0.515886	-2.469306	0.000633
12	h	0.754395	2.450374	0.000143
13	h	-2.467322	-0.621456	0.004011

No.66



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.852183	0.669657	-0.001085
2	c	2.284973	-0.660699	0.006384
3	c	1.354287	-1.697518	0.004393
4	c	-0.017014	-1.401524	-0.000830
5	c	-0.446718	-0.075580	-0.006119
6	c	0.489332	0.985826	-0.008271
7	o	-1.763301	0.326983	0.000017
8	c	-2.774575	-0.669460	0.004614
9	n	0.030430	2.304068	-0.078859
10	h	1.678870	-2.734262	0.007739
11	h	-0.738446	-2.211653	0.002577
12	h	2.578905	1.479726	-0.010182
13	h	3.349816	-0.877680	0.011569
14	h	-0.932268	2.429056	0.210040
15	h	0.650034	2.998651	0.319704
16	h	-3.724634	-0.131690	0.006957
17	h	-2.714670	-1.300185	-0.892062
18	h	-2.709013	-1.300526	0.901008

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.055734	-1.353534	-0.000119
2	c	-0.466368	-0.025084	-0.000045

3	c	0.505715	1.055917	-0.000000
4	c	1.889848	0.680940	0.000119
5	c	2.284290	-0.644067	0.000087
6	c	1.314509	-1.663104	-0.000067
7	o	-1.760638	0.386036	-0.000093
8	c	-2.797705	-0.590521	0.000165
9	n	0.186607	2.348976	-0.000083
10	h	1.619753	-2.706028	-0.000159
11	h	-0.781548	-2.159737	-0.000266
12	h	2.611393	1.492715	0.000237
13	h	3.339942	-0.900982	0.000163
14	h	-0.834447	2.446397	-0.000163
15	h	-3.732573	-0.028368	0.000362
16	h	-2.745698	-1.219207	-0.897314
17	h	-2.745298	-1.219183	0.897632

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.518734	0.979430	0.000030
2	c	-1.904313	0.645719	0.000038
3	c	-2.283692	-0.672689	0.000060
4	c	-1.302982	-1.708291	0.000055
5	c	0.057287	-1.421276	-0.000118
6	c	0.474686	-0.086369	-0.000185
7	o	1.731144	0.347407	-0.000440
8	c	2.835208	-0.592472	0.000318
9	n	-0.093451	2.246540	0.000047
10	h	-1.626735	-2.744655	0.000156
11	h	0.783371	-2.225425	-0.000233
12	h	-2.640739	1.444207	-0.000007
13	h	-3.336570	-0.935544	0.000050
14	h	0.899313	2.458691	0.000102
15	h	-0.743356	3.025293	0.000459
16	h	3.731460	0.025039	0.001430
17	h	2.795883	-1.208853	0.902459
18	h	2.797621	-1.208106	-0.902418

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.488207	1.101792	-0.000302
2	c	1.869904	0.693935	0.000528
3	c	2.273798	-0.637763	0.000472
4	c	1.342027	-1.687507	-0.000185
5	c	-0.031009	-1.346702	-0.000617
6	c	-0.439435	-0.021577	-0.000648
7	o	-1.784420	0.369148	-0.001128
8	c	-2.761645	-0.635126	0.001164
9	n	0.141462	2.389192	0.000079
10	h	1.651747	-2.730486	-0.000410
11	h	-0.768385	-2.147671	-0.001012
12	h	2.607533	1.495235	0.000894
13	h	3.341582	-0.865952	0.001001
14	h	-0.879093	2.452414	0.000143
15	h	-3.731813	-0.125777	0.001689
16	h	-2.694820	-1.279875	-0.891606
17	h	-2.692700	-1.277727	0.895297

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	0.490390	0.972680	-0.010230
2	c	1.838819	0.653210	0.001758
3	c	2.264691	-0.672774	0.010195
4	c	1.334661	-1.692984	0.006386
5	c	-0.027601	-1.389638	-0.006030
6	c	-0.448684	-0.072605	-0.016501
7	o	-1.746798	0.321067	-0.030439
8	c	-2.769040	-0.644239	0.023017
9	n	0.052453	2.299415	-0.081080
10	h	1.647351	-2.722672	0.014033

11	h	-0.742249	-2.192216	-0.007543
12	h	2.562905	1.451570	0.003633
13	h	3.318313	-0.893051	0.021084
14	h	-0.853913	2.444533	0.318868
15	h	0.708656	2.954601	0.300391
16	h	-3.699495	-0.096053	0.023969
17	h	-2.735883	-1.295795	-0.843147
18	h	-2.697885	-1.237257	0.928220

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.332999	-1.651718	-0.000104
2	c	-0.043529	-1.350927	-0.000039
3	c	-0.468546	-0.028250	0.000024
4	c	0.493753	1.047523	0.000024
5	c	1.881621	0.701330	0.000112
6	c	2.292104	-0.625316	0.000049
7	o	-1.758277	0.365450	0.000070
8	c	-2.788515	-0.597174	0.000033
9	n	0.154143	2.335003	-0.000111
10	h	1.643110	-2.681985	-0.000251
11	h	-0.751775	-2.158977	-0.000023
12	h	2.596635	1.506324	0.000211
13	h	3.340723	-0.866796	0.000052
14	h	-0.850038	2.438353	-0.000392
15	h	-3.714508	-0.042183	-0.000118
16	h	-2.738033	-1.218132	-0.886886
17	h	-2.738233	-1.218035	0.887025

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.055869	-1.404958	0.000197
2	c	0.485940	-0.086689	-0.000105
3	c	-0.494575	0.972259	-0.000048

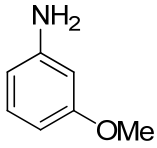
4	c	-1.896476	0.652503	-0.000269
5	c	-2.288667	-0.662794	-0.000136
6	c	-1.320495	-1.692796	0.000194
7	o	1.743847	0.341700	-0.000033
8	c	2.816859	-0.588768	-0.000183
9	n	-0.097934	2.213202	0.000302
10	h	-1.637733	-2.720271	0.000573
11	h	0.762820	-2.214221	0.000502
12	h	-2.606507	1.461807	-0.000700
13	h	-3.334899	-0.910896	-0.000299
14	h	0.882753	2.450702	0.000295
15	h	-0.758580	2.978037	0.000472
16	h	3.716198	0.006078	-0.000628
17	h	2.780307	-1.204637	0.889364
18	h	2.779675	-1.205155	-0.889337

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.438609	-0.024747	-0.001240
2	c	0.483772	1.078749	-0.000395
3	c	1.849336	0.702859	-0.000364
4	c	2.266951	-0.622074	0.000195
5	c	1.349846	-1.658225	0.000489
6	c	-0.016422	-1.333306	-0.000268
7	n	0.111441	2.368064	0.001614
8	o	-1.759136	0.346693	-0.003144
9	c	-2.754858	-0.637904	0.001799
10	h	1.661281	-2.688531	0.001322
11	h	-0.735955	-2.133431	-0.000309
12	h	2.582091	1.494930	-0.000012
13	h	3.324014	-0.837756	0.000663
14	h	-0.891244	2.426463	0.001733
15	h	-3.701833	-0.115953	0.000773
16	h	-2.693795	-1.267400	-0.880846
17	h	-2.691656	-1.260429	0.889231

No.67



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.713887	1.069011	-0.003196
2	c	-0.536347	1.808728	0.003539
3	c	0.721452	1.191847	0.005460
4	c	0.774731	-0.208290	-0.000232
5	c	-0.402267	-0.967183	-0.005836
6	c	-1.652623	-0.339185	-0.007485
7	o	1.935160	-0.936015	0.001664
8	c	3.172465	-0.238304	0.002225
9	n	-2.827318	-1.099081	-0.074987
10	h	1.620757	1.796052	0.011684
11	h	-2.679152	1.569861	-0.013126
12	h	-0.590722	2.894771	0.007991
13	h	-2.748926	-2.050241	0.264474
14	h	-3.657692	-0.643062	0.283352
15	h	-0.320764	-2.051022	-0.016560
16	h	3.946789	-1.007761	-0.001088
17	h	3.278045	0.389381	-0.892406
18	h	3.280479	0.383969	0.900431

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.419254	-1.010717	-0.000018
2	c	-1.718214	-0.414207	0.000009

3	c	-1.803103	1.018689	0.000015
4	c	-0.651359	1.781023	-0.000004
5	c	0.622600	1.179271	-0.000031
6	c	0.729960	-0.225484	-0.000038
7	n	-2.868531	-1.108983	0.000029
8	o	1.918029	-0.902174	-0.000063
9	c	3.131046	-0.159378	0.000069
10	h	1.506995	1.805954	-0.000062
11	h	-2.790800	1.468134	0.000036
12	h	-0.717097	2.865960	0.000000
13	h	-2.659950	-2.114908	0.000021
14	h	-0.317315	-2.092865	-0.000024
15	h	3.930689	-0.901896	0.000130
16	h	3.216533	0.467382	-0.897209
17	h	3.216369	0.467333	0.897397

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.638187	-0.375171	0.000057
2	c	1.730088	1.072006	0.000042
3	c	0.572802	1.824408	-0.000033
4	c	-0.680239	1.194732	-0.000051
5	c	-0.773726	-0.244069	-0.000078
6	c	0.382296	-1.012874	0.000018
7	o	-1.931064	-0.898550	-0.000290
8	c	-3.198045	-0.203960	0.000217
9	n	2.779081	-1.083206	0.000027
10	h	-1.581162	1.797292	-0.000027
11	h	2.707562	1.545638	-0.000154
12	h	0.627565	2.908198	-0.000127
13	h	2.774730	-2.098048	-0.000251
14	h	3.687698	-0.633007	0.000491
15	h	0.300624	-2.095119	0.000145
16	h	-3.946820	-0.994340	0.000567
17	h	-3.301335	0.404946	0.903195
18	h	-3.302091	0.404852	-0.902743

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.760155	-0.419799	0.000541
2	c	1.779683	1.030706	0.000631
3	c	0.619345	1.779334	-0.000241
4	c	-0.670914	1.195331	-0.001657
5	c	-0.717512	-0.210599	-0.001990
6	c	0.431611	-0.991494	-0.000749
7	o	-1.921609	-0.926327	-0.003800
8	c	-3.122650	-0.193946	0.003938
9	n	2.908623	-1.100039	0.001589
10	h	-1.560096	1.815550	-0.003238
11	h	2.754891	1.514542	0.001910
12	h	0.693126	2.868789	0.000123
13	h	2.694288	-2.104163	0.000608
14	h	0.318500	-2.075444	-0.000831
15	h	-3.932238	-0.932034	0.005781
16	h	-3.212670	0.440891	0.899406
17	h	-3.221609	0.445554	-0.887321

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-1.641435	-0.339219	-0.010177
2	c	-1.707010	1.060884	-0.004322
3	c	-0.538022	1.793869	0.003818
4	c	0.716071	1.185759	0.004300
5	c	0.771196	-0.202613	-0.002666
6	c	-0.398877	-0.959651	-0.009871
7	o	1.918521	-0.913154	-0.001475
8	c	3.158959	-0.245507	0.006876
9	n	-2.807848	-1.097108	-0.076013
10	h	1.602745	1.790850	0.011220

11	h	-2.664117	1.554518	-0.007685
12	h	-0.592345	2.869575	0.010416
13	h	-2.719263	-2.028428	0.283987
14	h	-3.616469	-0.646313	0.308153
15	h	-0.324208	-2.034744	-0.016771
16	h	3.913235	-1.018212	0.005269
17	h	3.274242	0.373320	-0.875628
18	h	3.267655	0.363282	0.897180

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.730581	-0.217210	-0.000607
2	c	-0.417591	-1.008192	-0.000767
3	c	-1.715395	-0.411164	-0.000020
4	c	-1.808054	1.016593	0.000148
5	c	-0.652964	1.784852	-0.000115
6	c	0.623520	1.184843	-0.000339
7	n	-2.846648	-1.126982	0.000764
8	o	1.908712	-0.886695	-0.000641
9	c	3.122554	-0.172339	0.000982
10	h	1.495245	1.812354	-0.000310
11	h	-2.783226	1.472314	0.000479
12	h	-0.721571	2.858820	-0.000022
13	h	-2.639101	-2.118273	0.000691
14	h	-0.322017	-2.081786	-0.000956
15	h	3.905973	-0.915563	0.000934
16	h	3.213546	0.445956	-0.885086
17	h	3.212082	0.444318	0.888354

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.365023	-1.005432	-0.000087
2	c	-1.646063	-0.371326	0.000037
3	c	-1.751233	1.066015	0.000102

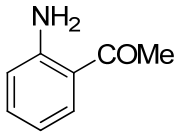
4	c	-0.590885	1.810426	-0.000023
5	c	0.675106	1.187038	-0.000146
6	c	0.774981	-0.232729	-0.000144
7	n	-2.731209	-1.095928	0.000074
8	o	1.939650	-0.892691	-0.000218
9	c	3.169266	-0.191590	0.000269
10	h	1.554633	1.803024	-0.000143
11	h	-2.725855	1.522543	0.000031
12	h	-0.644304	2.884255	-0.000060
13	h	-2.693168	-2.106453	0.000016
14	h	-3.650434	-0.675169	0.000296
15	h	-0.301574	-2.081056	-0.000085
16	h	3.936404	-0.950157	0.000108
17	h	3.264487	0.421131	-0.888014
18	h	3.264172	0.420489	0.889032

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.187834	-1.206294	-0.216670
2	c	1.192783	-1.197997	-0.028722
3	c	1.964074	0.024009	0.088374
4	c	1.166670	1.226760	-0.032043
5	c	-0.208624	1.203523	-0.219963
6	c	-0.909807	-0.010865	-0.309949
7	n	3.284882	0.110686	0.280588
8	o	-2.303055	-0.024550	-0.533611
9	c	-3.070483	-0.000619	0.657798
10	h	-0.721035	-2.154084	-0.307280
11	h	1.694476	2.177392	0.026674
12	h	-0.762032	2.139033	-0.314671
13	h	3.670290	-0.839632	0.334712
14	h	1.726867	-2.148421	0.029939
15	h	-4.128502	-0.010394	0.362995
16	h	-2.862200	-0.879102	1.289149
17	h	-2.868267	0.905705	1.250304

No.68



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.612121	0.973334	-0.000074
2	c	-2.019089	0.800389	-0.000102
3	c	-2.587904	-0.461019	-0.000050
4	c	-1.781176	-1.613032	0.000056
5	c	-0.403711	-1.461964	0.000064
6	c	0.220740	-0.193098	-0.000031
7	c	1.691468	-0.082084	-0.000041
8	o	2.269731	1.013609	-0.000067
9	n	-0.089690	2.229795	0.000203
10	c	2.541812	-1.345068	0.000005
11	h	-2.228309	-2.602431	0.000163
12	h	0.218382	-2.351077	0.000162
13	h	-2.652240	1.685396	-0.000135
14	h	-3.671194	-0.556074	-0.000074
15	h	0.918942	2.337972	0.000034
16	h	-0.696630	3.035213	0.000038
17	h	2.344652	-1.961852	0.884928
18	h	2.344129	-1.962215	-0.884577
19	h	3.592137	-1.047110	-0.000391

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.364315	-1.409369	-0.000033

2	c	0.230766	-0.144483	0.000028
3	c	-0.636833	1.031277	0.000061
4	c	-2.058132	0.808102	0.000049
5	c	-2.602928	-0.461340	-0.000032
6	c	-1.754434	-1.582159	-0.000085
7	c	1.718936	-0.026608	0.000037
8	o	2.282474	1.066856	-0.000275
9	n	-0.247577	2.307086	0.000101
10	c	2.568279	-1.290001	0.000164
11	h	-2.170681	-2.585670	-0.000165
12	h	0.260345	-2.296695	-0.000075
13	h	-2.682013	1.696791	0.000091
14	h	-3.681511	-0.594878	-0.000055
15	h	0.776868	2.346617	0.000072
16	h	2.371960	-1.906635	0.885366
17	h	2.372392	-1.906397	-0.885310
18	h	3.617840	-0.990099	0.000422

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.235894	-0.215483	0.000006
2	c	-0.635996	0.951866	-0.000007
3	c	-2.065317	0.786615	-0.000045
4	c	-2.619659	-0.473458	-0.000028
5	c	-1.778239	-1.604824	0.000027
6	c	-0.371049	-1.459009	0.000043
7	n	-0.124261	2.179053	0.000037
8	c	1.738001	-0.068069	0.000000
9	c	2.608347	-1.297761	-0.000031
10	o	2.234686	1.055831	-0.000014
11	h	-2.210066	-2.601094	0.000056
12	h	0.238659	-2.355899	0.000069
13	h	-2.692458	1.674363	-0.000070
14	h	-3.697955	-0.596828	-0.000057
15	h	0.903397	2.269069	0.000128
16	h	-0.718585	3.003895	0.000029
17	h	2.422741	-1.916407	0.886415
18	h	2.422568	-1.916525	-0.886355
19	h	3.652148	-0.979855	-0.000157

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.240863	-0.131815	0.000003
2	c	-0.621654	1.075200	0.000004
3	c	-2.059299	0.805578	-0.000006
4	c	-2.588983	-0.455113	-0.000015
5	c	-1.743112	-1.607591	-0.000015
6	c	-0.376119	-1.416614	-0.000006
7	n	-0.241735	2.333242	0.000053
8	c	1.680111	-0.029302	-0.000009
9	c	2.535325	-1.312703	0.000061
10	o	2.313358	1.053030	-0.000110
11	h	-2.167266	-2.609806	-0.000022
12	h	0.260728	-2.298810	-0.000006
13	h	-2.699302	1.686010	0.000012
14	h	-3.672508	-0.585948	-0.000022
15	h	0.778908	2.363608	0.000222
16	h	2.348355	-1.935479	0.885086
17	h	2.348257	-1.935641	-0.884830
18	h	3.585319	-1.006715	-0.000034

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.374478	-1.451385	-0.006221
2	c	0.220864	-0.176295	0.007121
3	c	-0.620987	0.960286	0.015960
4	c	-2.016011	0.762145	0.004328
5	c	-2.557973	-0.499356	-0.012504
6	c	-1.736863	-1.631007	-0.015740
7	c	1.698876	-0.058294	-0.008634

8	o	2.255424	1.016716	-0.061765
9	n	-0.156335	2.245001	0.089110
10	c	2.546750	-1.312181	0.036218
11	h	-2.159917	-2.619526	-0.027949
12	h	0.252211	-2.323132	-0.013075
13	h	-2.658229	1.626898	0.012347
14	h	-3.629109	-0.611886	-0.022188
15	h	0.795909	2.405526	-0.152671
16	h	-0.793895	2.965504	-0.184975
17	h	2.326224	-1.905010	0.917792
18	h	2.369283	-1.931993	-0.837044
19	h	3.587405	-1.018603	0.054943

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.748268	-1.585441	-0.000163
2	c	0.355821	-1.406845	-0.000480
3	c	-0.232882	-0.135871	-0.000241
4	c	0.641962	1.030588	-0.000089
5	c	2.057541	0.808866	0.000313
6	c	2.600627	-0.468759	0.000269
7	c	-1.724190	-0.023637	-0.000059
8	c	-2.564018	-1.280962	0.000461
9	n	0.245423	2.305130	-0.000066
10	o	-2.273026	1.052442	-0.000138
11	h	2.153904	-2.581852	-0.000267
12	h	-0.261129	-2.284874	-0.000791
13	h	2.690706	1.679323	0.000588
14	h	3.668442	-0.602593	0.000546
15	h	-0.756299	2.368942	-0.000414
16	h	-2.360737	-1.885683	-0.877422
17	h	-2.361248	-1.884439	0.879302
18	h	-3.606172	-0.991911	-0.000034

2.3 cation radical

Charge = 1 Multiplicity = 2

Center	Atomic	Coordinates (Angstroms)

Number	Name	X	Y	Z
1	c	0.335804	-1.455331	-0.001247
2	c	-0.249949	-0.200767	-0.000350
3	c	0.643271	0.954580	0.000514
4	c	2.067473	0.759507	0.001193
5	c	2.596613	-0.516199	0.000158
6	c	1.736922	-1.630950	-0.001186
7	c	-1.739591	-0.041353	-0.000519
8	o	-2.226413	1.061440	-0.003142
9	n	0.195093	2.179102	0.000796
10	c	-2.611893	-1.268784	0.002817
11	h	2.141784	-2.626870	-0.002159
12	h	-0.280431	-2.334059	-0.002049
13	h	2.699442	1.631472	0.002453
14	h	3.662994	-0.653397	0.000399
15	h	-0.794358	2.370720	0.000091
16	h	0.833648	2.964865	0.001672
17	h	-2.422941	-1.877851	-0.875495
18	h	-2.421434	-1.874058	0.883430
19	h	-3.644957	-0.950275	0.002930

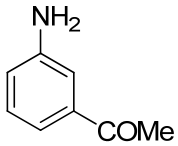
2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.378184	-1.408111	0.000222
2	c	-0.233917	-0.121916	0.000279
3	c	0.614788	1.063141	-0.000086
4	c	2.047484	0.798403	0.000413
5	c	2.566667	-0.450709	-0.000024
6	c	1.726303	-1.602199	-0.000573
7	c	-1.679542	-0.028148	0.000075
8	o	-2.289822	1.037555	-0.000234
9	n	0.238924	2.317568	-0.000205
10	c	-2.521421	-1.297477	0.000128
11	h	2.148112	-2.591988	-0.000774
12	h	-0.251865	-2.278771	0.000460
13	h	2.694688	1.660455	0.000846
14	h	3.637876	-0.578333	0.000075
15	h	-0.758722	2.371549	-0.000184

16	h	-2.324662	-1.906679	-0.876405
17	h	-2.325560	-1.906088	0.877255
18	h	-3.565029	-1.011465	-0.000568

No.69



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.834049	-0.413921	0.008607
2	c	2.096760	0.969723	0.000248
3	c	1.048143	1.887540	-0.008500
4	c	-0.280321	1.455756	-0.007356
5	c	-0.555272	0.078363	0.001368
6	c	0.500287	-0.842942	0.008323
7	c	-1.957153	-0.459519	-0.002533
8	o	-2.165580	-1.666314	-0.014482
9	n	2.881439	-1.337087	0.078294
10	c	-3.121589	0.516889	0.008842
11	h	-1.082908	2.185553	-0.014574
12	h	3.126666	1.321051	0.007493
13	h	1.271422	2.951400	-0.016377
14	h	2.657060	-2.275937	-0.228265
15	h	3.772332	-1.022906	-0.286603
16	h	0.258788	-1.902387	0.018113
17	h	-3.097457	1.169064	-0.872812
18	h	-4.054743	-0.049856	0.012187
19	h	-3.086025	1.162797	0.894638

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.507451	0.061147	-0.000007
2	c	0.509683	-0.891503	0.000248
3	c	1.888216	-0.510807	0.000249
4	c	2.190233	0.891406	-0.000177
5	c	1.176556	1.833274	-0.000532
6	c	-0.170105	1.430690	-0.000396
7	n	2.915976	-1.376415	0.000583
8	c	-1.934629	-0.418431	-0.000060
9	o	-2.184162	-1.615487	-0.001357
10	c	-3.056527	0.604315	0.001238
11	h	-0.948390	2.187090	-0.000697
12	h	3.237019	1.180447	-0.000210
13	h	1.418557	2.892708	-0.000902
14	h	2.553723	-2.337679	0.000832
15	h	0.238767	-1.944209	0.000448
16	h	-3.002619	1.250072	-0.884089
17	h	-4.012376	0.077027	0.003747
18	h	-2.999071	1.252800	0.884268

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.453520	-0.858956	-0.000125
2	c	-1.824117	-0.441270	-0.000098
3	c	-2.152382	0.957248	-0.000056
4	c	-1.134075	1.879736	0.000104
5	c	0.219523	1.456103	0.000183
6	c	0.558998	0.081831	0.000016
7	n	-2.795127	-1.362065	-0.000010
8	c	1.997371	-0.434016	0.000001
9	c	3.133625	0.556277	-0.000287
10	o	2.167041	-1.637996	0.000282
11	h	1.001835	2.208506	0.000425
12	h	-3.193663	1.267400	-0.000167
13	h	-1.362117	2.940970	0.000154
14	h	-2.584284	-2.356688	-0.000053
15	h	-3.778766	-1.105911	-0.000004

16	h	-0.191665	-1.914571	-0.000255
17	h	3.094390	1.202594	0.886222
18	h	4.078264	0.010153	-0.001445
19	h	3.093025	1.204251	-0.885480

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.534189	-0.880969	-0.000265
2	c	-1.933816	-0.515349	-0.000132
3	c	-2.161317	0.915225	-0.000036
4	c	-1.125926	1.837237	0.000194
5	c	0.224686	1.445460	0.000165
6	c	0.504771	0.055259	-0.000089
7	n	-2.966491	-1.357997	0.000028
8	c	1.906404	-0.439133	-0.000047
9	c	3.048326	0.582471	-0.000332
10	o	2.203535	-1.635756	0.000441
11	h	1.013366	2.190807	0.000366
12	h	-3.197566	1.249905	-0.000087
13	h	-1.367991	2.901663	0.000355
14	h	-2.605814	-2.318736	0.000027
15	h	-0.270772	-1.936851	-0.000459
16	h	2.997839	1.229881	0.883478
17	h	3.998597	0.041763	-0.002030
18	h	2.995867	1.232397	-0.882118

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	-0.504878	-0.840158	-0.008949
2	c	-1.826077	-0.407593	-0.009636
3	c	-2.080228	0.966404	-0.005256

