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羟烷基胺功能化离子液体吸收 SO_2 的量子化学计算

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QuantumChemical Calculation of Hydroxyalkyl Ammonium Functionalized Ionic Liquids for Absorbing SO_2

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Calculation Method for thermodynamic properties of Absorption Reaction

Standard Gibbs free energy Change (ΔG^{Θ}) value can be calculated in kJ mol^{-1} for the absorption reaction of ammonium ionic liquid with SO_2 using the following formula:

$$\Delta G^{T}/\text{kJ mol}^{-1} = G^{T}_{products} - G^{T}_{reactants}$$

$$= [(G^{T}_{corr,\ products} + E_{total,\ products}) - (G^{T}_{corr,\ reactants} + E_{total,\ reactants})]/\text{kJ mol}^{-1}$$

G^{T}_{corr} represents the temperature corrections for the free energy computed from 25 to 1000 K in steps of 25 K, and E_{total} of all the substances have been shown in Table S1. The unit of total energy is Hatree, and E_{total} can be converted from Hartree to kJ mol^{-1} (1 Hartree = 2625.50 kJ mol^{-1}). And the enthalpy and entropy changes are calculated by the similar way.

Table S1 Total Energy of all the Substances

substance	total energy/Ha	substance	total energy/Ha
primary ammonium acetate IL (g)	-439.511069	SO_2 (g)	-548.664311
secondary ammonium acetate IL (g)	-593.358958	primary ammonium acetate IL (l)	-439.541860
tertiary ammonium acetate IL (g)	-747.150469	secondary ammonium acetate IL (l)	-593.363524
$HO(CH_2)_2$-NH_2–SO_2 (g)	-759.079907	tertiary ammonium acetate IL (l)	-747.189592
$(HO(CH_2)_2)_2$-NH–SO_2 (g)	-912.916643	$HO(CH_2)_2$-NH_2-SO_2 +CH_3COOH (l)	-988.241412
$(HO(CH_2)_2)_3$-N–SO_2 (g)	-1066.754881	$(HO(CH_2)_2)_2$-NH–SO_2 +CH_3COOH (l)	-1142.044597
CH_3COOH (g)	-229.108725	$(HO(CH_2)_2)_3$-N–SO_2 +CH_3COOH (l)	-1295.879274

Minimum Energy Structures on MEP–2 and MEP–3

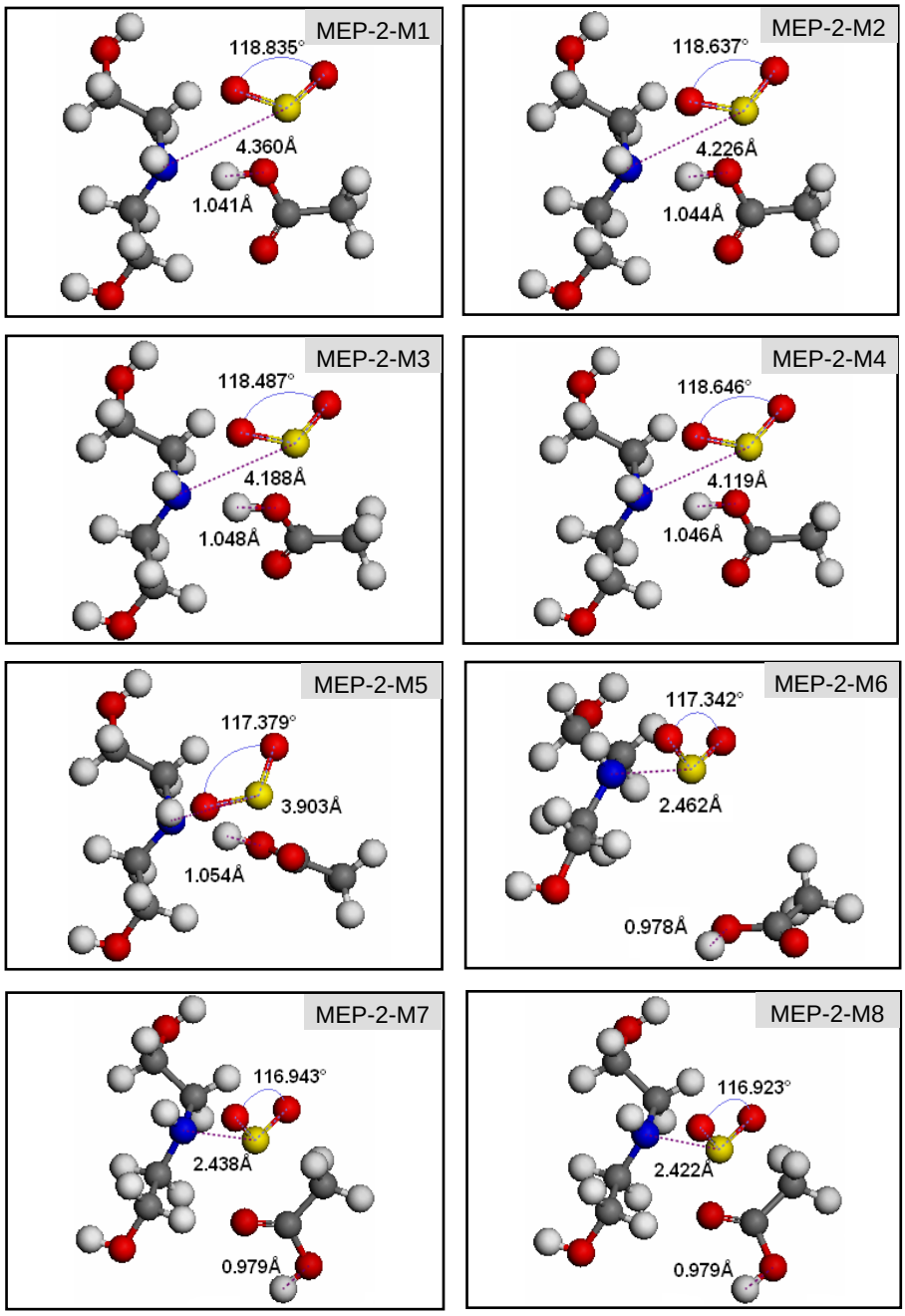

Fig.S1 Structures of minimum points on MEP–2

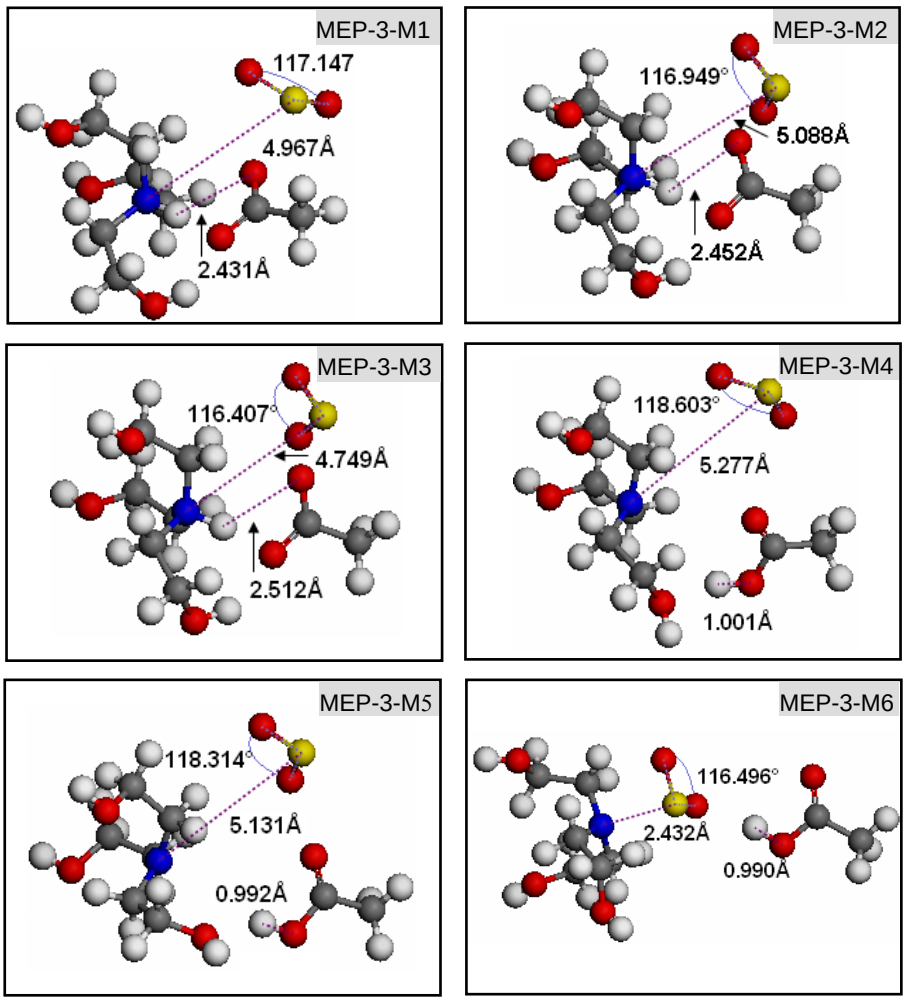

Fig.S2 Structures of minimum points on MEP–3

Geometry Characterization & Thermodynamic Properties

(1) 2-hydroxyethyl ammonium acetate ionic liquid of liquid state model

** GEOMETRY OPTIMIZATION IN DELOCALIZED COORDINATES **

Searching for a Minimum

Note: One or more atoms were translated into the central cell

Input Coordinates (Angstroms)

