

**金属、配体和溶剂之间的协同性：基于密度泛函理论研究含
双锌离子配合物催化磷酸二酯裂解的反应机理**

范育波¹ 高毅勤^{1,2,*}

(¹Department of Chemistry, Texas A&M University, College Station, TX 77843-3255, USA;

²北京大学化学与分子工程学院, 北京 100871)

**Cooperativity between Metals, Ligands and Solvent: a DFT Study
on the Mechanism of a Dizinc Complex-Mediated
Phosphodiester Cleavage**

FAN Yu-Bo¹ GAO Yi-Qin^{1,2,*}

(¹Department of Chemistry, Texas A&M University, College Station, TX 77843-3255, USA;

²College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China)

*Corresponding author. Email: yiqin@mail.chem.tamu.edu.

Complete description for Reference (41):

Gaussian 03, Revision C.02 and D.02 Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Cartesian coordinates for all species
shown in Scheme 4 and 5:

1a

Zn	-1.980842	-1.468177	0.291198
Zn	-0.502773	1.683542	-0.068280
O	-1.943002	0.330239	-0.628840
N	-4.011950	-1.479373	-0.637246
N	-2.664759	-3.421285	0.963467
N	-1.510392	-2.642213	-1.503609
N	-2.131746	3.104078	-0.628334
N	0.474802	3.738609	0.192641
N	0.137739	2.105107	-2.116487
H	-2.522523	-3.452983	1.975274
H	-0.561246	-2.399867	-1.814085
H	1.131205	3.673689	0.970983
H	0.361816	1.195141	-2.538156
C	-3.182390	0.857365	-1.087758
C	-4.384725	-0.036571	-0.636754
C	-3.384502	2.297954	-0.528702
H	-3.181082	0.894723	-2.196114
H	-4.646403	0.217813	0.400071
H	-5.267195	0.158078	-1.272711
H	-4.229929	2.803525	-1.030294
H	-3.612093	2.212330	0.542396
C	-4.831207	-2.308654	0.295704
C	-4.111870	-3.643153	0.637956
H	-5.833891	-2.529412	-0.110465
H	-4.958127	-1.723202	1.215444
H	-4.634707	-4.118829	1.479331
H	-4.173958	-4.335885	-0.210553
C	-3.910210	-2.076982	-2.009274
C	-2.453510	-2.124457	-2.538920
H	-4.535425	-1.513486	-2.720252
H	-4.317204	-3.095470	-1.965677
H	-2.435490	-2.739381	-3.454259
H	-2.099565	-1.119541	-2.789138
C	-1.717795	-4.380795	0.308610
C	-1.628908	-4.107831	-1.216796
H	-2.013542	-5.429146	0.474422
H	-0.740511	-4.207911	0.773664
H	-0.766280	-4.654788	-1.620978
H	-2.522047	-4.496879	-1.724906
C	-2.039204	4.140892	0.440539
C	-0.598691	4.729828	0.558202
H	-2.293354	3.630082	1.376413
H	-2.753855	4.968484	0.283635
H	-0.494332	5.623279	-0.073398
H	-0.455016	5.054414	1.596935
C	-1.870069	3.653071	-1.994303
C	-0.998156	2.707936	-2.870568
H	-1.359181	4.615407	-1.877248
H	-2.817491	3.855675	-2.521316
H	-1.607023	1.871831	-3.232171
H	-0.646881	3.272134	-3.750770
C	1.391395	2.902319	-2.023595
C	1.246751	4.098401	-1.050004
H	1.711530	3.285733	-3.007139
H	2.158431	2.211796	-1.652803
H	2.250015	4.460956	-0.786349
H	0.728645	4.926459	-1.550146
O	-2.505261	-0.541645	2.219813
H	-3.373296	-0.147417	2.398638
H	-1.828731	0.277980	2.134399
P	1.130008	-0.793877	1.052199
O	1.639422	-0.169463	2.484268
O	-0.108037	-1.709689	1.175136
O	1.173162	0.274402	-0.095396

C	0.674566	0.309364	3.506565
H	-0.057079	-0.484422	3.699326
H	1.303172	0.474331	4.387691
C	-0.021474	1.600976	3.046130
H	0.767323	2.323371	2.765882
O	-0.843912	1.320467	1.895134
C	-0.866643	2.194628	4.192876
H	-0.244061	2.440664	5.065010
H	-1.362381	3.112577	3.850402
H	-1.643048	1.482558	4.506561
O	0.836657	-0.909238	-2.540393
H	1.059904	-0.562247	-1.633991
H	1.685139	-1.183580	-2.924392
O	2.396899	-1.865545	0.745921
C	3.694741	-1.505186	0.429473
C	4.452519	-2.492215	-0.231823
C	5.779549	-2.233522	-0.583168
C	6.331335	-0.983016	-0.268478
C	5.592532	0.001749	0.400637
C	4.264949	-0.259275	0.755207
N	7.729465	-0.693877	-0.652431
O	8.180379	0.429287	-0.378191
O	8.364322	-1.588839	-1.229693
H	3.991708	-3.453912	-0.454588
H	6.387138	-2.978216	-1.093423
H	6.063531	0.952475	0.642932
H	3.684659	0.484182	1.296805

TS1

Zn	-1.880867	-1.538407	0.301865
Zn	-0.660189	1.743823	0.027825
O	-2.107592	0.349796	-0.423379
N	-4.070151	-1.596736	-0.123853
N	-2.337183	-3.561319	0.998557
N	-1.822743	-2.618047	-1.619364
N	-2.518423	3.113808	-0.403126
N	0.058698	3.843331	0.400314
N	-0.256308	2.381398	-2.020067
H	-1.954553	-3.626402	1.944243
H	-0.963426	-2.359267	-2.124817
H	0.894280	3.829597	0.989145
H	0.213246	1.563749	-2.415862
C	-3.449806	0.796101	-0.607212
C	-4.477947	-0.175127	0.054642
C	-3.635063	2.211096	0.002056
H	-3.675976	0.843753	-1.692736
H	-4.497033	0.014973	1.136779
H	-5.490459	0.013353	-0.346817
H	-4.618034	2.629755	-0.287400
H	-3.592043	2.125415	1.096140
C	-4.627690	-2.506123	0.921610
C	-3.811788	-3.825478	1.013574
H	-5.690566	-2.744819	0.741563
H	-4.556598	-1.973559	1.878427
H	-4.107894	-4.357649	1.928498
H	-4.055708	-4.481646	0.168566
C	-4.283952	-2.111914	-1.516064
C	-2.990603	-2.079932	-2.373378
H	-5.069392	-1.529565	-2.024034
H	-4.650012	-3.144319	-1.444737
H	-3.177919	-2.638281	-3.306392
H	-2.734560	-1.047494	-2.635270
C	-1.551621	-4.449281	0.085681
C	-1.846002	-4.099758	-1.396177
H	-1.766671	-5.516048	0.259180
H	-0.495723	-4.257124	0.308082
H	-1.097457	-4.595544	-2.029511
H	-2.828721	-4.491109	-1.693702
C	-2.421454	4.341951	0.453961