4	c	-1.035385	1.872727	0.003106
5	c	0.284104	1.438018	0.004439
6	c	0.547716	0.072061	-0.001813
7	n	-2.877955	-1.323632	-0.078125
8	c	1.952031	-0.460713	0.000810
9	c	3.109245	0.509592	0.006754
10	o	2.154585	-1.647373	-0.002352
11	h	1.077170	2.162040	0.010997
12	h	-3.098731	1.318287	-0.009370
13	h	-1.250099	2.927585	0.008770
14	h	-2.656641	-2.229080	0.291633
15	h	-3.737026	-0.990572	0.317837
16	h	-0.288667	-1.893252	-0.015432
17	h	3.072016	1.145666	0.885597
18	h	4.035357	-0.049047	0.007517
19	h	3.076471	1.150753	-0.868587

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.182126	1.427128	-0.000931
2	c	-0.510819	0.053926	-0.000293
3	c	0.516418	-0.899279	0.000332
4	c	1.889207	-0.501205	0.000524
5	c	2.189461	0.897543	-0.000378
6	c	1.164053	1.835748	-0.001139
7	c	-1.929166	-0.419733	-0.000352
8	c	-3.048467	0.592987	0.002812
9	n	2.902339	-1.376464	0.001527
10	o	-2.170855	-1.600998	-0.002929
11	h	-0.951635	2.176469	-0.001449
12	h	3.221993	1.202605	-0.000436
13	h	1.396634	2.886397	-0.001832
14	h	2.551794	-2.326803	0.001706
15	h	0.275142	-1.947600	0.000838
16	h	-2.991864	1.230215	-0.874519
17	h	-3.995071	0.069722	0.004649
18	h	-2.987890	1.229536	0.880344

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.560301	0.061981	-0.000196
2	c	-0.465873	-0.880636	-0.000279
3	c	-1.832295	-0.441788	-0.000112
4	c	-2.141545	0.959654	-0.000445
5	c	-1.105432	1.869863	-0.000103
6	c	0.239999	1.438068	0.000140
7	n	-2.793611	-1.327182	0.000603
8	c	1.977336	-0.436013	-0.000238
9	o	2.181255	-1.620802	-0.000359
10	c	3.108332	0.558773	0.000423
11	h	1.015822	2.180413	0.000552
12	h	-3.172347	1.270503	-0.000641
13	h	-1.322035	2.923041	-0.000004
14	h	-2.601875	-2.322029	0.000806
15	h	-3.769159	-1.053386	0.000773
16	h	-0.251499	-1.934056	-0.000434
17	h	3.058698	1.192571	0.880944
18	h	4.046964	0.021908	-0.002814
19	h	3.055724	1.198320	-0.875675

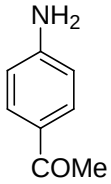
2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.492842	0.064363	-0.002293
2	c	-0.534793	-0.869335	-0.000633
3	c	-1.911455	-0.498679	0.001572
4	c	-2.148362	0.909896	-0.001734
5	c	-1.120593	1.826800	-0.003703
6	c	0.218766	1.433219	-0.003367
7	n	-2.935782	-1.361393	0.006795
8	c	1.910030	-0.435626	-0.001561
9	o	2.155767	-1.616634	-0.009761
10	c	3.046679	0.561899	0.010498

11	h	0.997049	2.172664	-0.004276
12	h	-3.171439	1.252390	-0.001475
13	h	-1.359342	2.878664	-0.005243
14	h	-2.576152	-2.304162	0.007499
15	h	-0.285007	-1.916604	0.000563
16	h	2.992959	1.194024	0.891129
17	h	3.985856	0.024559	0.011437
18	h	3.001734	1.206073	-0.861788

No.70



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	2.153007	0.044610	-0.004856
2	c	1.479464	-1.195091	-0.006850
3	c	0.094107	-1.242972	-0.004685
4	c	-0.679499	-0.066317	-0.001680
5	c	-0.001822	1.166038	-0.001195
6	c	1.387374	1.226436	-0.002871
7	c	-2.163546	-0.178075	0.003411
8	o	-2.716473	-1.274212	0.009559
9	n	3.539167	0.096589	-0.059635
10	c	-3.000639	1.093308	0.000205
11	h	-0.559460	2.098066	0.001889
12	h	2.056422	-2.117676	-0.014748
13	h	-0.422579	-2.197867	-0.003969
14	h	3.979173	0.956214	0.242384
15	h	4.040655	-0.731056	0.236006
16	h	1.889237	2.191759	-0.007901
17	h	-2.790519	1.704663	-0.886197
18	h	-4.056667	0.815849	0.002002

19	h	-2.789320	1.710006	0.882640

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.048753	1.188716	0.000157
2	c	1.428007	1.260003	0.000133
3	c	2.230804	0.068407	-0.000023
4	c	1.538386	-1.194629	-0.000131
5	c	0.162142	-1.248864	-0.000085
6	c	-0.612307	-0.062118	0.000049
7	n	3.558498	0.210033	-0.000038
8	c	-2.102673	-0.185375	0.000162
9	o	-2.631379	-1.291679	0.000212
10	c	-2.951495	1.074015	-0.000319
11	h	-0.527796	2.108643	0.000293
12	h	2.125426	-2.110909	-0.000250
13	h	-0.361454	-2.199737	-0.000150
14	h	4.005377	-0.715132	-0.000138
15	h	1.947346	2.213557	0.000214
16	h	-2.745541	1.690400	-0.884123
17	h	-4.004414	0.785777	-0.001312
18	h	-2.747099	1.689668	0.884384

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.660212	-0.047574	0.006047
2	c	-0.010407	1.203810	-0.046646
3	c	-1.383701	1.262830	-0.047498
4	c	-2.145755	0.044287	0.001403
5	c	-1.469349	-1.221510	0.049601
6	c	-0.099410	-1.253175	0.045533
7	n	-3.480689	0.093247	0.002849
8	c	2.170914	-0.170603	-0.007625
9	c	3.025899	1.067156	0.092063

10	o	2.640655	-1.291629	-0.114837
11	h	0.559786	2.125889	-0.084353
12	h	-2.051222	-2.138469	0.089172
13	h	0.440373	-2.194231	0.075056
14	h	-3.985520	0.974472	-0.029743
15	h	-4.045516	-0.751050	0.034391
16	h	-1.902293	2.217086	-0.083796
17	h	2.783637	1.648341	0.990561
18	h	4.074615	0.767739	0.128270
19	h	2.875304	1.719197	-0.778070

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.422153	1.251229	0.000405
2	c	2.271103	0.072802	-0.000140
3	c	1.540598	-1.187757	0.000274
4	c	0.168631	-1.247595	0.000199
5	c	-0.647565	-0.077184	0.000023
6	c	0.050573	1.170675	0.000289
7	n	3.587531	0.204694	-0.000563
8	c	-2.086091	-0.191570	-0.000159
9	c	-2.929933	1.094313	-0.000298
10	o	-2.701639	-1.280715	-0.000050
11	h	-0.518466	2.099505	0.000571
12	h	2.124355	-2.110301	0.000539
13	h	-0.337564	-2.210788	0.000273
14	h	4.013716	-0.729517	-0.000654
15	h	1.922451	2.217901	0.000700
16	h	-2.726082	1.714789	-0.883151
17	h	-3.985831	0.809225	-0.002313
18	h	-2.729004	1.712565	0.884820

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	c	1.375409	1.218379	-0.004709
2	c	2.140140	0.047166	-0.006921
3	c	1.476611	-1.188447	-0.008803
4	c	0.100292	-1.238706	-0.005602
5	c	-0.673882	-0.073312	-0.002717
6	c	-0.004474	1.152036	-0.002083
7	n	3.516154	0.103717	-0.063636
8	c	-2.154217	-0.179149	0.003654
9	c	-2.984677	1.084809	0.001215
10	o	-2.700469	-1.257232	0.010962
11	h	-0.553704	2.076379	0.001586
12	h	2.051611	-2.099341	-0.013233
13	h	-0.391881	-2.194132	-0.004623
14	h	3.934094	0.952644	0.265774
15	h	4.002070	-0.707577	0.267404
16	h	1.868249	2.176037	-0.005679
17	h	-2.769991	1.685173	-0.877512
18	h	-4.032650	0.816808	0.003014
19	h	-2.768345	1.689187	0.876819

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.616785	-0.070229	-0.000756
2	c	-0.034791	1.185844	-0.001915
3	c	-1.421173	1.264796	-0.001736
4	c	-2.223621	0.079560	0.000052
5	c	-1.550671	-1.187055	0.000938
6	c	-0.166174	-1.251968	0.000454
7	n	-3.552688	0.207662	0.001072
8	c	2.101915	-0.189025	-0.000339
9	c	2.948862	1.061046	0.003048
10	o	2.619744	-1.279979	-0.002301
11	h	0.534697	2.096812	-0.002967
12	h	-2.138033	-2.091221	0.002187
13	h	0.326759	-2.205921	0.001338
14	h	-3.998823	-0.701751	0.002812

15	h	-1.916281	2.220747	-0.002603
16	h	2.740451	1.664349	0.881377
17	h	3.992725	0.777621	0.003720
18	h	2.742572	1.667751	-0.873433

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.001985	1.188364	-0.002408
2	c	-1.376725	1.262090	-0.002730
3	c	-2.148184	0.048342	0.000131
4	c	-1.480484	-1.225162	0.003569
5	c	-0.104875	-1.264596	0.003196
6	c	0.663255	-0.066874	0.000021
7	n	-3.450618	0.104341	-0.000416
8	c	2.154936	-0.176288	-0.001025
9	o	2.660554	-1.270238	-0.007418
10	c	2.994238	1.075476	0.005845
11	h	0.562359	2.104278	-0.004669
12	h	-2.071274	-2.125269	0.006260
13	h	0.401097	-2.210883	0.005438
14	h	-3.945831	0.988096	-0.002901
15	h	-4.019223	-0.734096	0.001565
16	h	-1.889207	2.208914	-0.005291
17	h	2.781362	1.675608	0.885463
18	h	4.038697	0.795516	0.008084
19	h	2.787034	1.681243	-0.871289

2.4 anion

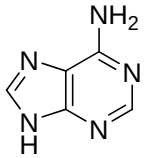
Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.045836	1.166333	-0.000702
2	c	-1.406783	1.253767	-0.000280
3	c	-2.249927	0.081354	0.000256
4	c	-1.537466	-1.178425	0.000260
5	c	-0.175420	-1.234629	-0.000249

6	c	0.638802	-0.075288	-0.000504
7	n	-3.555644	0.199469	0.000318
8	c	2.080147	-0.191532	0.000021
9	o	2.656137	-1.273714	-0.000222
10	c	2.927215	1.069471	0.000678
11	h	0.514831	2.085613	-0.000690
12	h	-2.114776	-2.090583	0.000384
13	h	0.306674	-2.196965	0.000025
14	h	-3.983807	-0.714648	0.000534
15	h	-1.887287	2.218897	-0.000307
16	h	2.722492	1.677685	0.876432
17	h	3.972690	0.790140	0.002473
18	h	2.725198	1.676993	-0.876181

The Cartesian Coordinates of the nucleobases and the metabolites.

No.1



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.229142	-0.609172	-0.003121
2	c	0.179500	-0.520809	-0.003391
3	c	0.711476	0.773925	-0.002205
4	n	0.024001	1.923367	-0.000631
5	c	-1.294809	1.702661	0.002827
6	n	-1.948177	0.527851	0.003558
7	n	1.182137	-1.477841	0.000761
8	c	2.291747	-0.777884	0.002565
9	n	2.077086	0.586196	0.000611

10	n	-1.883241	-1.797661	-0.031337
11	h	3.290847	-1.193949	0.005810
12	h	-2.885369	-1.799579	0.095656
13	h	-1.369171	-2.656882	0.099219
14	h	-1.927019	2.587249	0.007204
15	h	2.775436	1.317455	0.001333

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.219384	-0.590762	0.000015
2	c	-0.206863	-0.536855	0.000002
3	c	-0.810733	0.780928	-0.000022
4	n	-0.117989	1.902640	-0.000012
5	c	1.230837	1.705710	0.000000
6	n	1.920387	0.563911	0.000004
7	n	-1.142617	-1.475831	-0.000037
8	c	-2.321381	-0.692943	0.000013
9	n	-2.189369	0.613600	0.000036
10	n	1.887343	-1.753530	-0.000002
11	h	-3.287108	-1.185376	-0.000019
12	h	2.899540	-1.747021	0.000039
13	h	1.385958	-2.632389	0.000035
14	h	1.829860	2.612780	-0.000026

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-2.108062	0.560208	0.000073
2	c	-0.737332	0.778510	-0.000037
3	c	-0.185998	-0.543777	0.000073
4	n	-1.141848	-1.484004	0.000063
5	c	-2.292315	-0.782001	-0.000121
6	n	-0.068548	1.897957	-0.000147
7	c	1.299992	1.699379	0.000074
8	n	1.956164	0.556503	0.000060

9	c	1.249826	-0.603892	0.000092
10	n	1.911986	-1.752196	-0.000123
11	h	-3.275918	-1.235405	-0.000086
12	h	2.930100	-1.741542	-0.000176
13	h	1.426275	-2.645559	0.000173
14	h	1.895380	2.607391	-0.000077
15	h	-2.828713	1.276522	0.000197

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	2.143100	0.683241	0.009867
2	c	0.784777	0.796982	-0.006707
3	c	0.217960	-0.511254	-0.021007
4	n	1.221761	-1.451917	-0.006439
5	c	2.314997	-0.662482	0.011373
6	n	0.029752	1.928236	0.001623
7	c	-1.277207	1.690649	0.007550
8	n	-1.930449	0.502349	0.002793
9	c	-1.177399	-0.609031	-0.018624
10	n	-1.828607	-1.842989	-0.074146
11	h	3.313718	-1.093787	0.026051
12	h	-2.759116	-1.821900	0.327776
13	h	-1.255020	-2.612514	0.253380
14	h	-1.927248	2.566570	0.021393

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.228926	-0.599914	-0.020614
2	c	0.188728	-0.532999	0.005117
3	c	0.719936	0.781739	0.027816
4	n	0.029604	1.927791	0.005687
5	c	-1.322441	1.709832	-0.002805
6	n	-1.957554	0.533948	-0.011087
7	n	1.165085	-1.480403	-0.014107

8	c	2.345179	-0.794350	-0.104165
9	n	2.080954	0.606947	0.065509
10	n	-1.902370	-1.840299	-0.079477
11	h	3.266079	-1.198519	0.313531
12	h	-2.822370	-1.781911	0.350122
13	h	-1.345661	-2.585666	0.333463
14	h	-1.948297	2.600423	-0.012592
15	h	2.725352	1.343942	-0.182294

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.226128	-0.610944	-0.000028
2	c	-0.176954	-0.514488	0.000029
3	c	-0.710028	0.754325	-0.000005
4	n	-0.017660	1.899237	-0.000022
5	c	1.279392	1.688885	0.000000
6	n	1.928997	0.528815	0.000034
7	n	-1.187965	-1.460915	-0.000006
8	c	-2.274242	-0.764527	-0.000009
9	n	-2.055375	0.578196	0.000062
10	n	1.876237	-1.772169	-0.000097
11	h	-3.272573	-1.167750	-0.000033
12	h	2.888046	-1.786707	0.000279
13	h	1.372935	-2.649415	0.000238
14	h	1.905864	2.567715	-0.000012
15	h	-2.769689	1.304506	-0.000192

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.236087	-0.597161	0.000104
2	c	-0.214309	-0.538484	-0.000010

3	c	-0.820722	0.779553	-0.000148
4	n	-0.106305	1.899989	-0.000056
5	c	1.200214	1.700829	-0.000120
6	n	1.893533	0.557258	0.000020
7	n	-1.148889	-1.453893	-0.000201
8	c	-2.286840	-0.711289	-0.000204
9	n	-2.142375	0.618786	0.000396
10	n	1.864796	-1.740330	0.000092
11	h	-3.256396	-1.180973	0.000323
12	h	2.883243	-1.764620	0.000096
13	h	1.353172	-2.620253	0.000053
14	h	1.808089	2.592483	0.000036

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-2.077261	0.561768	0.000355
2	c	-0.746673	0.780069	-0.000061
3	c	-0.180883	-0.541637	-0.000025
4	n	-1.145136	-1.472883	0.000158
5	c	-2.262751	-0.785127	-0.000529
6	n	-0.068350	1.877776	-0.000032
7	c	1.281131	1.678609	-0.000073
8	n	1.942177	0.563780	-0.000066
9	c	1.254062	-0.609098	-0.000013
10	n	1.893328	-1.731015	0.000096
11	h	-3.249406	-1.219216	-0.000319
12	h	2.921601	-1.739531	0.000143
13	h	1.393296	-2.628965	0.000138
14	h	1.868562	2.583894	-0.000117
15	h	-2.816680	1.270938	0.000790

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	2.106451	0.686681	0.005788

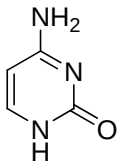
2	c	0.761534	0.777018	0.002373
3	c	0.221138	-0.504594	-0.004724
4	n	1.251727	-1.420317	-0.005463
5	c	2.313001	-0.643295	0.000768
6	n	0.012694	1.903962	0.004946
7	c	-1.274293	1.670574	0.001619
8	n	-1.904756	0.492986	-0.003022
9	c	-1.171311	-0.624940	-0.006976
10	n	-1.811109	-1.816644	-0.058839
11	h	3.312639	-1.049475	0.001759
12	h	-2.793183	-1.819893	0.211207
13	h	-1.282512	-2.641054	0.219142
14	h	-1.922414	2.535162	0.005661

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.214337	-0.594042	-0.004570
2	c	0.179291	-0.539256	0.008678
3	c	0.729793	0.765478	0.025702
4	n	0.041748	1.892648	0.012166
5	c	-1.295106	1.699826	-0.006056
6	n	-1.929187	0.557438	-0.013327
7	n	1.147423	-1.483010	-0.007497
8	c	2.341488	-0.801759	-0.121077
9	n	2.060362	0.595116	0.046811
10	n	-1.921063	-1.797513	-0.082713
11	h	3.229684	-1.178901	0.370321
12	h	-2.853489	-1.716698	0.289714
13	h	-1.442468	-2.564190	0.361247
14	h	-1.898689	2.591176	-0.017600
15	h	2.723213	1.334373	-0.107820

No.2



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.082394	-1.050834	0.002699
2	c	-1.185638	-0.529491	0.000231
3	n	-1.283832	0.894505	0.003162
4	c	-0.204250	1.715646	0.001292
5	c	1.050353	1.188256	-0.001944
6	c	1.133776	-0.250719	-0.002171
7	o	-2.222033	-1.180445	-0.000055
8	n	2.360979	-0.843671	-0.037687
9	h	-0.400114	2.783456	0.001371
10	h	1.930357	1.820101	-0.013811
11	h	2.393459	-1.847097	0.086417
12	h	3.198210	-0.316356	0.159695
13	h	-2.227877	1.261305	0.005116

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.326002	1.702383	0.002560
2	c	-0.980560	1.191042	-0.001440
3	c	-1.117585	-0.238674	-0.001403
4	n	-0.066287	-1.031830	0.004487
5	c	1.192313	-0.454888	0.000040
6	n	1.403058	0.938525	-0.000187
7	n	-2.359532	-0.805264	-0.044505

8	o	2.198304	-1.183259	0.001709
9	h	0.487829	2.779889	0.004779
10	h	-1.844804	1.848821	-0.011103
11	h	-2.410784	-1.807185	0.089874
12	h	-3.180360	-0.264647	0.185679

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.174787	-0.221800	0.000011
2	n	-0.110041	-1.050398	-0.001339
3	c	1.137576	-0.542716	-0.000150
4	n	1.329934	0.865640	0.001409
5	c	0.295471	1.709679	0.000002
6	c	-0.998758	1.204524	-0.001386
7	o	2.165140	-1.240931	-0.000306
8	n	-2.383242	-0.784119	0.001107
9	h	0.507503	2.774411	0.000078
10	h	-1.842629	1.886189	-0.003650
11	h	-2.456554	-1.796596	0.001229
12	h	-3.239314	-0.244198	0.002602
13	h	2.296309	1.191657	0.003090

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.105681	-0.222520	-0.019645
2	n	0.046172	-1.009251	-0.000753
3	c	-1.231035	-0.430806	0.001437
4	n	-1.375852	0.965744	0.021369
5	c	-0.270199	1.693107	0.007755
6	c	1.034362	1.185477	-0.020002
7	o	-2.238523	-1.162404	-0.002900
8	n	2.362393	-0.872335	-0.078661
9	h	-0.416309	2.779744	0.018422
10	h	1.912436	1.824829	-0.062184

11	h	2.263661	-1.844470	0.201279
12	h	3.086555	-0.401525	0.454725

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.082817	-1.060020	-0.012331
2	c	-1.165841	-0.534341	-0.010576
3	n	-1.308841	0.873689	-0.109964
4	c	-0.232899	1.773081	0.106672
5	c	1.053496	1.185769	0.019641
6	c	1.145225	-0.196353	-0.028960
7	o	-2.219745	-1.204724	0.052212
8	n	2.409638	-0.856303	-0.101237
9	h	-0.420266	2.809152	-0.169233
10	h	1.943464	1.812216	0.014828
11	h	2.283715	-1.822906	0.192113
12	h	3.114130	-0.407751	0.479106
13	h	-2.248270	1.176586	0.109548

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-0.066112	-1.039580	-0.000208
2	c	1.167442	-0.496662	-0.000174
3	n	1.281222	0.872647	0.000085
4	c	0.201574	1.688880	0.000056
5	c	-1.039599	1.178218	-0.000084
6	c	-1.134105	-0.257606	-0.000255
7	o	2.189666	-1.175166	0.000176
8	n	-2.330450	-0.829766	0.000058
9	h	0.407444	2.746558	0.000275
10	h	-1.921203	1.798619	0.000084

11	h	-2.411599	-1.839183	0.000891
12	h	-3.175199	-0.272108	0.000580
13	h	2.218738	1.267356	-0.000032

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.307734	1.709391	-0.000142
2	c	-0.990272	1.180743	0.000951
3	c	-1.106423	-0.275919	0.000085
4	n	-0.047490	-1.045296	-0.000188
5	c	1.182216	-0.466830	-0.000060
6	n	1.373016	0.940389	-0.001049
7	n	-2.312962	-0.800065	-0.000392
8	o	2.191592	-1.139094	0.000712
9	h	0.462742	2.779588	-0.000454
10	h	-1.871969	1.805846	0.002120
11	h	-2.429951	-1.809053	-0.001088
12	h	-3.141036	-0.213132	0.000121

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.148157	-0.270076	-0.000025
2	n	0.103574	-1.074407	-0.000078
3	c	-1.132222	-0.568251	0.000042
4	n	-1.294473	0.870741	0.000019
5	c	-0.309687	1.703624	-0.000007
6	c	1.009730	1.192200	-0.000014
7	o	-2.153873	-1.195879	0.000010
8	n	2.356527	-0.755339	0.000029
9	h	-0.523172	2.762908	-0.000023
10	h	1.898570	1.863390	-0.000037
11	h	2.502588	-1.764494	0.000030
12	h	3.169796	-0.141916	0.000160
13	h	-2.272064	1.215199	0.000027

2.4 anion

Charge = -1 Multiplicity = 1

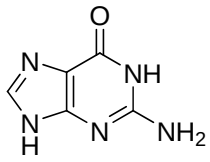
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.103754	-0.243751	-0.007520
2	n	0.018309	-1.000505	-0.004091
3	c	-1.205904	-0.404768	0.000621
4	n	-1.357416	0.945920	0.004078
5	c	-0.247202	1.678313	0.004082
6	c	1.024668	1.165860	-0.001901
7	o	-2.223161	-1.133364	0.003019
8	n	2.305577	-0.868789	-0.058543
9	h	-0.391077	2.753217	0.008458
10	h	1.906211	1.789110	-0.003490
11	h	2.324372	-1.855443	0.199023
12	h	3.128602	-0.330280	0.210054

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.056878	-1.050230	-0.003055
2	c	-1.157219	-0.515792	-0.006481
3	n	-1.312990	0.854328	-0.079538
4	c	-0.231827	1.745658	0.057166
5	c	1.050405	1.173220	0.025159
6	c	1.153606	-0.195220	-0.013911
7	o	-2.201574	-1.196883	0.031127
8	n	2.390527	-0.867004	-0.107668
9	h	-0.447666	2.792396	-0.027392
10	h	1.927547	1.799052	0.044791
11	h	2.384031	-1.719306	0.431062
12	h	3.164030	-0.296496	0.195232
13	h	-2.246052	1.192570	0.067515

No.3



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.528891	-0.853226	-0.000659
2	n	1.732760	-1.507865	-0.004202
3	c	2.717192	-0.533148	0.000880
4	n	2.227393	0.680271	0.008232
5	c	0.856533	0.503970	0.008259
6	n	-0.697104	-1.438775	0.007853
7	c	-1.676242	-0.565034	-0.001767
8	n	-1.477946	0.792585	-0.003474
9	c	-0.209896	1.471365	0.003160
10	o	-0.189615	2.692310	-0.003723
11	n	-2.980923	-1.005533	-0.068583
12	h	3.768702	-0.787796	-0.001005
13	h	-2.271483	1.420733	-0.080173
14	h	-3.690943	-0.447772	0.389927
15	h	-3.075410	-2.000668	0.095998
16	h	1.857928	-2.511318	-0.012982

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.178601	1.468370	0.000527
2	c	0.894829	0.491824	0.002424
3	c	0.576241	-0.936179	-0.001741
4	n	-0.658160	-1.450375	-0.001709