	ATOM	X	Y	Z
1	H	0.132114	4.264337	3.991228
2	N	5.182810	3.697715	5.161560
3	H	4.320870	4.250978	5.139635
4	C	4.853547	2.253310	5.269130
5	C	3.699357	1.842400	4.374226
6	O	3.475392	0.439700	4.583208
7	H	2.673923	0.178299	4.099882

8	H	2.792927	2.422839	4.651566
9	H	3.938447	2.063221	3.317910
10	H	5.752263	1.679562	4.983821
11	H	4.601859	1.980204	6.306655
12	H	5.630418	3.960039	6.050854
13	C	0.759415	4.649605	2.111406
14	C	1.833711	5.397357	1.363735
15	O	0.874286	4.778586	3.432638
16	O	5.890948	3.972590	1.554195
17	H	1.933345	6.423860	1.734345
18	H	1.620231	5.420231	0.290743
19	H	2.807805	4.905811	1.516945

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-439.541858Ha	-3.0041013Ha	3.84E-04	113.2m	1
Ef	-439.541860Ha	-3.0041031Ha	3.94E-05	113.3m	2
Ef	-439.541860Ha	-3.0041036Ha	6.50E-05	113.4m	3
Ef	-439.541860Ha	-3.0041030Ha	1.38E-05	113.6m	4
Ef	-439.541860Ha	-3.0041031Ha	4.38E-06	113.7m	5

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	H	0.249659	-4.490487	-5.006587	-0.000091	0.000011	0.000398
df	N	-1.544265	-5.561247	-2.794980	0.000087	0.000092	-0.000462
df	H	-3.173096	-4.515731	-2.836413	0.000012	0.000037	0.000460
df	C	-2.166482	4.258139	-2.591703	-0.000683	-0.000409	0.000656
df	C	-4.347585	3.481632	-4.282827	0.000612	0.000860	-0.000299
df	O	-4.770818	0.830913	-3.887907	-0.000046	-0.000215	-0.000153
df	H	5.052981	0.336936	-4.801262	-0.000059	0.000167	0.000159
df	H	5.277868	4.578502	-3.758729	-0.000176	-0.000087	0.000352
df	H	-3.895770	3.898922	6.269940	-0.000045	-0.000056	0.000234
df	H	-0.468155	3.173912	-3.130858	0.000128	0.000173	-0.000155
df	H	-2.642104	3.742043	-0.631064	-0.000097	0.000098	-0.000085
df	H	-0.698408	-5.065526	-1.114458	0.000558	-0.000064	-0.000270
df	C	1.435086	-3.762436	3.989979	0.000119	0.000151	-0.000719
df	C	3.465212	-2.349388	2.577085	-0.000164	0.000272	0.001979
df	O	1.652162	-3.518697	-6.062170	-0.000031	-0.000323	0.000102
df	O	-0.206078	-5.041808	2.937003	-0.000040	-0.000022	-0.000141
df	H	3.653492	-0.409579	3.277437	-0.000267	-0.000053	-0.000465
df	H	3.061792	-2.306163	0.549424	0.000520	-0.000397	-0.000423
df	H	5.305982	-3.278276	2.856611	-0.000338	-0.000236	-0.001167

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T (K)	Entropy S	Heat_Capacity (cal/mol.K) Cp	Enthalpy H	Free_Energy (kcal/mol) G
				(ZPVE is included)	
1	25.00	1.107	3.201	98.788	98.760
2	50.00	5.284	9.268	98.947	98.683
3	75.00	9.893	13.498	99.235	98.493
4	100.00	14.223	16.627	99.613	98.191
5	125.00	18.218	19.220	100.062	97.785
6	150.00	21.929	21.516	100.572	97.283
7	175.00	25.407	23.651	101.137	96.690
8	200.00	28.701	25.726	101.754	96.014
9	225.00	31.851	27.809	102.423	95.257
10	250.00	34.891	29.935	103.145	94.422
11	275.00	37.846	32.114	103.920	93.513
12	298.15	40.523	34.170	104.687	92.605
13	300.00	40.735	34.335	104.751	92.530
14	325.00	43.572	36.581	105.637	91.476
15	350.00	46.365	38.828	106.580	90.352
16	375.00	49.120	41.054	107.578	89.158
17	400.00	51.840	43.240	108.632	87.896
18	425.00	54.525	45.372	109.740	86.567
19	450.00	57.177	47.440	110.900	85.170
20	475.00	59.796	49.436	112.111	83.708
21	500.00	62.381	51.357	113.371	82.181
22	525.00	64.932	53.202	114.679	80.589
23	550.00	67.448	54.971	116.031	78.935
24	575.00	69.929	56.666	117.427	77.217
25	600.00	72.375	58.290	118.864	75.438
26	625.00	74.787	59.845	120.340	73.599
27	650.00	77.163	61.334	121.855	71.699
28	675.00	79.505	62.761	123.407	69.741
29	700.00	81.812	64.129	124.993	67.724
30	725.00	84.086	65.440	126.613	65.651
31	750.00	86.325	66.699	128.264	63.520
32	775.00	88.532	67.908	129.947	61.335
33	800.00	90.707	69.069	131.659	59.094
34	825.00	92.849	70.185	133.400	56.800

35	850.00	94.961	71.257	135.168	54.452
36	875.00	97.041	72.289	136.963	52.052
37	900.00	99.092	73.281	138.782	49.600
38	925.00	101.113	74.237	140.627	47.097
39	950.00	103.105	75.156	142.494	44.545
40	975.00	105.068	76.042	144.384	41.942
41	1000.00	107.004	76.894	146.296	39.291

$HO(CH_2)_2$-NH_2-SO_2 +CH_3COOH (l)

** GEOMETRY OPTIMIZATION IN DELOCALIZED COORDINATES **
Searching for a Minimum
Note: One or more atoms were translated into the central cell

Input Coordinates (Angstroms)

	ATOM	X	Y	Z
1	H	0.797596	3.758200	6.129745
2	N	1.730052	3.396750	5.816567
3	H	2.269989	3.182939	6.658420
4	C	1.606115	2.213508	4.936692
5	C	0.398371	1.355266	5.314139
6	O	0.454299	0.935957	6.674031
7	H	1.070836	0.171612	6.679244
8	S	2.611028	5.098229	4.906522
9	O	2.520051	6.012629	6.126822
10	O	1.561473	5.385320	3.886065
11	H	5.614076	1.946871	5.194759
12	H	0.345057	0.496769	4.629723
13	H	1.511243	2.566640	3.900930
14	H	2.532654	1.626540	5.023215
15	C	4.985860	4.381215	0.659784
16	C	5.676721	3.655270	1.770577
17	O	5.383349	4.409257	6.733028
18	O	3.874221	5.023388	1.041365
19	H	5.024344	3.541338	2.639969
20	H	0.408247	4.245541	2.081465
21	H	6.023998	2.681913	1.405436
22	H	3.491472	5.485528	0.237249

Total Energy	Binding E	Cnvgnce	Time	Iter

Ef		-988.241406Ha	-3.4770371Ha	9.00E-04	238.1m	1
Ef		-988.241408Ha	-3.4770387Ha	4.50E-04	238.3m	2
Ef		-988.241426Ha	-3.4770565Ha	7.60E-04	238.5m	3
Ef		-988.241414Ha	-3.4770448Ha	1.52E-04	238.7m	4
Ef		-988.241412Ha	-3.4770428Ha	2.68E-05	238.9m	5
Ef		-988.241412Ha	-3.4770428Ha	1.61E-05	239.1m	6
Ef		-988.241412Ha	-3.4770430Ha	6.48E-06	239.3m	7

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	H	1.507238	-6.013864	-2.099212	-0.000123	-0.000117	0.000324
df	N	3.269325	6.418927	-2.691033	0.000158	0.000225	-0.000659
df	H	4.289658	6.014882	-1.100160	-0.000208	0.000004	0.000189
df	C	3.035117	4.182924	-4.353756	0.000730	-0.000108	-0.000258
df	C	0.752813	2.561082	-3.640484	-0.000091	-0.000338	0.000001
df	O	0.858501	1.768702	-1.070661	0.000100	0.000105	-0.000034
df	H	2.023586	0.324299	-1.060808	0.000052	-0.000088	-0.000036
df	S	4.934127	-3.481577	-4.410768	-0.000188	0.000152	0.000141
df	O	4.762207	-1.753612	-2.104736	-0.000112	-0.000011	-0.000216
df	O	2.950757	-2.939054	-6.339153	-0.000263	-0.000179	-0.000155
df	H	-0.994986	3.679053	-3.866080	-0.000008	-0.000083	-0.000062
df	H	0.652063	0.938758	-4.933843	0.000163	0.000025	-0.000015
df	H	2.855835	4.850246	-6.311061	-0.000210	0.000150	0.000071
df	H	4.786022	3.073715	-4.190250	-0.000094	-0.000031	0.000261
df	C	-2.182142	-4.836538	1.246811	0.000015	-0.000020	-0.000204
df	C	-0.876604	-6.208374	3.345906	-0.000058	-0.000039	0.000079
df	O	-1.430997	-4.783546	-0.959172	0.000041	0.000047	0.000146
df	O	-4.282836	-3.623005	1.967896	0.000839	-0.001364	0.002528
df	H	-2.109418	-6.423674	4.988818	0.000104	0.000196	0.000091
df	H	0.771475	-5.092923	3.933399	0.000047	0.000114	0.000032
df	H	-0.220346	5.068080	2.655889	-0.000122	0.000059	0.000136
df	H	-5.006126	-2.749688	0.438336	-0.000773	0.001298	-0.002358

