Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Structural and energetic aspects of the substrate binding and mechanism of action of the DapE-encoded N-succinyl-$_{L,L}$-diaminopimelic acid desuccinylase (DapE) from hybrid QM/MM method

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Table S1: The pKa of the side chains of the active site residues obtained from PropKa program.

Residue	pKa
Asp100	1.57
Glu134	2.55
Glu135	2.41
Glu163	3.17
His67	10.55
His349	7.73

Table S2: The convergence of energy (in a.u.) and geometry (rmsd in Å) for iterative optimization, during the linear transit scan along O6-H1 (step 1), C1-O5 (step 2) and N3-H1 (step 3) distances, with improved partial charges obtained from each iteration of restrained electrostatic potential calculation of the QM atoms.

Distance (Å)	Iteration 1 (a.u.)	Iteration 2 (a.u.)	Iteration 3 (a.u.)	Δ_{12} (kcal/mol)	Δ_{23} (kcal/mol)	$RMSD_{12}$	$RMSD_{23}$
			Step 1				
1.30	-6272.893867	-6272.894923	-6272.894911	0.664	0.008	0.012	0.002
1.25	-6272.895759	-6272.894259	-6272.894240	0.941	0.012	0.003	0.001
1.20	-6272.893497	-6272.891342	-6272.891488	1.352	0.092	0.012	0.003
1.15	-6272.896473	-6272.898590	-6272.898431	1.328	0.010	0.007	0.003
1.10	-6272.900364	-6272.894310	-6272.895091	3.800	0.490	0.018	0.005
			Step 2				
3.40	-6272.882562	-6272.892781	-6272.892551	6.412	0.144	0.055	0.015
3.00	-6272.879434	-6272.880139	-6272.880427	0.442	0.181	0.067	0.014
2.70	-6272.864735	-6272.864146	-6272.864150	0.370	0.004	0.041	0.012
2.60	-6272.845060	-6272.860427	-6272.860342	9.643	0.053	0.071	0.025
2.50	-6272.856002	-6272.856519	-6272.856385	0.324	0.084	0.054	0.017
2.40	-6272.851197	-6272.849856	-6272.850728	0.841	0.547	0.069	0.028
2.30	-6272.844000	-6272.845614	-6272.846067	1.013	0.284	0.055	0.019
2.20	-6272.897370	-6272.897850	-6272.898721	0.301	0.548	0.054	0.013
2.10	-6272.894712	-6272.893417	-6272.893272	0.813	0.092	0.067	0.021
2.00	-6272.883851	-6272.884347	-6272.884845	0.311	0.312	0.055	0.012
1.90	-6272.889251	-6272.878362	-6272.879267	6.833	0.569	0.526	0.057
1.80	-6272.873637	-6272.866076	-6272.865913	4.745	0.102	0.325	0.037
1.70	-6272.864269	-6272.862890	-6272.862210	0.865	0.428	0.426	0.033
1.60	-6272.872698	-6272.864107	-6272.864033	5.391	0.046	0.038	0.031
1.50	-6272.865224	-6272.897856	-6272.900260	20.477	1.51	0.558	0.049
			Step 3				
1.91	-6272.898319	-6272.907361	-6272.906551	5.674	0.508	0.196	0.026
1.81	-6272.895228	-6272.904376	-6272.903121	5.740	0.788	0.028	0.004
1.71	-6272.900878	-6272.890715	-6272.892065	6.377	0.847	0.052	0.006
1.61	-6272.901178	-6272.890105	-6272.890913	6.948	0.507	0.046	0.004
1.51	-6272.900992	-6272.890878	-6272.890763	6.347	0.072	0.041	0.005
1.41	-6272.900492	-6272.890389	-6272.890446	6.340	0.036	0.042	0.004
1.31	-6272.900077	-6272.889873	-6272.889922	6.403	0.031	0.038	0.003
1.21	-6272.900830	-6272.890257	-6272.891307	6.635	0.659	0.039	0.006
1.11	-6272.902262	-6272.907702	-6272.909184	3.414	0.930	0.062	0.006

Table S3: The convergence of NBO charges of the reactant state for iterative optimization with improved partial charges obtained from each iteration of restrained electrostatic potential calculation of the QM atoms.