5	c	-1.639431	-0.551376	-0.000589
6	n	-1.449205	0.806174	0.000831
7	n	2.207344	0.653424	0.004324
8	c	2.658617	-0.666115	0.001500
9	n	1.745535	-1.634719	-0.001884
10	n	-2.911384	-1.012060	-0.019584
11	o	-0.142055	2.685992	-0.002502
12	h	3.722234	-0.875306	0.002066
13	h	-2.241840	1.440194	-0.020962
14	h	-3.715526	-0.415451	0.108155
15	h	-3.037260	-2.013627	0.044178

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.239318	1.484409	-0.000061
2	c	-0.858560	0.520474	-0.000099
3	c	-0.530506	-0.882145	0.000163
4	n	0.659378	-1.438260	0.000171
5	c	1.687874	-0.547283	-0.000195
6	n	1.506485	0.801203	-0.000082
7	n	-2.181881	0.711990	0.000069
8	c	-2.702036	-0.522578	-0.000183
9	n	-1.753967	-1.508901	0.000017
10	n	2.916011	-1.059259	0.000004
11	o	0.194642	2.690114	0.000112
12	h	-3.763162	-0.738796	-0.000202
13	h	2.307256	1.430332	0.000413
14	h	3.758517	-0.496271	-0.000478
15	h	3.015678	-2.069187	0.000192
16	h	-1.914148	-2.511663	0.000172

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.139326	1.449373	0.003158

2	c	0.895059	0.466747	0.015665
3	c	0.575367	-0.921627	-0.005776
4	n	-0.708210	-1.442636	0.000256
5	c	-1.644565	-0.547710	-0.010973
6	n	-1.424392	0.810282	-0.004542
7	n	2.263394	0.605728	0.021149
8	c	2.670121	-0.670057	0.004591
9	n	1.715446	-1.645195	-0.011361
10	n	-3.007127	-0.933138	-0.074513
11	o	-0.114476	2.689059	-0.011671
12	h	3.726469	-0.927567	0.004445
13	h	-2.202251	1.446304	-0.135754
14	h	-3.568957	-0.511119	0.662960
15	h	-3.053170	-1.945744	0.004806

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.527554	-0.851881	0.012517
2	n	1.738646	-1.502333	0.011116
3	c	2.719551	-0.527012	-0.003492
4	n	2.228281	0.687450	-0.015591
5	c	0.852811	0.508143	-0.007368
6	n	-0.684108	-1.446041	0.009308
7	c	-1.681967	-0.574818	-0.009746
8	n	-1.479056	0.788098	-0.000567
9	c	-0.225304	1.463298	0.002232
10	o	-0.189294	2.692226	0.010230
11	n	-2.970639	-1.011591	-0.084274
12	h	3.771727	-0.782653	-0.006670
13	h	-2.300207	1.396857	0.037162
14	h	-3.706261	-0.377200	0.254467
15	h	-3.102282	-1.982676	0.201884
16	h	1.863636	-2.507604	0.026521

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.540703	-0.844293	-0.000560
2	n	1.739484	-1.468278	0.001261
3	c	2.696038	-0.493698	0.001890
4	n	2.201333	0.694563	0.000997
5	c	0.830241	0.498031	-0.000841
6	n	-0.672463	-1.431985	0.000503
7	c	-1.658884	-0.574320	-0.002868
8	n	-1.473127	0.775233	-0.001182
9	c	-0.247221	1.424595	0.000063
10	o	-0.202124	2.642781	0.001936
11	n	-2.927037	-1.001512	-0.045742
12	h	3.744133	-0.738396	0.003218
13	h	-2.300024	1.374781	-0.006913
14	h	-3.679614	-0.358722	0.174226
15	h	-3.093423	-1.984263	0.135148
16	h	1.903325	-2.473701	0.001873

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.217069	1.434004	0.000144
2	c	0.878518	0.470837	0.000066
3	c	0.577072	-0.950776	-0.000087
4	n	-0.651219	-1.450796	-0.000017
5	c	-1.629930	-0.556367	0.000136
6	n	-1.437335	0.799809	0.000083
7	n	2.187210	0.644590	-0.000283
8	c	2.649191	-0.615800	0.000398
9	n	1.728861	-1.604176	-0.000131
10	n	-2.877401	-0.966601	-0.000198
11	o	-0.113917	2.631161	-0.000076

12	h	3.705488	-0.826309	-0.000033
13	h	-2.265998	1.402070	-0.000170
14	h	-3.655525	-0.312460	0.000616
15	h	-3.070135	-1.963763	0.000077

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.291265	1.449866	-0.000184
2	c	-0.830823	0.517086	-0.000050
3	c	-0.543977	-0.895997	-0.000040
4	n	0.626359	-1.444651	-0.000038
5	c	1.659369	-0.567307	0.000045
6	n	1.500308	0.781903	-0.000002
7	n	-2.149068	0.734126	0.000006
8	c	-2.683973	-0.465231	0.000129
9	n	-1.756762	-1.469864	-0.000051
10	n	2.864371	-1.045771	0.000052
11	o	0.215269	2.644009	0.000068
12	h	-3.741584	-0.670782	0.000160
13	h	2.346095	1.365902	0.000070
14	h	3.683965	-0.436649	0.000113
15	h	2.999896	-2.056685	-0.000005
16	h	-1.958155	-2.474561	-0.000049

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.176623	1.402296	-0.000472
2	c	0.870490	0.453951	-0.001710
3	c	0.572816	-0.899890	-0.001546
4	n	-0.687884	-1.432662	-0.001034
5	c	-1.639653	-0.552837	-0.005710
6	n	-1.421562	0.792941	-0.004092
7	n	2.242655	0.606388	0.002377
8	c	2.662700	-0.633977	0.004172

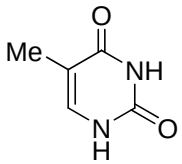
9	n	1.716450	-1.599922	0.002418
10	n	-2.940157	-0.938100	-0.068145
11	o	-0.104682	2.629111	0.003311
12	h	3.711968	-0.883756	0.007028
13	h	-2.237036	1.416838	-0.013253
14	h	-3.631508	-0.278221	0.288444
15	h	-3.110871	-1.905521	0.202225

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.548098	-0.827803	-0.014417
2	n	1.752878	-1.477543	-0.053792
3	c	2.709680	-0.524330	-0.010023
4	n	2.215065	0.673373	0.064027
5	c	0.841448	0.503049	0.062248
6	n	-0.688267	-1.438724	-0.012948
7	c	-1.662644	-0.573003	0.003577
8	n	-1.497140	0.757905	0.055123
9	c	-0.223117	1.482546	0.236936
10	o	-0.215656	2.698770	-0.207061
11	n	-2.949698	-1.027624	-0.102381
12	h	3.754383	-0.767450	-0.040507
13	h	-2.322244	1.332082	0.073328
14	h	-3.662729	-0.453127	0.315942
15	h	-3.058149	-2.005041	0.108121
16	h	1.903329	-2.471087	-0.120536

No.4



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.727859	1.032273	0.000029
2	c	1.681132	0.027355	0.000015
3	n	1.120969	-1.243017	-0.000663
4	c	-0.239370	-1.482961	-0.000098
5	c	-1.158598	-0.488694	0.000108
6	c	-0.673275	0.897035	-0.000040
7	o	2.886215	0.226212	0.000397
8	c	-2.642795	-0.720244	0.000306
9	o	-1.386406	1.892676	-0.000252
10	h	-0.518728	-2.532001	-0.000158
11	h	-2.874751	-1.790392	0.000600
12	h	-3.110485	-0.261541	0.879188
13	h	-3.110667	-0.262005	-0.878729
14	h	1.087416	1.981818	-0.000061
15	h	1.784384	-2.006722	0.000693

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.121159	-0.482529	-0.000031
2	c	0.632199	0.907288	-0.000070
3	n	-0.750252	1.014203	-0.000061
4	c	-1.664511	-0.046947	-0.000158
5	n	-1.151030	-1.354060	-0.000016
6	c	0.157136	-1.516011	0.000018
7	o	1.365920	1.890814	0.000056
8	o	-2.864846	0.172734	0.000136
9	c	2.588228	-0.729884	0.000032
10	h	0.505547	-2.549643	0.000060
11	h	2.815489	-1.799549	-0.000068
12	h	3.058607	-0.261557	-0.874764
13	h	3.058481	-0.261751	0.875003
14	h	-1.143005	1.951606	0.000024

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.668512	0.919302	0.000024
2	n	-0.725089	1.075318	0.000043
3	c	-1.673109	0.081771	0.000083
4	n	-1.101120	-1.248017	-0.000010
5	c	0.196513	-1.526318	-0.000011
6	c	1.156356	-0.492525	0.000000
7	o	-2.868639	0.211219	-0.000050
8	c	2.608888	-0.744694	0.000000
9	o	1.422554	1.868087	-0.000047
10	h	0.481959	-2.575397	-0.000037
11	h	2.855426	-1.808059	-0.000184
12	h	3.075621	-0.253601	-0.868716
13	h	3.075543	-0.253952	0.868964
14	h	-1.077873	2.032645	-0.000022
15	h	-1.801487	-1.992406	-0.000047

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.647453	0.885444	-0.000726
2	n	0.745361	0.972534	-0.000426
3	c	1.676087	-0.091489	-0.000825
4	n	1.165150	-1.356735	-0.000086
5	c	-0.173991	-1.475331	0.000054
6	c	-1.129801	-0.468608	-0.000156
7	o	2.887663	0.193953	0.000834
8	c	-2.611306	-0.728930	0.000254
9	o	-1.341862	1.925920	0.000459
10	h	-0.531989	-2.511035	0.000447
11	h	-2.812647	-1.809059	0.000786
12	h	-3.107651	-0.291026	0.878994
13	h	-3.107995	-0.291842	-0.878698
14	h	1.139065	1.906878	0.000098

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.730320	1.022109	-0.015423
2	c	1.671283	0.021511	-0.010706
3	n	1.145876	-1.240738	-0.066927
4	c	-0.247215	-1.541987	0.081239
5	c	-1.165853	-0.459387	0.006723
6	c	-0.711969	0.872623	-0.008156
7	o	2.898101	0.240461	0.034694
8	c	-2.644519	-0.733159	0.014987
9	o	-1.373782	1.948370	-0.009395
10	h	1.826704	-1.966085	0.108078
11	h	-3.194446	0.195144	-0.171035
12	h	-2.992216	-1.142440	0.980653
13	h	-2.932384	-1.467257	-0.757788
14	h	-0.520708	-2.529536	-0.292320
15	h	1.074756	1.972318	0.001944

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.732215	1.019640	-0.000249
2	c	1.643616	0.004284	0.000004
3	n	1.104824	-1.235988	-0.000089
4	c	-0.248123	-1.461477	-0.000091
5	c	-1.149465	-0.473643	-0.000173
6	c	-0.638511	0.892907	-0.000901
7	o	2.839484	0.209847	0.000374
8	c	-2.636888	-0.699245	0.000267
9	o	-1.334707	1.886405	0.000409
10	h	-0.528397	-2.501980	0.000147

11	h	-2.854192	-1.762657	0.000762
12	h	-3.100160	-0.255008	0.877057
13	h	-3.100539	-0.255749	-0.876697
14	h	1.112016	1.967346	0.000101
15	h	1.750008	-2.024484	0.000092

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.120421	-0.466131	-0.000004
2	c	0.597841	0.909062	-0.000056
3	n	-0.766831	1.009134	-0.000001
4	c	-1.636769	-0.045824	0.000028
5	n	-1.120831	-1.348707	0.000002
6	c	0.175548	-1.518402	0.000006
7	o	1.301310	1.887525	0.000023
8	o	-2.825500	0.127262	-0.000009
9	c	2.598011	-0.695860	0.000002
10	h	0.530232	-2.541071	-0.000015
11	h	2.815899	-1.758112	-0.000081
12	h	3.052690	-0.243010	-0.877575
13	h	3.052658	-0.243159	0.877675
14	h	-1.174630	1.946989	0.000014

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.641031	0.923825	-0.000197
2	n	-0.727854	1.065093	-0.000125
3	c	-1.635854	0.062464	-0.000290
4	n	-1.083166	-1.245979	-0.000038
5	c	0.182433	-1.512761	0.000006
6	c	1.146848	-0.469366	-0.000076
7	o	-2.815723	0.198192	0.000265
8	c	2.614297	-0.732895	0.000075
9	o	1.371472	1.871028	0.000148

10	h	0.474464	-2.554971	0.000150
11	h	2.811970	-1.798784	0.000053
12	h	3.067886	-0.281921	-0.879207
13	h	3.067682	-0.282006	0.879511
14	h	-1.104932	2.021837	0.000100
15	h	-1.778445	-2.019321	0.000116

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.603696	0.877857	0.000000
2	n	-0.762158	0.962963	0.000000
3	c	-1.636318	-0.101244	0.000000
4	n	-1.136837	-1.338682	0.000000
5	c	0.206572	-1.463718	0.000000
6	c	1.125601	-0.458347	0.000000
7	o	-2.849641	0.147449	0.000000
8	c	2.615111	-0.686796	0.000000
9	o	1.275384	1.910034	0.000000
10	h	0.561145	-2.488372	-0.000001
11	h	2.830650	-1.751824	-0.000001
12	h	3.090619	-0.249355	-0.875778
13	h	3.090618	-0.249379	0.875789
14	h	-1.173979	1.902584	0.000000

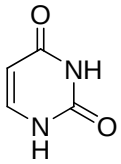
2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.733892	1.010867	0.044799
2	c	1.645785	0.015315	-0.003191
3	n	1.143087	-1.232141	-0.037434
4	c	-0.241472	-1.526355	0.092167
5	c	-1.158372	-0.441224	-0.001879
6	c	-0.690354	0.853277	-0.003012
7	o	2.854868	0.237277	-0.017484
8	c	-2.641338	-0.722399	-0.010741

9	o	-1.344826	1.942289	-0.018930
10	h	1.813094	-1.979391	0.012641
11	h	-3.168307	-0.048633	-0.678910
12	h	-3.090953	-0.610020	0.975366
13	h	-2.839169	-1.739003	-0.340591
14	h	-0.508414	-2.532550	-0.182846
15	h	1.089068	1.950308	0.014028

No.5



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.221686	-0.405210	0.000028
2	n	1.176027	0.987754	-0.000629
3	c	0.004829	1.711967	0.000117
4	c	-1.205467	1.109687	0.000144
5	c	-1.291382	-0.347314	-0.000126
6	n	-0.033632	-0.989600	-0.000262
7	o	-2.320011	-1.008172	0.000126
8	o	2.269328	-1.030465	0.000334
9	h	0.126782	2.790080	0.000710
10	h	-2.127653	1.675461	0.000248
11	h	-0.046086	-2.005091	-0.000196
12	h	2.077657	1.446785	0.000806

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	c	1.253504	-0.352649	-0.000784
2	n	0.015466	-0.981840	-0.000255
3	c	-1.231923	-0.345314	-0.000139
4	n	-1.259539	1.062947	-0.000095
5	c	-0.110242	1.715902	0.000038
6	c	1.155825	1.106215	0.000100
7	o	-2.260886	-1.000139	0.000325
8	o	2.311238	-0.974200	0.000443
9	h	-0.180906	2.802920	0.000410
10	h	2.077343	1.677277	0.000560
11	h	0.006284	-1.998158	0.000048

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.052676	-1.033167	-0.000033
2	c	-1.198096	-0.467690	-0.000340
3	n	-1.166226	0.991914	0.000033
4	c	-0.072837	1.737890	0.000027
5	c	1.187110	1.111190	-0.000045
6	c	1.282563	-0.356051	0.000154
7	o	-2.261434	-1.024375	0.000131
8	o	2.348695	-0.941698	-0.000006
9	h	-0.192241	2.818713	0.000028
10	h	2.108324	1.684487	-0.000084
11	h	0.086252	-2.053262	0.000110
12	h	-2.098013	1.415392	0.000166

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	0.007209	-0.933912	-0.000045
2	c	-1.256498	-0.300995	-0.000512
3	n	-1.271599	1.067028	0.000017
4	c	-0.080403	1.686001	0.000077
5	c	1.178950	1.103976	-0.000010

6	c	1.268416	-0.326232	0.000079
7	o	-2.269377	-1.023033	0.000253
8	o	2.299812	-1.030821	0.000024
9	h	-0.140889	2.779021	0.000158
10	h	2.090826	1.691177	-0.000014
11	h	-0.005470	-1.947669	0.000027

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.212243	-0.403886	0.009709
2	n	1.205644	0.964744	0.080933
3	c	0.036339	1.775072	-0.112887
4	c	-1.215051	1.104362	-0.007489
5	c	-1.318174	-0.293882	0.001148
6	n	-0.034673	-0.978214	-0.053985
7	o	-2.336241	-1.037646	0.035760
8	o	2.266869	-1.069233	0.001174
9	h	-2.135440	1.679078	0.014690
10	h	2.116756	1.373395	-0.070621
11	h	0.155105	2.794905	0.249972
12	h	-0.070387	-1.988062	-0.021032

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.190993	-0.389045	-0.000085
2	n	-1.171519	0.968461	0.000017
3	c	-0.012902	1.691516	0.000024
4	c	1.190574	1.106629	-0.000008
5	c	1.258906	-0.341368	-0.000206
6	n	0.038422	-0.981544	-0.000044
7	o	2.283137	-0.992445	0.000126

8	o	-2.217880	-1.032030	0.000074
9	h	-0.142844	2.761081	0.000110
10	h	2.105228	1.676332	0.000095
11	h	0.045868	-2.002686	0.000042
12	h	-2.072139	1.446260	0.000004

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.228411	-0.355245	0.000069
2	n	0.013968	-0.986498	0.000034
3	c	-1.200720	-0.355669	-0.000019
4	n	-1.242290	1.048736	-0.000039
5	c	-0.114901	1.719453	-0.000008
6	c	1.152479	1.105859	0.000046
7	o	-2.225933	-0.979482	0.000004
8	o	2.265837	-0.968922	-0.000071
9	h	-0.188068	2.798505	-0.000026
10	h	2.069987	1.676040	0.000030
11	h	0.005486	-2.009363	0.000045

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-0.072168	-1.019230	-0.000057
2	c	1.159684	-0.461906	-0.000031
3	n	1.179965	0.962348	0.000004
4	c	0.128423	1.713675	0.000012
5	c	-1.164857	1.127401	-0.000015
6	c	-1.270687	-0.337427	-0.000156
7	o	2.188152	-1.055335	0.000054
8	o	-2.322697	-0.911407	0.000111
9	h	0.271937	2.785674	0.000104
10	h	-2.087465	1.752754	0.000054
11	h	-0.106611	-2.046675	0.000003
12	h	2.128544	1.389894	0.000024

2.4 anion

Charge = -1 Multiplicity = 1

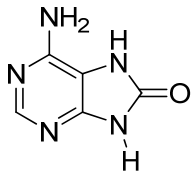
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-0.005989	-0.939902	-0.000199
2	c	-1.220165	-0.289153	-0.000033
3	n	-1.237749	1.051324	-0.000038
4	c	-0.051913	1.681041	0.000042
5	c	1.177381	1.088340	0.000042
6	c	1.224914	-0.337773	-0.000773
7	o	-2.245725	-0.978195	0.000207
8	o	2.242208	-1.032925	0.000416
9	h	-0.110879	2.763444	0.000369
10	h	2.093814	1.658259	0.000539
11	h	-0.029934	-1.967423	0.000102

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.186038	-0.401816	0.000886
2	n	1.213025	0.942132	0.048853
3	c	0.058694	1.760309	-0.100309
4	c	-1.202806	1.097579	0.007482
5	c	-1.289357	-0.273637	0.002184
6	n	-0.043511	-0.968428	-0.064155
7	o	-2.314315	-1.014538	0.034804
8	o	2.209055	-1.080979	0.019022
9	h	-2.108277	1.678513	0.041106
10	h	2.124992	1.363637	0.008318
11	h	0.200351	2.784482	0.200152
12	h	-0.076997	-1.973034	-0.034523

No.6



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.557325	-1.073619	0.040582
2	c	-0.182183	-0.951424	0.016996
3	c	0.105894	0.418374	-0.007119
4	n	-1.116848	1.094748	0.014993
5	c	-2.175862	0.181798	0.002098
6	n	0.718854	-1.928729	0.012295
7	c	1.979678	-1.466306	-0.019899
8	n	2.383681	-0.194257	-0.023693
9	c	1.452087	0.781948	-0.005111
10	n	1.893258	2.089349	-0.047487
11	o	-3.368919	0.426026	-0.033145
12	h	2.887811	2.186793	0.124234
13	h	1.329627	2.790512	0.417080
14	h	2.765293	-2.216882	-0.036962
15	h	-2.077182	-1.940348	0.034621
16	h	-1.283227	2.072925	-0.172436

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.424835	0.798499	0.000046
2	c	0.044086	0.433996	-0.000057
3	c	-0.222068	-0.978789	-0.000095

4	n	0.694644	-1.933823	-0.000043
5	c	1.954609	-1.441795	0.000009
6	n	2.362723	-0.168063	0.000051
7	n	-1.062044	1.175433	-0.000211
8	c	-2.123517	0.250979	0.000020
9	n	-1.575785	-1.069336	-0.000039
10	o	-3.317278	0.491616	0.000113
11	n	1.803219	2.088134	0.000030
12	h	2.787552	2.319589	0.000289
13	h	1.109754	2.824378	0.000051
14	h	2.746123	-2.186660	0.000054
15	h	-2.132182	-1.913982	0.000645

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.486069	0.781681	0.000177
2	c	-0.089061	0.442867	0.000171
3	c	0.219190	-0.969903	0.000309
4	n	-0.668645	-1.927919	0.000191
5	c	-1.954789	-1.477956	-0.000518
6	n	-2.382760	-0.221835	-0.000330
7	n	1.081531	1.107948	-0.000358
8	c	2.185986	0.182756	-0.000327
9	n	1.580331	-1.074657	0.000447
10	o	3.347697	0.482425	-0.000202
11	n	-1.947864	2.035627	0.000370
12	h	-2.956393	2.170366	-0.000555
13	h	-1.360946	2.860597	0.000428
14	h	-2.721149	-2.247488	-0.000193
15	h	2.109064	-1.942248	0.000550
16	h	1.258158	2.108559	0.000280

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	c	1.399171	0.794905	-0.017977
2	c	0.050563	0.427733	-0.026630
3	c	-0.189621	-0.967478	-0.014385
4	n	0.741877	-1.927634	0.001571
5	c	1.993444	-1.431809	0.015101
6	n	2.368751	-0.145954	0.009362
7	n	-1.106754	1.165706	-0.015036
8	c	-2.123962	0.257601	0.002847
9	n	-1.552650	-1.070578	-0.006013
10	o	-3.355751	0.425502	0.024670
11	n	1.782777	2.136886	-0.075249
12	h	2.682756	2.315688	0.355904
13	h	1.049396	2.767800	0.232193
14	h	2.798803	-2.164659	0.036439
15	h	-2.100530	-1.917546	0.021913

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.555930	-1.068952	0.009225
2	c	-0.174336	-0.949003	0.071557
3	c	0.108172	0.414526	0.092137
4	n	-1.120520	1.085895	-0.033458
5	c	-2.171583	0.187125	-0.037336
6	n	0.717460	-1.947753	0.016420
7	c	1.989744	-1.465827	-0.004488
8	n	2.388882	-0.197097	-0.055654
9	c	1.461850	0.792515	-0.054661
10	n	1.880953	2.115136	-0.073673
11	o	-3.384315	0.417361	-0.027764
12	h	2.871695	2.198930	0.173228
13	h	1.303331	2.747794	0.514728
14	h	2.777624	-2.216933	-0.022372
15	h	-2.075112	-1.934282	-0.003551
16	h	-1.262021	2.078980	0.116807

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.438931	0.780709	-0.004287
2	c	0.105474	0.409753	-0.001984
3	c	-0.180112	-0.936967	0.004811
4	n	0.715240	-1.907525	0.005437
5	c	1.957726	-1.451403	-0.001606
6	n	2.357684	-0.196675	-0.005831
7	n	-1.119483	1.082388	-0.003833
8	c	-2.133854	0.182102	-0.000189
9	n	-1.541146	-1.059327	0.008250
10	o	-3.323788	0.407996	-0.003776
11	n	1.870038	2.061330	-0.053222
12	h	2.836792	2.214665	0.171083
13	h	1.249702	2.795020	0.238208
14	h	2.736343	-2.194151	-0.002130
15	h	-2.061528	-1.921275	0.012264
16	h	-1.276322	2.075262	-0.025300

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.586129	-1.039141	0.000008
2	c	0.233224	-0.950580	0.000396
3	c	-0.054219	0.433683	0.000584
4	n	1.050915	1.167371	0.000523
5	c	2.107596	0.239440	-0.000022
6	n	-0.655531	-1.910375	0.000647
7	c	-1.910945	-1.452841	0.000234
8	n	-2.328502	-0.199575	-0.001363
9	c	-1.427660	0.789741	-0.000204
10	n	-1.840016	2.049092	-0.000111
11	o	3.272245	0.523562	-0.000558

12	h	-2.823114	2.254377	-0.000690
13	h	-1.190693	2.814191	0.003081
14	h	-2.681456	-2.203199	0.000755
15	h	2.138364	-1.882116	-0.002545

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.560071	-1.065589	0.000307
2	c	-0.219691	-0.974377	0.000113
3	c	0.087051	0.430937	-0.000726
4	n	-1.075284	1.092821	-0.000069
5	c	-2.137747	0.190289	0.000229
6	n	0.665871	-1.909591	0.000053
7	c	1.939720	-1.449068	-0.000301
8	n	2.366153	-0.219826	-0.000068
9	c	1.469886	0.789701	-0.000266
10	n	1.886920	2.018962	0.000687
11	o	-3.292889	0.459907	-0.000161
12	h	2.882481	2.203446	0.001936
13	h	1.263141	2.815468	-0.001173
14	h	2.697171	-2.213053	-0.000697
15	h	-2.097290	-1.923850	0.002101
16	h	-1.222820	2.096409	-0.001542