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T (K)	Entropy S	Heat_Capacity (cal/mol.K) Cp	Enthalpy H	Free_Energy (kcal/mol) G
				(ZPVE is included)	
1	25.00	1.156	3.598	106.554	106.525
2	50.00	6.271	11.865	106.750	106.437
3	75.00	12.296	17.890	107.127	106.205

4	100.00	18.065	22.227	107.631	105.824
5	125.00	23.410	25.717	108.231	105.305
6	150.00	28.375	28.790	108.913	104.657
7	175.00	33.030	31.665	109.669	103.889
8	200.00	37.441	34.460	110.496	103.008
9	225.00	41.661	37.241	111.392	102.018
10	250.00	45.729	40.034	112.358	100.926
11	275.00	49.676	42.839	113.394	99.733
12	298.15	53.242	45.435	114.416	98.542
13	300.00	53.524	45.642	114.500	98.443
14	325.00	57.287	48.420	115.676	97.058
15	350.00	60.976	51.150	116.921	95.579
16	375.00	64.596	53.812	118.233	94.009
17	400.00	68.151	56.388	119.610	92.350
18	425.00	71.645	58.868	121.051	90.602
19	450.00	75.077	61.246	122.553	88.768
20	475.00	78.450	63.517	124.113	86.849
21	500.00	81.764	65.682	125.728	84.846
22	525.00	85.019	67.744	127.396	82.761
23	550.00	88.216	69.706	129.114	80.596
24	575.00	91.356	71.573	130.880	78.351
25	600.00	94.440	73.350	132.692	76.028
26	625.00	97.469	75.042	134.547	73.629
27	650.00	100.444	76.656	136.444	71.155
28	675.00	103.366	78.195	138.379	68.608
29	700.00	106.236	79.666	140.353	65.987
30	725.00	109.057	81.071	142.362	63.296
31	750.00	111.828	82.416	144.406	60.535
32	775.00	114.551	83.705	146.483	57.705
33	800.00	117.229	84.940	148.591	54.808
34	825.00	119.861	86.124	150.729	51.844
35	850.00	122.449	87.262	152.897	48.815
36	875.00	124.994	88.354	155.092	45.722
37	900.00	127.498	89.404	157.314	42.566
38	925.00	129.961	90.414	159.562	39.348
39	950.00	132.385	91.385	161.834	36.068
40	975.00	134.771	92.320	164.131	32.729
41	1000.00	137.120	93.220	166.450	29.330

(2) di(2-hydroxyethyl) ammonium acetate ionic liquid of liquid state model

** GEOMETRY OPTIMIZATION IN DELOCALIZED COORDINATES **

Searching for a Minimum

Note: One or more atoms were translated into the central cell

Input Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	6.694655	4.056077	4.411331
2	N	7.454150	5.151536	5.038247
3	C	7.285621	2.687416	4.744617
4	O	6.581491	1.634837	4.088823
5	C	6.786336	6.459232	4.890371
6	C	7.439858	7.547774	5.739149
7	O	8.729365	7.925808	5.307368
8	H	6.717199	4.198745	3.322841
9	H	5.630891	4.084831	4.722716
10	H	7.557009	4.954170	6.038655
11	H	7.302312	2.535299	5.839849
12	H	8.321387	2.628633	4.390497
13	H	5.680049	1.611503	4.448811
14	H	5.716319	6.382483	5.167087
15	H	6.840515	6.749265	3.832693
16	H	7.436039	7.230432	6.801800
17	H	6.808967	8.445725	5.669526
18	H	9.380231	7.230034	5.561172
19	H	8.954257	5.124356	4.380359
20	C	0.877859	5.428669	4.576980
21	C	2.210857	5.131275	3.944054
22	O	0.757098	6.051953	5.635645
23	O	9.855080	4.947066	3.875915
24	H	3.013617	5.615551	4.506883
25	H	2.215430	5.476441	2.903279
26	H	2.374878	4.045990	3.914556

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-593.363523Ha	-4.1232742Ha	3.37E-04	286.9m	1
Ef	-593.363524Ha	-4.1232757Ha	2.06E-05	287.1m	2
Ef	-593.363524Ha	-4.1232759Ha	5.55E-05	287.3m	3
Ef	-593.363524Ha	-4.1232757Ha	5.43E-06	287.5m	4

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	C	-6.246196	7.664874	8.336207	-0.000125	0.000255	0.000103
df	N	-4.810959	-9.162270	-9.376355	-0.000020	0.000356	-0.000224
df	C	-5.129433	5.078479	8.966027	-0.000373	-0.000016	-0.000081
df	O	-6.460046	3.089395	7.726755	0.000267	-0.000126	-0.000147

df	C	-6.072945	-6.691082	9.241462	0.000009	-0.000664	-0.000026
df	C	-4.837968	-4.634035	-8.051841	-0.000492	0.000138	0.000228
df	O	-2.401152	-3.919655	-8.867790	-0.000085	-0.000042	-0.000166
df	H	-6.203595	7.934478	6.279260	0.000138	-0.000264	0.000062
df	H	-8.256419	7.719212	8.924639	0.000011	-0.000051	0.000177
df	H	-4.616583	9.362025	-7.485858	-0.000002	-0.000047	0.000060
df	H	-5.097892	4.791021	-7.861546	-0.000014	-0.000253	0.000045
df	H	-3.172120	4.967397	8.296838	0.000114	0.000102	0.000200
df	H	-8.163525	3.045299	8.407035	-0.000041	0.000034	-0.000196
df	H	-8.094984	-6.836117	-9.132882	-0.000173	0.000153	0.000050
df	H	-5.970562	-6.143000	7.242740	0.000211	-0.000033	0.000205
df	H	-4.845185	-5.233724	-6.043722	0.000097	-0.000251	0.000234
df	H	-6.030178	-2.937155	-8.183410	0.000092	-0.000042	-0.000134
df	H	-1.171193	-5.234477	-8.388169	0.000027	0.000040	0.000259
df	H	-1.976168	-9.213633	8.277678	-0.000415	0.000257	0.000109
df	C	1.658914	-8.638563	8.649239	0.000285	0.000400	-0.000172
df	C	4.177913	-9.200557	7.453181	-0.000066	0.000716	0.000876
df	O	1.430708	-7.460727	-8.247435	0.000227	-0.000070	0.000112
df	O	-0.273859	9.348599	7.324417	0.000272	-0.000022	-0.000335
df	H	5.694911	-8.285409	8.516774	-0.000062	0.000189	-0.000125
df	H	4.186556	-8.548287	5.486403	0.000088	-0.000598	-0.000339
df	H	4.487868	7.645813	7.387439	0.000031	-0.000162	-0.000776

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T (K)	Entropy S	Heat_Capacity (cal/mol.K) Cp	Enthalpy H	Free_Energy (kcal/mol) G
					(ZPVE is included)
1	25.00	3.229	5.806	137.322	137.242
2	50.00	9.388	12.489	137.554	137.085
3	75.00	15.462	17.569	137.933	136.773
4	100.00	21.075	21.499	138.423	136.315
5	125.00	26.233	24.766	139.002	135.723
6	150.00	31.009	27.669	139.658	135.007
7	175.00	35.481	30.418	140.385	134.175
8	200.00	39.721	33.159	141.179	133.235
9	225.00	43.789	35.982	142.043	132.191
10	250.00	47.731	38.924	142.979	131.047
11	275.00	51.583	41.982	143.990	129.805
12	298.15	55.092	44.895	144.996	128.570
13	300.00	55.371	45.130	145.079	128.468

14	325.00	59.109	48.330	146.247	127.037
15	350.00	62.808	51.542	147.496	125.513
16	375.00	66.473	54.729	148.824	123.897
17	400.00	70.106	57.861	150.232	122.189
18	425.00	73.706	60.914	151.717	120.392
19	450.00	77.272	63.872	153.277	118.504
20	475.00	80.802	66.725	154.909	116.528
21	500.00	84.295	69.467	156.612	114.465
22	525.00	87.748	72.096	158.382	112.314
23	550.00	91.161	74.615	160.216	110.077
24	575.00	94.531	77.024	162.112	107.756
25	600.00	97.858	79.329	164.066	105.351
26	625.00	101.141	81.534	166.077	102.864
27	650.00	104.381	83.644	168.142	100.295
28	675.00	107.576	85.663	170.259	97.645
29	700.00	110.726	87.597	172.424	94.916
30	725.00	113.833	89.450	174.638	92.109
31	750.00	116.895	91.227	176.896	89.225
32	775.00	119.915	92.932	179.198	86.265
33	800.00	122.891	94.568	181.542	83.230
34	825.00	125.825	96.139	183.926	80.121
35	850.00	128.718	97.649	186.349	76.939
36	875.00	131.569	99.100	188.808	73.685
37	900.00	134.381	100.495	191.303	70.360
38	925.00	137.153	101.837	193.833	66.966
39	950.00	139.886	103.128	196.395	63.503
40	975.00	142.581	104.371	198.989	59.972
41	1000.00	145.238	105.568	201.613	56.374