C	-1.055540	4.440609	1.199266	H	-3.432059	0.886262	-2.046788
H	-3.218157	4.333378	1.209398	H	-4.653318	0.181456	0.660787
H	-2.584003	5.235038	-0.165920	H	-5.406584	0.088816	-0.953935
H	-0.865548	5.495995	1.456516	H	-4.431650	2.746414	-0.770539
H	-1.101206	3.856332	2.126027	H	-3.671604	2.154487	0.737643
C	-2.545248	3.431990	-1.870714	C	-4.793536	-2.322954	0.637627
C	-1.556809	2.578838	-2.711925	C	-4.037432	-3.640569	0.958122
H	-2.303779	4.493875	-1.998408	H	-5.828986	-2.561382	0.337151
H	-3.562163	3.288876	-2.272215	H	-4.839037	-1.705716	1.544035
H	-1.966218	1.574731	-2.868723	H	-4.464635	-4.075303	1.872745
H	-1.432193	3.058899	-3.697811	H	-4.193390	-4.370730	0.154260
C	0.700070	3.522581	-2.005615	C	-4.127823	-2.153135	-1.759246
C	0.371941	4.546239	-0.884415	C	-2.733383	-2.232117	-2.437621
H	0.731502	4.046126	-2.975217	H	-4.818140	-1.599206	-2.415110
H	1.690489	3.088223	-1.819537	H	-4.537865	-3.165453	-1.647908
H	1.223792	5.231572	-0.766568	H	-2.820495	-2.860668	-3.340000
H	-0.492365	5.158441	-1.164461	H	-2.406995	-1.230469	-2.740014
O	-2.016405	-0.821343	2.369359	C	-1.708325	-4.405634	0.387540
H	-1.396142	0.034977	2.275391	C	-1.821733	-4.195328	-1.142786
H	-2.835419	-0.498072	2.775518	H	-1.978491	-5.444134	0.638292
P	1.275219	-0.707987	0.505522	H	-0.677525	-4.217741	0.709208
O	1.931108	-0.296548	1.959318	H	-1.026397	-4.766859	-1.637741
O	0.138214	-1.745588	0.628570	H	-2.783443	-4.575951	-1.512835
O	1.102734	0.533723	-0.418624	C	-2.200732	4.146844	0.551237
C	1.866493	1.120988	2.379018	C	-0.786561	4.803989	0.579893
H	2.643731	1.209511	3.145621	H	-2.362331	3.612862	1.494744
H	2.117375	1.748265	1.514213	H	-2.965163	4.938744	0.458137
C	0.474360	1.480584	2.937797	H	-0.768589	5.709765	-0.042802
H	0.501021	2.573195	3.135584	H	-0.589182	5.122459	1.611706
O	-0.559808	1.192681	1.973246	C	-2.188351	3.693243	-1.899067
C	0.187670	0.757566	4.268694	C	-1.333725	2.801731	-2.847757
H	0.933504	1.036829	5.026198	H	-1.724090	4.681889	-1.810179
H	-0.805824	1.038679	4.641887	H	-3.181187	3.847464	-2.353562
H	0.216819	-0.329454	4.127185	H	-1.926676	1.940690	-3.176658
O	0.697550	-1.689516	-3.015587	H	-1.071919	3.391060	-3.742480
H	1.294606	-1.485835	-2.271917	C	1.098277	3.099603	-2.154943
H	1.255577	-2.160793	-3.654976	C	0.969548	4.277319	-1.156942
O	2.517736	-1.679681	-0.136376	H	1.334998	3.505675	-3.152938
C	3.853751	-1.307835	-0.177601	H	1.912652	2.434439	-1.845351
C	4.787726	-2.354375	-0.061958	H	1.972410	4.681539	-0.959671
C	6.155164	-2.076048	-0.134616	H	0.382350	5.086799	-1.608811
C	6.566589	-0.747987	-0.318811	O	-2.285229	-0.598546	2.289543
C	5.646675	0.301900	-0.438078	H	-1.650657	0.251745	2.172026
C	4.277989	0.020547	-0.371270	H	-3.139227	-0.246742	2.586504
N	8.012906	-0.444238	-0.392474	P	1.204818	-0.639448	0.696434
O	8.343261	0.742015	-0.545796	O	1.851292	-0.152465	2.128470
O	8.805291	-1.392328	-0.297156	O	0.028004	-1.628088	0.867233
H	4.429213	-3.371149	0.092958	O	1.120099	0.520527	-0.333868
H	6.900181	-2.863888	-0.043141	C	0.971072	0.265871	3.249265
H	6.009926	1.316774	-0.587703	H	0.266727	-0.546650	3.464367
H	3.540183	0.813187	-0.482065	H	1.671711	0.395595	4.080419

1b

Zn	-1.953229	-1.480045	0.284729	H	-1.197315	1.367369	4.583421
Zn	-0.604643	1.751804	-0.096271	H	-1.031065	3.023929	3.956140
O	-2.040508	0.341079	-0.606520	H	0.246991	2.334724	4.991504
N	-4.078522	-1.519288	-0.400342	O	1.174854	-3.047758	-2.101484
N	-2.564127	-3.411845	1.110605	H	1.686297	-2.644130	-1.369413
N	-1.699044	-2.741807	-1.491946	H	1.812655	-3.172639	-2.820918
N	-2.321624	3.118547	-0.524851	O	2.468778	-1.667093	0.180538
N	0.301878	3.869155	0.128220	C	3.804737	-1.308834	0.058281
N	-0.126771	2.255071	-2.170714	C	4.700914	-2.378367	-0.133841
H	-2.308082	-3.399013	2.100069	C	6.065238	-2.122843	-0.294139
H	-0.762176	-2.599124	-1.893330	C	6.513543	-0.794922	-0.255327
H	1.010806	3.818776	0.860010	C	5.631814	0.275490	-0.056831
H	0.113951	1.347892	-2.573434	C	4.265702	0.019977	0.098692
C	-3.331491	0.837945	-0.943556	N	7.955326	-0.514084	-0.426881
C	-4.471288	-0.082079	-0.390641	O	8.318164	0.671853	-0.387107
C	-3.531553	2.264188	-0.346331	O	8.712449	-1.479766	-0.602776

H	4.319837	-3.399214	-0.141187
H	6.779780	-2.930447	-0.440009
H	6.021841	1.290985	-0.027157
H	3.565606	0.837938	0.249479

O	1.099021	0.785403	0.012423
C	2.016853	0.639028	3.206865
H	2.600567	0.357166	4.087937
H	2.437331	1.549887	2.756321
C	0.508957	0.784379	3.497950
H	0.280502	1.823405	3.786311
O	-0.135925	0.512335	2.214809
C	0.032418	-0.182886	4.594877
H	0.517511	0.062669	5.550794
H	-1.054228	-0.119534	4.734185
H	0.288716	-1.215463	4.324640
O	1.092850	-1.890002	-2.439404
H	1.528800	-1.754494	-1.558101
H	1.767481	-2.311022	-2.994133
O	2.283017	-1.457217	0.055102
C	3.604432	-1.157263	-0.102521
C	4.456477	-2.239106	-0.430803
C	5.815904	-2.029576	-0.666588
C	6.329556	-0.727006	-0.565000
C	5.505927	0.359208	-0.232698
C	4.144556	0.146682	-0.004286
N	7.760569	-0.492083	-0.814509
O	8.184366	0.672249	-0.708667
O	8.464479	-1.468874	-1.119542
H	4.032148	-3.242153	-0.480234
H	6.482736	-2.853040	-0.915108
H	5.942135	1.354312	-0.164719
H	3.488682	0.981571	0.230231