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.552693	-1.033896	0.004883
2	c	-0.200507	-0.932566	0.001924
3	c	0.061213	0.428588	-0.007459
4	n	-1.117926	1.160598	-0.008795
5	c	-2.092815	0.258179	-0.000501
6	n	0.705259	-1.902136	0.006043
7	c	1.944058	-1.439221	0.002518
8	n	2.333345	-0.178914	-0.004005

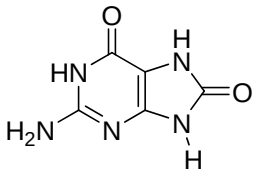
9	c	1.398424	0.785663	-0.008734
10	n	1.822095	2.083709	-0.065998
11	o	-3.320401	0.441113	0.002614
12	h	2.765514	2.241396	0.245426
13	h	1.171919	2.777431	0.260247
14	h	2.728866	-2.176414	0.007498
15	h	-2.095893	-1.880702	0.014523

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.447549	0.811628	-0.211608
2	c	-0.101913	0.393953	-0.044156
3	c	0.188736	-0.927290	0.037996
4	n	-0.717562	-1.953410	0.036106
5	c	-1.964612	-1.465724	0.014504
6	n	-2.386102	-0.232938	-0.063129
7	n	1.125384	1.072008	-0.079063
8	c	2.148536	0.185550	-0.008392
9	n	1.580356	-1.046106	0.035194
10	o	3.348026	0.444832	0.016037
11	h	2.111545	-1.894778	0.132111
12	h	1.263915	2.067247	-0.073589
13	n	-1.834948	2.142064	0.114353
14	h	-2.668378	2.400401	-0.390133
15	h	-2.060472	2.225055	1.099451
16	h	-2.739903	-2.216614	0.069575

No.7



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.735215	1.463624	0.002565
2	c	0.397750	0.609067	0.007988
3	c	0.245957	-0.765905	0.000216
4	n	-0.917116	-1.458086	0.008529
5	c	-1.987502	-0.692616	-0.001036
6	n	-1.932161	0.675978	-0.003072
7	n	1.766271	0.878694	0.007179
8	c	2.494370	-0.301268	0.000419
9	n	1.508883	-1.310477	-0.002682
10	o	3.704719	-0.456149	-0.001888
11	n	-3.233610	-1.273602	-0.068541
12	o	-0.799837	2.691537	-0.003307
13	h	-2.783167	1.224023	-0.078909
14	h	-4.006745	-0.795906	0.377925
15	h	-3.220614	-2.273681	0.092685
16	h	1.737068	-2.294818	-0.010188
17	h	2.196368	1.792310	0.009236

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.494618	-1.336931	-0.000418
2	c	-0.213984	-0.820748	0.000005
3	c	-0.353199	0.594796	0.000530
4	n	-1.680743	0.876494	0.000363
5	c	-2.445958	-0.309650	-0.000030
6	n	0.925787	-1.455713	-0.000230
7	c	2.014300	-0.576991	0.000005
8	n	2.023515	0.745695	0.000075
9	c	0.836962	1.442849	-0.000033
10	o	0.737484	2.675498	-0.000425

11	n	3.205151	-1.219303	0.000027
12	o	-3.654650	-0.404921	0.000010
13	h	4.057396	-0.677475	0.000744
14	h	3.236789	-2.227827	0.000431
15	h	-1.748355	-2.315998	0.000166
16	h	-2.090873	1.803453	0.000399

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.507034	-1.333808	-0.000167
2	c	0.254191	-0.809172	-0.000139
3	c	0.409052	0.614767	0.000294
4	n	1.725252	0.892450	0.000418
5	c	2.484407	-0.314039	-0.000131
6	n	-0.891876	-1.456798	-0.000239
7	c	-1.992928	-0.676898	-0.000108
8	n	-1.946548	0.691763	-0.000046
9	c	-0.755771	1.471733	-0.000333
10	o	-0.775880	2.685830	-0.000156
11	n	-3.175262	-1.289871	0.000273
12	o	3.679113	-0.420134	0.000069
13	h	-2.803455	1.241440	-0.000576
14	h	-4.061981	-0.800682	0.001283
15	h	-3.188910	-2.304286	0.000397
16	h	1.747742	-2.320320	-0.000489
17	h	2.156829	1.813775	0.000921

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.493667	-1.314960	0.002069
2	c	0.203487	-0.779164	-0.009356
3	c	0.342034	0.590252	-0.012790
4	n	1.723144	0.864461	-0.002014
5	c	2.454936	-0.300384	0.004315

6	n	-0.954931	-1.457912	-0.009939
7	c	-2.003581	-0.601104	-0.014758
8	n	-2.012505	0.730277	-0.004217
9	c	-0.815325	1.438754	-0.002712
10	o	-0.756639	2.690767	0.012133
11	n	-3.267469	-1.220734	-0.073132
12	o	3.685444	-0.444172	0.011774
13	h	-3.996673	-0.616661	0.288425
14	h	-3.267835	-2.144108	0.345400
15	h	1.734879	-2.294346	-0.002390
16	h	2.136530	1.784302	-0.000250

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.741370	1.454025	0.000221
2	c	0.384758	0.605538	-0.022681
3	c	0.237602	-0.778663	0.033616
4	n	-0.909508	-1.471189	0.022236
5	c	-1.995659	-0.703732	-0.040302
6	n	-1.939231	0.680735	-0.011366
7	n	1.766765	0.873357	-0.035063
8	c	2.490930	-0.299117	-0.004946
9	n	1.526416	-1.309875	0.025221
10	o	3.716759	-0.443562	-0.000943
11	n	-3.249069	-1.263338	-0.109815
12	o	-0.783462	2.696362	0.028843
13	h	-2.808335	1.200933	0.140003
14	h	-3.991599	-0.718372	0.377712
15	h	-3.249669	-2.238175	0.202571
16	h	1.763983	-2.289280	0.071922
17	h	2.194071	1.786356	-0.049354

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.504818	-1.282818	0.000621
2	c	-0.250316	-0.748938	-0.000811
3	c	-0.391241	0.606604	-0.002796
4	n	-1.768083	0.877749	-0.001283
5	c	-2.454970	-0.282244	0.000384
6	n	0.890112	-1.448470	0.000202
7	c	1.965060	-0.696363	0.000180
8	n	1.914438	0.660715	0.000890
9	c	0.749557	1.429127	-0.000024
10	o	0.819157	2.644655	0.001307
11	n	3.170237	-1.260284	-0.003338
12	o	-3.658738	-0.444512	0.001207
13	h	2.780029	1.181355	0.002378
14	h	4.014054	-0.716298	0.011388
15	h	3.240349	-2.261085	0.005700
16	h	-1.732292	-2.263448	0.003356
17	h	-2.207219	1.780968	-0.004177

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.841467	1.430153	0.000233
2	c	0.358979	0.605133	0.000242
3	c	0.221885	-0.813400	-0.000677
4	n	-0.897747	-1.434554	-0.000793
5	c	-1.995162	-0.587562	0.000408
6	n	-2.004731	0.730941	0.000570
7	n	1.686201	0.879596	0.001039
8	c	2.412026	-0.292420	0.000340
9	n	1.483552	-1.314834	-0.001023
10	o	3.602522	-0.402884	0.000486
11	n	-3.153152	-1.224036	0.000865
12	o	-0.776837	2.643036	-0.001590
13	h	-4.012990	-0.706511	0.000517
14	h	-3.181952	-2.226760	0.000368
15	h	1.737102	-2.291697	-0.003139
16	h	2.115937	1.792533	0.003202

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.776298	1.446983	-0.000116
2	c	0.401977	0.616602	0.000619
3	c	0.260318	-0.811209	-0.000617
4	n	-0.856591	-1.454031	-0.001272
5	c	-1.965617	-0.680739	0.000056
6	n	-1.930455	0.672963	-0.000246
7	n	1.719150	0.892158	0.000865
8	c	2.446444	-0.285292	0.000283
9	n	1.506270	-1.307867	-0.000853
10	o	3.629022	-0.400390	0.000461
11	n	-3.120228	-1.276451	0.001461
12	o	-0.801727	2.643062	-0.000927
13	h	-2.807322	1.184109	-0.001072
14	h	-3.990547	-0.764410	0.001207
15	h	-3.154124	-2.284475	0.001703
16	h	1.754090	-2.289259	-0.002466
17	h	2.151589	1.807193	0.003322

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.808191	1.411764	-0.000778
2	c	0.350657	0.595882	-0.008146
3	c	0.211954	-0.755051	-0.005376
4	n	-0.938476	-1.426369	-0.006477
5	c	-1.989044	-0.605637	-0.009161
6	n	-1.985228	0.720405	-0.003815
7	n	1.732921	0.864767	0.000311
8	c	2.418257	-0.294048	0.003519
9	n	1.476816	-1.294541	0.001697
10	o	3.629617	-0.451619	0.006956
11	n	-3.220871	-1.209877	-0.066642

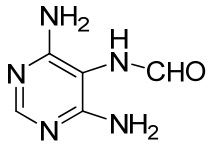
12	o	-0.780985	2.653290	0.008237
13	h	-3.985428	-0.646985	0.260734
14	h	-3.246596	-2.157676	0.265395
15	h	1.710350	-2.274605	0.003506
16	h	2.174701	1.767745	-0.007045

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.714017	1.407857	0.052400
2	c	0.381205	0.619550	0.220241
3	c	0.266509	-0.795433	0.390429
4	n	-0.915155	-1.455898	0.050268
5	c	-1.952602	-0.700812	-0.013117
6	n	-1.932913	0.654234	0.199342
7	n	1.753717	0.875685	-0.004268
8	c	2.438734	-0.283269	-0.086243
9	n	1.534402	-1.306528	-0.014788
10	o	3.650222	-0.406303	-0.201345
11	n	-3.181952	-1.229291	-0.322683
12	o	-0.827184	2.652895	-0.153629
13	h	-2.757079	1.164617	-0.069715
14	h	-3.976976	-0.726110	0.036916
15	h	-3.250386	-2.218922	-0.156870
16	h	1.863942	-2.216010	0.260193
17	h	2.210529	1.768918	0.031911

No.8



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.298428	-1.750854	0.026209
2	c	-0.087532	-1.173829	-0.142769
3	c	0.037418	0.232523	-0.176478
4	c	-1.135542	0.977632	0.032421
5	n	-2.336855	0.396524	0.190103
6	c	-2.341322	-0.937794	0.157232
7	n	0.975651	-2.011299	-0.332216
8	n	1.231917	0.933178	-0.510228
9	c	2.493835	0.724028	-0.040249
10	o	2.820386	-0.123709	0.782657
11	n	-1.109024	2.361361	0.002202
12	h	0.752798	-2.985935	-0.166026
13	h	1.870689	-1.699316	0.039272
14	h	-3.312654	-1.415871	0.265873
15	h	1.136249	1.653053	-1.221703
16	h	3.224685	1.415789	-0.495768
17	h	-1.985513	2.777522	0.297414
18	h	-0.293314	2.806696	0.406257

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-2.289719	-1.057628	0.023064
2	n	-1.190203	-1.800299	-0.030286
3	c	-0.002911	-1.154399	-0.048259
4	c	0.074251	0.301641	-0.046493
5	c	-1.234636	0.947443	0.029213
6	n	-2.391301	0.275446	0.066954
7	n	1.094196	-1.920699	-0.083480
8	n	1.110353	1.146363	-0.162501
9	c	2.449052	0.900956	-0.112637
10	o	3.052349	-0.108018	0.285984
11	n	-1.277563	2.288711	0.058576
12	h	0.953758	-2.922806	-0.043813
13	h	2.015367	-1.498949	0.084905
14	h	-3.230932	-1.603523	0.037702
15	h	3.034020	1.774403	-0.437188

16	h	-2.173858	2.754129	0.078486
17	h	-0.411741	2.806159	-0.022139

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	2.309170	-1.054409	0.142522
2	n	1.223934	-1.802505	0.057326
3	c	0.028221	-1.186593	-0.033459
4	c	-0.044076	0.271911	0.025740
5	c	1.247104	0.945312	-0.074184
6	n	2.386153	0.287594	0.034691
7	n	-1.039948	-1.969835	-0.138529
8	n	-1.136799	1.070032	0.288088
9	c	-2.521623	0.856571	0.192011
10	o	-3.046393	-0.155215	-0.218393
11	n	1.286358	2.296894	-0.211548
12	h	-0.878839	-2.974425	-0.139545
13	h	-1.982465	-1.588798	-0.260312
14	h	3.252986	-1.576898	0.272823
15	h	-0.895165	1.993220	0.648510
16	h	-3.088091	1.736968	0.525132
17	h	2.221103	2.694933	-0.260205
18	h	0.590960	2.784701	-0.765234

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-2.260857	-1.054951	0.212512
2	n	-1.168404	-1.791217	0.037315
3	c	-0.001078	-1.124158	-0.160208
4	c	0.067172	0.294980	-0.156469
5	c	-1.191680	0.931604	-0.007513
6	n	-2.352315	0.276901	0.198862
7	n	1.109223	-1.899879	-0.426834
8	n	1.159445	1.133603	-0.390159

9	c	2.397746	0.862828	-0.000214
10	o	2.876369	-0.107637	0.661896
11	n	-1.255527	2.310933	-0.109673
12	h	0.952751	-2.871111	-0.178853
13	h	1.976625	-1.491467	-0.045436
14	h	-3.189307	-1.600154	0.386819
15	h	3.108168	1.655922	-0.313634
16	h	-2.027116	2.739079	0.384653
17	h	-0.346839	2.754619	-0.023955

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.243262	-1.800091	0.008010
2	c	-0.071999	-1.170889	-0.115146
3	c	0.033397	0.249379	-0.052102
4	c	-1.214109	0.948055	0.015093
5	n	-2.378980	0.321692	0.156239
6	c	-2.348446	-1.023303	0.167727
7	n	1.046005	-1.956306	-0.353612
8	n	1.192333	0.993342	-0.362287
9	c	2.501676	0.799732	-0.049070
10	o	2.983478	-0.141584	0.617213
11	n	-1.215343	2.356419	-0.061475
12	h	0.864586	-2.931739	-0.144563
13	h	1.915340	-1.588712	0.041596
14	h	-3.299334	-1.540398	0.267152
15	h	1.015734	1.855064	-0.887599
16	h	3.134224	1.614826	-0.440517
17	h	-2.156271	2.705185	0.121230
18	h	-0.550482	2.795208	0.597855

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center	Atomic	Coordinates (Angstroms)

Number	Name	X	Y	Z
1	c	2.418566	-0.008451	0.411257
2	n	1.874974	1.176076	0.242778
3	c	0.589869	1.189429	-0.145546
4	c	-0.114623	0.002088	-0.349073
5	c	0.580726	-1.191035	-0.147756
6	n	1.865975	-1.188498	0.240208
7	n	0.014647	2.397911	-0.295119
8	n	-1.474030	0.007456	-0.749424
9	c	-2.514397	0.006314	0.103397
10	o	-2.436561	-0.000026	1.307262
11	n	-0.004063	-2.394640	-0.299211
12	h	0.622938	3.194800	-0.322070
13	h	-0.846356	2.482509	-0.798940
14	h	3.449269	-0.012654	0.725124
15	h	-1.694235	0.013710	-1.731795
16	h	-3.474845	0.011546	-0.408184
17	h	0.597928	-3.196268	-0.327276
18	h	-0.865566	-2.471637	-0.803233

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-2.342951	0.322241	0.137742
2	c	-2.283871	-0.994555	0.116402
3	n	-1.216741	-1.755143	0.009794
4	c	-0.029903	-1.150254	-0.095099
5	c	0.066769	0.275916	-0.104461
6	c	-1.186809	0.971916	0.020802
7	n	1.032744	-1.958693	-0.245054
8	n	1.144740	1.036219	-0.309781
9	c	2.467220	0.718039	-0.227696
10	o	2.982935	0.100332	0.668007
11	n	-1.219214	2.299058	0.019520
12	h	0.855918	-2.939873	-0.123536
13	h	1.942644	-1.656421	0.025929
14	h	-3.224902	-1.510806	0.201023
15	h	3.057662	1.158168	-1.027230
16	h	-2.100202	2.770633	0.105835

17	h	-0.385088	2.843485	-0.071314

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-2.191791	0.566023	0.288243
2	c	-2.259013	-0.745317	0.426850
3	n	-1.341119	-1.662178	0.194574
4	c	-0.158000	-1.237260	-0.239903
5	c	0.120113	0.196543	-0.336315
6	c	-1.024071	1.075828	-0.085899
7	n	0.740345	-2.099713	-0.607942
8	n	1.377680	0.696285	-0.640498
9	c	2.449142	0.567642	0.200262
10	o	2.411675	-0.034946	1.232992
11	n	-0.886496	2.363702	-0.198226
12	h	0.519767	-3.084977	-0.562490
13	h	1.624010	-1.841052	-1.012193
14	h	-3.207780	-1.121550	0.769811
15	h	1.479926	1.295364	-1.451325
16	h	3.337090	1.067887	-0.174820
17	h	-1.680543	2.959113	-0.007499
18	h	-0.025232	2.811336	-0.468442

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-2.252618	0.392917	0.249084
2	c	-2.258217	-0.921240	0.268530
3	n	-1.238819	-1.720125	0.062253
4	c	-0.054784	-1.137127	-0.195581
5	c	0.098450	0.248839	-0.243656
6	c	-1.077408	0.977510	-0.020824
7	n	0.986001	-1.986272	-0.471700
8	n	1.259612	0.944977	-0.635738
9	c	2.382327	0.746076	-0.004642

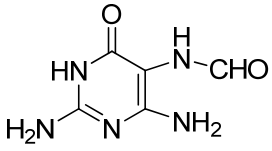
10	o	2.643710	-0.026212	0.941349
11	n	-1.083477	2.335053	-0.114889
12	h	0.797915	-2.940245	-0.214638
13	h	1.873219	-1.669681	-0.133080
14	h	-3.203594	-1.393452	0.480207
15	h	3.200482	1.357451	-0.390675
16	h	-1.855199	2.804822	0.324193
17	h	-0.199606	2.800613	-0.042823

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.889332	-1.234484	0.212343
2	c	-0.634421	-1.199603	-0.133292
3	c	0.119640	0.004415	-0.155095
4	c	-0.654288	1.195869	-0.127528
5	n	-1.909913	1.207933	0.217866
6	c	-2.432629	-0.018764	0.643236
7	n	-0.050170	-2.382661	-0.553149
8	n	1.454015	0.016191	-0.660662
9	c	2.573233	0.013414	0.070161
10	o	2.654877	0.000328	1.279671
11	n	-0.090664	2.389934	-0.543845
12	h	-0.512238	-3.202400	-0.199599
13	h	0.944607	-2.443946	-0.455330
14	h	-3.505624	-0.028090	0.766410
15	h	1.600375	0.026958	-1.658366
16	h	3.471069	0.025242	-0.547143
17	h	-0.567122	3.200707	-0.188985
18	h	0.903153	2.468530	-0.447119

No.9



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	2.146480	-0.380974	0.072215
2	n	1.812550	0.941467	0.091207
3	c	0.479776	1.388093	-0.014130
4	c	-0.490394	0.339426	-0.102224
5	c	-0.064830	-0.990768	-0.173555
6	n	1.261696	-1.333141	-0.042146
7	o	0.239459	2.602226	-0.054023
8	n	-1.810855	0.829691	-0.273974
9	c	-3.001175	0.301283	0.100528
10	o	-3.193007	-0.816861	0.581750
11	n	-0.899824	-2.037134	-0.407597
12	n	3.485434	-0.695575	0.128200
13	h	2.515957	1.672189	0.082155
14	h	4.092971	-0.089154	0.665223
15	h	3.659887	-1.683385	0.269470
16	h	-1.815211	1.816705	-0.523982
17	h	-3.835043	0.996746	-0.093436
18	h	-0.480496	-2.949395	-0.279126
19	h	-1.871833	-1.926149	-0.108957

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.289517	-1.333463	0.000119
2	c	-2.164186	-0.282899	0.000034
3	n	-1.911290	1.023712	-0.000307
4	c	-0.611114	1.395642	-0.000219
5	c	0.439728	0.325842	-0.000096
6	c	0.007503	-1.054889	0.000056
7	n	-3.465902	-0.651414	0.000218
8	o	-0.212180	2.574905	-0.000161

9	n	1.703118	0.866830	0.000586
10	c	2.983393	0.370676	0.000235
11	o	3.320859	-0.807467	-0.000613
12	n	0.876646	-2.082188	0.000154
13	h	-4.179925	0.062390	-0.000506
14	h	-3.713587	-1.629450	0.000081
15	h	1.599138	1.894101	0.000861
16	h	3.724677	1.183591	0.000951
17	h	0.492562	-3.017741	-0.000368
18	h	1.884375	-1.922962	-0.000286

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.253842	-1.340719	0.000072
2	c	-2.169742	-0.386536	0.000006
3	n	-1.851642	0.948112	0.000018
4	c	-0.536227	1.399409	0.000061
5	c	0.497761	0.346378	0.000279
6	c	0.057470	-1.040358	0.000291
7	n	-3.459952	-0.734426	-0.000446
8	o	-0.259653	2.589819	-0.000344
9	n	1.755878	0.886836	0.000685
10	c	3.045296	0.351667	0.000073
11	o	3.320649	-0.831848	-0.000980
12	n	0.904418	-2.061736	0.000380
13	h	-2.563275	1.674624	-0.000679
14	h	-4.220259	-0.067098	0.000718
15	h	-3.688849	-1.721658	-0.000173
16	h	1.709331	1.912187	0.000818
17	h	3.807042	1.142278	0.000577
18	h	0.517532	-3.000169	0.000414
19	h	1.919150	-1.913770	-0.000303

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	n	1.308280	-1.319144	-0.061780
2	c	2.146474	-0.279305	0.064192
3	n	1.875658	1.022139	0.080346
4	c	0.554325	1.382012	-0.028716
5	c	-0.433051	0.317036	-0.100158
6	c	-0.007434	-1.003714	-0.175897
7	n	3.507560	-0.622141	0.152033
8	o	0.179474	2.587204	-0.077347
9	n	-1.755426	0.817462	-0.233353
10	c	-2.955847	0.324449	0.110390
11	o	-3.224648	-0.808745	0.546259
12	n	-0.861970	-2.071471	-0.425427
13	h	4.053094	0.100414	0.607221
14	h	3.653924	-1.547289	0.538795
15	h	-1.694862	1.826200	-0.403639
16	h	-3.760157	1.066227	-0.056202
17	h	-0.429204	-2.955963	-0.183004
18	h	-1.806917	-1.948031	-0.056063

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	2.210574	-0.354586	-0.161179
2	n	1.803573	0.973569	0.123614
3	c	0.481381	1.380038	-0.021957
4	c	-0.472068	0.324406	-0.121057
5	c	-0.015092	-1.025338	-0.180565
6	n	1.276570	-1.347583	-0.121419
7	o	0.189840	2.605153	-0.056867
8	n	-1.802575	0.804429	-0.259865
9	c	-3.000975	0.316184	0.111825
10	o	-3.262244	-0.807310	0.583016
11	n	-0.912566	-2.070392	-0.391601
12	n	3.546618	-0.602999	0.289134
13	h	2.489999	1.705333	-0.011739
14	h	3.572552	-0.657853	1.327235
15	h	3.823753	-1.521796	-0.049336
16	h	-1.784816	1.799684	-0.481294
17	h	-3.808514	1.047732	-0.080820

18	h	-0.485597	-2.966864	-0.186305
19	h	-1.832400	-1.932370	0.031623

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.509596	1.185151	0.066262
2	c	-2.112982	0.030863	0.165681
3	n	-1.470933	-1.143674	-0.003282
4	c	-0.114243	-1.238516	-0.294398
5	c	0.546509	0.008850	-0.397952
6	c	-0.184842	1.177258	-0.213947
7	n	-3.413584	-0.014020	0.441644
8	o	0.373585	-2.349198	-0.436434
9	n	1.931095	0.047115	-0.688232
10	c	2.899161	-0.093565	0.229751
11	o	2.740605	-0.158113	1.426130
12	n	0.382889	2.385757	-0.291888
13	h	-1.977776	-2.012308	0.076303
14	h	-3.910628	-0.881952	0.527025
15	h	-3.914918	0.844881	0.571780
16	h	2.225152	0.009521	-1.648843
17	h	3.893261	-0.131442	-0.212581
18	h	-0.198782	3.200058	-0.243480
19	h	1.329456	2.498089	-0.594115

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.008506	-1.048843	0.000240
2	n	1.276020	-1.314431	0.000112
3	c	2.156285	-0.292141	0.000471
4	n	1.894523	1.007207	-0.000300

5	c	0.613076	1.388513	0.000071
6	c	-0.451716	0.343307	0.001166
7	n	3.433472	-0.651811	0.000434
8	o	0.261268	2.557128	-0.002380
9	n	-1.725264	0.870173	0.002335
10	c	-2.980864	0.357184	0.001121
11	o	-3.296099	-0.804118	-0.001433
12	n	-0.849233	-2.060144	-0.000825
13	h	4.152849	0.046219	0.000867
14	h	3.687233	-1.621283	-0.000012
15	h	-1.701881	1.877404	0.001955
16	h	-3.724367	1.148215	0.000825
17	h	-0.471323	-2.991700	-0.003144
18	h	-1.840150	-1.928018	-0.000693