$(HO(CH_2)_2)_2$-NH–SO_2 +CH_3COOH (l)

** GEOMETRY OPTIMIZATION IN DELOCALIZED COORDINATES **

Searching for a Minimum

Note: One or more atoms were translated into the central cell

Input Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	6.529018	3.845971	1.752715
2	N	6.479789	4.927928	2.748137
3	C	5.810916	2.588903	2.252847
4	O	5.819382	1.546957	1.276843
5	C	7.171429	6.183033	2.418089
6	C	6.234520	7.308592	1.976453
7	O	7.044363	8.459820	1.777431

8	H	7.581308	3.611529	1.553195
9	H	6.082978	4.168950	0.796464
10	H	5.519684	5.099143	3.059355
11	H	4.781177	2.841951	2.555988
12	H	6.321502	2.192726	3.136760
13	H	5.188106	1.799201	0.575489
14	H	7.908721	5.982655	1.633433
15	H	7.715772	6.518588	3.313971
16	H	5.481317	7.473010	2.767853
17	H	5.698704	7.022130	1.053130
18	H	6.483905	9.234837	1.591189
19	S	7.120226	4.237326	4.944298
20	O	7.929599	5.446306	5.269007
21	O	5.717686	4.199341	5.471370
22	C	2.777135	3.333056	9.000003
23	C	3.730151	4.195538	8.236396
24	H	3.171629	4.944866	7.673517
25	H	4.423761	4.693608	8.924250
26	H	4.338046	3.599803	7.546040
27	O	1.570030	3.430713	9.040062
28	O	3.430585	2.338165	9.713599
29	H	2.715363	1.831935	0.150440

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-1142.044590Ha	-4.5715625Ha	6.00E-04	487.6m	1
Ef	-1142.044599Ha	-4.5715715Ha	2.99E-04	487.9m	2
Ef	-1142.044601Ha	-4.5715734Ha	5.03E-04	488.2m	3
Ef	-1142.044595Ha	-4.5715675Ha	1.12E-04	488.5m	4
Ef	-1142.044597Ha	-4.5715692Ha	1.32E-05	488.7m	5
Ef	-1142.044597Ha	-4.5715692Ha	1.28E-05	489.0m	6
Ef	-1142.044597Ha	-4.5715692Ha	3.34E-06	489.4m	7

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	C	-6.559206	7.267831	3.312152	-0.000024	0.000116	0.000008
df	N	-6.652234	9.312434	5.193226	0.000095	-0.000090	0.000077
df	C	-7.916221	4.892317	4.257264	0.000058	0.000075	0.000070
df	O	-7.900223	2.923325	2.412884	0.000069	-0.000068	-0.000046
df	C	-5.345224	-7.213023	4.569525	0.000168	-0.000020	0.000001
df	C	-7.115726	-5.086024	3.734954	-0.000094	-0.000177	0.000018
df	O	-5.585345	-2.910518	3.358857	0.000033	0.000065	0.000158
df	H	-4.570665	6.824801	2.935114	0.000005	-0.000086	-0.000034

df	H	-7.402098	7.878174	1.505099	-0.000071	-0.000013	-0.000038
df	H	-8.466570	-9.261278	5.781343	0.000038	-0.000026	-0.000043
df	H	9.035115	5.370508	4.830117	0.000035	-0.000052	-0.000009
df	H	-6.951353	4.143652	5.927618	0.000060	-0.000019	-0.000016
df	H	-9.093162	3.399997	1.087517	-0.000048	-0.000010	0.000023
df	H	-3.951945	-7.591682	3.086742	-0.000095	-0.000025	-0.000168
df	H	-4.316565	-6.578916	6.262497	0.000084	-0.000016	-0.000069
df	H	-8.539074	-4.775319	5.230485	0.000073	-0.000021	0.000107
df	H	-8.128271	-5.627359	1.990127	0.000004	0.000060	0.000003
df	H	-6.644457	-1.445949	3.006912	-0.000005	-0.000044	-0.000106
df	S	-5.441984	8.007385	9.343369	-0.000023	0.000088	0.000086
df	O	-3.912492	-8.605235	-8.940282	-0.000107	0.000150	0.000095
df	O	-8.092401	7.935604	-8.557870	-0.000034	0.000032	-0.000028
df	C	5.248024	6.298563	-1.889721	-0.000677	-0.000249	0.000069
df	C	7.048964	7.928417	-3.332728	0.000486	0.000164	-0.000067
df	H	5.993511	9.344442	-4.396416	-0.000061	-0.000084	-0.000081
df	H	8.359696	8.869634	-2.032874	-0.000251	0.000098	0.000002
df	H	8.197719	6.802642	-4.637312	-0.000147	-0.000050	-0.000016
df	O	2.966927	6.483108	-1.814021	0.000198	0.000159	0.000160
df	O	6.482866	4.418491	-0.541219	-0.001114	-0.001219	0.001021
df	H	5.131293	3.461856	0.274290	0.001346	0.001262	-0.001178

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T (K)	Entropy S (cal/mol.K)	Heat_Capacity Cp	Enthalpy H (kcal/mol)	Free_Energy G
				(ZPVE is included)	
1	25.00	11.653	14.022	141.890	141.599
2	50.00	24.180	22.192	142.353	141.144
3	75.00	34.169	27.117	142.973	140.411
4	100.00	42.512	30.985	143.701	139.450
5	125.00	49.810	34.521	144.520	138.294
6	150.00	56.405	37.916	145.426	136.965
7	175.00	62.500	41.247	146.415	135.478
8	200.00	68.226	44.582	147.488	133.843
9	225.00	73.671	47.968	148.645	132.069
10	250.00	78.904	51.427	149.887	130.161
11	275.00	83.970	54.951	151.217	128.125
12	298.15	88.543	58.247	152.527	126.128
13	300.00	88.904	58.511	152.635	125.964
14	325.00	93.728	62.071	154.142	123.681

15	350.00	98.457	65.594	155.738	121.278
16	375.00	103.101	69.046	157.421	118.759
17	400.00	107.665	72.401	159.190	116.124
18	425.00	112.152	75.639	161.040	113.376
19	450.00	116.564	78.749	162.971	110.517
20	475.00	120.902	81.725	164.977	107.548
21	500.00	125.167	84.565	167.056	104.472
22	525.00	129.359	87.271	169.204	101.291
23	550.00	133.478	89.846	171.418	98.005
24	575.00	137.527	92.298	173.695	94.617
25	600.00	141.505	94.631	176.032	91.129
26	625.00	145.413	96.854	178.426	87.543
27	650.00	149.253	98.974	180.874	83.859
28	675.00	153.027	100.996	183.374	80.081
29	700.00	156.735	102.927	185.923	76.208
30	725.00	160.379	104.774	188.519	72.244
31	750.00	163.961	106.542	191.161	68.190
32	775.00	167.483	108.235	193.846	64.047
33	800.00	170.945	109.858	196.572	59.816
34	825.00	174.349	111.416	199.338	55.500
35	850.00	177.698	112.912	202.142	51.099
36	875.00	180.992	114.349	204.983	46.616
37	900.00	184.233	115.732	207.859	42.050
38	925.00	187.422	117.061	210.769	37.404
39	950.00	190.561	118.341	213.712	32.679
40	975.00	193.651	119.573	216.686	27.877
41	1000.00	196.693	120.760	219.690	22.997

(3) tri(2-hydroxyethyl) ammonium acetate ionic liquid of liquid state model

** GEOMETRY OPTIMIZATION IN DELOCALIZED COORDINATES **

Searching for a Minimum

Note: One or more atoms were translated into the central cell

Input Coordinates (Angstroms)

	ATOM	X	Y	Z
1	N	7.850167	4.544242	5.147745
2	C	6.999984	3.909423	6.200540
3	C	7.823333	3.213624	7.281087
4	O	8.628297	2.143242	6.781930
5	H	9.473500	2.543121	6.506094
6	H	8.445450	3.947840	7.819133
7	H	7.126201	2.776952	8.011071
8	H	6.373903	4.678394	6.669646

9	H	6.325152	3.185026	5.728941
10	C	7.875357	3.802156	3.864639
11	C	6.741563	4.013206	2.872872
12	O	5.489666	3.603420	3.442174
13	H	4.813425	3.666978	2.749379
14	H	6.701368	5.069505	2.555391
15	H	6.978825	3.414127	1.977958
16	H	7.943768	2.739309	4.126987
17	H	8.810044	4.078977	3.351837
18	C	7.702690	6.009530	5.015500
19	C	6.296942	6.598225	4.883015
20	O	5.761231	6.810198	6.202629
21	H	8.163915	6.477421	5.897527
22	H	8.313348	6.306155	4.152338
23	H	6.375695	7.561653	4.351331
24	H	5.640676	5.931279	4.305607
25	H	4.854805	7.139812	6.098960
26	H	9.361639	4.447916	5.552246
27	C	1.275524	4.727914	5.039103
28	C	2.678245	4.668603	5.591919
29	O	1.006191	5.130726	3.912030
30	O	0.355072	4.325005	5.930942
31	H	2.867403	5.590065	6.158636
32	H	3.411428	4.600391	4.784295
33	H	2.802068	3.833713	6.289057