Atoms	iteration 1	iteration 2	iteration 3	ΔNBO_{12}	ΔNBO_{23}
Zn1	1.31590	1.31672	1.31385	0.00082	0.00287
Zn2	1.28721	1.30887	1.31014	0.02166	0.00127
O1	-0.83187	-0.83955	-0.83946	0.00768	0.00000
O2	-0.81573	-0.80279	-0.80939	0.01294	0.00660
O3	-0.79645	-0.78904	-0.78983	0.00741	0.00079
O4	-0.73126	-0.74569	-0.74610	0.01443	0.00041
O5	-1.06531	-1.09662	-1.09642	0.03131	0.00020
O6	-0.77292	-0.77475	-0.77365	0.00183	0.00110
N1	-0.61879	-0.59503	-0.59313	0.02376	0.00190
N2	-0.56142	-0.55093	-0.55102	0.01049	0.00000
H1	0.53655	0.53150	0.53193	0.00505	0.00043
H2	0.50757	0.51386	0.51440	0.00629	0.00054
O7	-0.84418	-0.82955	-0.82831	0.01463	0.00124
O8	-0.73244	-0.79833	-0.79751	0.06589	0.00082
C1	0.73439	0.73068	0.72971	0.00371	0.00097
N3	-0.64318	-0.61930	-0.61834	0.02388	0.00096

Table S4: The convergence of energy (in a.u.) and geometry (rmsd in Å) for iterative optimization, of the critical points along the enzymatic reaction with improved partial charges obtained from each iteration of restrained electrostatic potential calculation of the QM atoms from B3LYP, CAM-B3LYP, and M06-2X functionals when only one water molecule (the catalytic water molecule) is treated in QM region (model 1).

Point	Iteration 1 (a.u.)	Iteration 2 (a.u.)	Iteration 3 (a.u.)	Δ_{12} (kcal/mol)	Δ_{23} (kcal/mol)	$RMSD_{12}$	$RMSD_{23}$
			B3LYP				
R	-6272.903834	-6272.896167	-6272.895543	4.811	0.392	0.182	0.017
TS1	-6272.905157	-6272.893152	-6272.891728	7.533	0.984	0.214	0.041
IN1	-6272.902969	-6272.906505	-6272.907701	2.970	0.750	0.153	0.027
TS2	-6272.848537	-6272.849342	-6272.849694	0.505	0.221	0.128	0.007
IN2	-6272.906568	-6272.903176	-6272.902215	2.128	0.603	0.178	0.012
TS3	-6272.861238	-6272.863776	-6272.862668	1.593	0.695	0.078	0.021
TD	-6272.908362	-6272.907309	-6272.907315	0.661	0.004	0.012	0.002
TS4	-6272.894029	-6272.889916	-6272.889927	2.581	0.007	0.029	0.005
P	-6272.899004	-6272.897127	-6272.898082	1.178	0.600	0.121	0.011
			CAM-B3LYP				
R	-6271.905144	-6271.906796	-6271.906362	1.036	-0.272	0.006	0.001
TS1	-6271.889713	-6271.899945	-6271.899712	6.420	-0.146	0.319	0.118
IN1	-6271.921943	-6271.921414	-6271.921457	-0.331	0.026	0.007	0.003
TS2	-6271.882017	-6271.876902	-6271.877521	-3.209	0.388	0.053	0.010
IN2	-6271.919555	-6271.917616	-6271.917064	-1.216	-0.346	0.019	0.008
TS3	-6271.907056	-6271.904520	-6271.904936	-1.591	0.261	0.310	0.102
TD	-6271.922532	-6271.923957	-6271.924219	0.894	0.164	0.073	0.002
TS4	-6271.902572	-6271.907904	-6271.909910	3.345	1.258	0.090	0.018
P	-6271.906791	-6271.914214	-6271.914521	4.657	0.192	0.081	0.009
			M06-2X				
R	-6271.742353	-6271.731217	-6271.729312	6.987	1.195	0.034	0.006
TS1	-6271.732100	-6271.721797	-6271.721350	6.465	0.280	0.050	0.021
IN1	-6271.751422	-6271.750767	-6271.750489	0.411	0.174	0.019	0.006
TS2	-6271.697691	-6271.708264	-6271.708026	6.634	0.149	0.025	0.003
IN2	-6271.739226	-6271.734650	-6271.734720	2.871	0.043	0.055	0.009
TS3	-6271.714182	-6271.714516	-6271.714815	0.209	0.187	0.061	0.012
TD	-6271.764109	-6271.760596	-6271.761250	2.204	0.410	0.022	0.004
TS4	-6271.760606	-6271.752135	-6271.753641	5.315	0.945	0.110	0.060
P	-6271.749584	-6271.757185	-6271.759562	4.769	1.491	0.122	0.014

Table S5: The convergence of energy (in a.u.) and geometry (rmsd in Å) for iterative optimization, of the critical points along the enzymatic reaction with improved partial charges obtained from each iteration of restrained electrostatic potential calculation of the QM atoms from B3LYP, CAM-B3LYP, and M06-2X functionals when nine water molecules in the active site are in treated in QM region (model 2).