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.053052	-1.048731	-0.001070
2	n	-1.241004	-1.341544	-0.000158
3	c	-2.152089	-0.388945	0.000484
4	n	-1.838278	0.929005	-0.000275
5	c	-0.550827	1.385445	-0.000090
6	c	0.496810	0.348939	-0.000899
7	n	-3.420064	-0.714859	0.001996
8	o	-0.291092	2.556353	-0.000789
9	n	1.760927	0.882299	-0.001057
10	c	3.021337	0.359759	0.001523
11	o	3.318552	-0.802355	0.002416
12	n	0.888716	-2.045452	-0.002587
13	h	-2.571710	1.628787	-0.000853
14	h	-4.152073	-0.022463	0.001601
15	h	-3.676077	-1.688296	0.003133
16	h	1.753688	1.891509	-0.000396
17	h	3.768183	1.146994	0.002520
18	h	0.514408	-2.981906	-0.001702
19	h	1.882115	-1.911547	-0.002442

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.504287	0.021189	-0.380644
2	c	-0.243720	1.167252	-0.210827
3	n	-1.558886	1.130501	0.062202
4	c	-2.095803	-0.081463	0.150738
5	n	-1.492682	-1.244228	-0.003484
6	c	-0.157322	-1.246215	-0.285478
7	n	0.289460	2.417174	-0.357704
8	n	-3.445338	-0.117247	0.388935
9	o	0.439490	-2.322347	-0.451991
10	n	1.891783	0.086813	-0.679193
11	c	2.871659	-0.083531	0.212587
12	o	2.745309	-0.166513	1.415244
13	h	-3.793213	-0.979632	0.767406
14	h	-3.830806	0.704470	0.818290
15	h	2.175879	0.062574	-1.644500
16	h	3.857275	-0.122300	-0.249719
17	h	-0.233974	3.157634	0.074640
18	h	1.281492	2.513642	-0.265691

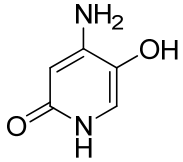
2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-2.282976	-0.079928	-0.171237
2	n	-1.483934	-1.220747	0.091923
3	c	-0.131395	-1.210302	-0.154125
4	c	0.444529	0.075114	-0.279240
5	c	-0.382962	1.214542	-0.098501
6	n	-1.683975	1.159159	0.028320
7	o	0.482045	-2.285249	-0.208115
8	n	0.192008	2.465275	-0.108837
9	h	-1.929673	-2.114094	-0.019835
10	h	-0.391349	3.188233	0.273852
11	h	1.145845	2.530258	0.190009

12	n	-3.616283	-0.268454	0.283938
13	h	-3.660611	-0.221892	1.296964
14	h	-4.202855	0.472041	-0.066339
15	n	1.849159	0.205077	-0.463222
16	h	2.219598	0.325467	-1.393091
17	c	2.740124	-0.107373	0.477540
18	o	3.942829	-0.166535	0.307405
19	h	2.297298	-0.300221	1.452643

No.10



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.623638	0.779227	-0.000549
2	n	0.643269	1.139697	-0.000011
3	c	1.645318	0.197970	0.000150
4	n	1.229094	-1.156802	-0.001649
5	c	-0.083650	-1.547816	-0.000247
6	c	-1.054888	-0.602195	0.000004
7	o	2.845518	0.446181	0.001479
8	o	-2.417119	-0.820406	0.001609
9	n	-1.579570	1.738718	-0.003459
10	h	-0.283288	-2.615468	0.000136
11	h	-1.292629	2.707268	0.006856
12	h	-2.559276	1.498787	0.009218
13	h	1.974708	-1.841364	-0.000205
14	h	-2.615111	-1.769828	-0.001034

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.116092	0.683475	0.000133
2	c	0.698471	-0.756406	-0.000155
3	n	-0.548004	-1.173611	0.000283
4	c	-1.574972	-0.269516	0.000151
5	n	-1.228524	1.124760	-0.000920
6	c	0.032138	1.595221	-0.000536
7	n	1.710375	-1.634466	-0.001601
8	o	-2.765895	-0.544656	0.000833
9	o	2.325891	1.014207	0.001214
10	h	0.195845	2.667282	-0.000699
11	h	1.520850	-2.627262	0.001828
12	h	2.660542	-1.284959	0.001715
13	h	-2.024518	1.755096	-0.001121

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.039178	-0.614120	-0.000076
2	c	0.655191	0.804086	-0.000120
3	n	-0.611013	1.168362	-0.000180
4	c	-1.611754	0.255330	0.000018
5	n	-1.237570	-1.158009	0.000166
6	c	0.019786	-1.577813	0.000136
7	n	1.623911	1.720925	0.000183
8	o	-2.807695	0.478974	-0.000116
9	o	2.335591	-0.880096	-0.000182
10	h	0.218442	-2.646860	0.000320
11	h	1.367154	2.702914	0.000459
12	h	2.605470	1.474155	0.000655
13	h	-2.019304	-1.814680	0.000427
14	h	2.563368	-1.830398	-0.000412

1.4 anion

Charge = -1 Multiplicity = 1

Center	Atomic	Coordinates (Angstroms)

Number	Name	X	Y	Z
1	c	1.149622	0.679717	-0.005064
2	c	0.667943	-0.724419	-0.019083
3	n	-0.586007	-1.141558	0.001073
4	c	-1.605465	-0.217137	0.003897
5	n	-1.225083	1.113872	-0.013346
6	c	0.095848	1.577004	-0.007237
7	n	1.678874	-1.644508	-0.064620
8	o	-2.820581	-0.514499	0.017776
9	o	2.417375	0.916551	0.025851
10	h	0.234810	2.652879	0.012200
11	h	1.468858	-2.589745	0.223524
12	h	2.590970	-1.238885	0.132757
13	h	-1.991163	1.773699	-0.014316

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.641844	0.753572	-0.064028
2	n	-0.663500	1.150519	-0.074439
3	c	-1.629306	0.201118	-0.000322
4	n	-1.236182	-1.155823	-0.046769
5	c	0.103954	-1.600736	0.020620
6	c	1.055615	-0.568488	-0.048281
7	o	-2.855168	0.434634	0.089264
8	o	2.430771	-0.867016	0.005428
9	n	1.590027	1.800673	-0.071902
10	h	0.300817	-2.587014	-0.399165
11	h	1.209140	2.625054	0.386274
12	h	2.482759	1.514736	0.321819
13	h	-1.987827	-1.798066	0.164181
14	h	2.525232	-1.576028	0.673188

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.050191	-0.601324	-0.000078
2	c	-0.621022	0.780336	-0.000324
3	n	0.646973	1.120028	-0.000387
4	c	1.613753	0.171807	0.000164
5	n	1.223064	-1.138002	-0.000630
6	c	-0.088847	-1.523802	-0.000322
7	n	-1.546572	1.730332	-0.001620
8	o	2.807228	0.443686	0.000901
9	o	-2.389315	-0.816014	0.000834
10	h	-0.280229	-2.583351	-0.000248
11	h	-1.267754	2.694493	0.003750
12	h	-2.523382	1.512488	0.004594
13	h	1.944461	-1.838667	-0.000496
14	h	-2.602820	-1.754939	0.000339

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.024660	1.577022	0.000120
2	c	1.092803	0.686520	-0.000291
3	c	0.710047	-0.755661	-0.000599
4	n	-0.532448	-1.148690	-0.000377
5	c	-1.548493	-0.243691	-0.000640
6	n	-1.236584	1.103935	-0.000451
7	o	2.288670	1.035476	0.000603
8	n	1.690437	-1.633177	-0.000255
9	o	-2.715755	-0.569559	0.001084
10	h	0.169011	2.643030	0.000578
11	h	1.484720	-2.616977	0.001336
12	h	2.650197	-1.341977	0.001691
13	h	-2.011172	1.748970	-0.001063

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.009182	-1.562382	0.001650
2	c	1.037977	-0.609576	-0.001323
3	c	0.644042	0.812954	-0.000049
4	n	-0.612224	1.165254	-0.001313
5	c	-1.590793	0.243465	-0.000624
6	n	-1.216978	-1.143148	0.002717
7	o	2.306527	-0.879011	-0.002909
8	n	1.598031	1.706515	0.002550
9	o	-2.764885	0.469098	-0.002150
10	h	0.205100	-2.625777	0.003381
11	h	1.357894	2.685439	0.004684
12	h	2.571681	1.457208	0.003060
13	h	-1.982436	-1.815604	0.005963
14	h	2.530376	-1.829079	-0.002220

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.092240	-1.547251	0.000326
2	c	1.115567	-0.675914	0.000348
3	c	0.679027	0.729669	-0.000277
4	n	-0.577020	1.117387	0.000421
5	c	-1.572511	0.197792	0.000114
6	n	-1.223279	-1.108337	0.000270
7	o	2.393443	-0.954523	-0.000302
8	n	1.632101	1.654607	-0.005216
9	o	-2.763660	0.519311	-0.000205
10	h	0.229547	-2.613403	0.000346
11	h	1.396250	2.628331	0.015879
12	h	2.593268	1.378794	0.016361
13	h	-1.965886	-1.783406	0.000071

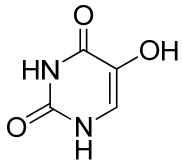
2.5 anion radical

Charge = -1 Multiplicity = 2

Center	Atomic	Coordinates (Angstroms)

Number	Name	X	Y	Z
1	c	0.667050	0.741797	0.015153
2	n	-0.669967	1.131211	-0.043317
3	c	-1.605921	0.199733	0.003708
4	n	-1.249045	-1.132778	0.132271
5	c	0.074540	-1.569115	-0.063185
6	c	1.056474	-0.577222	-0.024352
7	o	-2.829026	0.447828	-0.038394
8	o	2.393708	-0.894792	-0.098803
9	n	1.588299	1.806713	-0.057278
10	h	0.268004	-2.622849	0.011074
11	h	1.256467	2.602778	0.464065
12	h	2.498516	1.550264	0.284865
13	h	-1.991260	-1.790405	-0.020367
14	h	2.612943	-1.571245	0.548275

No.11



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.736346	-0.839073	-0.000491
2	n	-0.635402	-1.058757	-0.000256
3	c	-1.645489	-0.094966	-0.000497
4	n	-1.158496	1.197752	-0.000029
5	c	0.189751	1.534723	0.000079
6	c	1.134156	0.568461	-0.000102
7	o	-2.834603	-0.374211	0.000417
8	o	2.467173	0.823317	0.000107
9	o	1.560553	-1.752630	0.000402
10	h	0.426428	2.591784	0.000396
11	h	-0.949868	-2.024323	0.000135

12	h	-1.865012	1.921605	0.000324
13	h	2.912156	-0.048709	-0.000212

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.250442	-0.579021	-0.000160
2	c	0.809077	0.880541	-0.000446
3	n	-0.586682	1.064344	-0.000276
4	c	-1.584031	0.105476	-0.000662
5	n	-1.100711	-1.208923	-0.000073
6	c	0.215743	-1.554533	0.000021
7	o	1.562806	1.828416	0.000348
8	o	-2.776428	0.353319	0.000561
9	o	2.456077	-0.881832	0.000212
10	h	0.459623	-2.610553	0.000384
11	h	-0.910483	2.028056	0.000194
12	h	-1.824413	-1.919459	0.000376

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.741316	-0.875680	0.000019
2	n	-0.622471	-1.108816	-0.000014
3	c	-1.625391	-0.148922	-0.000116
4	n	-1.137841	1.204766	0.000016
5	c	0.144570	1.572268	0.000011
6	c	1.122391	0.567798	-0.000006
7	o	-2.806396	-0.366951	0.000044
8	o	2.390497	0.862961	-0.000013
9	o	1.606919	-1.726787	0.000022
10	h	0.392735	2.630058	0.000036
11	h	-0.937217	-2.079796	0.000024
12	h	-1.880893	1.905086	0.000072
13	h	2.922083	0.026438	-0.000008

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.291650	-0.581673	-0.000026
2	c	-0.793229	0.852999	-0.000210
3	n	0.608431	1.019249	-0.000083
4	c	1.605940	0.053277	-0.000055
5	n	1.105314	-1.203797	-0.000017
6	c	-0.272861	-1.533936	0.000014
7	o	-1.497664	1.860674	0.000129
8	o	2.821343	0.339315	0.000101
9	o	-2.538928	-0.812082	0.000048
10	h	-0.492527	-2.595055	0.000077
11	h	0.932993	1.980016	-0.000000
12	h	1.796099	-1.940381	0.000053

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.770652	-0.796396	0.011775
2	n	0.643654	-1.059030	0.055206
3	c	1.636600	-0.108436	0.014865
4	n	1.191910	1.187796	0.077586
5	c	-0.181737	1.600612	-0.077947
6	c	-1.119657	0.554548	-0.020565
7	o	2.846651	-0.399521	-0.057952
8	o	-2.482196	0.834243	-0.024265
9	o	-1.588303	-1.778953	-0.001736
10	h	-0.409495	2.580347	0.338221
11	h	1.916285	1.854074	-0.150580
12	h	-2.885701	-0.058540	-0.011927
13	h	0.933427	-2.025366	-0.002406

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.228820	-1.489974	0.010110
2	c	1.145151	-0.525812	0.003003
3	c	0.705465	0.867998	-0.006847
4	n	-0.660210	1.035869	0.006595
5	c	-1.613949	0.052588	0.002385
6	n	-1.117935	-1.206708	0.002989
7	o	2.471053	-0.795879	-0.079824
8	o	1.449225	1.817483	-0.012436
9	o	-2.796020	0.304068	0.000056
10	h	0.488409	-2.533721	0.010362
11	h	-1.002736	1.985479	0.003806
12	h	-1.784340	-1.961798	-0.001078
13	h	2.958701	-0.328262	0.605563

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.216169	-1.542777	0.000220
2	c	-1.216485	-0.573293	-0.000403
3	c	-0.782484	0.867803	0.000642
4	n	0.575659	1.055146	-0.000148
5	c	1.553835	0.090157	-0.000419
6	n	1.101349	-1.195380	-0.000105
7	o	-2.428718	-0.852220	0.000046
8	o	-1.548165	1.786094	-0.000197
9	o	2.722486	0.369837	0.000204
10	h	-0.448266	-2.592623	0.000743
11	h	0.905853	2.010512	0.000736
12	h	1.806357	-1.917279	-0.000376

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.134833	-0.534030	0.000255
2	c	-0.720668	0.890253	-0.000522
3	n	0.634794	1.085245	-0.000093
4	c	1.596452	0.119321	0.000107
5	n	1.106767	-1.205128	-0.001822
6	c	-0.154025	-1.535947	-0.000280
7	o	-1.519401	1.773975	-0.001112
8	o	2.762989	0.325289	0.001566
9	o	-2.378995	-0.874072	0.001426
10	h	-0.415216	-2.584807	0.000135
11	h	0.966723	2.044621	0.001721
12	h	1.819719	-1.935072	-0.002588
13	h	-3.000449	-0.124681	0.001725

2.4 anion

Charge = -1 Multiplicity = 1

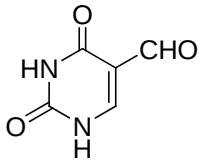
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.271994	-1.505381	-0.005827
2	c	1.237580	-0.570923	0.001462
3	c	0.759637	0.842150	-0.002415
4	n	-0.605774	1.020974	0.005164
5	c	-1.573938	0.050583	0.001755
6	n	-1.095800	-1.195325	-0.009181
7	o	2.518479	-0.789289	0.011938
8	o	1.484720	1.809129	-0.010219
9	o	-2.759244	0.336181	0.006763
10	h	0.491115	-2.556978	-0.007082
11	h	-0.935927	1.973265	0.008281
12	h	-1.767445	-1.942582	-0.010791

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.756221	0.805448	-0.008416
2	n	0.657163	1.037703	0.038004
3	c	1.612906	0.086045	-0.003158
4	n	1.170074	-1.188049	-0.041673
5	c	-0.196376	-1.554895	0.075483
6	c	-1.133810	-0.516872	0.006835
7	o	2.810749	0.359521	-0.009984
8	o	-2.465513	-0.859555	-0.018668
9	o	-1.515977	1.836219	-0.016341
10	h	-0.429686	-2.583633	-0.121426
11	h	1.874616	-1.901760	0.022813
12	h	-2.994452	-0.063857	0.050570
13	h	0.965802	1.993838	0.009210

No.12



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.253104	0.941737	-0.000188
2	c	-1.921077	-0.267920	-0.000275
3	n	-1.055436	-1.373164	0.000005
4	c	0.299901	-1.269007	0.000131
5	c	0.938397	-0.063633	0.000054
6	c	0.141325	1.166500	-0.000106
7	o	-3.131297	-0.392781	0.000174
8	c	2.412728	-0.004405	0.000220
9	o	3.125792	-0.996757	-0.000282
10	o	0.577888	2.307147	0.000070

11	h	0.865737	-2.196086	0.000333
12	h	-1.840618	1.770607	-0.000048
13	h	-1.514424	-2.276528	0.000222
14	h	2.842381	1.011909	0.000927

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.229266	0.943188	0.390082
2	c	0.099993	1.190759	-0.013580
3	c	0.890487	-0.063617	0.032447
4	c	0.249657	-1.268791	-0.064289
5	n	-1.102542	-1.358243	-0.072142
6	c	-1.910059	-0.208661	0.057353
7	o	0.559475	2.290315	-0.248264
8	c	2.368131	0.003193	0.066934
9	o	3.074421	-0.991000	0.033836
10	o	-3.120554	-0.250610	-0.083321
11	h	2.795430	1.018428	0.116762
12	h	0.814213	-2.191829	-0.157116
13	h	-1.582976	-2.228146	-0.276427

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.200242	1.077196	0.000171
2	n	-1.172629	1.012068	0.000059
3	c	-1.945851	-0.154242	0.000027
4	n	-1.170999	-1.354549	0.000238
5	c	0.162276	-1.400362	0.000257
6	c	0.889494	-0.221467	0.000294
7	o	-3.144301	-0.172568	-0.000434
8	c	2.310129	-0.053248	0.000104
9	o	3.186298	-0.896432	-0.000506
10	o	0.822359	2.139651	0.000013
11	h	0.628739	-2.381977	0.000243

12	h	-1.696331	1.887457	-0.000329
13	h	-1.726932	-2.208490	0.000070
14	h	2.587330	1.047900	0.000235

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.068364	1.171798	0.000244
2	n	-1.299011	1.053597	0.000087
3	c	-1.916389	-0.132554	0.000126
4	n	-1.088880	-1.329700	0.000009
5	c	0.253609	-1.281539	0.000002
6	c	0.897957	-0.073484	0.000068
7	o	-3.138536	-0.355638	-0.000157
8	c	2.349281	-0.022788	-0.000049
9	o	3.107414	-1.002121	-0.000034
10	o	0.634656	2.281463	-0.000182
11	h	0.802253	-2.221200	-0.000089
12	h	-1.597995	-2.204398	-0.000068
13	h	2.765778	1.000079	0.000122

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.230655	0.928460	0.014412
2	c	-1.921369	-0.275185	-0.007209
3	n	-1.110858	-1.369831	-0.013636
4	c	0.296734	-1.329722	0.049816
5	c	0.966454	-0.074030	0.015945
6	c	0.181484	1.135694	0.007881
7	o	-3.163349	-0.333323	-0.016936
8	c	2.393343	0.006920	-0.010407
9	o	3.175481	-0.977190	-0.015442
10	o	0.570540	2.314696	-0.004198
11	h	-1.797918	1.766536	0.001170
12	h	2.803389	1.033611	-0.027031

13	h	-1.596429	-2.255121	0.010580
14	h	0.820301	-2.270960	-0.033703

---

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.123377	1.145859	0.000651
2	n	-1.241437	0.931898	-0.000185
3	c	-1.885648	-0.270290	0.000326
4	n	-1.051900	-1.362734	0.000160
5	c	0.288715	-1.262764	0.000118
6	c	0.926445	-0.069521	0.000434
7	o	-3.081538	-0.376299	-0.000456
8	c	2.390241	0.002728	0.000793
9	o	3.107156	-0.963099	-0.001141
10	o	0.559403	2.270214	-0.000332
11	h	0.828778	-2.192562	-0.000000
12	h	-1.832869	1.751165	-0.001867
13	h	-1.495170	-2.270514	0.001394
14	h	2.813669	1.005155	0.002145

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.900108	-0.244247	0.025117
2	n	-1.250013	0.932681	0.418085
3	c	0.093635	1.161187	0.032620
4	c	0.906047	-0.051341	0.040005
5	c	0.263147	-1.243090	0.013974
6	n	-1.082758	-1.349363	0.010719
7	o	0.462816	2.273611	-0.200706
8	c	2.370517	0.022264	-0.008488
9	o	3.085635	-0.943216	-0.021441

10	o	-3.066520	-0.274849	-0.206840
11	h	2.792796	1.025728	-0.027424
12	h	0.803781	-2.171479	-0.035510
13	h	-1.522043	-2.250487	-0.126166

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.936822	-0.039071	0.000179
2	c	0.102572	1.181653	0.000464
3	n	-1.257694	0.963971	-0.000337
4	c	-1.884691	-0.236581	-0.000218
5	n	-1.004864	-1.370116	0.001593
6	c	0.278979	-1.314269	0.000731
7	o	0.576026	2.276733	0.000871
8	o	-3.050375	-0.419788	-0.001551
9	c	2.391507	0.031462	-0.000141
10	o	3.040630	-1.002731	-0.001577
11	h	0.833613	-2.239279	0.001146
12	h	-1.859922	1.782281	-0.002216
13	h	-1.477721	-2.280434	0.003556
14	h	2.860549	1.007582	0.000681

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.888745	-0.070291	0.000148
2	c	-0.068016	1.149144	0.000127
3	n	1.279725	1.028170	0.000143
4	c	1.878460	-0.162290	-0.000139
5	n	1.089549	-1.315193	-0.000182
6	c	-0.243089	-1.262690	0.000069
7	o	-0.602242	2.258002	-0.000255
8	o	3.093870	-0.325544	0.000127
9	c	-2.343722	-0.014774	0.000046
10	o	-3.069331	-0.982736	-0.000047

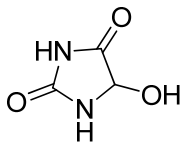
11	h	-0.765455	-2.203006	0.000029
12	h	1.567443	-2.204491	-0.000429
13	h	-2.774620	0.984280	0.000571

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.210143	0.925110	0.039949
2	c	-1.885184	-0.267043	-0.010898
3	n	-1.121880	-1.365548	-0.025652
4	c	0.281217	-1.357612	0.126021
5	c	0.956703	-0.084302	0.020512
6	c	0.166709	1.113647	0.016063
7	o	-3.105221	-0.292122	-0.044324
8	c	2.353639	0.014590	-0.032533
9	o	3.153117	-0.937472	-0.022957
10	o	0.571732	2.268450	-0.008790
11	h	-1.780769	1.756280	0.028144
12	h	-1.612248	-2.244531	-0.020504
13	h	2.753004	1.025883	-0.087417
14	h	0.768651	-2.281084	-0.126714

No.13



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.797323	0.787369	0.115249
2	n	-0.509236	1.132158	-0.126240

3	c	-1.395547	0.036471	-0.006951
4	n	-0.623829	-1.019186	0.430518
5	c	0.781504	-0.729521	0.427465
6	o	-2.587670	0.061277	-0.221752
7	o	1.427962	-1.461520	-0.601006
8	o	1.788119	1.487043	0.059013
9	h	-0.992022	-1.960798	0.403372
10	h	-0.822949	2.047956	-0.423042
11	h	1.252275	-0.931815	1.398749
12	h	2.367183	-1.206469	-0.613641

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.871350	-0.751028	0.072157
2	n	0.431358	-1.117030	-0.104768
3	c	1.370475	-0.057740	0.005202
4	n	0.650465	1.047879	0.384934
5	c	-0.798135	0.845118	0.336623
6	o	2.560601	-0.169903	-0.189179
7	o	-1.478124	1.513316	-0.581304
8	o	-1.869058	-1.420012	0.056187
9	h	1.053031	1.965359	0.236750
10	h	0.721523	-2.068287	-0.300684
11	h	-1.260603	0.981673	1.333250

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-0.659630	1.135598	0.006330
2	c	-1.420649	-0.074048	-0.002107
3	n	-0.493471	-1.115942	0.125323
4	c	0.838378	-0.748434	0.391379
5	c	0.672094	0.986747	0.011392
6	o	-2.603854	-0.148594	-0.132353
7	o	1.617425	1.699634	-0.082284

8	o	1.827759	-1.398499	-0.220335
9	h	-0.776242	-2.066659	-0.107917
10	h	-1.117662	2.045080	-0.072580
11	h	1.092447	-0.605552	1.453048
12	h	1.603585	-1.716376	-1.118337

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.905278	-0.698861	0.091536
2	n	0.403324	-1.113983	-0.097389
3	c	1.349513	-0.076702	0.034013
4	n	0.680575	0.997735	0.526876
5	c	-0.877335	0.858223	0.319540
6	o	2.544463	-0.208463	-0.245615
7	o	-1.345160	1.573843	-0.662521
8	o	-1.876030	-1.441452	0.048873
9	h	1.064061	1.905182	0.284316
10	h	0.670085	-2.035065	-0.422026
11	h	-1.309027	1.056230	1.334880

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.788746	0.803483	0.044390
2	n	-0.587982	1.107129	-0.116907
3	c	-1.408518	0.002985	0.011374
4	n	-0.574993	-1.016988	0.414650
5	c	0.843681	-0.662630	0.374151
6	o	-2.627913	-0.053748	-0.198719
7	o	1.576343	-1.419230	-0.593550
8	o	1.700507	1.654056	0.058933
9	h	-0.878235	-1.977253	0.340219
10	h	-0.932110	2.011175	-0.403595
11	h	1.326043	-0.871504	1.359533
12	h	2.090181	-2.105060	-0.093158