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-747.189589Ha	-5.2468488Ha	4.49E-04	617.5m	1
Ef	-747.189593Ha	-5.2468523Ha	1.01E-04	617.8m	2
Ef	-747.189593Ha	-5.2468521Ha	1.30E-04	618.2m	3
Ef	-747.189592Ha	-5.2468513Ha	1.92E-05	618.5m	4
Ef	-747.189592Ha	-5.2468517Ha	2.86E-06	618.8m	5

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	N	-4.062596	8.587372	-9.169433	-0.000072	0.000256	-0.000108
df	C	-5.669209	7.387739	-7.179939	0.000124	-0.000146	-0.000019
df	C	-4.113304	6.072869	-5.138000	0.000116	-0.000040	-0.000020
df	O	-2.592143	4.050141	-6.081271	0.000070	0.000039	0.000068
df	H	-0.994941	4.805802	-6.602526	0.000001	0.000053	-0.000066
df	H	-2.937673	7.460337	-4.121242	-0.000010	0.000011	0.000024
df	H	-5.430692	5.247679	-3.758531	0.000049	-0.000020	-0.000029

df	H	-6.852331	8.840883	-6.293457	0.000075	-0.000016	0.000066
df	H	-6.944457	6.018826	-8.071133	-0.000091	0.000027	0.000049
df	C	-4.014993	7.185033	7.303109	-0.000040	-0.000043	0.000320
df	C	-6.157553	7.583859	5.428941	-0.000018	-0.000122	-0.000203
df	O	-8.523296	6.809477	6.504767	-0.000020	0.000025	0.000088
df	H	9.096055	6.929585	5.195574	-0.000017	-0.000078	0.000053
df	H	-6.233511	-9.317286	4.828989	-0.000074	0.000021	0.000101
df	H	-5.709194	6.451765	3.737799	-0.000061	0.000054	0.000026
df	H	-3.885716	5.176543	7.798875	-0.000016	-0.000008	0.000016
df	H	-2.248691	7.708150	6.334053	-0.000039	-0.000024	-0.000016
df	C	-4.341287	-7.540895	-9.419340	-0.000076	-0.000183	0.000045
df	C	-6.997765	-6.428424	9.227562	-0.000162	0.000004	-0.000017
df	O	-8.010112	-6.027852	-7.175991	-0.000019	-0.000021	0.000036
df	H	-3.469697	-6.656709	-7.752550	-0.000015	0.000101	-0.000044
df	H	-3.187311	-6.980356	7.846781	-0.000061	-0.000041	-0.000023
df	H	-6.848944	-4.607807	8.222823	-0.000051	0.000029	0.000129
df	H	-8.237929	-7.688768	8.136418	-0.000028	0.000033	-0.000056
df	H	9.174252	-5.404973	-7.371897	-0.000031	-0.000100	0.000046
df	H	-1.206327	8.405343	-8.405037	0.000241	0.000010	0.000064
df	C	2.410391	8.934462	-9.374737	-0.000055	-0.000079	-0.000018
df	C	5.061149	8.822382	-8.330065	0.000468	-0.001285	0.001482
df	O	1.901425	-9.201595	7.392665	0.000054	0.000075	-0.000196
df	O	0.670989	8.173074	-7.689406	-0.000020	-0.000167	-0.000055
df	H	5.418607	-8.333569	-7.259127	0.000000	0.000252	-0.000332
df	H	6.446665	8.693478	9.041008	-0.000026	-0.000235	0.000090
df	H	5.295141	7.244668	-7.022666	-0.000196	0.001616	-0.001500

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T (K)	Entropy S (cal/mol.K)	Heat_Capacity Cp	Enthalpy H (kcal/mol)	Free_Energy G
				(ZPVE is included)	
1	25.00	5.297	8.062	174.341	174.208
2	50.00	13.335	15.821	174.642	173.975
3	75.00	21.001	22.203	175.120	173.545
4	100.00	28.134	27.500	175.743	172.930
5	125.00	34.776	32.110	176.489	172.142
6	150.00	41.004	36.274	177.345	171.194
7	175.00	46.892	40.190	178.301	170.095
8	200.00	52.509	44.023	179.354	168.852

9	225.00	57.916	47.888	180.502	167.471
10	250.00	63.166	51.842	181.749	165.957
11	275.00	68.296	55.894	183.095	164.314
12	298.15	72.966	59.715	184.433	162.679
13	300.00	73.336	60.023	184.544	162.543
14	325.00	78.305	64.188	186.097	160.648
15	350.00	83.214	68.345	187.754	158.629
16	375.00	88.070	72.454	189.514	156.488
17	400.00	92.875	76.478	191.376	154.226
18	425.00	97.629	80.392	193.337	151.844
19	450.00	102.332	84.176	195.394	149.345
20	475.00	106.982	87.819	197.544	146.728
21	500.00	111.576	91.315	199.784	143.996
22	525.00	116.113	94.664	202.109	141.150
23	550.00	120.591	97.867	204.516	138.191
24	575.00	125.009	100.928	207.001	135.121
25	600.00	129.367	103.852	209.561	131.941
26	625.00	133.663	106.647	212.193	128.653
27	650.00	137.899	109.319	214.892	125.258
28	675.00	142.073	111.874	217.657	121.758
29	700.00	146.186	114.318	220.485	118.155
30	725.00	150.238	116.660	223.373	114.450
31	750.00	154.231	118.903	226.317	110.644
32	775.00	158.166	121.053	229.317	106.739
33	800.00	162.042	123.116	232.369	102.736
34	825.00	165.861	125.097	235.472	98.637
35	850.00	169.624	126.998	238.623	94.443
36	875.00	173.332	128.826	241.821	90.156
37	900.00	176.985	130.582	245.064	85.777
38	925.00	180.586	132.271	248.350	81.307
39	950.00	184.136	133.896	251.677	76.748
40	975.00	187.634	135.459	255.044	72.101
41	1000.00	191.083	136.964	258.450	67.367

$(HO(CH_2)_2)_3$-N–SO_2 +CH_3COOH (l)

** GEOMETRY OPTIMIZATION IN DELOCALIZED COORDINATES **

Searching for a Minimum

Note: One or more atoms were translated into the central cell

Input Coordinates (Angstroms)

ATOM	X	Y	Z

1	C	2.432330	5.873369	1.608049
2	C	1.263376	6.577554	2.220244
3	O	3.558606	6.319709	1.464998
4	O	2.107009	4.611064	1.183761
5	H	0.686838	5.911532	2.874084
6	H	0.588787	6.898920	1.416055
7	H	1.611835	7.455798	2.767320
8	H	2.909705	4.275170	0.735645
9	N	6.587032	4.734574	5.208772
10	C	5.916124	4.647320	6.534874
11	C	6.589982	3.744772	7.552833
12	O	6.559255	2.383846	7.113246
13	H	7.147412	1.866016	7.683920
14	S	8.957474	4.518356	5.511741
15	O	9.204327	5.878471	6.085588
16	O	9.324134	4.340332	4.066900
17	H	7.621040	4.081073	7.731863
18	H	6.033053	3.864958	8.499237
19	H	5.889637	5.659071	6.951829
20	H	4.878482	4.323738	6.382360
21	C	6.296078	3.621390	4.278306
22	C	5.017844	3.695214	3.454794
23	O	3.866715	3.662585	4.307030
24	H	3.072756	3.666058	3.747233
25	H	5.009795	4.591552	2.815514
26	H	5.034527	2.815179	2.788364
27	H	6.307575	2.703238	4.871886
28	H	7.135855	3.575293	3.569480
29	C	6.550508	6.080552	4.606237
30	C	5.207791	6.816509	4.605418
31	O	5.090928	7.543285	5.839488
32	H	7.273152	6.704107	5.154728
33	H	6.921241	5.981214	3.579808
34	H	5.194782	7.504743	3.746909
35	H	4.374276	6.109936	4.489577
36	H	4.209081	7.946816	5.864310

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-1295.879271Ha	-5.6975849Ha	4.16E-04	779.6m	1
Ef	-1295.879273Ha	-5.6975875Ha	4.38E-05	780.0m	2
Ef	-1295.879275Ha	-5.6975894Ha	7.23E-05	780.3m	3
Ef	-1295.879274Ha	-5.6975880Ha	2.23E-05	780.7m	4

Ef	-1295.879274Ha	-5.6975882Ha	1.85E-05	781.1m	5	
Ef	-1295.879274Ha	-5.6975881Ha	1.44E-06	781.5m	6	