TS2

Zn	-1.892028	-1.518371	0.198857
Zn	-0.616439	1.772032	-0.100211
O	-2.072104	0.466522	-0.330667
N	-4.010537	-1.499916	-0.549702
N	-2.501590	-3.496574	0.846435
N	-1.588341	-2.587551	-1.669656
N	-2.476377	3.244461	-0.568856
N	-0.049512	3.659002	0.727942
N	-0.006810	2.632843	-1.961217
H	-2.276579	-3.555998	1.841637
H	-0.644122	-2.360436	-2.031637
H	0.687915	3.478733	1.413448
H	0.513810	1.892416	-2.438965
C	-3.309718	0.890761	-0.899787
C	-4.447434	-0.078160	-0.461417
C	-3.643968	2.327091	-0.418167
H	-3.240654	0.885808	-2.005758
H	-4.684508	0.119098	0.593509
H	-5.358910	0.105715	-1.058615
H	-4.532436	2.717667	-0.948185
H	-3.873227	2.272654	0.654794
C	-4.727080	-2.392104	0.416287
C	-3.965010	-3.727835	0.629755
H	-5.759177	-2.608987	0.089048
H	-4.773737	-1.853698	1.370955
H	-4.412487	-4.249651	1.487048
H	-4.088595	-4.380619	-0.243246
C	-4.022232	-2.038590	-1.952210
C	-2.613414	-2.046122	-2.603658
H	-4.713106	-1.454091	-2.580677
H	-4.412381	-3.063710	-1.918693
H	-2.666939	-2.620085	-3.544137
H	-2.299963	-1.024194	-2.847841
C	-1.597455	-4.404320	0.071663
C	-1.670714	-4.067933	-1.439604
H	-1.845575	-5.466875	0.224529
H	-0.583356	-4.215183	0.442987
H	-0.844824	-4.576729	-1.954743
H	-2.606365	-4.449045	-1.872202
C	-2.453872	4.340608	0.456931
C	-1.246870	4.210150	1.434214
H	-3.378676	4.330465	1.049552
H	-2.420027	5.313624	-0.051555
H	-1.045991	5.193631	1.888674
H	-1.479689	3.499391	2.237339
C	-2.289539	3.748860	-1.970227
C	-1.192613	3.002038	-2.784875
H	-2.028959	4.813312	-1.919227
H	-3.237872	3.679485	-2.528325
H	-1.591357	2.057537	-3.175425
H	-0.914344	3.631427	-3.646979
C	0.963202	3.709580	-1.589931
C	0.484753	4.539929	-0.369665
H	1.158088	4.392616	-2.431961
H	1.897686	3.194309	-1.336976
H	1.321887	5.151444	-0.005226
H	-0.311740	5.229832	-0.667304
O	-2.354878	-0.866284	2.336405
H	-1.467289	-0.352742	2.373691
H	-3.025619	-0.172883	2.440921
P	1.066571	-0.469194	0.993354
O	2.168806	-0.463640	2.258733
O	0.006826	-1.618640	0.834063

2

Zn	2.497294	-0.479546	0.141700
Zn	-0.502722	1.292886	-0.608077
O	1.465003	1.247267	-0.247142
N	4.167975	1.036888	0.261313
N	4.195634	-1.833316	0.339212
N	2.751466	-0.411636	2.306357
N	0.062230	3.509952	-0.974354
N	-2.238547	2.099298	-1.621011
N	-1.424107	2.058013	1.106300
H	4.145634	-2.514631	-0.420344
H	1.796158	-0.530288	2.677035
H	-2.731388	1.298329	-2.024454
H	-1.327147	1.367673	1.865572
C	2.193858	2.473523	-0.209300
C	3.681476	2.190562	-0.552205
C	1.543974	3.474802	-1.195018
H	2.154515	2.914733	0.806534
H	3.759097	1.898205	-1.608308
H	4.299136	3.092666	-0.390550
H	1.989689	4.480476	-1.089742
H	1.710687	3.118652	-2.220646
C	5.323340	0.315860	-0.355900
C	5.500138	-1.095304	0.266763
H	6.267390	0.878813	-0.249681
H	5.095273	0.208177	-1.422764
H	6.230286	-1.652990	-0.335989
H	5.913426	-1.020397	1.280519
C	4.400342	1.388168	1.701199
C	3.223885	0.962393	2.624370
H	4.571017	2.471512	1.810196
H	5.320056	0.888510	2.031240
H	3.551408	1.058227	3.673693
H	2.363064	1.623573	2.478527
C	3.929519	-2.533787	1.635960
C	3.662534	-1.506792	2.766982
H	4.761269	-3.193750	1.930380
H	3.031714	-3.141792	1.474215
H	3.230538	-2.035921	3.627532
H	4.607432	-1.058625	3.104344

O	-7.591838	-0.896951	1.907130
H	-2.887361	-0.998490	2.868078
H	-5.391887	-0.957423	2.918118
H	-5.491728	-1.076234	-1.386652
H	-2.985305	-1.126895	-1.455484

3

Zn	2.395882	-0.533516	0.495535
Zn	-0.617842	1.195762	-0.392739
O	1.383573	1.117415	-0.118838
N	4.071276	0.892684	0.556701
N	4.029198	-1.946334	0.796134
N	2.493550	-0.393828	2.607388
N	0.234745	3.277237	-1.558343
N	-2.087971	1.732727	-1.865698
N	-1.522024	2.898727	0.679111
H	3.991858	-2.669847	0.075574
H	1.532527	-0.458320	3.004212
H	-2.650277	0.893050	-2.025782
H	-1.587096	2.552764	1.639445
C	2.156096	2.321971	-0.252427
C	3.673443	1.991820	-0.371278
C	1.706643	3.068077	-1.534149
H	1.994142	2.964959	0.632446
H	3.875157	1.629974	-1.386505
H	4.270978	2.903125	-0.193224
H	2.252512	4.026001	-1.633248
H	1.967667	2.431550	-2.389835
C	5.252939	0.120768	0.055706
C	5.360405	-1.253889	0.764392
H	6.195277	0.678727	0.191995
H	5.085805	-0.037180	-1.016066
H	6.107966	-1.865469	0.240668
H	5.712216	-1.130786	1.796246
C	4.224409	1.334535	1.985356
C	2.981027	0.998900	2.851057
H	4.415502	2.418091	2.030657
H	5.108877	0.837333	2.403833
H	3.233184	1.160145	3.911646
H	2.145547	1.661210	2.598368
C	3.670479	-2.566018	2.114951
C	3.376267	-1.468648	3.169751
H	4.466588	-3.230049	2.487568
H	2.767001	-3.161681	1.936832
H	2.898032	-1.936014	4.041404
H	4.313577	-1.015588	3.520016
C	-0.360843	3.234799	-2.933042
C	-1.333465	2.033499	-3.125309
H	0.430807	3.154710	-3.691001
H	-0.886335	4.179892	-3.130250
H	-2.014810	2.259537	-3.961633
H	-0.777499	1.119317	-3.362450
C	-0.192680	4.472513	-0.768483
C	-0.689145	4.130587	0.660937
H	-1.001126	4.976868	-1.312032
H	0.635749	5.197099	-0.686709
H	0.162277	3.939253	1.325883
H	-1.237025	5.001984	1.059307
C	-2.914468	3.020137	0.143621
C	-2.978143	2.848572	-1.397502
H	-3.366619	3.987326	0.417142
H	-3.499188	2.223888	0.618587
H	-4.020651	2.657737	-1.686829
H	-2.667927	3.770323	-1.900592
O	2.770991	-0.426554	-2.127548
H	2.510706	-1.231809	-2.618065
H	1.918074	0.036889	-1.978664
P	0.196917	-1.972170	-1.221775
O	-0.970461	-3.147096	-1.075597