Point	Iteration 1 (a.u.)	Iteration 2 (a.u.)	Iteration 3 (a.u.)	Δ_{12} (kcal/mol)	Δ_{23} (kcal/mol)	$RMSD_{12}$	$RMSD_{23}$
			B3LYP				
R	-6807.901321	-6807.870378	-6807.864347	19.42	3.78(Δ_{34}=0.110)	0.582	0.344 ($RMSD_{34}$=0.008)
TS1	-6807.872243	-6807.857124	-6807.859987	9.49	1.80	0.303	0.012
IN1	-6807.915289	-6807.881070	-6807.881217	21.47	0.09	0.635	0.005
TS2	-6807.820519	-6807.841286	-6807.843492	13.03	1.38	0.457	0.038
IN2	-6807.888386	-6807.873486	-6807.870528	9.35	1.86	0.219	0.027
TS3	-6807.859333	-6807.843625	-6807.841012	9.86	1.64	0.378	0.014
TD	-6807.909580	-6807.880809	-6807.880731	18.05	0.06	0.568	0.009
TS4	-6807.891017	-6807.873219	-6807.871212	11.17	1.26	0.498	0.091
PDT	-6807.900955	-6807.887655	-6807.884942	8.35	1.70	0.312	0.031
			CAM-B3LYP				
R	-6806.678757	-6806.690355	-6806.689846	7.28	0.32	0.434	0.045
TS1	-6806.673399	-6806.684666	-6806.685277	7.07	0.38	0.478	0.034
IN1	-6806.694484	-6806.709312	-6806.709886	9.30	0.38	0.612	0.056
TS2	-6806.679377	-6806.676878	-6806.674461	1.57	1.52	0.192	0.080
IN2	-6806.701058	-6806.691250	-6806.693456	6.15	1.38	0.209	0.049
TS3	-6806.662592	-6806.676789	-6806.676543	8.91	0.15	0.581	0.009
TD	-6806.705544	-6806.714942	-6806.715263	5.89	0.20	0.375	0.018
TS4	-6806.712786	-6806.705131	-6806.705263	4.80	0.08	0.212	0.008
PDT	-6806.718777	-6806.720497	-6806.721685	1.08	0.74	0.159	0.027
			M06-2X				
R	-6806.470088	-6806.462884	-6806.462953	4.52	0.04	0.309	0.009
TS1	-6806.467743	-6806.459212	-6806.459375	5.35	0.10	0.387	0.027
IN1	-6806.489615	-6806.485444	-6806.484788	2.61	0.41	0.293	0.019
TS2	-6806.463099	-6806.452072	-6806.453111	6.92	0.65	0.505	0.030
IN2	-6806.484319	-6806.472948	-6806.472392	7.13	0.35	0.769	0.012
TS3	-6806.455824	-6806.451912	-6806.456376	2.45	0.96	0.270	0.018
TD	-6806.498988	-6806.496132	-6806.495366	1.79	0.48	0.193	0.021
TS4	-6806.480136	-6806.486245	-6806.484255	3.83	1.25	0.275	0.034
PDT	-6806.498940	-6806.507756	-6806.508192	5.53	0.27	0.412	0.023

Table S6: Geometric characterization of the active site of DapE during its enzymatic action on SDAP. The important bond distances in the active site of DapE crystal structure (C) and in the critical points during the hydrolysis of SDAP by DapE are given in Å. The reactant state, the tetrahedral intermediate, and the product states are referred as R, TD, and P, respectively. TS1 through TS4 represent four transition states while IN1 and IN2 represent two intermediates observed during the (B3LYP/CAM-B3LYP/M06-2X)//Amber study of the reaction. The coordination number (CN) of both the Zn atoms are shown for the crystal structure, all intermediates, and transition states (model 1).