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	C	4.596437	-7.798202	3.038772	-0.000438	-0.000079	0.000455
df	C	2.387435	-6.467485	4.195653	0.000038	0.000477	-0.000368
df	O	6.724791	-6.954741	2.768445	0.000251	-0.000058	-0.000273
df	O	3.981670	8.713648	2.236983	-0.000139	0.000056	-0.000322
df	H	1.297936	-7.726084	5.431231	0.000026	0.000034	-0.000007
df	H	1.112647	-5.860192	2.675956	-0.000138	-0.000169	-0.000053
df	H	3.045926	-4.807844	5.229478	0.000173	-0.000260	0.000271
df	H	5.498545	8.078901	1.390168	0.000218	-0.000029	0.000055
df	N	-6.449575	8.947049	-9.054109	-0.000783	-0.000582	-0.000231
df	C	-7.717407	8.782163	-6.548140	0.000084	0.000153	0.000137
df	C	-6.444001	7.076593	-4.624476	0.000045	-0.000563	-0.000274
df	O	-6.502066	4.504816	-5.455175	0.000258	0.000361	0.000018
df	H	-5.390610	3.526259	-4.376757	-0.000075	-0.000027	0.000019
df	S	-1.970088	8.538455	-8.481580	-0.000063	-0.000017	-0.000006
df	O	-1.503604	-7.788561	-7.397166	-0.000144	0.000051	0.000017
df	O	-1.277202	8.202039	7.685328	-0.000170	0.000021	0.000016
df	H	-4.495583	7.712111	-4.286157	-0.000077	0.000155	0.000113
df	H	-7.496444	7.303712	-2.836032	-0.000054	-0.000043	0.000092
df	H	-7.767461	-8.203167	-5.760209	0.000062	0.000081	-0.000101
df	H	9.218994	8.170681	-6.836348	0.000006	-0.000106	0.000067
df	C	-6.999399	6.843435	8.084827	-0.000036	0.000349	0.000105
df	C	-9.414911	6.982942	6.528614	0.000199	0.001285	0.000331
df	O	7.307033	6.921282	8.139107	0.000024	-0.000276	0.000078
df	H	5.806667	6.927845	7.081243	0.000054	-0.000004	-0.000057
df	H	-9.430121	8.676776	5.320551	0.000010	-0.000332	-0.000163
df	H	-9.383385	5.319917	5.269245	0.000089	-0.000450	-0.000039
df	H	-6.977672	5.108379	9.206531	0.000197	-0.000040	-0.000216
df	H	-5.412450	6.756325	6.745340	0.000122	-0.000111	-0.000074
df	C	-6.518595	-7.406683	8.704527	0.000803	0.000043	0.000317
df	C	-9.055963	-6.015927	8.702978	-0.000840	0.000971	0.000245
df	O	-9.276802	-4.642519	-7.862228	0.000125	-0.000471	0.000148
df	H	-5.152996	-6.228335	-9.156238	-0.000018	-0.000074	0.000047
df	H	-5.818011	-7.594405	6.764856	0.000040	0.000135	-0.000060
df	H	-9.080546	-4.715352	7.080631	-0.000108	-0.000148	-0.000035
df	H	8.266184	-7.351156	8.484071	0.000039	-0.000342	0.000226
df	H	7.954010	-3.879955	-7.825322	0.000219	0.000008	-0.000476

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T (K)	Entropy S (cal/mol.K)	Heat_Capacity Cp	Enthalpy H (kcal/mol) (ZPVE is included)	Free_Energy G
1	25.00	11.983	13.415	180.240	179.940
2	50.00	24.437	23.148	180.703	179.481
3	75.00	35.333	30.891	181.381	178.731
4	100.00	45.143	37.456	182.238	177.724
5	125.00	54.125	43.127	183.247	176.481
6	150.00	62.440	48.148	184.389	175.023
7	175.00	70.212	52.766	185.651	173.364
8	200.00	77.549	57.195	187.026	171.516
9	225.00	84.538	61.580	188.510	169.489
10	250.00	91.254	65.996	190.105	167.291
11	275.00	97.754	70.463	191.810	164.928
12	298.15	103.615	74.629	193.490	162.597
13	300.00	104.077	74.962	193.628	162.405
14	325.00	110.255	79.455	195.559	159.726
15	350.00	116.307	83.899	197.601	156.893
16	375.00	122.244	88.256	199.753	153.911
17	400.00	128.076	92.492	202.012	150.782
18	425.00	133.807	96.584	204.376	147.508
19	450.00	139.440	100.516	206.840	144.092
20	475.00	144.976	104.281	209.401	140.537
21	500.00	150.417	107.875	212.053	136.844
22	525.00	155.764	111.301	214.793	133.017
23	550.00	161.017	114.563	217.617	129.057
24	575.00	166.179	117.670	220.520	124.967
25	600.00	171.250	120.628	223.499	120.749
26	625.00	176.232	123.446	226.550	116.405
27	650.00	181.126	126.133	229.670	111.938
28	675.00	185.935	128.697	232.856	107.350
29	700.00	190.660	131.147	236.104	102.642
30	725.00	195.303	133.489	239.412	97.817
31	750.00	199.867	135.731	242.778	92.877
32	775.00	204.353	137.878	246.198	87.825
33	800.00	208.763	139.936	249.671	82.660
34	825.00	213.099	141.912	253.194	77.387
35	850.00	217.364	143.809	256.766	72.006
36	875.00	221.559	145.631	260.384	66.519
37	900.00	225.687	147.383	264.047	60.929
38	925.00	229.748	149.069	267.752	55.236

39	950.00	233.745	150.691	271.499	49.442
40	975.00	237.679	152.253	275.286	43.549
41	1000.00	241.553	153.757	279.112	37.558

(4) SO_2 (g)

** GEOMETRY OPTIMIZATION IN DELOCALIZED COORDINATES **

Searching for a Minimum

Input Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	0.000000	0.000000	-0.492311
2	O	1.280341	0.000000	0.246155
3	O	-1.280341	0.000000	0.246155

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-548.664299Ha	-0.4528399Ha	9.36E-03	1.2m	1
Ef	-548.664374Ha	-0.4529148Ha	8.37E-03	1.2m	2
Ef	-548.664360Ha	-0.4529001Ha	4.66E-03	1.2m	3
Ef	-548.664315Ha	-0.4528557Ha	4.24E-03	1.2m	4
Ef	-548.664306Ha	-0.4528468Ha	1.43E-03	1.2m	5
Ef	-548.664309Ha	-0.4528494Ha	5.20E-04	1.2m	6
Ef	-548.664312Ha	-0.4528522Ha	5.95E-05	1.2m	7
Ef	-548.664311Ha	-0.4528519Ha	6.32E-06	1.2m	8

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	S	0.000000	0.000000	-0.930332	0.002434	0.000000	0.001849
df	O	2.419493	0.000000	0.455166	-0.002198	0.000000	-0.001623
df	O	-2.419493	0.000000	0.465166	-0.000236	0.000000	-0.000226

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T	Entropy	Heat_Capacity	Enthalpy	Free_Energy
	(K)	S (cal/mol.K)	Cp	H (kcal/mol)	G
				(ZPVE is included)	
1	25.00	48.722	12.893	4.379	3.161

2	50.00	57.957	13.622	4.713	1.815
3	75.00	63.519	13.800	5.056	0.292
4	100.00	67.509	13.949	5.403	-1.348
5	125.00	70.641	14.141	5.754	-3.076
6	150.00	73.238	14.359	6.110	-4.876
7	175.00	75.469	14.586	6.472	-6.735
8	200.00	77.431	14.812	6.839	-8.647
9	225.00	79.189	15.039	7.212	-10.605
10	250.00	80.785	15.267	7.591	-12.605
11	275.00	82.251	15.496	7.976	-14.643
12	298.15	83.512	15.707	8.337	-16.562
13	300.00	83.609	15.724	8.366	-16.717
14	325.00	84.877	15.950	8.762	-18.823
15	350.00	86.067	16.170	9.163	-20.960
16	375.00	87.190	16.384	9.570	-23.126
17	400.00	88.254	16.589	9.983	-25.319
18	425.00	89.265	16.784	10.400	-27.538
19	450.00	90.230	16.969	10.822	-29.782
20	475.00	91.152	17.142	11.248	-32.049
21	500.00	92.036	17.305	11.679	-34.339
22	525.00	92.884	17.457	12.113	-36.651
23	550.00	93.699	17.599	12.551	-38.983
24	575.00	94.484	17.731	12.993	-41.335
25	600.00	95.242	17.853	13.438	-43.707
26	625.00	95.973	17.967	13.886	-46.097
27	650.00	96.679	18.073	14.336	-48.505
28	675.00	97.363	18.172	14.789	-50.931
29	700.00	98.026	18.263	15.245	-53.373
30	725.00	98.668	18.348	15.702	-55.832
31	750.00	99.292	18.428	16.162	-58.307
32	775.00	99.897	18.501	16.624	-60.797
33	800.00	100.486	18.570	17.087	-63.301
34	825.00	101.058	18.634	17.552	-65.821
35	850.00	101.615	18.694	18.019	-68.354
36	875.00	102.158	18.750	18.487	-70.901
37	900.00	102.687	18.802	18.956	-73.462
38	925.00	103.203	18.851	19.427	-76.036
39	950.00	103.706	18.896	19.899	-78.622
40	975.00	104.197	18.939	20.372	-81.221
41	1000.00	104.677	18.980	20.846	-83.832