O	1.099172	-2.015434	0.047137
O	-0.334290	-0.583022	-1.670601
C	-1.055797	-3.909857	-2.342707
H	-1.462468	-4.889167	-2.079432
H	-1.732446	-3.385451	-3.027667
C	0.387726	-3.984822	-2.900987
H	0.385554	-4.016214	-3.996133
O	0.984199	-2.658560	-2.552837
C	1.232631	-5.114136	-2.308106
H	0.845436	-6.086033	-2.645174
H	2.274166	-5.023767	-2.640498
H	1.202366	-5.085389	-1.211087
O	-0.187145	-0.143207	3.435379
H	-0.714501	-0.086339	2.577413
H	-0.690730	-0.742137	4.008020
O	-1.498853	0.103236	1.130371
C	-2.777494	-0.282371	1.144929
C	-3.566674	-0.113745	2.322571
C	-4.910615	-0.486355	2.354237
C	-5.499541	-1.036830	1.203100
C	-4.750224	-1.235360	0.030774
C	-3.405644	-0.865054	0.004155
N	-6.916050	-1.413272	1.224563
O	-7.409372	-1.880004	0.181296
O	-7.547987	-1.242761	2.281945
H	-3.103828	0.328683	3.206940
H	-5.514950	-0.351536	3.249869
H	-5.231302	-1.688784	-0.834708
H	-2.797405	-1.065948	-0.877659

1'a

Zn	-1.678869	-1.747124	0.304580
Zn	-0.718716	1.720919	-0.167415
O	-1.941237	0.090711	-0.460144
N	-3.663540	-2.063742	-0.581765
N	-1.976675	-3.841391	0.881814
N	-1.015189	-2.754251	-1.540474
N	-2.559063	2.757301	-0.879788
N	-0.118110	4.006594	-0.264972
N	-0.120829	1.975893	-2.242403
H	-1.822844	-3.907540	1.889449
H	-0.127050	-2.346926	-1.865787
H	0.531190	4.181431	0.501411
H	0.270070	1.075951	-2.551213
C	-3.233652	0.353015	-1.015753
C	-4.261913	-0.695833	-0.505252
C	-3.674068	1.788837	-0.630606
H	-3.189260	0.276035	-2.121580
H	-4.477694	-0.498445	0.552480
H	-5.201626	-0.631872	-1.082621
H	-4.585874	2.084609	-1.180420
H	-3.877433	1.805154	0.447457
C	-4.314186	-3.059261	0.322115
C	-3.378968	-4.275994	0.564725
H	-5.277582	-3.416375	-0.081732
H	-4.497439	-2.551516	1.275538
H	-3.793373	-4.878762	1.384285
H	-3.347373	-4.919229	-0.324106
C	-3.498023	-2.569872	-1.982980
C	-2.060544	-2.366576	-2.537030
H	-4.214788	-2.074738	-2.657798
H	-3.743577	-3.639648	-1.989438
H	-1.962507	-2.943617	-3.471784
H	-1.881550	-1.311709	-2.766063
C	-0.901401	-4.600001	0.172018
C	-0.881145	-4.233833	-1.334715
H	-1.019157	-5.690285	0.279991
H	0.044865	-4.300716	0.639161
H	0.054775	-4.602211	-1.776546

H	-1.704585	-4.738718	-1.857956	H	0.631111	4.099961	0.725826
C	-2.657395	3.955085	0.007700	H	0.383799	1.443564	-2.428755
C	-1.360831	4.819896	-0.031350	C	-3.352886	0.538742	-0.792451
H	-2.805506	3.566052	1.021201	C	-4.356571	-0.459417	-0.150976
H	-3.521755	4.591825	-0.252993	C	-3.697054	1.980461	-0.348140
H	-1.437155	5.593497	-0.809059	H	-3.458903	0.470597	-1.895131
H	-1.280850	5.343812	0.930088	H	-4.423196	-0.249983	0.924101
C	-2.394747	3.125797	-2.321960	H	-5.358738	-0.339189	-0.600956
C	-1.335508	2.257282	-3.063854	H	-4.673482	2.288922	-0.767157
H	-2.100925	4.180192	-2.370934	H	-3.743577	2.000962	0.747728
H	-3.356702	3.037986	-2.853718	C	-4.435616	-2.797231	0.712067
H	-1.769102	1.283085	-3.315912	C	-3.568358	-4.077975	0.846491
H	-1.072160	2.759210	-4.009919	H	-5.472286	-3.082222	0.461601
C	0.970141	2.990295	-2.298919	H	-4.440588	-2.266081	1.670273
C	0.578592	4.292328	-1.562945	H	-3.892619	-4.627592	1.740972
H	1.246714	3.236250	-3.338070	H	-3.728477	-4.741277	-0.013346
H	1.837101	2.527428	-1.810388	C	-3.944019	-2.382546	-1.701278
H	1.483905	4.894292	-1.399606	C	-2.595589	-2.284064	-2.466794
H	-0.092150	4.889299	-2.194045	H	-4.718016	-1.838641	-2.266116
O	-2.526713	-1.417122	2.400713	H	-4.262078	-3.431946	-1.654653
H	-2.835430	-0.467527	2.544880	H	-2.686087	-2.851407	-3.408459
H	-1.625638	-1.418424	2.776288	H	-2.374994	-1.239718	-2.713780
H	-3.317174	1.534986	3.498261	C	-1.225169	-4.600329	0.073947
O	-3.100869	1.155726	2.632099	C	-1.429012	-4.250623	-1.421532
P	1.227477	-0.532563	1.152269	H	-1.407923	-5.676628	0.225487
O	1.795917	0.228111	2.488715	H	-0.194433	-4.373081	0.371854
O	0.062697	-1.516076	1.442089	H	-0.620091	-4.706262	-2.008552
O	1.118714	0.422095	-0.081302	H	-2.373057	-4.677509	-1.786033
C	0.946191	1.017585	3.413885	C	-2.676460	4.234600	-0.033847
H	0.189675	0.352216	3.849031	C	-1.372846	4.539269	0.764950
H	1.658053	1.333578	4.183680	H	-3.510245	4.218253	0.679524
C	0.273183	2.218591	2.725832	H	-2.884649	5.044034	-0.748427
H	1.056966	2.754244	2.157329	H	-1.298693	5.628246	0.923855
O	-0.750150	1.751213	1.831985	H	-1.420563	4.044149	1.742267
H	-2.135365	1.461483	2.390436	C	-2.552460	3.100263	-2.255056
C	-0.307089	3.170659	3.796646	C	-1.439695	2.260782	-2.939166
H	0.485315	3.587721	4.433986	H	-2.387060	4.162269	-2.472421
H	-0.834893	4.000553	3.308971	H	-3.521388	2.830900	-2.707133
H	-1.025129	2.642840	4.441551	H	-1.751420	1.212901	-3.012411
O	1.128822	-0.824616	-2.477083	H	-1.285067	2.648003	-3.960955
H	1.274652	-0.432386	-1.570740	C	0.671962	3.473774	-2.210046
H	2.014572	-0.985195	-2.840604	C	0.171560	4.575312	-1.237223
O	2.533857	-1.564456	0.881483	H	0.729688	3.886261	-3.230711
C	3.816028	-1.194982	0.517040	H	1.680773	3.160257	-1.912049
C	4.672156	-2.263251	0.181923	H	0.943740	5.353457	-1.148515
C	5.989237	-2.007130	-0.204384	H	-0.724866	5.060960	-1.636657
C	6.434096	-0.677549	-0.251344	O	-2.164361	-1.297082	2.449802
C	5.596052	0.392147	0.088839	H	-1.209214	-1.171194	2.615870
C	4.276608	0.135128	0.476676	H	-2.550418	-0.391305	2.645099
N	7.824076	-0.395514	-0.669348	H	-3.022099	1.558671	3.710318
O	8.181888	0.791890	-0.710457	O	-2.908880	1.248125	2.798266
O	8.544946	-1.362112	-0.957074	P	1.303605	-0.592473	0.686545
H	4.292895	-3.282950	0.237576	O	1.964877	0.037982	2.055429
H	6.670935	-2.814228	-0.465166	O	0.196694	-1.629020	1.005486
H	5.983959	1.408313	0.052290	O	1.084461	0.497228	-0.397288
H	3.618862	0.954239	0.756406	C	1.905181	1.509230	2.235779