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.804344	-0.684005	0.385196
2	c	0.715454	0.818255	0.093367
3	n	-0.598501	1.090835	-0.112856
4	c	-1.387501	-0.043896	-0.027202
5	n	-0.558229	-1.087975	0.175662
6	o	1.627504	1.591071	0.049390
7	o	-2.586439	-0.057932	-0.124426
8	o	1.652031	-1.323572	-0.506446
9	h	-0.920482	-1.969424	0.511904
10	h	-0.971665	2.000839	-0.334865
11	h	1.130597	-0.843540	1.435990
12	h	2.520107	-1.426546	-0.108980

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.794001	-0.759193	0.340205
2	c	0.793380	0.754568	0.083142
3	n	-0.507292	1.093844	-0.095582
4	c	-1.358429	0.002546	-0.029958
5	n	-0.586138	-1.097113	0.122699
6	o	1.746071	1.471690	0.045811
7	o	-2.555640	0.060047	-0.103525
8	o	1.680518	-1.416404	-0.461468
9	h	-0.993136	-1.950049	0.483955
10	h	-0.833884	2.030193	-0.281584
11	h	1.139735	-0.967448	1.400928

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.852174	-0.678418	0.403889
2	c	0.761935	0.804726	0.084499
3	n	-0.595774	1.090308	-0.082457
4	c	-1.416735	-0.049973	-0.020788
5	n	-0.544363	-1.056206	0.195967
6	o	1.618701	1.631134	-0.001446
7	o	-2.604123	-0.059892	-0.141456
8	o	1.729804	-1.396889	-0.341248
9	h	-0.868930	-2.030437	0.285560
10	h	-0.970422	2.041382	-0.216615
11	h	1.101372	-0.806598	1.496234
12	h	1.579640	-1.295895	-1.292141

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.849228	-0.774502	0.341854
2	c	0.801541	0.744470	0.082882
3	n	-0.501630	1.090231	-0.096555
4	c	-1.352773	-0.002424	-0.016151
5	n	-0.591453	-1.072318	0.207364
6	o	1.735616	1.500032	0.041538
7	o	-2.556869	0.065838	-0.133899
8	o	1.641735	-1.448370	-0.497039
9	h	-0.994366	-1.979204	0.385007
10	h	-0.827700	2.018461	-0.310726
11	h	1.121820	-0.909907	1.413743

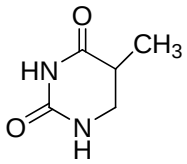
2.5 anion radical

Charge = -1 Multiplicity = 2

Center	Atomic	Coordinates (Angstroms)

Number	Name	X	Y	Z
1	c	0.761594	0.820034	-0.190867
2	n	-0.668167	1.090864	-0.125583
3	c	-1.388068	-0.040463	-0.011586
4	n	-0.524393	-1.077668	0.158915
5	c	0.841672	-0.615719	0.313929
6	o	-2.608131	-0.138319	-0.055780
7	o	1.749404	-1.371495	-0.439174
8	o	1.589900	1.726941	0.191584
9	h	-0.857128	-1.908063	0.636984
10	h	-1.080854	1.907021	-0.544133
11	h	1.147565	-0.655063	1.377134
12	h	1.997760	-2.156390	0.054801

No.14



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.647604	0.945267	-0.046476
2	n	0.728597	1.052522	0.105816
3	c	1.693090	0.034829	-0.005819
4	n	1.167838	-1.223982	-0.128727
5	c	-0.215402	-1.516573	0.239727
6	c	-1.154322	-0.462515	-0.361062
7	o	2.887920	0.293197	-0.006436
8	c	-2.607610	-0.650923	0.082327
9	o	-1.365611	1.927610	0.035877
10	h	-0.337305	-1.544885	1.334449
11	h	1.104246	1.988286	0.224691
12	h	1.861014	-1.958921	-0.064126
13	h	-1.096707	-0.551960	-1.457305

14	h	-0.470726	-2.506650	-0.148757
15	h	-3.244218	0.122867	-0.352897
16	h	-2.978953	-1.631658	-0.235888
17	h	-2.699778	-0.583818	1.172495

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.145249	-0.421868	-0.356382
2	c	-0.568373	0.969672	-0.014000
3	n	0.682407	0.922082	0.612379
4	c	1.656472	0.048580	0.065835
5	n	1.167941	-1.208146	-0.170803
6	c	-0.220121	-1.550094	0.128519
7	o	-1.157915	2.008554	-0.235989
8	o	2.801353	0.422056	-0.127191
9	c	-2.580932	-0.560106	0.163773
10	h	-0.359981	-1.722400	1.205840
11	h	1.856982	-1.929314	-0.347713
12	h	-1.155419	-0.439472	-1.456243
13	h	-0.464394	-2.480973	-0.390634
14	h	-3.198278	0.263590	-0.203478
15	h	-3.020542	-1.503974	-0.179313
16	h	-2.609100	-0.546996	1.259479

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.654486	0.951030	-0.065325
2	n	0.749692	1.084777	0.106961
3	c	1.669030	0.082467	-0.017994
4	n	1.147104	-1.196837	-0.186611
5	c	-0.191524	-1.504761	0.258171
6	c	-1.175047	-0.453757	-0.360444
7	o	2.887785	0.206914	0.063743
8	c	-2.608097	-0.686866	0.130864

9	o	-1.351693	1.931792	-0.007217
10	h	-0.244148	-1.432390	1.357365
11	h	1.105412	2.025896	0.276357
12	h	1.821238	-1.920745	-0.445380
13	h	-1.144468	-0.557594	-1.456160
14	h	-0.436008	-2.527633	-0.033626
15	h	-3.288004	0.025955	-0.341433
16	h	-2.936254	-1.695383	-0.140342
17	h	-2.683333	-0.572011	1.216929

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.112053	-0.464673	-0.358503
2	c	-0.582079	0.966353	-0.042957
3	n	0.745510	1.176708	0.096890
4	c	1.645865	0.161982	-0.003532
5	n	1.187198	-1.171181	-0.204078
6	c	-0.158626	-1.502395	0.228614
7	o	-1.427082	1.880849	0.034654
8	o	2.880385	0.319395	0.049956
9	c	-2.554304	-0.672078	0.106502
10	h	-0.258022	-1.501179	1.333124
11	h	1.916114	-1.830681	0.044779
12	h	-1.072890	-0.568793	-1.455374
13	h	-0.413704	-2.513968	-0.120603
14	h	-3.204001	0.100201	-0.313572
15	h	-2.927983	-1.662650	-0.195479
16	h	-2.627717	-0.598705	1.199811

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.670839	0.921133	-0.116247
2	n	-0.760916	1.056498	0.007473
3	c	-1.689824	0.057198	0.016492

4	n	-1.163735	-1.219877	0.010303
5	c	0.247294	-1.548758	-0.165454
6	c	1.155599	-0.421112	0.356145
7	o	-2.922602	0.254013	0.018789
8	c	2.610975	-0.673376	-0.048583
9	o	1.362371	1.987383	-0.071731
10	h	0.479213	-1.741082	-1.224606
11	h	-1.120858	2.002523	-0.018903
12	h	-1.858524	-1.940116	-0.129158
13	h	1.102350	-0.455806	1.476597
14	h	0.458326	-2.474621	0.398487
15	h	3.248744	0.127737	0.337612
16	h	2.966612	-1.635733	0.348081
17	h	2.709240	-0.680934	-1.143134

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.146146	-0.446601	-0.363236
2	c	-0.624205	0.937842	-0.040716
3	n	0.735173	1.039004	0.105025
4	c	1.662706	0.017386	-0.006351
5	n	1.153179	-1.215432	-0.101576
6	c	-0.229564	-1.503951	0.244717
7	o	-1.315950	1.917705	0.050279
8	o	2.848021	0.276961	-0.026708
9	c	-2.599653	-0.628064	0.065287
10	h	-0.353104	-1.536035	1.328275
11	h	1.116752	1.964586	0.220306
12	h	1.827211	-1.965797	-0.063039
13	h	-1.076727	-0.522712	-1.452709
14	h	-0.477244	-2.481327	-0.154625
15	h	-3.239882	0.101996	-0.412791
16	h	-2.941986	-1.618515	-0.216824
17	h	-2.708884	-0.524196	1.140477

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.238974	-1.520812	0.153989
2	c	-1.147187	-0.400874	-0.362858
3	c	-0.562639	0.955356	-0.009625
4	n	0.688583	0.895401	0.631834
5	c	1.645259	0.014710	0.062141
6	n	1.152844	-1.201268	-0.143150
7	c	-2.588128	-0.534761	0.133108
8	o	-1.080594	2.008285	-0.221404
9	o	2.767746	0.397959	-0.155865
10	h	-0.372030	-1.663872	1.225882
11	h	1.792125	-1.924662	-0.444747
12	h	-1.135933	-0.426439	-1.455731
13	h	-0.479191	-2.451792	-0.346434
14	h	-3.212037	0.246165	-0.283425
15	h	-2.991584	-1.493652	-0.174857
16	h	-2.638531	-0.476344	1.216134

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.145129	-0.438192	-0.372369
2	c	-0.630757	0.943915	-0.033961
3	n	0.751203	1.071811	0.075284
4	c	1.677015	0.091975	-0.013112
5	n	1.140393	-1.233319	-0.025510
6	c	-0.258897	-1.522363	0.238982
7	o	-1.314848	1.911442	0.088653
8	o	2.856409	0.221844	-0.048011
9	c	-2.602712	-0.629759	0.040708
10	h	-0.337770	-1.556355	1.334569
11	h	1.116560	2.011399	0.183239
12	h	1.835426	-2.000968	-0.138997
13	h	-1.064259	-0.509062	-1.462590

14	h	-0.469908	-2.508706	-0.164437
15	h	-3.231407	0.103313	-0.446346
16	h	-2.936772	-1.618260	-0.254864
17	h	-2.722644	-0.530555	1.114384

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.185644	-1.488341	0.242519
2	c	-1.105654	-0.439987	-0.363879
3	c	-0.569391	0.951217	-0.029856
4	n	0.752067	1.145915	0.099597
5	c	1.628437	0.117539	-0.005284
6	n	1.176951	-1.164704	-0.121623
7	c	-2.558141	-0.643643	0.056442
8	o	-1.359302	1.886740	0.072845
9	o	2.846935	0.318065	-0.011994
10	h	-0.308853	-1.512503	1.329894
11	h	1.882417	-1.869628	0.046996
12	h	-1.036390	-0.524175	-1.453600
13	h	-0.424183	-2.476696	-0.142061
14	h	-3.211604	0.068931	-0.430304
15	h	-2.884997	-1.644503	-0.213340
16	h	-2.678225	-0.529059	1.130146

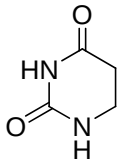
2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.676764	0.928065	0.221084
2	n	0.774377	1.037669	0.078123
3	c	1.659577	0.034884	-0.007451
4	n	1.150161	-1.214890	-0.116222
5	c	-0.241901	-1.524026	0.178350
6	c	-1.156706	-0.407108	-0.319007
7	o	2.879570	0.231381	-0.025316
8	c	-2.608159	-0.694643	0.056893

9	o	-1.309793	2.021685	-0.057547
10	h	-0.382585	-1.667709	1.251919
11	h	1.164912	1.958496	0.170784
12	h	1.829318	-1.954890	0.000449
13	h	-1.084427	-0.378638	-1.415897
14	h	-0.482760	-2.462479	-0.315589
15	h	-3.262110	0.086425	-0.313247
16	h	-2.938974	-1.641048	-0.364527
17	h	-2.729632	-0.747170	1.136498

No.15



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.255223	-0.448175	-0.013491
2	n	0.001148	-1.032411	0.103756
3	c	-1.254533	-0.408979	-0.023128
4	n	-1.200956	0.957083	-0.121207
5	c	-0.020249	1.713101	0.293861
6	c	1.231112	1.047853	-0.280990
7	o	-2.284137	-1.066569	-0.057738
8	o	2.275376	-1.110658	0.065344
9	h	0.048554	1.765711	1.391297
10	h	-0.029541	-2.042823	0.199276
11	h	-2.110127	1.399150	-0.068077
12	h	1.263526	1.184136	-1.370466
13	h	-0.116638	2.734574	-0.083999
14	h	2.143651	1.481558	0.135766

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.226621	1.030326	-0.231048
2	c	1.205561	-0.477938	0.043959
3	n	0.003113	-0.929083	0.609813
4	c	-1.201074	-0.449690	0.031170
5	n	-1.205462	0.908655	-0.147973
6	c	-0.058138	1.733151	0.225879
7	o	2.143480	-1.217033	-0.176655
8	o	-2.117456	-1.208689	-0.235463
9	h	-0.039021	1.909101	1.310515
10	h	-2.106649	1.328687	-0.342069
11	h	1.362013	1.140312	-1.314280
12	h	-0.156905	2.703579	-0.267193
13	h	2.110992	1.451997	0.257332

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.257680	-0.444742	0.001394
2	n	-0.005709	-1.089212	-0.029951
3	c	1.216058	-0.455692	-0.000828
4	n	1.194238	0.919824	-0.210475
5	c	0.016600	1.758448	-0.152202
6	c	-1.202250	1.025531	0.394424
7	o	2.286600	-1.018487	0.181053
8	o	-2.269488	-1.067154	-0.205110
9	h	-0.134193	2.138869	-1.181525
10	h	0.002800	-2.108546	-0.076865
11	h	2.117638	1.338647	-0.344397
12	h	-1.189311	1.033088	1.493696
13	h	0.234372	2.651527	0.452762
14	h	-2.124274	1.515991	0.075036

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.207366	1.021598	-0.258718
2	c	1.189532	-0.503843	-0.007241
3	n	0.007694	-1.153308	0.088912
4	c	-1.175294	-0.491166	-0.026218
5	n	-1.186389	0.925519	-0.197298
6	c	-0.047220	1.683126	0.297119
7	o	2.296236	-1.073796	0.072315
8	o	-2.288112	-1.050627	-0.012260
9	h	-0.000047	1.690583	1.404260
10	h	-2.102619	1.291203	0.036936
11	h	1.258908	1.186719	-1.345302
12	h	-0.135207	2.727848	-0.034094
13	h	2.118541	1.435263	0.186815

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.257610	-0.409968	-0.095827
2	n	0.012473	-1.051817	0.021247
3	c	1.236913	-0.429114	0.016992
4	n	1.190591	0.933502	-0.181983
5	c	-0.011087	1.766492	-0.188494
6	c	-1.201856	1.001377	0.404066
7	o	2.315862	-1.046514	0.116480
8	o	-2.298038	-1.121651	-0.180956
9	h	-0.241386	2.087512	-1.213345
10	h	0.022983	-2.065339	0.054881
11	h	2.094617	1.381395	-0.126895
12	h	-1.086635	1.006525	1.519302
13	h	0.187347	2.675970	0.412420
14	h	-2.139124	1.514740	0.174177

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.223654	1.037144	-0.289315
2	c	1.231489	-0.442908	-0.012033
3	n	-0.002066	-1.024774	0.106795
4	c	-1.230069	-0.394386	-0.020362
5	n	-1.192501	0.941030	-0.099069
6	c	-0.014749	1.704660	0.288262
7	o	2.233080	-1.105224	0.069863
8	o	-2.244353	-1.058095	-0.069431
9	h	0.058016	1.767207	1.373772
10	h	-0.033403	-2.027602	0.203387
11	h	-2.092357	1.397634	-0.070814
12	h	1.245989	1.150619	-1.373128
13	h	-0.120174	2.709322	-0.105138
14	h	2.132137	1.468519	0.115063

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.033522	1.711233	0.230676
2	c	1.244059	1.013867	-0.234127
3	c	1.196486	-0.470855	0.042035
4	n	-0.007079	-0.899842	0.632783
5	c	-1.201031	-0.417701	0.031988
6	n	-1.187372	0.898980	-0.144268
7	o	2.071395	-1.247652	-0.186562
8	o	-2.093452	-1.182860	-0.236686
9	h	-0.018189	1.868320	1.307378
10	h	-2.042808	1.339707	-0.455824
11	h	1.374764	1.121874	-1.309417
12	h	-0.134239	2.674864	-0.254251
13	h	2.122132	1.426095	0.255052

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.223467	1.036987	0.300684
2	c	-1.243052	-0.439588	0.011107
3	n	-0.001896	-1.058609	-0.080608
4	c	1.214304	-0.475998	0.022582
5	n	1.196287	0.954154	0.029740
6	c	0.005362	1.736879	-0.261336
7	o	-2.235326	-1.091612	-0.091582
8	o	2.265503	-1.024544	0.075301
9	h	-0.022974	1.805528	-1.356793
10	h	0.003171	-2.068255	-0.174280
11	h	2.122397	1.414831	0.154404
12	h	-1.258780	1.146113	1.384779
13	h	0.154566	2.729031	0.154337
14	h	-2.119409	1.483511	-0.114345

2.4 anion

Charge = -1 Multiplicity = 1

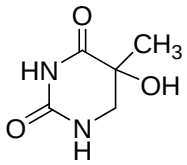
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.025661	1.682170	-0.279518
2	c	-1.204004	1.001190	0.288905
3	c	-1.174163	-0.490140	0.005406
4	n	-0.002361	-1.128615	-0.100951
5	c	1.170696	-0.454052	0.016540
6	n	1.182671	0.906444	0.121400
7	o	-2.245498	-1.089296	-0.087157
8	o	2.246100	-1.058724	0.049940
9	h	-0.046764	1.745139	-1.368643
10	h	2.093199	1.323469	-0.026243
11	h	-1.234034	1.124225	1.372251
12	h	0.129231	2.691985	0.108492
13	h	-2.117752	1.419541	-0.119266

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.280009	-0.368077	-0.245670
2	n	0.006829	-1.031244	-0.054415
3	c	1.209425	-0.439700	0.020269
4	n	1.222424	0.912581	0.090651
5	c	0.061823	1.738722	-0.219399
6	c	-1.204493	1.050207	0.271684
7	o	2.258943	-1.090427	0.062602
8	o	-2.307130	-1.112212	0.019491
9	h	-0.002062	1.917856	-1.293974
10	h	0.017869	-2.032859	-0.137243
11	h	2.138423	1.328036	-0.021234
12	h	-1.215162	1.044552	1.368140
13	h	0.198524	2.699595	0.270539
14	h	-2.077342	1.607657	-0.057923

No.16



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.069678	-0.369435	0.041760
2	c	0.448831	1.039481	-0.095182
3	n	-0.926490	1.084049	-0.187669
4	c	-1.833547	0.010413	-0.042805
5	n	-1.248723	-1.217529	-0.072193
6	c	0.122394	-1.439671	-0.506797

7	o	1.125871	2.055984	-0.060690
8	o	-3.028738	0.219210	0.105397
9	c	2.427343	-0.429867	-0.657036
10	o	1.195863	-0.625433	1.447829
11	h	0.189173	-1.447476	-1.604776
12	h	-1.890141	-1.996141	-0.003879
13	h	3.098601	0.329055	-0.245032
14	h	2.871381	-1.420037	-0.508980
15	h	2.332266	-0.238222	-1.731615
16	h	1.776556	0.053026	1.832356
17	h	-1.356285	2.004146	-0.163237
18	h	0.452770	-2.413616	-0.135734

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.151842	-1.409000	-0.598516
2	c	1.091629	-0.425365	0.156958
3	c	0.492520	1.045657	-0.085505
4	n	-0.875894	1.093641	-0.136542
5	c	-1.794354	0.017892	-0.042517
6	n	-1.234203	-1.205108	-0.226364
7	c	2.533292	-0.484160	-0.357288
8	o	0.977866	-0.561053	1.498880
9	o	1.207886	2.015511	-0.193731
10	o	-2.977144	0.234448	0.165942
11	h	0.297681	-1.286720	-1.681584
12	h	-1.853846	-1.990722	-0.083036
13	h	3.139015	0.256821	0.167591
14	h	2.942848	-1.480770	-0.158785
15	h	2.590139	-0.285848	-1.432998
16	h	-1.303001	2.015274	-0.148307
17	h	0.439409	-2.429159	-0.330060

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	c	0.105961	-1.352920	-0.674279
2	c	1.111989	-0.369989	0.072489
3	c	0.416928	1.074849	-0.065218
4	n	-0.947127	1.106068	-0.145981
5	c	-1.832607	0.009652	-0.036660
6	n	-1.210854	-1.213051	-0.143618
7	c	2.500376	-0.391158	-0.543272
8	o	1.064747	-0.697767	1.415778
9	o	1.124681	2.054624	-0.057207
10	o	-3.019223	0.161984	0.144594
11	h	0.150195	-1.073680	-1.736398
12	h	-1.763819	-2.021598	0.131255
13	h	3.178234	0.277360	-0.003867
14	h	2.898212	-1.411051	-0.498262
15	h	2.480172	-0.069825	-1.588408
16	h	1.928354	-0.568952	1.853797
17	h	-1.393020	2.024008	-0.127443
18	h	0.450025	-2.380710	-0.547169

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.189688	-1.415574	-0.591114
2	c	1.074641	-0.390521	0.190450
3	c	0.519554	1.020806	-0.130113
4	n	-0.884926	1.083952	-0.200702
5	c	-1.768441	0.016434	-0.055277
6	n	-1.235376	-1.207304	-0.323739
7	c	2.527689	-0.511544	-0.331428
8	o	0.949104	-0.526952	1.524880
9	o	1.158041	2.068637	-0.198426
10	o	-2.958935	0.200530	0.230131
11	h	0.363433	-1.370233	-1.680724
12	h	-1.795316	-1.972173	0.023412
13	h	3.142502	0.245514	0.163945
14	h	2.910189	-1.504068	-0.058684
15	h	2.617495	-0.376479	-1.421633
16	h	-1.301369	1.999724	-0.070565
17	h	0.460722	-2.414148	-0.232445

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.098324	-0.351375	0.027451
2	c	0.455824	1.028081	0.211769
3	n	-0.967260	1.055713	-0.116514
4	c	-1.856851	0.030137	-0.025314
5	n	-1.228751	-1.207270	0.091090
6	c	0.081659	-1.355257	-0.546842
7	o	1.091395	2.124401	0.044795
8	o	-3.099396	0.157794	-0.005715
9	c	2.336495	-0.280384	-0.868086
10	o	1.563792	-0.872555	1.315895
11	h	0.004345	-1.205173	-1.640479
12	h	-1.883717	-1.967434	-0.045970
13	h	3.031674	0.454263	-0.455025
14	h	2.833827	-1.259068	-0.921541
15	h	2.067042	0.041207	-1.882449
16	h	1.103156	-0.321657	1.979090
17	h	-1.365515	1.986796	-0.127649
18	h	0.442227	-2.372373	-0.361686

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.140243	-1.394657	-0.573294
2	c	1.062065	-0.362199	0.059410
3	c	0.441320	1.032979	-0.099285
4	n	-0.923331	1.075228	-0.121757
5	c	-1.793190	-0.001334	-0.034275
6	n	-1.227017	-1.204889	-0.127597
7	c	2.451496	-0.425315	-0.556805

8	o	1.096849	-0.623764	1.443114
9	o	1.092035	2.041609	-0.143458
10	o	-2.980043	0.195915	0.123352
11	h	0.201977	-1.317308	-1.658856
12	h	-1.858047	-1.992504	-0.137487
13	h	3.115817	0.279931	-0.072026
14	h	2.850209	-1.426031	-0.428455
15	h	2.421543	-0.192859	-1.615727
16	h	1.730914	-0.049990	1.882240
17	h	-1.354336	1.986751	-0.106097
18	h	0.462021	-2.387283	-0.276698

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.202780	-1.210126	-0.088372
2	c	0.157782	-1.395723	-0.560435
3	c	1.071223	-0.361808	0.087333
4	c	0.457765	1.037210	-0.067639
5	n	-0.906893	1.075828	-0.098395
6	c	-1.777571	-0.002227	-0.030860
7	c	2.489903	-0.425073	-0.469676
8	o	1.148311	-0.625923	1.459077
9	o	1.112309	2.040755	-0.109650
10	o	-2.966031	0.190602	0.093880
11	h	0.214512	-1.289690	-1.644366
12	h	-1.838674	-1.993413	-0.142284
13	h	3.136850	0.264109	0.056872
14	h	2.872840	-1.432532	-0.357470
15	h	2.485676	-0.160394	-1.520490
16	h	-1.340162	1.987013	-0.097934
17	h	0.485348	-2.392748	-0.285766

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	c	0.195474	-1.361914	-0.687664
2	c	1.054320	-0.362112	0.076586
3	c	0.476278	1.046377	-0.114698
4	n	-0.908279	1.121862	-0.071690
5	c	-1.775321	0.084420	-0.021023
6	n	-1.190249	-1.194590	-0.276346
7	c	2.505729	-0.447274	-0.361025
8	o	0.866834	-0.689925	1.428336
9	o	1.128676	2.034237	-0.224874
10	o	-2.946020	0.139297	0.167837
11	h	0.209020	-1.182087	-1.770625
12	h	-1.839702	-2.008847	-0.230184
13	h	3.106339	0.253332	0.205951
14	h	2.870550	-1.451700	-0.178959
15	h	2.608835	-0.216417	-1.415109
16	h	1.439592	-0.169270	2.003342
17	h	-1.322394	2.046740	-0.026007
18	h	0.482650	-2.388510	-0.475602