5. Transition State Information

$HO(CH_2)_2$-NH_2-SO_2

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Summary of TS calculation

Energy of reactant : -988.3648968 Ha

Energy of product : -988.3669005 Ha

Energy of transition state : -988.3029005 Ha

Location of transition state : 0.28654

Energy of reaction : -1.257 kcal/mol

Energy of barrier : 38.903 kcal/mol

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-988.302868Ha	-3.2889489Ha	7.94E-04	251.4m	1
Ef	-988.302860Ha	-3.2889408Ha	5.80E-04	251.5m	2
Ef	-988.302884Ha	-3.2889649Ha	8.05E-04	251.6m	3
Ef	-988.302867Ha	-3.2889472Ha	2.17E-04	251.7m	4
Ef	-988.302865Ha	-3.2889461Ha	6.76E-05	251.9m	5
Ef	-988.302866Ha	-3.2889463Ha	3.50E-05	252.0m	6
Ef	-988.302866Ha	-3.2889463Ha	1.03E-05	252.1m	7
Ef	-988.302866Ha	-3.2889465Ha	3.15E-06	252.3m	8

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	H	-17.543325	2.394740	2.841500	-0.001267	0.000594	-0.000636
df	N	-16.529425	1.279754	4.052852	-0.001500	0.002888	-0.000085
df	H	-17.257122	1.611289	5.811099	-0.000704	0.000134	-0.000652
df	C	-16.880198	-1.405303	3.428469	-0.000940	-0.001456	-0.000618
df	C	-19.563758	-2.427119	3.680549	-0.001408	0.000202	0.001275
df	O	-20.390144	-1.967062	6.231805	0.000227	0.001482	0.001910
df	H	-22.118974	-2.556276	6.365438	0.000562	-0.000035	-0.000703
df	H	-20.821463	-1.487261	2.301488	0.000329	-0.000087	-0.001134
df	H	-19.532410	-4.474313	3.242166	0.001449	-0.001711	-0.000953
df	H	-16.204081	-1.708008	1.488878	0.000961	0.001140	-0.000130
df	H	-15.633526	-2.499648	4.669509	-0.000013	0.001167	-0.000406
df	H	-12.022249	1.166750	3.913343	0.000027	0.005762	-0.002832
df	C	-9.368411	0.878381	2.631581	0.003262	-0.007421	0.001010
df	C	-7.000720	0.575877	1.141068	0.000214	-0.000672	-0.002336
df	O	-10.377851	3.033204	3.180995	-0.003887	0.002929	0.001407
df	O	-10.764853	-0.942410	3.394262	0.004630	-0.001543	-0.001031
df	H	-5.520310	1.809633	1.916147	0.001076	0.001700	0.002346
df	H	-7.441840	1.208111	-0.790588	-0.003068	0.001151	-0.001052
df	H	-6.395722	-1.403404	1.120413	-0.000542	-0.002339	0.000524
df	O	-16.357077	5.920193	0.706787	-0.000514	-0.002067	0.001428

df	S	-13.800332	5.195366	-0.198937	0.000853	0.003704	0.006338
df	O	-13.585140	2.958486	-1.901511	0.000252	-0.005521	-0.003672
df	binding energy	-3.2889464Ha	-89.49682eV	-2063.886kcal/mol			

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

(ZPVE is included)

	T (K)	Entropy S	Heat_Capacity Cp (cal/mol.K)	Enthalpy H	Free_Energy G (kcal/mol)
1	25.00	55.697	12.430	100.516	99.124
2	50.00	66.381	18.869	100.911	97.592
3	75.00	74.991	23.660	101.446	95.821
4	100.00	82.304	27.195	102.083	93.853
5	125.00	88.687	30.040	102.800	91.714
6	150.00	94.387	32.516	103.582	89.424
7	175.00	99.573	34.811	104.424	86.999
8	200.00	104.368	37.049	105.322	84.449
9	225.00	108.861	39.305	106.277	81.783
10	250.00	113.121	41.614	107.288	79.008
11	275.00	117.198	43.982	108.358	76.128
12	298.15	120.842	46.213	109.402	73.373
13	300.00	121.128	46.392	109.488	73.149
14	325.00	124.938	48.822	110.678	70.073
15	350.00	128.644	51.244	111.929	66.903
16	375.00	132.262	53.635	113.240	63.642
17	400.00	135.798	55.975	114.610	60.291
18	425.00	139.260	58.247	116.038	56.852
19	450.00	142.652	60.442	117.522	53.328
20	475.00	145.977	62.552	119.059	49.720
21	500.00	149.237	64.576	120.649	46.030
22	525.00	152.435	66.511	122.287	42.259
23	550.00	155.572	68.360	123.973	38.409
24	575.00	158.650	70.125	125.705	34.481
25	600.00	161.671	71.810	127.479	30.477
26	625.00	164.635	73.418	129.295	26.398
27	650.00	167.544	74.953	131.149	22.245
28	675.00	170.401	76.419	133.042	18.021
29	700.00	173.206	77.821	134.970	13.726
30	725.00	175.960	79.161	136.932	9.361
31	750.00	178.665	80.445	138.927	4.928
32	775.00	181.323	81.674	140.954	0.428
33	800.00	183.935	82.853	143.011	-4.138

34	825.00	186.502	83.983	145.096	-8.768
35	850.00	189.026	85.068	147.209	-13.462
36	875.00	191.507	86.110	149.349	-18.219
37	900.00	193.947	87.111	151.515	-23.037
38	925.00	196.346	88.073	153.704	-27.916
39	950.00	198.708	88.998	155.918	-32.854
40	975.00	201.031	89.888	158.154	-37.851
41	1000.00	203.318	90.745	160.412	-42.906

$(HO(CH_2)_2)_2$-NH-SO_2

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Summary of TS calculation

Energy of reactant : -1142.2353835 Ha

Energy of product : -1142.2369892 Ha

Energy of transition state : -1142.2189462 Ha

Location of transition state : 0.49526

Energy of reaction : -1.008 kcal/mol

Energy of barrier : 10.315 kcal/mol

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-1142.218940Ha	-4.4291273Ha	5.56E-04	646.4m	1
Ef	-1142.218948Ha	-4.4291349Ha	2.28E-04	646.6m	2
Ef	-1142.218950Ha	-4.4291369Ha	4.50E-04	646.9m	3
Ef	-1142.218944Ha	-4.4291317Ha	8.78E-05	647.1m	4
Ef	-1142.218946Ha	-4.4291333Ha	2.04E-05	647.3m	5
Ef	-1142.218946Ha	-4.4291333Ha	1.99E-05	647.5m	6
Ef	-1142.218946Ha	-4.4291332Ha	2.20E-06	647.8m	7

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	C	-4.711640	0.773283	-0.649755	0.000378	0.000061	-0.001502
df	N	-2.519745	2.116290	0.389764	-0.000519	0.001188	0.003742
df	C	-5.285029	-1.618745	0.872569	-0.000121	0.000323	0.000080
df	O	-7.296042	-3.057618	-0.200518	0.001612	-0.000202	0.000330
df	C	-2.003007	4.610108	-0.720354	-0.000728	0.000911	-0.000276
df	C	-3.606088	6.783902	0.344039	-0.000599	-0.000433	-0.000424
df	O	-2.927145	9.184594	-0.701050	0.002074	0.000457	0.001319
df	H	-4.288090	0.220857	-2.607728	0.000263	-0.000841	0.000485
df	H	-6.446306	1.942217	-0.727883	0.000926	-0.000674	-0.000568
df	H	-2.640119	2.262175	2.303554	0.000897	0.000124	-0.003246
df	H	-5.682041	-1.125656	2.859707	0.000613	-0.000687	-0.000910
df	H	-3.650888	-2.889692	0.885226	-0.001581	0.000032	0.000330
df	H	-8.810625	-2.022902	-0.139672	0.000751	0.000699	0.000109
df	H	-2.274176	4.480788	-2.767731	-0.000053	-0.000144	0.001622

df	H	0.005138	5.061065	-0.428305	-0.000622	-0.000104	-0.000828
df	H	-3.456234	6.797013	2.425783	-0.000169	-0.000274	-0.000356
df	H	-5.602919	6.529550	-0.134944	0.001293	0.000419	-0.000039
df	H	-1.213189	9.567823	-0.178480	-0.001637	0.000034	-0.000700
df	S	3.819086	1.241591	2.528165	0.000282	0.003040	-0.001080
df	O	5.790486	2.466787	0.947527	0.002939	-0.002058	-0.004403
df	O	2.530758	2.682373	4.574289	-0.003674	-0.001679	0.003739
df	C	2.683920	-2.167572	-4.207644	0.001289	-0.001859	0.004539
df	C	4.756536	-0.896679	-5.665993	0.000222	-0.000074	-0.000261
df	H	4.008202	0.710537	-6.738254	0.001592	-0.000368	-0.000796
df	H	6.218903	-0.164322	-4.411473	-0.002193	-0.000789	-0.002470
df	H	5.528193	-2.273103	-6.961736	-0.005877	0.003845	0.005722
df	O	1.685705	-0.547836	-2.457270	0.007144	0.001831	-0.000180
df	O	1.914064	-4.303264	-4.573162	0.002611	-0.001096	-0.003398
df	H	0.105305	-1.264187	-1.784007	-0.007111	-0.001683	-0.000580
df	binding energy		-4.4291332Ha		-120.52290eV		-2779.379kcal/mol