TS1'

Zn	-1.738307	-1.677743	0.253230
Zn	-0.692874	1.771013	-0.086092
O	-2.006845	0.217038	-0.421057
N	-3.857333	-1.858907	-0.297793
N	-2.107552	-3.748310	0.923609
N	-1.451467	-2.764944	-1.634755
N	-2.612442	2.923153	-0.763850
N	-0.162065	3.979461	0.092349
N	-0.178578	2.251931	-2.151843
H	-1.796081	-3.791269	1.895469
H	-0.574010	-2.483094	-2.096280

C	4.845330	-2.229320	0.293162
C	6.204507	-1.942650	0.138814
C	6.581897	-0.654759	-0.267686
C	5.637625	0.347307	-0.525424
C	4.277021	0.056684	-0.377268
N	8.019686	-0.342661	-0.434374
O	8.319357	0.810119	-0.780838
O	8.833412	-1.251722	-0.219035
H	4.512525	-3.214434	0.617429
H	6.968405	-2.692818	0.333417
H	5.975692	1.331197	-0.844868
H	3.520046	0.808691	-0.592949

1'b

Zn	-1.767657	-1.657916	0.239173
Zn	-0.674528	1.795420	-0.095687
O	-2.004707	0.251840	-0.439778
N	-3.889482	-1.794749	-0.305685
N	-2.186496	-3.715074	0.940056
N	-1.511048	-2.779748	-1.625336
N	-2.583197	2.975860	-0.755651
N	-0.124768	4.001694	0.112063
N	-0.159145	2.310342	-2.155174
H	-1.877762	-3.755850	1.912861
H	-0.610557	-2.553974	-2.068119
H	0.670631	4.105078	0.745805
H	0.399853	1.501595	-2.435909
C	-3.345933	0.595829	-0.808177
C	-4.365745	-0.387149	-0.169021
C	-3.675030	2.037496	-0.351093
H	-3.453952	0.535997	-1.911183
H	-4.433339	-0.172363	0.905051
H	-5.364530	-0.253200	-0.622608
H	-4.648852	2.358803	-0.766640
H	-3.721241	2.047544	0.745014
C	-4.489312	-2.710626	0.713272
C	-3.654508	-4.009547	0.863833
H	-5.532847	-2.972032	0.465309
H	-4.481708	-2.168821	1.665621
H	-3.994662	-4.540305	1.763847
H	-3.829443	-4.678659	0.011535
C	-3.986278	-2.327396	-1.705843
C	-2.632551	-2.270188	-2.468639
H	-4.743869	-1.767345	-2.276893
H	-4.331837	-3.367686	-1.652172
H	-2.736754	-2.839315	-3.407834
H	-2.384632	-1.232175	-2.718181
C	-1.330085	-4.601240	0.098255
C	-1.534025	-4.264907	-1.398324
H	-1.540090	-5.670167	0.265873
H	-0.291705	-4.397462	0.384798
H	-0.737281	-4.740588	-1.983182
H	-2.493352	-4.665481	-1.752608
C	-2.636338	4.277458	-0.006623
C	-1.330209	4.559140	0.795714
H	-3.470152	4.257855	0.706587
H	-2.837894	5.098529	-0.709676
H	-1.247964	5.644773	0.972708
H	-1.380793	4.048466	1.764826
C	-2.525365	3.173775	-2.244086
C	-1.421091	2.333684	-2.940301
H	-2.350539	4.236997	-2.447456
H	-3.497311	2.919030	-2.698013
H	-1.741209	1.288712	-3.021006
H	-1.267002	2.728962	-3.959045
C	0.698524	3.527624	-2.199692
C	0.209884	4.617413	-1.207692
H	0.754234	3.954536	-3.214514
H	1.706744	3.204043	-1.910378

H	0.989146	5.387136	-1.108473
H	-0.683554	5.116880	-1.596794
O	-2.156078	-1.246362	2.435147
H	-1.198819	-1.118640	2.587251
H	-2.537742	-0.339452	2.630152
H	-2.976734	1.617893	3.708073
O	-2.873655	1.310655	2.793704
P	1.298867	-0.597265	0.618518
O	1.986527	0.011921	1.985252
O	0.182501	-1.621782	0.941374
O	1.088294	0.506666	-0.450129
C	1.945829	1.481661	2.180945
H	2.761751	1.679957	2.884212
H	2.151805	1.964996	1.218031
C	0.587024	1.934660	2.751930
H	0.639171	3.045356	2.801679
O	-0.493913	1.516567	1.897764
H	-1.886860	1.492640	2.516135
C	0.374042	1.403199	4.184850
H	1.181575	1.741516	4.849608
H	-0.577589	1.767565	4.593925
H	0.361096	0.305829	4.183016
O	1.368118	-2.969908	-2.253235
H	1.865540	-2.604253	-1.491803
H	2.033957	-3.139744	-2.937083
O	2.546830	-1.648290	0.097428
C	3.877011	-1.246757	-0.017055
C	4.845415	-2.149556	0.455537
C	6.202669	-1.843181	0.316434
C	6.562710	-0.631739	-0.290132
C	5.605883	0.274462	-0.764721
C	4.248374	-0.037908	-0.632903
N	7.998871	-0.298116	-0.438063
O	8.283056	0.785386	-0.970542
O	8.825370	-1.121570	-0.022145
H	4.524637	-3.075300	0.931213
H	6.976892	-2.518938	0.674485
H	5.931595	1.199039	-1.237223
H	3.479226	0.636196	-1.006156