2.4 anion

Charge = -1 Multiplicity = 1

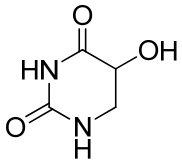
Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.773396	-0.002375	-0.033583
2	n	-1.217785	-1.214128	-0.089069
3	c	0.162917	-1.415277	-0.501620
4	c	1.090778	-0.377472	0.151180
5	c	0.473590	1.011546	-0.074598
6	n	-0.899347	1.064535	-0.087815
7	c	2.456471	-0.448762	-0.539455
8	o	1.172106	-0.533283	1.507096
9	o	1.103972	2.037008	-0.151545
10	o	-2.970105	0.201754	0.064634
11	h	0.232824	-1.374226	-1.589616
12	h	-1.869090	-1.976898	-0.193688
13	h	3.134501	0.268404	-0.093205
14	h	2.869810	-1.443405	-0.396330
15	h	2.397710	-0.250167	-1.606274
16	h	-1.325740	1.976700	-0.081258
17	h	0.469962	-2.403042	-0.174457

2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.097975	-0.338782	0.029215
2	c	0.408650	1.008510	0.272520
3	n	-0.970192	1.032866	-0.220838
4	c	-1.826851	0.012811	-0.027852
5	n	-1.216392	-1.192311	0.140949
6	c	0.086381	-1.363839	-0.494020
7	o	1.038475	2.124713	0.137495
8	o	-3.048294	0.145285	-0.001316
9	c	2.267863	-0.242836	-0.941716
10	o	1.661505	-0.811833	1.254098
11	h	-0.012514	-1.260662	-1.576044
12	h	-1.850888	-1.977653	0.068794
13	h	3.026227	0.420698	-0.547152
14	h	2.710475	-1.223984	-1.097411
15	h	1.941543	0.144146	-1.901274
16	h	1.024839	-0.685537	1.959209
17	h	-1.392723	1.945092	-0.219167
18	h	0.441525	-2.366492	-0.278844

No.17



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.131610	-0.527943	0.378212
2	c	-0.695596	0.898487	0.038494

3	n	0.662657	1.087803	-0.060646
4	c	1.663568	0.090905	0.013695
5	n	1.181037	-1.187792	0.069475
6	c	-0.193791	-1.533889	-0.288465
7	o	-1.511332	1.797212	-0.105501
8	o	2.845161	0.394944	0.039649
9	o	-2.456256	-0.747345	-0.036311
10	h	-0.409740	-2.541914	0.073460
11	h	1.004593	2.036076	-0.184249
12	h	1.900511	-1.897810	0.019724
13	h	-0.354346	-1.516970	-1.375999
14	h	-1.040887	-0.632852	1.473606
15	h	-2.882004	0.129549	-0.102659

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.202250	-1.566709	-0.252331
2	c	-1.214758	-0.547482	0.296112
3	c	-0.761525	0.930534	0.028022
4	n	0.605972	1.067977	-0.136573
5	c	1.615286	0.090863	0.007333
6	n	1.147926	-1.187707	0.151833
7	o	-2.487623	-0.773860	-0.099580
8	o	-1.524736	1.867836	-0.010097
9	o	2.792537	0.410594	0.024291
10	h	-0.430065	-2.554408	0.155110
11	h	0.951847	2.016742	-0.249907
12	h	1.878629	-1.888612	0.134161
13	h	-0.305523	-1.616149	-1.346272
14	h	-1.234107	-0.599260	1.408370

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.861322	0.937103	-0.144892

2	n	-0.453821	1.168056	-0.011839
3	c	-1.513639	0.186001	0.066766
4	n	-1.078408	-1.096455	-0.144397
5	c	0.141054	-1.354747	-0.894974
6	c	1.312056	-0.660745	-0.158930
7	o	-2.626299	0.549022	0.344175
8	o	1.506418	-1.049910	1.128512
9	o	1.763559	1.738130	-0.233735
10	h	0.099971	-0.984277	-1.927284
11	h	-0.768438	2.135809	0.086515
12	h	-1.817952	-1.794670	-0.146738
13	h	0.337324	-2.430863	-0.913414
14	h	2.261165	-0.692798	-0.693970
15	h	0.659366	-1.278018	1.569097

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.271252	-1.521471	-0.281090
2	c	-1.299169	-0.512020	0.330618
3	c	-0.757129	0.927152	0.014346
4	n	0.654237	1.050145	-0.068541
5	c	1.620301	0.052323	0.020312
6	n	1.125180	-1.214253	0.071214
7	o	-2.540648	-0.771052	-0.026555
8	o	-1.419431	1.945472	-0.101117
9	o	2.828434	0.326492	0.055814
10	h	-0.517240	-2.512662	0.108105
11	h	1.020457	1.993871	-0.142803
12	h	1.839844	-1.927735	0.005899
13	h	-0.411607	-1.534980	-1.373358
14	h	-1.090717	-0.552938	1.453188

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	c	-1.123108	-0.504205	0.351511
2	c	-0.728744	0.852469	-0.179016
3	n	0.685032	1.091052	0.029492
4	c	1.658456	0.138134	0.021057
5	n	1.196494	-1.171298	0.011989
6	c	-0.190937	-1.584109	-0.203238
7	o	-1.549940	1.839124	-0.071961
8	o	2.882318	0.385654	0.028755
9	o	-2.475000	-0.774270	-0.011893
10	h	-0.356506	-2.538164	0.319347
11	h	0.998661	2.052497	-0.013665
12	h	1.936413	-1.845002	-0.124417
13	h	-0.421081	-1.730567	-1.268116
14	h	-1.049679	-0.521286	1.466634
15	h	-2.831514	0.126444	-0.171247

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.219674	-1.517043	-0.269438
2	c	-1.145591	-0.491863	0.360477
3	c	-0.673312	0.912856	0.024508
4	n	0.681450	1.062911	-0.083161
5	c	1.632962	0.059764	0.013311
6	n	1.152568	-1.187447	0.076936
7	o	-2.434670	-0.720161	-0.107589
8	o	-1.416984	1.848748	-0.095013
9	o	2.810445	0.346113	0.050675
10	h	-0.443417	-2.503535	0.120024
11	h	1.038542	1.999885	-0.188895
12	h	1.845548	-1.920993	0.050472
13	h	-0.360598	-1.527910	-1.350759
14	h	-1.092314	-0.571672	1.474674
15	h	-3.062521	-0.183912	0.380337

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.129866	-1.179160	0.084377
2	c	-0.229459	-1.540655	-0.277078
3	c	-1.181900	-0.517494	0.327704
4	c	-0.735191	0.904832	0.022256
5	n	0.617841	1.064719	-0.089401
6	c	1.586467	0.077593	0.013697
7	o	-2.482968	-0.737227	-0.045371
8	o	-1.486524	1.833150	-0.080204
9	o	2.757381	0.385388	0.052830
10	h	-0.444866	-2.523025	0.126971
11	h	0.962530	2.007129	-0.190385
12	h	1.838572	-1.898108	0.054671
13	h	-0.352511	-1.571485	-1.360414
14	h	-1.180285	-0.609554	1.466814

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.135051	-1.211477	-0.023059
2	c	-0.260815	-1.534461	-0.254920
3	c	-1.151935	-0.470789	0.388438
4	c	-0.681177	0.927330	0.028866
5	n	0.697774	1.092115	-0.033290
6	c	1.642993	0.126751	0.017497
7	o	-2.477854	-0.683464	0.074640
8	o	-1.402161	1.857351	-0.142593
9	o	2.818730	0.278683	0.060882
10	h	-0.447330	-2.524066	0.152358
11	h	1.044422	2.041480	-0.120216
12	h	1.851735	-1.965644	0.042170
13	h	-0.377671	-1.560487	-1.348114
14	h	-1.054801	-0.542810	1.505275
15	h	-2.650242	-0.526497	-0.859749

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.120265	-1.191810	0.066930
2	c	-0.255732	-1.512396	-0.287762
3	c	-1.228799	-0.510766	0.341927
4	c	-0.731032	0.901312	0.017473
5	n	0.635330	1.050122	-0.080846
6	c	1.590440	0.057657	0.017020
7	o	-2.512222	-0.736705	-0.023508
8	o	-1.434481	1.871941	-0.098287
9	o	2.770009	0.352179	0.064180
10	h	-0.475904	-2.505543	0.086771
11	h	0.989451	1.988444	-0.171459
12	h	1.818658	-1.918429	0.028107
13	h	-0.383818	-1.517750	-1.371281
14	h	-1.073259	-0.569071	1.454247

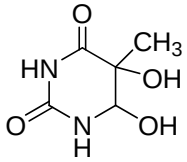
2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.139670	-0.465887	0.316532
2	c	-0.729371	0.881499	-0.234247
3	n	0.703481	1.065653	-0.059175
4	c	1.629767	0.095195	0.009194
5	n	1.170427	-1.175588	0.092472
6	c	-0.206022	-1.551826	-0.189601
7	o	-1.452833	1.919990	0.032077
8	o	2.838421	0.341201	0.037653
9	o	-2.446111	-0.810679	-0.081997
10	h	-0.409403	-2.494492	0.311948
11	h	1.055006	2.003098	-0.146522
12	h	1.881052	-1.889323	0.001653
13	h	-0.364156	-1.694457	-1.259543
14	h	-1.093785	-0.435214	1.429448

15	h	-3.030110	-0.078052	0.116800

No.18



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.152319	-1.339123	0.096503
2	c	1.046169	-0.106376	0.322267
3	c	0.410373	1.144253	-0.328748
4	n	-0.969337	1.138408	-0.407258
5	c	-1.842216	0.145906	0.062596
6	n	-1.226146	-1.032788	0.396345
7	c	2.470474	-0.323927	-0.175907
8	o	1.011339	0.107632	1.740831
9	o	1.065740	2.113968	-0.671712
10	o	-3.042669	0.344754	0.157891
11	o	0.337997	-1.734164	-1.259616
12	h	-1.417504	1.998375	-0.708577
13	h	-1.824918	-1.723524	0.829239
14	h	3.072745	0.567133	0.026094
15	h	2.909593	-1.183195	0.341677
16	h	2.487681	-0.509172	-1.252001
17	h	1.624161	0.830693	1.954451
18	h	0.471504	-2.132572	0.782082
19	h	-0.356858	-2.368999	-1.496000

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	n	-1.217830	-1.074438	0.320957
2	c	0.174090	-1.350347	0.056744
3	c	1.056473	-0.129577	0.452919
4	c	0.425648	1.154938	-0.284516
5	n	-0.944615	1.147291	-0.342043
6	c	-1.824670	0.123664	0.063926
7	o	0.432079	-1.616388	-1.315006
8	c	2.527327	-0.276467	0.048932
9	o	0.883426	0.182996	1.758702
10	o	1.112789	2.054889	-0.704265
11	o	-3.022621	0.329996	0.151065
12	h	-1.396363	1.987226	-0.691786
13	h	-1.815840	-1.777516	0.734958
14	h	3.069261	0.621974	0.349343
15	h	2.952622	-1.141167	0.570153
16	h	2.630226	-0.424974	-1.027871
17	h	0.463365	-2.202918	0.682779
18	h	-0.164743	-2.317797	-1.621968

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.203765	-1.093095	0.335128
2	c	0.149142	-1.338230	-0.093470
3	c	1.095163	-0.199239	0.419963
4	c	0.345251	1.176622	-0.309172
5	n	-0.988009	1.158419	-0.308282
6	c	-1.856448	0.082735	0.108318
7	o	0.327611	-1.340115	-1.482901
8	c	2.541012	-0.303696	-0.010594
9	o	0.874609	-0.010109	1.750519
10	o	1.109289	2.038343	-0.664635
11	o	-3.034676	0.300552	0.229934
12	h	-1.480785	2.000004	-0.612272
13	h	-1.770326	-1.844614	0.714980
14	h	3.130818	0.535032	0.372028
15	h	2.950120	-1.237818	0.393689
16	h	2.627614	-0.329567	-1.097500
17	h	1.655852	0.368467	2.200586

18	h	0.491077	-2.267633	0.379547
19	h	-0.121330	-2.099654	-1.892576

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.250051	-1.018529	0.493597
2	c	0.181015	-1.419179	-0.003176
3	c	1.065398	-0.144418	0.257271
4	c	0.406334	1.139100	-0.274378
5	n	-0.963084	1.159933	-0.258577
6	c	-1.852210	0.114399	0.091150
7	o	0.190370	-1.858181	-1.230763
8	c	2.441150	-0.350422	-0.360364
9	o	1.177372	0.051313	1.691594
10	o	1.047388	2.137637	-0.612426
11	o	-3.070152	0.337871	0.033784
12	h	-1.414013	2.016430	-0.558722
13	h	-1.891618	-1.804398	0.505360
14	h	3.073717	0.535067	-0.221870
15	h	2.912889	-1.218861	0.114622
16	h	2.333183	-0.558618	-1.427878
17	h	1.780365	0.800764	1.828871
18	h	0.487470	-2.146211	0.793950

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.149447	-1.315391	0.085680
2	c	1.045142	-0.087791	0.302084
3	c	0.421449	1.139427	-0.304943
4	n	-0.989395	1.162776	-0.301289
5	c	-1.850849	0.161706	0.076151
6	n	-1.220164	-1.011330	0.432640
7	c	2.466768	-0.312078	-0.212550
8	o	1.119936	0.040756	1.789671

9	o	1.059139	2.142130	-0.735037
10	o	-3.088331	0.307871	0.112445
11	o	0.302308	-1.728689	-1.283085
12	h	-1.420796	2.030551	-0.594994
13	h	-1.849317	-1.796227	0.556223
14	h	3.084962	0.554141	0.043454
15	h	2.888587	-1.208602	0.259175
16	h	2.479527	-0.439420	-1.296997
17	h	1.316824	0.976906	1.963599
18	h	0.472994	-2.141783	0.738585
19	h	-0.042028	-2.647468	-1.338990

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-1.207472	-1.019399	0.422142
2	c	0.151357	-1.325385	0.051307
3	c	1.040801	-0.114429	0.334843
4	c	0.408076	1.124627	-0.315854
5	n	-0.957706	1.142123	-0.339063
6	c	-1.803873	0.135130	0.089558
7	o	0.267734	-1.606951	-1.311817
8	c	2.471873	-0.329121	-0.132305
9	o	0.981014	0.089961	1.724902
10	o	1.046761	2.056990	-0.719909
11	o	-2.996456	0.333365	0.156662
12	h	-1.404923	1.992469	-0.645706
13	h	-1.825552	-1.782420	0.659757
14	h	3.088171	0.510349	0.168190
15	h	2.861199	-1.230557	0.328608
16	h	2.528726	-0.430687	-1.206920
17	h	1.611161	0.763099	1.995310
18	h	0.477828	-2.181731	0.666291
19	h	-0.182185	-2.431439	-1.511074

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.790282	0.133565	0.103933
2	n	-1.185653	-1.024182	0.436221
3	c	0.164253	-1.327371	0.023766
4	c	1.043112	-0.121113	0.356767
5	c	0.421913	1.144794	-0.252997
6	n	-0.943661	1.160016	-0.278611
7	o	0.266751	-1.534710	-1.349959
8	c	2.500207	-0.302967	-0.059492
9	o	1.050037	0.048180	1.743147
10	o	1.066276	2.081690	-0.629489
11	o	-2.983350	0.315776	0.147155
12	h	-1.392338	2.013526	-0.576556
13	h	-1.809153	-1.798984	0.620293
14	h	3.095977	0.527205	0.296777
15	h	2.879300	-1.225545	0.363809
16	h	2.571977	-0.349181	-1.136763
17	h	0.497482	-2.210419	0.598999
18	h	-0.170968	-2.356369	-1.588525

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.821571	0.096985	0.095616
2	n	-1.203844	-1.038106	0.402709
3	c	0.161257	-1.333535	0.026193
4	c	1.050775	-0.132690	0.365113
5	c	0.338894	1.082324	-0.296894
6	n	-0.949145	1.137691	-0.370478
7	o	0.288392	-1.543299	-1.338280
8	c	2.483957	-0.295279	-0.119205
9	o	0.948284	0.094565	1.725508
10	o	1.058173	2.047164	-0.700088
11	o	-2.985369	0.348602	0.178481

12	h	-1.410902	1.976458	-0.724311
13	h	-1.797295	-1.798708	0.716349
14	h	3.089671	0.545704	0.203918
15	h	2.884438	-1.198952	0.325233
16	h	2.534839	-0.379979	-1.195508
17	h	1.661516	0.652587	2.059029
18	h	0.489468	-2.206938	0.626852
19	h	-0.136521	-2.370345	-1.587084

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	-0.958854	1.143497	-0.264938
2	c	-1.801002	0.102010	0.088223
3	n	-1.203891	-1.056959	0.365680
4	c	0.173067	-1.366229	-0.083839
5	c	1.040680	-0.150727	0.301286
6	c	0.405642	1.116262	-0.278851
7	o	-3.000983	0.302217	0.143142
8	o	0.234087	-1.659704	-1.394436
9	c	2.480223	-0.317086	-0.152914
10	o	0.978095	-0.010722	1.707192
11	o	1.034394	2.065894	-0.669179
12	h	-1.409086	2.002519	-0.536502
13	h	-1.832539	-1.837338	0.480574
14	h	3.081660	0.524349	0.174009
15	h	2.884385	-1.223616	0.285972
16	h	2.547664	-0.390886	-1.229248
17	h	1.620671	0.633516	2.010829
18	h	0.490067	-2.201171	0.571984

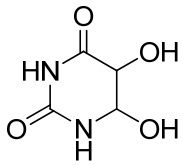
2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	0.142555	-1.324709	0.163598
2	c	1.039923	-0.086119	0.256229

3	c	0.456604	1.044878	-0.573158
4	n	-0.984645	1.136728	-0.390919
5	c	-1.806738	0.178834	0.050468
6	n	-1.221517	-0.974318	0.459794
7	c	2.472885	-0.403229	-0.154771
8	o	1.033242	0.256212	1.643224
9	o	1.061836	2.187989	-0.608485
10	o	-3.028888	0.333831	0.125616
11	o	0.272101	-1.874570	-1.123519
12	h	-1.421035	1.993804	-0.679632
13	h	-1.860054	-1.725401	0.684207
14	h	3.096199	0.467890	0.012298
15	h	2.858849	-1.222887	0.444932
16	h	2.538116	-0.676441	-1.199967
17	h	1.397908	1.137151	1.735861
18	h	0.457851	-2.066478	0.913320
19	h	-0.162423	-2.730138	-1.142024

No.19



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.249414	0.427170	0.144232
2	c	-0.855510	-0.965201	-0.363461
3	n	0.491494	-1.261876	-0.322997
4	c	1.522890	-0.447465	0.171533
5	n	1.137989	0.835567	0.473417
6	c	-0.102580	1.431268	0.035465
7	o	-1.693316	-1.782567	-0.708457
8	o	2.653054	-0.879306	0.328165
9	o	-0.083542	1.822777	-1.335013
10	o	-1.612711	0.333634	1.516971

11	h	0.768754	-2.208513	-0.565068
12	h	1.869942	1.413042	0.866896
13	h	-2.362364	-0.279771	1.593473
14	h	-0.308499	2.287805	0.686612
15	h	0.708176	2.358377	-1.503541
16	h	-2.082583	0.782293	-0.471245

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.141947	1.446739	0.058459
2	c	-1.265481	0.439144	0.388254
3	c	-0.912384	-0.963725	-0.286848
4	n	0.430048	-1.246534	-0.300018
5	c	1.499318	-0.416912	0.096687
6	n	1.145987	0.876294	0.371747
7	o	-1.375387	0.160894	1.702205
8	o	-1.769563	-1.706097	-0.699684
9	o	2.631923	-0.859222	0.174502
10	o	-0.312047	1.754485	-1.317908
11	h	0.704388	-2.168603	-0.626859
12	h	1.899635	1.458051	0.714580
13	h	-0.267146	2.339036	0.681963
14	h	0.365042	2.390825	-1.598597
15	h	-2.210612	0.740419	-0.085415

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.173102	1.423639	-0.105765
2	c	-1.292551	0.426043	0.334716
3	c	-0.796057	-0.995454	-0.312457
4	n	0.517675	-1.235776	-0.275350
5	c	1.546603	-0.319600	0.153736
6	n	1.097105	0.946727	0.387053
7	o	-1.309933	0.268226	1.688804

8	o	-1.689832	-1.722290	-0.697489
9	o	2.671629	-0.731518	0.285891
10	o	-0.295516	1.439661	-1.499506
11	h	0.858609	-2.153728	-0.566165
12	h	1.781138	1.594204	0.767283
13	h	-2.205394	0.086425	2.033956
14	h	-0.381808	2.393986	0.358265
15	h	0.176273	2.193931	-1.893363
16	h	-2.252419	0.668135	-0.124872

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.145553	1.517997	-0.110325
2	c	-1.259483	0.444313	0.045016
3	c	-0.824637	-0.966459	-0.340991
4	n	0.504679	-1.252924	-0.196893
5	c	1.543820	-0.376389	0.210940
6	n	1.134237	0.862747	0.536197
7	o	-1.751843	0.377489	1.402082
8	o	-1.636279	-1.833182	-0.680653
9	o	2.696113	-0.828467	0.270757
10	o	0.043864	1.901636	-1.343047
11	h	0.806577	-2.194665	-0.418916
12	h	1.912306	1.510868	0.600351
13	h	-2.453174	-0.294757	1.414817
14	h	-0.370940	2.316228	0.642022
15	h	-2.066903	0.736972	-0.634359

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.260411	0.376996	0.145022
2	c	-0.853211	-0.969743	-0.349023
3	n	0.523389	-1.267990	-0.227315
4	c	1.531207	-0.431962	0.181046

5	n	1.111931	0.853832	0.465422
6	c	-0.143434	1.404335	0.006313
7	o	-1.647226	-1.850473	-0.791107
8	o	2.715415	-0.800656	0.310085
9	o	-0.124612	1.795234	-1.381235
10	o	-1.644750	0.379757	1.585768
11	h	0.799191	-2.214455	-0.458813
12	h	1.872169	1.503288	0.628553
13	h	-2.123145	-0.455626	1.726434
14	h	-0.348777	2.295373	0.618506
15	h	0.448879	2.590313	-1.443254
16	h	-2.131081	0.711570	-0.426408

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.120254	0.847712	0.446443
2	c	-0.123764	1.419908	-0.014588
3	c	-1.245437	0.425773	0.223657
4	c	-0.863650	-0.935888	-0.344920
5	n	0.463987	-1.249392	-0.268637
6	c	1.479083	-0.416807	0.167589
7	o	-0.110621	1.669276	-1.389505
8	o	-1.427979	0.273929	1.605033
9	o	-1.668997	-1.719325	-0.770089
10	o	2.602341	-0.848521	0.296831
11	h	0.743029	-2.181709	-0.533820
12	h	1.880698	1.472398	0.675128
13	h	-2.339871	0.031304	1.782800
14	h	-0.304629	2.343263	0.561019
15	h	0.463207	2.415700	-1.580196
16	h	-2.167465	0.770013	-0.278155

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.110120	0.825820	0.494216
2	c	-0.110435	1.425008	0.006488
3	c	-1.252612	0.449567	0.238336
4	c	-0.903139	-0.942991	-0.280224
5	n	0.425370	-1.254740	-0.256079
6	c	1.458226	-0.436709	0.173406
7	o	-0.073809	1.657783	-1.369892
8	o	-1.596231	0.361309	1.574768
9	o	-1.730427	-1.730179	-0.645336
10	o	2.578293	-0.878725	0.266476
11	h	0.689812	-2.189824	-0.528412
12	h	1.884492	1.439231	0.710610
13	h	-0.282970	2.357228	0.572369
14	h	0.568932	2.343919	-1.568243
15	h	-2.183539	0.801135	-0.289447

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.103668	0.876553	0.444275
2	c	-0.152281	1.423866	-0.027552
3	c	-1.266424	0.424326	0.244158
4	c	-0.777789	-0.918403	-0.328148
5	n	0.475874	-1.230801	-0.316507
6	c	1.506907	-0.362494	0.176714
7	o	-0.149361	1.620635	-1.402054
8	o	-1.424297	0.216380	1.600698
9	o	-1.655274	-1.732630	-0.749372
10	o	2.597241	-0.827755	0.317619
11	h	0.784560	-2.154069	-0.621903
12	h	1.823043	1.514914	0.766187
13	h	-2.353676	0.073289	1.811643
14	h	-0.349233	2.355757	0.537239
15	h	0.436208	2.348405	-1.633192
16	h	-2.206646	0.724631	-0.280511

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	n	1.106709	0.909598	0.380452
2	c	-0.160303	1.457110	-0.151605
3	c	-1.248052	0.439347	0.189013
4	c	-0.846059	-0.939501	-0.313041
5	n	0.483515	-1.229543	-0.215927
6	c	1.486910	-0.350985	0.164990
7	o	-0.113149	1.696954	-1.480022
8	o	-1.418352	0.347766	1.584090
9	o	-1.633881	-1.758860	-0.713322
10	o	2.622073	-0.769951	0.296552
11	h	0.778652	-2.166636	-0.438300
12	h	1.866616	1.556838	0.525337
13	h	-2.287124	-0.007483	1.780055
14	h	-0.350271	2.364004	0.454393
15	h	-2.187945	0.729789	-0.307683

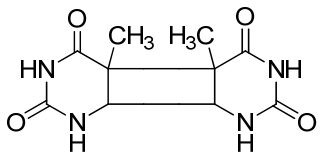
2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.192469	0.528160	0.160537
2	c	-0.960094	-0.751942	-0.600400
3	n	0.359511	-1.294897	-0.320932
4	c	1.424221	-0.610429	0.114557
5	n	1.216322	0.690067	0.442003
6	c	0.030145	1.432525	0.105402
7	o	-1.907726	-1.631703	-0.673105
8	o	2.535219	-1.129019	0.251777
9	o	0.092005	1.974682	-1.191723
10	o	-1.459744	0.296724	1.539855
11	h	0.523901	-2.252977	-0.574248
12	h	2.047344	1.210695	0.690336
13	h	-2.156851	-0.355926	1.608487
14	h	-0.068948	2.247576	0.838029