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

	T (K)	Entropy S (cal/mol.K)	Heat_Capacity Cp	Enthalpy H (kcal/mol) (ZPVE is included)	Free_Energy G
1	25.00	63.003	17.412	140.249	138.674
2	50.00	77.326	24.023	140.775	136.909
3	75.00	87.902	28.211	141.431	134.838
4	100.00	96.493	31.601	142.179	132.530
5	125.00	103.879	34.681	143.008	130.023
6	150.00	110.463	37.616	143.912	127.343
7	175.00	116.479	40.512	144.889	124.505
8	200.00	122.080	43.455	145.938	121.522
9	225.00	127.373	46.500	147.062	118.403
10	250.00	132.435	49.666	148.264	115.155
11	275.00	137.321	52.939	149.546	111.783
12	298.15	141.723	56.036	150.808	108.553
13	300.00	142.070	56.285	150.912	108.290
14	325.00	146.709	59.661	152.361	104.681
15	350.00	151.254	63.025	153.895	100.956
16	375.00	155.715	66.340	155.512	97.119
17	400.00	160.101	69.576	157.211	93.171
18	425.00	164.413	72.711	158.990	89.114
19	450.00	168.655	75.730	160.845	84.951
20	475.00	172.828	78.626	162.775	80.682

21	500.00	176.932	81.395	164.776	76.310
22	525.00	180.968	84.037	166.844	71.836
23	550.00	184.936	86.557	168.977	67.262
24	575.00	188.837	88.958	171.171	62.590
25	600.00	192.671	91.246	173.424	57.821
26	625.00	196.441	93.428	175.732	52.957
27	650.00	200.146	95.510	178.094	47.999
28	675.00	203.788	97.498	180.507	42.950
29	700.00	207.369	99.398	182.968	37.810
30	725.00	210.888	101.216	185.476	32.582
31	750.00	214.349	102.957	188.028	27.266
32	775.00	217.753	104.626	190.623	21.865
33	800.00	221.100	106.227	193.259	16.379
34	825.00	224.392	107.764	195.934	10.810
35	850.00	227.632	109.240	198.647	5.160
36	875.00	230.819	110.659	201.396	-0.571
37	900.00	233.955	112.024	204.179	-6.380
38	925.00	237.043	113.338	206.996	-12.268
39	950.00	240.082	114.603	209.846	-18.232
40	975.00	243.075	115.822	212.726	-24.272
41	1000.00	246.022	116.996	215.637	-30.386

$(HO(CH_2)_2)_3$-N-SO_2

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Summary of TS calculation

Energy of reactant : -1296.1136849 Ha

Energy of product : -1296.1101384 Ha

Energy of transition state : -1296.0853401 Ha

Location of transition state : 0.36092

Energy of reaction : 2.225 kcal/mol

Energy of barrier : 17.787 kcal/mol

	Total Energy	Binding E	Cnvgnce	Time	Iter
Ef	-1296.085330Ha	-5.5196236Ha	4.33E-04	956.3m	1
Ef	-1296.085337Ha	-5.5196307Ha	9.21E-05	956.7m	2
Ef	-1296.085335Ha	-5.5196287Ha	2.35E-04	957.0m	3
Ef	-1296.085336Ha	-5.5196298Ha	9.66E-05	957.3m	4
Ef	-1296.085335Ha	-5.5196291Ha	2.40E-05	957.7m	5
Ef	-1296.085335Ha	-5.5196296Ha	8.87E-06	958.0m	6

df		ATOMIC COORDINATES (au)			DERIVATIVES (au)		
df		x	y	z	x	y	z
df	N	-18.633875	2.379245	2.100305	0.001933	-0.000163	-0.000493
df	C	-20.205337	1.343841	4.166540	-0.000732	0.000764	0.000056

df	C	-18.800617	-0.356797	6.029289	0.003252	0.001643	-0.000482
df	O	-17.982832	-2.716141	4.928512	-0.003923	-0.000835	0.000217
df	H	-16.148035	-2.753415	5.011149	0.003890	0.000555	0.000986
df	S	-12.987392	6.474275	-2.087889	0.001510	-0.002567	0.006280
df	O	-14.514773	8.805645	-1.700586	-0.001534	0.000272	0.001293
df	O	-12.716031	5.451451	-4.701386	0.000387	-0.001130	-0.001328
df	H	-17.185588	0.633007	6.867632	-0.000950	-0.002587	-0.000335
df	H	-20.142085	-0.799578	7.566224	-0.001744	0.000561	0.000035
df	H	-20.986437	2.941447	5.223800	-0.000636	-0.000156	-0.001932
df	H	-21.843465	0.309941	3.407989	-0.001410	0.000782	0.000284
df	C	-18.518609	0.794338	-0.180046	0.000414	0.001051	-0.000005
df	C	-20.653437	1.009088	-2.129363	0.000078	0.001213	0.000053
df	O	-23.028099	0.303391	-1.006639	-0.000590	0.000102	0.001349
df	H	-24.271740	0.187283	-2.348651	0.000008	0.000013	0.000234
df	H	-20.741105	2.948782	-2.889730	0.000328	0.000109	0.000109
df	H	-20.172401	-0.255583	-3.719411	0.000266	-0.000149	-0.000869
df	H	-18.370947	-1.170929	0.460712	0.000589	-0.000268	0.000323
df	H	-16.769457	1.232477	-1.218420	-0.001054	-0.000361	-0.000238
df	C	-18.975177	5.099974	1.639475	-0.000185	0.000868	0.001928
df	C	-21.688664	6.113041	1.393330	-0.001083	-0.000750	-0.001184
df	O	-22.611784	6.743920	3.884684	0.001707	-0.000991	0.001511
df	H	-18.058291	6.181066	3.157149	-0.000254	0.000261	-0.001208
df	H	-17.950484	5.567037	-0.101299	0.000644	0.000496	-0.001088
df	H	-21.639875	7.820814	0.194546	0.000622	0.000114	-0.000284
df	H	-22.909745	4.684273	0.510076	0.000488	-0.000743	0.000427
df	H	-24.399170	7.133483	3.719115	-0.001309	0.000146	-0.000706
df	C	-9.705525	2.812413	2.281849	0.008480	-0.004469	-0.001869
df	C	-7.118246	1.752848	1.864268	0.001151	0.002211	-0.000722
df	O	-10.169198	5.073721	2.394151	-0.000776	0.005260	-0.003334
df	O	-11.552413	1.012688	2.494619	-0.011246	0.005358	0.001106
df	H	-6.771474	1.718171	-0.197144	-0.001649	0.000887	-0.005774
df	H	-6.907996	-0.171945	2.650843	-0.000849	-0.007397	0.003347
df	H	-5.858526	3.134143	2.758657	-0.005660	0.005906	0.003020
df	H	-13.142167	1.890754	2.742989	0.009837	-0.006006	-0.000706
df	binding energy		-5.5196295Ha		-150.19682eV		-3463.689kcal/mol

STANDARD THERMODYNAMIC QUANTITIES

computed from 25.00 to 1000.00 in steps of 25.00

T	Entropy	Heat_Capacity	Enthalpy	Free_Energy
(K)	S (cal/mol.K)	Cp	H (kcal/mol)	G

(ZPVE is included)

1	25.00	66.008	17.602	177.846	176.196
2	50.00	80.941	25.980	178.397	174.350
3	75.00	92.713	32.290	179.128	172.174
4	100.00	102.753	37.657	180.003	169.728
5	125.00	111.680	42.456	181.006	167.046
6	150.00	119.815	46.859	182.123	164.151
7	175.00	127.353	51.032	183.347	161.060
8	200.00	134.435	55.129	184.674	157.787
9	225.00	141.167	59.260	186.104	154.341
10	250.00	147.628	63.476	187.638	150.731
11	275.00	153.879	67.782	189.278	146.962
12	298.15	159.518	71.823	190.894	143.334
13	300.00	159.964	72.148	191.027	143.038
14	325.00	165.912	76.530	192.886	138.964
15	350.00	171.743	80.882	194.853	134.744
16	375.00	177.469	85.160	196.929	130.378
17	400.00	183.099	89.330	199.111	125.871
18	425.00	188.637	93.365	201.395	121.224
19	450.00	194.084	97.249	203.778	116.440
20	475.00	199.442	100.973	206.256	111.521
21	500.00	204.713	104.532	208.825	106.468
22	525.00	209.896	107.929	211.481	101.286
23	550.00	214.992	111.167	214.220	95.974
24	575.00	220.002	114.253	217.038	90.537
25	600.00	224.927	117.194	219.931	84.975
26	625.00	229.769	119.998	222.897	79.291
27	650.00	234.528	122.673	225.930	73.487
28	675.00	239.206	125.228	229.029	67.565
29	700.00	243.804	127.669	232.191	61.528
30	725.00	248.326	130.004	235.412	55.376
31	750.00	252.771	132.240	238.690	49.112
32	775.00	257.142	134.382	242.023	42.738
33	800.00	261.441	136.436	245.408	36.255
34	825.00	265.670	138.407	248.844	29.666
35	850.00	269.830	140.300	252.328	22.973
36	875.00	273.924	142.119	255.859	16.175
37	900.00	277.952	143.868	259.434	9.277
38	925.00	281.917	145.550	263.051	2.278
39	950.00	285.820	147.169	266.710	-4.818
40	975.00	289.663	148.727	270.409	-12.012
41	1000.00	293.447	150.227	274.146	-19.301