TS2'a

Zn	-1.658973	-1.692905	0.193100
Zn	-0.716209	1.758669	-0.301918
O	-1.991797	0.230978	-0.445990
N	-3.749749	-1.908808	-0.480756
N	-2.014586	-3.752952	0.848157
N	-1.249993	-2.734151	-1.663808
N	-2.683666	2.940882	-0.783473
N	-0.252590	3.797170	0.236732
N	-0.252122	2.454181	-2.291603
H	-1.765828	-3.805593	1.837619
H	-0.337030	-2.447462	-2.052738
H	0.542769	3.787557	0.879530
H	0.313718	1.718237	-2.720243
C	-3.316836	0.518135	-0.911873
C	-4.315766	-0.534273	-0.357281
C	-3.739713	1.933106	-0.450339
H	-3.337981	0.473773	-2.019662
H	-4.465662	-0.346063	0.713286
H	-5.289096	-0.448727	-0.873364
H	-4.710319	2.213975	-0.898828
H	-3.828265	1.915928	0.642141
C	-4.356417	-2.875910	0.486783
C	-3.456576	-4.126809	0.670874
H	-5.363972	-3.194424	0.167296
H	-4.439199	-2.352856	1.445604
H	-3.821597	-4.692495	1.538990
H	-3.536591	-4.788514	-0.201041
C	-3.735805	-2.426060	-1.890940

C	-2.346186	-2.285027	-2.570441	Zn	-0.523562	1.303239	-0.468020
H	-4.492953	-1.904703	-2.498119	O	1.432007	1.240681	-0.019123
H	-4.021118	-3.485242	-1.865720	N	4.159782	0.992431	0.309076
H	-2.359255	-2.857025	-3.513423	N	4.182238	-1.870490	0.437269
H	-2.141651	-1.234844	-2.809651	N	2.762865	-0.415029	2.393392
C	-1.054948	-4.570420	0.044089	N	0.043463	3.457146	-0.892614
C	-1.192766	-4.222448	-1.457257	N	-2.311869	2.100610	-1.421646
H	-1.206570	-5.652371	0.186937	N	-1.395003	2.082790	1.268864
H	-0.049933	-4.306168	0.394507	H	4.124737	-2.563132	-0.311184
H	-0.333227	-4.634753	-2.000201	H	1.812801	-0.527172	2.776462
H	-2.101247	-4.677287	-1.874618	H	-2.849117	1.313375	-1.793236
C	-2.742052	4.151174	0.105534	H	-1.280831	1.400599	2.032364
C	-1.452032	4.315770	0.965422	C	2.187073	2.448655	-0.130684
H	-3.596237	4.072203	0.789350	C	3.653296	2.120131	-0.526828
H	-2.906214	5.047787	-0.508238	C	1.514776	3.377009	-1.169747
H	-1.337210	5.374683	1.247879	H	2.206174	2.972873	0.847218
H	-1.539281	3.715725	1.877981	H	3.677879	1.781799	-1.570932
C	-2.648685	3.298663	-2.243431	H	4.289778	3.018552	-0.429257
C	-1.522740	2.595942	-3.058109	H	1.976945	4.380551	-1.161551
H	-2.524208	4.385161	-2.328675	H	1.626390	2.929628	-2.165283
H	-3.614796	3.053180	-2.714005	C	5.310078	0.263199	-0.305829
H	-1.830123	1.575930	-3.319467	C	5.488492	-1.138041	0.338935
H	-1.375463	3.155087	-3.997837	H	6.254659	0.827673	-0.213662
C	0.608530	3.665254	-2.129815	H	5.073822	0.139588	-1.368944
C	0.102340	4.586614	-0.992150	H	6.210822	-1.708775	-0.261127
H	0.675701	4.248379	-3.062589	H	5.912089	-1.046852	1.347113
H	1.611141	3.294315	-1.883299	C	4.405446	1.373406	1.738491
H	0.872010	5.338324	-0.767398	C	3.237609	0.965552	2.680553
H	-0.792552	5.128773	-1.315013	H	4.576949	2.458734	1.823685
O	-2.323309	-1.360272	2.449435	H	5.328454	0.880210	2.069428
H	-1.347778	-1.250092	2.530035	H	3.575173	1.080865	3.724760
H	-2.658343	-0.442203	2.602212	H	2.375621	1.623082	2.528207
H	-2.709901	1.686735	3.569090	C	3.928718	-2.548289	1.747274
O	-2.673593	1.371773	2.651597	C	3.678168	-1.501077	2.863218
P	1.118380	-0.225149	0.998247	H	4.761079	-3.206685	2.044187
O	2.243875	0.100243	2.194206	H	3.027458	-3.156561	1.606364
O	0.090839	-1.405108	1.191493	H	3.259130	-2.013558	3.740415
O	1.026936	0.778129	-0.223868	H	4.628438	-1.048161	3.178128
C	2.101251	1.386227	2.875746	C	-0.744086	3.968022	-2.068594
H	2.760841	1.332313	3.746580	C	-1.812575	2.936790	-2.555350
H	2.436274	2.184698	2.198567	H	-0.063628	4.171576	-2.904538
C	0.614422	1.526662	3.240228	H	-1.221575	4.921419	-1.803410
H	0.362776	2.590367	3.388802	H	-2.628238	3.474721	-3.064220
O	-0.095211	1.033368	2.064575	H	-1.351335	2.243092	-3.267868
H	-1.689283	1.266625	2.429111	C	-0.272231	4.196756	0.383780
C	0.264941	0.718158	4.505215	C	-0.560777	3.278663	1.606891
H	0.770806	1.145621	5.383051	H	-1.144340	4.834679	0.200561
H	-0.815801	0.722969	4.698264	H	0.563080	4.866237	0.646278
H	0.589986	-0.323830	4.386715	H	0.374773	2.878546	2.012757
O	1.523657	-2.500390	-2.129369	H	-1.042714	3.888321	2.389079
H	1.834398	-2.098412	-1.279224	C	-2.853782	2.325686	1.027896
H	2.279364	-2.449774	-2.733547	C	-3.134981	2.840982	-0.409884
O	2.347178	-1.341475	0.266478	H	-3.263585	3.041647	1.757592
C	3.662376	-1.019102	0.056443	H	-3.353507	1.361306	1.173482
C	4.580222	-2.094445	0.061580	H	-4.207905	2.733637	-0.621064
C	5.933330	-1.872636	-0.203030	H	-2.895303	3.906835	-0.492902
C	6.367419	-0.564571	-0.467446	O	2.749810	-0.844998	-1.975941
C	5.474061	0.516928	-0.474655	H	2.116318	-1.615690	-2.081181
C	4.119832	0.290523	-0.216283	H	2.285593	-0.164987	-2.524009
N	7.792792	-0.318901	-0.749131	H	0.705247	0.125300	-4.312841
O	8.145769	0.852792	-0.967071	O	0.791364	0.545294	-3.441881
O	8.558701	-1.295646	-0.755057	P	-0.253936	-1.828644	-0.647731
H	4.213672	-3.095798	0.286792	O	-1.238604	-3.191039	-0.713227
H	6.653736	-2.688364	-0.197925	O	0.950520	-1.800855	0.368153
H	5.850325	1.515492	-0.689812	O	-0.653772	-0.461145	-1.409243
H	3.406761	1.111655	-0.242353	C	-1.028397	-4.075217	-1.870329
				H	-1.228977	-5.089814	-1.513837
				H	-1.748898	-3.796467	-2.648751
				C	0.426524	-3.864340	-2.332354
				H	0.513909	-4.012321	-3.415976
				O	0.642850	-2.438396	-2.091417
2'							
Zn	2.489689	-0.490002	0.220035				