15	h	0.779538	2.644273	-1.220300
16	h	-2.044665	1.064814	-0.284807

No.20



1. Gas phase

1.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.698706	1.086168	-0.624292
2	c	-0.751223	0.657412	0.481996
3	c	-0.461868	-0.836012	0.277680
4	n	-1.643396	-1.637672	0.501128
5	c	-2.714191	-1.258957	-0.301827
6	n	-2.608871	0.031008	-0.878646
7	c	0.817668	0.843075	0.632687
8	c	0.833059	-0.661323	1.109307
9	n	2.013700	-1.415441	0.771050
10	c	2.765028	-1.187454	-0.351481
11	n	2.438007	-0.011605	-1.048362
12	c	1.556107	1.008186	-0.702102
13	c	1.365608	1.910133	1.585683
14	o	3.663938	-1.919405	-0.735479
15	o	1.444315	1.996117	-1.401968
16	c	-1.482647	1.007237	1.801409
17	o	-3.686208	-1.962996	-0.519503
18	o	-1.808127	2.158864	-1.175618
19	h	0.665824	-0.732367	2.185445
20	h	2.236997	-2.273099	1.259751
21	h	2.992540	0.146805	-1.884812
22	h	-0.120735	-0.973349	-0.761525
23	h	-1.581567	-2.642821	0.624057
24	h	1.185177	2.908228	1.175709
25	h	2.447811	1.784606	1.709529

26	h	0.906116	1.843905	2.575174
27	h	-2.518006	0.657586	1.783408
28	h	-1.494955	2.094737	1.924334
29	h	-1.007316	0.564992	2.680484
30	h	-3.392336	0.265331	-1.481548

1.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.505088	0.992473	-0.726191
2	c	0.783093	0.859824	0.623299
3	c	0.823109	-0.625075	1.149804
4	n	2.013444	-1.370424	0.824592
5	c	2.727838	-1.187084	-0.329189
6	n	2.380667	-0.033615	-1.058095
7	c	-0.786318	0.674790	0.480718
8	c	-1.717696	1.012530	-0.670855
9	n	-2.576472	-0.086715	-0.909985
10	c	-2.634947	-1.336358	-0.247009
11	n	-1.619511	-1.626813	0.688510
12	c	-0.476821	-0.862140	0.353982
13	o	-1.839995	2.057879	-1.267846
14	c	-1.529868	1.098548	1.768584
15	o	-3.526537	-2.132134	-0.489386
16	c	1.323010	1.963443	1.538696
17	o	3.614008	-1.930732	-0.717407
18	o	1.376717	1.963124	-1.447577
19	h	0.665052	-0.665030	2.229410
20	h	2.211154	-2.239125	1.306010
21	h	2.921158	0.101093	-1.907996
22	h	-0.189788	-1.034955	-0.696600
23	h	1.130723	2.946947	1.100139
24	h	2.406940	1.850580	1.658061
25	h	0.872553	1.921236	2.533678
26	h	-2.572782	0.770016	1.755307
27	h	-1.522732	2.191291	1.832685
28	h	-1.071641	0.693334	2.673667
29	h	-3.330011	0.076767	-1.572814

1.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.488662	0.992547	-0.647595
2	c	0.794837	0.741455	0.709379
3	c	0.819447	-0.807484	1.046070
4	n	2.000630	-1.510014	0.622694
5	c	2.825367	-1.111354	-0.389536
6	n	2.478766	0.134165	-1.004734
7	c	-0.740502	0.580755	0.558810
8	c	-1.615162	1.073508	-0.590141
9	n	-2.601775	0.171711	-0.881574
10	c	-2.782796	-1.169159	-0.343465
11	n	-1.719424	-1.652263	0.391276
12	c	-0.495398	-0.906663	0.221050
13	o	-1.461087	2.150836	-1.152346
14	c	-1.506615	0.900264	1.862315
15	o	-3.810464	-1.755022	-0.583365
16	c	1.388976	1.727883	1.718640
17	o	3.787271	-1.723029	-0.796243
18	o	1.179580	1.969114	-1.323790
19	h	0.666037	-0.957672	2.116559
20	h	2.278565	-2.372457	1.078996
21	h	3.035242	0.358363	-1.828716
22	h	-0.170298	-0.977417	-0.829316
23	h	-1.745045	-2.651992	0.571676
24	h	1.185045	2.760643	1.421010
25	h	2.474173	1.597596	1.786153
26	h	0.971415	1.561301	2.715344
27	h	-2.550841	0.586487	1.810001
28	h	-1.479658	1.978788	2.043663
29	h	-1.055758	0.396624	2.721786
30	h	-3.339550	0.448849	-1.527998

1.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z

1	c	1.583853	1.034262	-0.636416
2	c	0.779609	0.834369	0.646869
3	c	0.776498	-0.673062	1.097886
4	n	1.977865	-1.435515	0.785505
5	c	2.721258	-1.210446	-0.332810
6	n	2.472114	0.013122	-0.973587
7	c	-0.787311	0.652207	0.446823
8	c	-1.710155	1.038780	-0.703301
9	n	-2.518995	-0.045236	-0.974935
10	c	-2.635964	-1.359400	-0.234051
11	n	-1.581968	-1.757960	0.467710
12	c	-0.504796	-0.857601	0.259163
13	o	-1.828456	2.137508	-1.243883
14	c	-1.560102	1.007369	1.737251
15	o	-3.740029	-1.910388	-0.396284
16	c	1.290273	1.886483	1.642021
17	o	3.587920	-1.970643	-0.762503
18	o	1.558024	2.053860	-1.306563
19	h	0.595804	-0.758784	2.172588
20	h	2.044756	-2.384889	1.132427
21	h	3.044276	0.180109	-1.794376
22	h	-0.122539	-0.945430	-0.781679
23	h	1.116573	2.893100	1.248730
24	h	2.369046	1.765373	1.807722
25	h	0.791354	1.794450	2.610290
26	h	-2.579253	0.616063	1.682301
27	h	-1.613127	2.096873	1.851060
28	h	-1.105894	0.582615	2.637865
29	h	-3.322765	0.139184	-1.566527

1.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.594494	1.071865	-0.729518
2	c	-0.730780	0.714308	0.455434
3	c	-0.458996	-0.796430	0.351057
4	n	-1.658283	-1.573378	0.605511
5	c	-2.697052	-1.226127	-0.270340
6	n	-2.567030	0.010272	-0.896028

7	c	0.828118	0.889107	0.625513
8	c	0.830160	-0.589156	1.180376
9	n	2.011185	-1.369850	0.883718
10	c	2.629736	-1.293613	-0.354939
11	n	2.383438	-0.126612	-1.046442
12	c	1.567764	0.987032	-0.713334
13	c	1.364200	1.969567	1.568725
14	o	3.383384	-2.183132	-0.782682
15	o	1.689693	2.039348	-1.365833
16	c	-1.498020	1.121117	1.746508
17	o	-3.667999	-1.964522	-0.474386
18	o	-1.744119	2.128402	-1.348878
19	h	0.663418	-0.600864	2.262918
20	h	2.103531	-2.283310	1.310427
21	h	2.903426	-0.026835	-1.910953
22	h	-0.108392	-0.996648	-0.671982
23	h	-1.587120	-2.579667	0.712626
24	h	1.211617	2.960917	1.130764
25	h	2.442139	1.826702	1.714543
26	h	0.883967	1.930725	2.555484
27	h	-2.544869	0.808477	1.694714
28	h	-1.472676	2.211555	1.843885
29	h	-1.071101	0.683082	2.659929
30	h	-3.340611	0.236047	-1.512317

2. Aqueous solution(UAHF)

2.1 neutral molecule

Charge = 0 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.568394	1.003835	-0.665311
2	c	0.808996	0.805433	0.637904
3	c	0.807352	-0.699042	1.061194
4	n	1.980762	-1.443733	0.701384
5	c	2.753213	-1.153825	-0.349550
6	n	2.468678	0.031449	-1.008592
7	c	-0.743967	0.634538	0.466255
8	c	-1.691964	1.078947	-0.616037
9	n	-2.615288	0.065119	-0.859392
10	c	-2.705551	-1.212899	-0.301894

11	n	-1.648740	-1.627717	0.442395
12	c	-0.465299	-0.841751	0.215761
13	o	-1.783852	2.135995	-1.166013
14	c	-1.474235	0.958523	1.792123
15	o	-3.696700	-1.876256	-0.500130
16	c	1.360443	1.831608	1.631742
17	o	3.668841	-1.847501	-0.735768
18	o	1.454415	1.988535	-1.340804
19	h	0.637477	-0.823987	2.145824
20	h	2.178806	-2.313600	1.175242
21	h	3.041235	0.216752	-1.818014
22	h	-0.153523	-0.985292	-0.842504
23	h	-1.587506	-2.630452	0.564269
24	h	1.132037	2.840226	1.307192
25	h	2.440226	1.734870	1.703649
26	h	0.950459	1.678807	2.620407
27	h	-2.513009	0.655380	1.757989
28	h	-1.446026	2.029815	1.958813
29	h	-1.020126	0.466596	2.640513
30	h	-3.403848	0.316687	-1.435354

2.2 radical

Charge = 0 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-0.475603	-0.871523	0.276580
2	c	-0.770378	0.622821	0.464350
3	c	-1.698860	1.025270	-0.648533
4	n	-2.607862	-0.007187	-0.881055
5	c	-2.677942	-1.254914	-0.279563
6	n	-1.624395	-1.668147	0.572761
7	c	0.780140	0.812805	0.639666
8	c	1.533247	0.996179	-0.672644
9	n	2.410301	0.007991	-1.027948
10	c	2.723515	-1.154679	-0.343078
11	n	1.988018	-1.413681	0.742215
12	c	0.806350	-0.681744	1.099129
13	o	1.418175	1.977352	-1.352126
14	c	1.307083	1.874691	1.608352
15	o	3.631385	-1.854463	-0.735514
16	c	-1.516458	0.981954	1.773440

17	o	-1.782497	2.059053	-1.236885
18	o	-3.604798	-1.985223	-0.481764
19	h	0.649653	-0.790836	2.190252
20	h	2.201916	-2.270982	1.232059
21	h	2.966930	0.179742	-1.851500
22	h	-0.202517	-1.091087	-0.791480
23	h	1.073745	2.870028	1.249374
24	h	2.386515	1.789435	1.696096
25	h	0.886781	1.748486	2.596271
26	h	-2.549951	0.656082	1.749293
27	h	-1.515077	2.059047	1.898351
28	h	-1.053543	0.534617	2.641460
29	h	-3.371569	0.203708	-1.507860

2.3 cation radical

Charge = 1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	1.761863	0.618627	1.166911
2	c	0.795017	0.788473	0.037143
3	c	1.040364	-0.254936	-1.053080
4	n	2.252660	-0.905549	-1.040700
5	c	3.169752	-0.903760	-0.044627
6	n	2.813743	-0.097260	1.079141
7	c	-0.684136	0.659717	0.571485
8	c	-0.805474	-0.719041	1.183403
9	n	-2.011236	-1.400856	1.067757
10	c	-2.934591	-1.163214	0.117557
11	n	-2.701492	-0.056060	-0.669760
12	c	-1.701819	0.866612	-0.560010
13	c	-1.042275	1.744946	1.620723
14	o	-1.698504	1.841618	-1.254127
15	o	-3.915242	-1.845065	-0.050104
16	c	1.195601	2.181545	-0.555217
17	o	0.246727	-0.464512	-1.913457
18	o	4.189772	-1.497749	-0.032553
19	h	1.637587	1.171861	2.087267
20	h	3.484256	-0.119235	1.852700
21	h	2.447591	-1.524954	-1.821695
22	h	-0.252582	-0.947914	2.085101
23	h	-2.166354	-2.213580	1.641805

24	h	0.555175	2.407086	-1.391219
25	h	2.227869	2.159281	-0.889498
26	h	1.094191	2.958469	0.191788
27	h	-2.070867	1.601604	1.934751
28	h	-0.950931	2.742058	1.211728
29	h	-0.424793	1.662089	2.507557
30	h	-3.404708	0.133167	-1.369150

2.4 anion

Charge = -1 Multiplicity = 1

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.724789	1.031847	-0.629649
2	c	-0.776968	0.612339	0.464029
3	c	-0.483685	-0.864171	0.201351
4	n	-1.591140	-1.751525	0.381582
5	c	-2.641262	-1.299899	-0.265981
6	n	-2.573580	-0.015242	-0.904339
7	c	0.773142	0.799687	0.639710
8	c	0.784973	-0.705592	1.049048
9	n	1.980314	-1.434117	0.707807
10	c	2.758557	-1.130222	-0.331568
11	n	2.474573	0.060904	-0.979608
12	c	1.540943	1.010279	-0.655337
13	c	1.314566	1.823864	1.641827
14	o	1.417650	1.988263	-1.340850
15	o	3.684651	-1.813381	-0.719055
16	c	-1.518841	0.921795	1.784531
17	o	-3.720214	-1.886659	-0.409679
18	o	-1.849916	2.105726	-1.159468
19	h	0.607733	-0.834381	2.130338
20	h	2.168458	-2.315646	1.162283
21	h	3.048220	0.254498	-1.785506
22	h	-0.139188	-0.942536	-0.848541
23	h	1.094889	2.834480	1.316581
24	h	2.393049	1.724428	1.732445
25	h	0.887907	1.672420	2.623695
26	h	-2.554913	0.610831	1.734759
27	h	-1.502476	1.991192	1.967969
28	h	-1.072383	0.423896	2.634191
29	h	-3.379640	0.209535	-1.461666

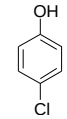
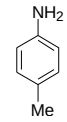
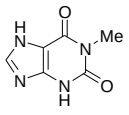
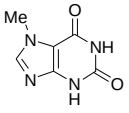
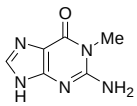
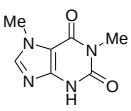
2.5 anion radical

Charge = -1 Multiplicity = 2

Center Number	Atomic Name	Coordinates (Angstroms) X	Y	Z
1	c	-1.731202	1.112243	-0.579886
2	c	-0.771592	0.624151	0.471377
3	c	-0.527385	-0.846637	0.169791
4	n	-1.724027	-1.626170	0.387218
5	c	-2.776665	-1.174211	-0.335730
6	n	-2.671818	0.116695	-0.854062
7	c	0.793980	0.764422	0.593408
8	c	0.771867	-0.759620	0.976648
9	n	1.908267	-1.536695	0.564055
10	c	2.820222	-1.143895	-0.352579
11	n	2.676186	0.091680	-0.851387
12	c	1.501078	0.961887	-0.752939
13	c	1.363563	1.716275	1.644653
14	o	3.756101	-1.883758	-0.672859
15	o	1.702773	2.146953	-1.217651
16	c	-1.488098	0.913008	1.812454
17	o	-3.779385	-1.820700	-0.554021
18	o	-1.831475	2.188292	-1.096621
19	h	0.621780	-0.915246	2.055141
20	h	2.003389	-2.481121	0.905156
21	h	3.345366	0.351688	-1.552022
22	h	-0.232161	-0.954690	-0.888463
23	h	-1.676855	-2.635299	0.472028
24	h	1.150116	2.745811	1.381525
25	h	2.443550	1.604191	1.683656
26	h	0.975827	1.522967	2.638155
27	h	-2.527189	0.606045	1.792168
28	h	-1.461838	1.980015	2.007353
29	h	-1.017797	0.405885	2.643022
30	h	-3.463177	0.399154	-1.412458

Part 2. The evaluation of different theoretical methods

Table S1 Experimental and theoretical redox potentials (vs NHE, V) in aqueous solution for 12 compounds

Molecule	HF//CPCM/UAHF		HF//CPCM/UAKS		HF//CPCM// COSMORS/UAHF		HF//CPCM// COSMORS/UAKS		Expt[a]
	Water[b]	Gas[c]	Water[b]	Gas[c]	Water[b]	Gas[c]	Water[b]	Gas[c]	
	0.65	0.47	0.65	0.47	0.81	0.65	0.81	0.65	0.86[d]
	0.72	0.57	0.72	0.57	0.88	0.77	0.88	0.77	0.93[d]
	0.82	0.67	0.82	0.67	0.94	0.82	0.94	0.82	0.88[d]
	0.66	0.54	0.66	0.54	0.82	0.70	0.82	0.70	0.85[d]
	0.91	0.92	0.84	0.86	0.89	0.90	0.82	0.82	0.87[e]
	0.83	0.84	0.77	0.79	0.80	0.82	0.74	0.73	0.84[e]
	0.86	0.87	0.80	0.80	0.84	0.86	0.78	0.78	0.85[e]
	0.69	0.70	0.63	0.64	0.67	0.69	0.60	0.61	0.78[e]
	0.93	0.93	1.03	0.98	0.65	0.93	1.2	0.93	0.70[d]
	0.89	0.83	0.98	0.91	0.97	0.90	1.08	1.00	0.98[d]
	0.90	0.92	0.96	0.98	1.05	0.77	1.11	0.82	1.06[f]
	1.08	1.09	1.14	1.15	1.23	0.94	1.30	1.00	1.22[f]

[a] from reference 42-43. [b] re-optimized solution geometries used for solvation energy calculations. [c] gas-phase geometries used for solvation energy calculations. [d] pH=12. [e] pH=5.6. [f] pH=7.

Table S2 The evaluation of different theoretical methods (all the gas phase calculations at the B3LYP/6-311++G(2df,2p)//B3LYP/6-31+G(d) level)

Method	*R (correlation coefficient)*	*RMSD (room-mean square deviation)*	*N (compounds number)*
method	0.969	0.04	12
1[a]	0.257	0.15	12
method 2[b]			
method	0.532	0.13	12
3[c]	0.405	0.20	12
method 4[d]			
method	0.570	0.16	12
5[e]	0.505	0.14	12
method 6[f]			
method	0.549	0.15	12
7[g]			
method	0.500	0.20	12
8[h]			

[a] the HF-COSMORS/UAHF for solvation energy calculations at the HF-CPCM/UAHF re-optimized solution geometries in aqueous solution.

[b] the HF-COSMORS/UAHF for solvation energy calculations at the gas optimized geometries in aqueous solution.

[c] the HF-CPCM /UAHF for solvation energy calculations at the HF-CPCM/UAHF re-optimized solution geometries in aqueous solution.

[d] the HF-COSMORS/UAHF for solvation energy calculations at the gas optimized geometries in aqueous solution.

[e] the HF-COSMORS/UAKS for solvation energy calculations at the HF-CPCM/UAKS re-optimized solution geometries in aqueous solution.

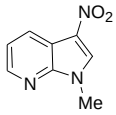
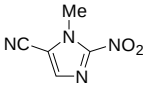
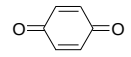
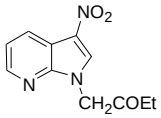
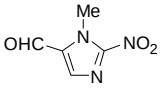
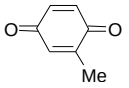
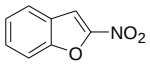
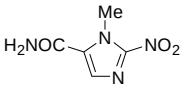
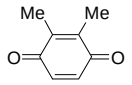
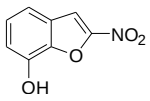
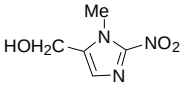
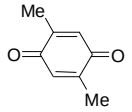
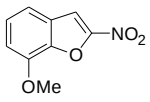
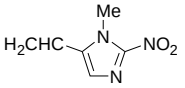
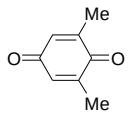
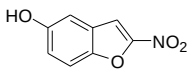
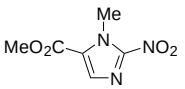
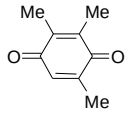
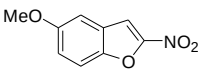
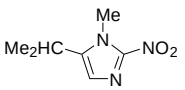
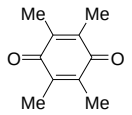
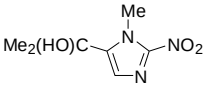
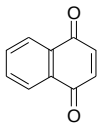
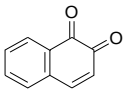
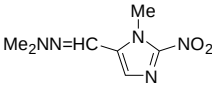
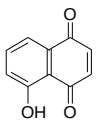
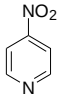
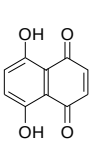
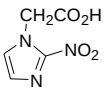
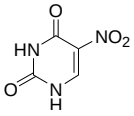
[f] the HF-COSMORS/UAKS for solvation energy calculations at the gas optimized geometries in aqueous solution.

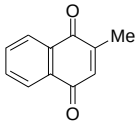
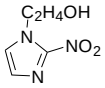
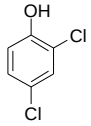
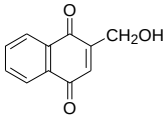
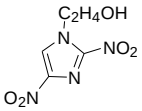
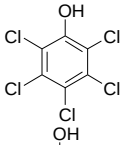
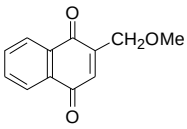
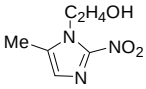
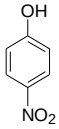
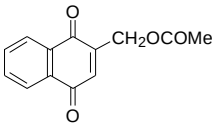
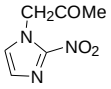
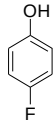
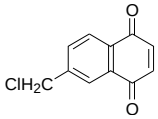
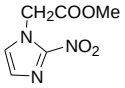
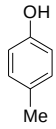
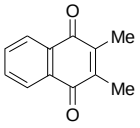
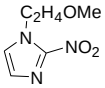
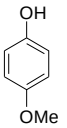
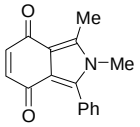
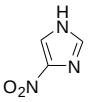
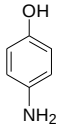
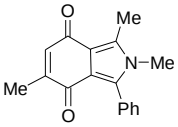
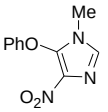
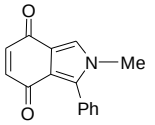
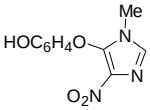
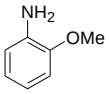
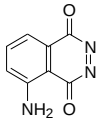
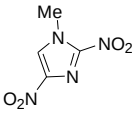
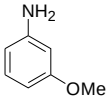
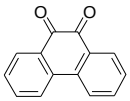
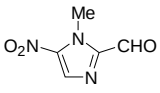
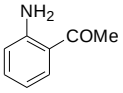
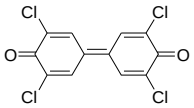
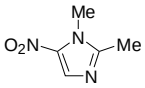
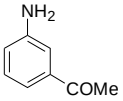
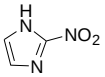
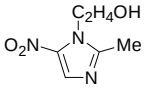
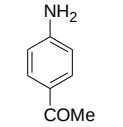
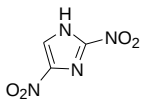
[g] the HF-CPCM /UAKS for solvation energy calculations at the HF-CPCM/UAKS re-optimized solution geometries in aqueous solution.

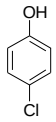
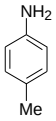
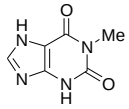
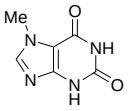
[h] the HF-COSMORS/UAKS for solvation energy calculations at the gas optimized geometries in aqueous solution.

Part 3. Experimental and theoretical redox potentials for 82 compounds

Table S3 Experimental[a] and theoretical redox potentials (vs NHE, V) in aqueous solution for 82 compounds

Molecule	Calc.	Exp.	Molecule	Calc.	Exp.	Molecule	Calc.	Exp.
	-0.735	-0.566		-0.072	-0.267		0.024	0.078
	-0.682	-0.616		-0.110	-0.243		-0.077	0.023
	-0.107	-0.292		-0.119	-0.321		-0.200	-0.074
	-0.118	-0.288		-0.318	-0.400		-0.188	-0.067
	-0.081	-0.296		-0.299	-0.392		-0.176	-0.080
	-0.074	-0.295		-0.105	-0.300		-0.287	-0.165
	-0.081	-0.292		-0.331	-0.439		-0.422	-0.260
	-0.434	-0.412		-0.250	-0.140		-0.010	-0.089
	-0.253	-0.386		-0.168	-0.093		-0.151	-0.191
	-0.212	-0.110		-0.363	-0.447		-0.374	-0.527

	-0.347	-0.206		-0.417	-0.398		0.906	0.88
	-0.228	-0.152		-0.514	-0.238		1.06	0.99
	-0.205	-0.129		-0.476	-0.423		1.30	1.28
	-0.193	-0.100		-0.387	-0.358		0.760	0.80
	-0.185	-0.094		-0.396	-0.355		0.862	0.770
	-0.462	-0.240		-0.385	-0.393		0.564	0.58
	-0.599	-0.440		-0.579	<= -0.527		0.436	0.410
	-0.673	-0.423		-0.644	-0.560		0.632	0.530
	-0.505	-0.419		-0.637	-0.565		0.651	0.74
	0.501	0.240		-0.103	-0.243		0.780	0.86
	-0.077	-0.124		-0.077	-0.360		1.187	1.09
	0.368	0.260		-0.634	-0.480		1.020	1.00
	-0.327	-0.418		-0.613	-0.488		1.064	1.06
	-0.003	-0.265		1.05	1.06		1.23	1.22

	0.81	0.86		0.88	0.93		0.94	0.88
	0.82	0.85		0.89	0.87		0.80	0.84
	0.84	0.85		0.67	0.78		0.65	0.70
	0.97	0.98						

[a] From ref 42, 43, 44.