H	0.211796	0.006754	-2.828026	C	-0.084906	4.254542	0.088880
C	1.444801	-4.737988	-1.583350	C	-0.299951	3.526564	1.445409
H	1.283994	-5.798652	-1.824143	H	-0.950897	4.894480	-0.116509
H	2.467145	-4.471276	-1.884389	H	0.786295	4.923018	0.189700
H	1.344552	-4.601177	-0.498767	H	0.653878	3.154285	1.834624
O	-0.207174	-0.240798	2.997485	H	-0.701595	4.256186	2.168785
H	-0.545717	-0.805534	2.245227	C	-2.651933	2.617666	1.177338
H	-0.592436	-0.630738	3.798354	C	-3.036609	2.941384	-0.293007
O	-1.418645	-1.383379	0.832811	H	-2.966905	3.451613	1.825139
C	-2.764360	-1.325869	0.784271	H	-3.180759	1.713669	1.499731
C	-3.473875	-1.309721	2.016449	H	-4.126693	2.855711	-0.400493
C	-4.862091	-1.172940	2.049789	H	-2.767552	3.973141	-0.544055
C	-5.566571	-1.056572	0.840506	O	2.816895	-1.146688	-1.936565
C	-4.899463	-1.108999	-0.394224	H	2.183713	-1.905480	-2.029280
C	-3.509783	-1.242631	-0.424613	H	2.422793	-0.498086	-2.578409
N	-7.024575	-0.877895	0.865391	H	1.007967	-0.053842	-4.411839
O	-7.611303	-0.753527	-0.224129	O	1.156581	0.356147	-3.544616
O	-7.586810	-0.848630	1.973032	P	-0.234626	-1.754259	-0.742376
H	-2.917343	-1.423118	2.946864	O	-1.399292	-2.935818	-0.556942
H	-5.408032	-1.161865	2.991557	O	0.872386	-1.751527	0.365617
H	-5.479934	-1.047238	-1.313734	O	-0.506963	-0.427617	-1.589211
H	-2.988456	-1.290883	-1.377638	C	-1.354930	-3.976527	-1.604716

TS3'

Zn	2.510693	-0.566430	0.241759	H	-2.047408	-3.687900	-2.404171
Zn	-0.521021	1.236968	-0.363923	C	0.103689	-4.045128	-2.102487
O	1.473699	1.166376	-0.039359	H	0.140364	-4.329747	-3.160702
N	4.190791	0.866305	0.204968	O	0.542853	-2.641155	-2.048633
N	4.169249	-1.971466	0.568999	H	0.462392	-0.033197	-2.936287
N	2.773156	-0.350041	2.400899	C	1.009948	-4.952360	-1.259922
N	0.108926	3.332693	-1.085152	H	0.689544	-5.999690	-1.354541
N	-2.333980	2.027158	-1.251901	H	2.048418	-4.879353	-1.609439
N	-1.191143	2.333793	1.331606	H	0.968421	-4.662304	-0.202053
H	4.101654	-2.720168	-0.122576	O	-0.163727	-0.086510	3.023415
H	1.820303	-0.413754	2.791821	H	-0.589739	-0.519249	2.223733
H	-2.946450	1.237242	-1.474729	H	-0.555135	-0.531835	3.791661
H	-1.043362	1.739983	2.159087	O	-1.469508	-0.794840	0.751043
C	2.249628	2.333558	-0.322191	C	-2.811789	-0.878189	0.754385
C	3.695072	1.927044	-0.723270	C	-3.520454	-0.853169	1.988254
C	1.555354	3.153821	-1.435128	C	-4.915714	-0.886050	2.025994
H	2.321490	2.965631	0.586917	C	-5.633208	-0.948444	0.820779
H	3.686856	1.493931	-1.731758	C	-4.968663	-1.000931	-0.415775
H	4.357677	2.811398	-0.721853	C	-3.573677	-0.966222	-0.447755
H	2.053951	4.130691	-1.574350	N	-7.101668	-0.964331	0.851187
H	1.597178	2.583388	-2.371313	O	-7.702988	-1.012441	-0.236328
C	5.335282	0.077828	-0.343579	O	-7.659511	-0.921246	1.960796
C	5.488310	-1.270566	0.411331	H	-2.956271	-0.816447	2.920691
H	6.286555	0.635307	-0.285739	H	-5.457517	-0.869831	2.970210
H	5.107970	-0.123594	-1.396652	H	-5.554496	-1.072240	-1.331179
H	6.200105	-1.901284	-0.139068	H	-3.048229	-1.037330	-1.399516
H	5.912864	-1.104641	1.409492				
C	4.438344	1.361216	1.600486				
C	3.264822	1.045446	2.570332	Zn	-2.428707	0.635749	0.415331
H	4.621087	2.447653	1.594447	Zn	0.540168	-1.249939	-0.307998
H	5.356165	0.888133	1.972709	O	-1.448530	-1.055713	-0.122073
H	3.601080	1.244017	3.602075	N	-4.149782	-0.715388	0.384135
H	2.410002	1.694234	2.356959	N	-4.001287	2.073836	0.943755
C	3.914594	-2.539976	1.930738	N	-2.518493	0.268452	2.547824
C	3.674930	-1.403262	2.959206	N	-0.315349	-3.256263	-1.488215
H	4.742974	-3.179043	2.276609	N	2.158827	-1.983405	-1.500374
H	3.009884	-3.153902	1.843143	N	1.106698	-2.915358	1.001922
H	3.250785	-1.838959	3.874860	H	-3.964444	2.878606	0.315908
H	4.630585	-0.938604	3.237458	H	-1.554814	0.232609	2.924365
C	-0.743306	3.709575	-2.264135	H	2.828533	-1.214462	-1.597848
C	-1.884188	2.673183	-2.522450	H	1.038001	-2.534575	1.951015
H	-0.121102	3.762137	-3.166363	C	-2.291063	-2.177921	-0.426601
H	-1.166222	4.711810	-2.106967	C	-3.753920	-1.708434	-0.658619
H	-2.713820	3.173657	-3.047161	C	-1.751719	-2.906569	-1.679871
H	-1.511235	1.862701	-3.159635	H	-2.292946	-2.883655	0.426506
				H	-3.826691	-1.199254	-1.627924

3'

P	1.195372	-0.919636	0.634717	H	-2.407966	-5.246583	-0.866832
O	2.087101	-1.427532	1.916871	H	-1.029532	-4.207522	-0.395678
O	-0.004549	-1.838411	0.326681	H	-1.292795	-3.997461	-2.805470
O	1.043772	0.621689	0.624847	H	-3.037409	-3.744734	-2.685690
C	2.208704	-0.571428	3.124699	C	-1.863032	4.489145	0.829663
H	3.201004	-0.807822	3.523849	C	-0.391135	5.007847	0.910041
H	2.163326	0.479139	2.813922	H	-2.145102	4.043951	1.790666
C	1.107392	-0.893758	4.149783	H	-2.533363	5.343952	0.629342
H	1.253665	-0.204473	5.000619	H	-0.251936	5.870471	0.242738
O	-0.208711	-0.676127	3.572043	H	-0.218404	5.368389	1.932856
H	-0.350210	0.261492	3.249932	C	-1.759692	3.882679	-1.580384
C	1.146987	-2.344294	4.643175	C	-0.911237	2.890608	-2.435797
H	2.097305	-2.553628	5.152571	H	-1.232559	4.840753	-1.510399
H	0.325408	-2.518318	5.348291	H	-2.709374	4.079313	-2.105379
H	1.042354	-3.032983	3.795283	H	-1.549616	2.079894	-2.802985
O	0.746158	-0.803923	-2.976803	H	-0.527142	3.435933	-3.314534
H	1.350649	-1.102105	-2.259730	C	1.485148	2.973665	-1.603406
H	1.243223	-0.944563	-3.798639	C	1.392127	4.223355	-0.697114
O	2.280264	-1.381363	-0.628441	H	1.832984	3.287949	-2.602366
C	3.635371	-1.073607	-0.632717	H	2.210051	2.262485	-1.190324
C	4.471956	-1.981803	-1.308183	H	2.409218	4.570275	-0.466067
C	5.843049	-1.726505	-1.401587	H	0.890176	5.038205	-1.234491
C	6.356855	-0.566667	-0.804709	O	-2.558593	-1.324515	2.176003
C	5.535664	0.340358	-0.122455	H	-1.617284	-1.075974	2.552737
C	4.161936	0.088628	-0.038527	H	-3.096345	-0.563752	2.451645
N	7.808126	-0.289201	-0.898039	H	-0.380152	2.484895	2.982220
O	8.230182	0.743312	-0.355738	O	-0.903030	1.880657	2.431417
O	8.509660	-1.103689	-1.514212	P	1.076970	-0.936749	0.834274
H	4.040879	-2.883851	-1.741291	O	2.012122	-1.499039	2.071596
H	6.514234	-2.411807	-1.915468	O	-0.129254	-1.813891	0.412261
H	5.976437	1.228337	0.326690	O	1.107344	0.613429	0.671357
H	3.500082	0.785369	0.472882	C	1.987114	-0.790209	3.368959

TS2'b

Zn	-2.089756	-1.373054	-0.002785	H	2.723942	-1.321015	3.979293
Zn	-0.492086	1.907594	0.374977	H	2.304885	0.247117	3.201667
O	-2.005244	0.634507	-0.234191	C	0.561510	-0.845158	3.949728
N	-4.189129	-1.026659	-0.696536	H	0.494827	-0.118867	4.778627
N	-2.864400	-3.404229	0.181651	O	-0.307305	-0.437586	2.868241
N	-1.888028	-2.059620	-2.093678	H	-0.564865	0.792359	2.730834
N	-2.020787	3.405892	-0.184389	C	0.176017	-2.246094	4.451254
N	0.623761	3.950954	0.569010	H	0.829274	-2.555734	5.279105
N	0.190387	2.242911	-1.669197	H	-0.861598	-2.247921	4.808863
H	-2.647476	-3.688042	1.138911	H	0.269894	-2.974757	3.635575
H	-0.943350	-1.794486	-2.403761	O	0.788939	-0.766285	-2.758856
H	1.290324	3.872153	1.337327	H	1.315941	-1.095274	-1.988377
H	0.367723	1.312692	-2.069054	H	1.352729	-0.924862	-3.533087
C	-3.211960	1.265011	-0.662094	O	2.177670	-1.505765	-0.417861
C	-4.441733	0.388055	-0.292755	C	3.534219	-1.249994	-0.445379
C	-3.315341	2.673572	-0.024290	C	4.314075	-2.144690	-1.207438
H	-3.209782	1.385638	-1.764816	C	5.690008	-1.941220	-1.338342
H	-4.574662	0.398169	0.797828	C	6.275598	-0.842015	-0.693437
H	-5.359920	0.787578	-0.761071	C	5.516470	0.050077	0.076011
H	-4.155226	3.244496	-0.460504	C	4.138093	-0.150902	0.199393
H	-3.479855	2.560847	1.055436	N	7.729100	-0.614735	-0.829202
C	-4.983153	-2.030985	0.073240	O	8.215022	0.366891	-0.245088
C	-4.346646	-3.444378	-0.037340	O	8.375394	-1.415566	-1.521121
H	-6.033263	-2.077892	-0.265779	H	3.830594	-3.001181	-1.676969
H	-4.973078	-1.713765	1.122537	H	6.311562	-2.620662	-1.918289
H	-4.833204	-4.104970	0.693697	H	6.010791	0.888530	0.563185
H	-4.538588	-3.868872	-1.030905	H	3.529143	0.539675	0.778691
C	-4.268211	-1.243739	-2.178613				
C	-2.875507	-1.257933	-2.867029				
H	-4.893520	-0.466321	-2.646767				
H	-4.769610	-2.203845	-2.356271				
H	-3.002085	-1.634331	-3.896731				
H	-2.468211	-0.243084	-2.925986				
C	-2.054810	-4.205947	-0.784361				
C	-2.079078	-3.542927	-2.186968				

Electronic energies (E), zero-point energies (ZPE), enthalpies (H), free energies (G) (in hartree) and solvation free energies (ΔG_{solv}) (in kcal/mol) for all species included in Scheme 4 and 5

	E	ZPE	H	G	ΔG_{solv}
H_2O	-76.43628312	-76.415386	-76.411606	-76.433054	-6.61
1a	-2539.13326685	-2538.380729	-2538.331776	-2538.461663	-43.11
TS1	-2539.12877683	-2538.376338	-2538.328210	-2538.455034	-43.22
1b	-2539.13908767	-2538.385521	-2538.337383	-2538.463694	-41.59
TS2	-2539.12064917	-2538.366361	-2538.318884	-2538.444603	-53.28
2	-2539.13257689	-2538.376375	-2538.328872	-2538.453667	-44.47
TS3	-2539.13197773	-2538.376806	-2538.329589	-2538.453880	-43.94
3	-2539.14342248	-2538.388896	-2538.339914	-2538.470859	-43.11
1'a	-2615.59350725	-2614.814015	-2614.763469	-2614.895527	-36.01
TS1'	-2615.58361204	-2614.804993	-2614.754644	-2614.885895	-36.81
1'b	-2615.58454542	-2614.805495	-2614.754449	-2614.887789	-37.88
TS2'a	-2615.57263191	-2614.792600	-2614.742730	-2614.872993	-46.03
2'	-2615.59300023	-2614.811663	-2614.761704	-2614.891342	-38.69
TS3'	-2615.59161458	-2614.811341	-2614.761741	-2614.890712	-39.08
3'	-2615.59926935	-2614.818659	-2614.767835	-2614.900842	-41.47
1'c	-2615.59003829	-2614.810085	-2614.759556	-2614.891317	-39.97
TS2'b	-2615.58355536	-2614.808290	-2614.758501	-2614.887946	-40.95