Bond	**C**	**R**	**TS1**	**IN1**	**TS2**	**IN2**	**TS3**	**TD**	**TS4**	**P**
Zn1-Zn2	3.58	3.68/ 3.66/ 3.59	3.66/ 3.63/ 3.58	3.61/ 3.56/ 3.46	3.76/ 3.72/ 3.81	4.59/ 4.62/ 3.98	3.83/ 3.53/ 3.38	3.51/ 3.46/ 3.50	3.53/ 3.49/ 3.65	3.58/ 3.53/ 3.46
Zn2-O2(E135)	1.99	1.96/ 1.95/ 1.98	1.96/ 1.94/ 1.98	1.95/ 1.93/ 1.96	1.95/ 1.94/ 1.93	1.89/ 1.88/ 1.93	1.96/ 1.95/ 2.00	1.95/ 1.93/ 1.95	1.94/ 1.92/ 2.19	1.93/ 1.92/ 1.94
Zn1-O1(E163)	2.05	1.99/ 1.97/ 2.07	2.00/ 1.97/ 2.07	2.04/ 2.04/ 2.04	2.12/ 2.09/ 2.05	2.00/ 1.97/ 1.99	2.09/ 1.99/ 2.05	1.97/ 1.95/ 1.97	1.97/ 1.95/ 2.00	1.97/ 1.95/ 2.02
Zn2-O4(D100)	1.97	1.99/ 1.98/ 2.02	1.99/ 2.00/ 2.02	2.01/ 2.00/ 2.01	2.09/ 2.06/ 2.05	3.30/ 3.38/ 2.29	2.09/ 2.08/ 2.11	2.12/ 2.09/ 2.09	2.08/ 2.06/ 2.19	2.05/ 2.04/ 2.02
Zn1-O3(D100)	2.01	2.04/ 2.01/ 2.05	2.05/ 2.01/ 2.06	2.02/ 2.01/ 2.07	1.99/ 1.97/ 2.00	1.94/ 1.92/ 1.93	1.99/ 1.98/ 2.00	1.98/ 1.96/ 1.99	1.99/ 1.97/ 2.00	1.99/ 1.97/ 2.03
Zn2-N2(H349)	2.22	2.13/ 2.12/ 2.16	2.14/ 2.10/ 2.16	2.16/ 2.15/ 2.16	2.12/ 2.10/ 2.12	2.06/ 2.03/ 2.10	2.15/ 2.14/ 2.13	2.17/ 2.14/ 2.14	2.19/ 2.15/ 2.12	2.17/ 2.16/ 2.18
Zn1-N1(H67)	2.15	2.25/ 2.20/ 2.18	2.26/ 2.18/ 2.19	2.22/ 2.12/ 2.17	2.13/ 2.11/ 2.08	2.07/ .045/ 2.06	2.09/ 2.07/ 2.13	2.12/ 2.09/ 2.11	2.09/ 2.07/ 2.11	2.07/ 2.05/ 2.06
Zn2-O5(WAT)	2.12	3.79/ 3.72/ 3.79	3.80/ 3.65/ 3.80	3.84/ 3.81/ 3.79	4.04/ 4.03/ 4.33	3.71/ 3.66/ 3.42	4.22/ 3.98/ 3.38	4.14/ 4.12/ 4.13	4.18/ 4.14/ 4.04	4.20/ 4.15/ 4.19
Zn1-O5(WAT)	2.22	1.98/ 1.95/ 2.00	1.96/ 1.95/ 2.00	1.93/ 1.92/ 1.95	1.95/ 1.94/ 2.09	1.93/ 1.92/ 1.89	2.03/ 2.38/ 2.05	2.60/ 2.59/ 2.54	2.67/ 2.62/ 2.18	2.71/ 2.66/ 2.81
H1(WAT)-O5(WAT)		1.07/ 1.04/ 1.12	1.19/ 1.13/ 1.14	1.46/ 1.51/ 1.50	1.45/ 1.46/ 1.77	1.58/ 1.45/ 1.53	1.86/ 1.59/ 1.90	3.32/ 3.05/ 3.00	2.85/ 2.86/ 2.72	2.78/ 2.74/ 2.76
H2(WAT)-O5(WAT)		0.97/ 0.97/ 0.97	0.97/ 0.97/ 0.97	0.97/ 0.97/ 0.96	0.97/ 0.97/ 0.96	0.97/ 0.96/ 0.97	0.97/ 0.95/ 0.97	1.03/ 1.03/ 1.04	1.05/ 1.04/ 1.07	1.05/ 1.04/ 1.05
H1(WAT)-O6(E134)		1.35/ 1.37/ 1.28	1.21/ 1.28/ 1.20	1.03/ 1.02/ 1.05	1.08/ 1.04/ 1.06	1.04/ 1.04/ 1.06	1.01/ 1.02/ 0.99	1.00/ 1.06/ 1.06	1.32/ 1.21/ 1.29	1.63/ 1.58/ 1.56
H2(WAT)-O9(SDAP)		8.77/ 6.77/ 6.74	6.83/ 6.73/ 6.76	5.97/ 5.92/ 5.85	4.97/ 5.22/ 5.10	4.46/ 4.42/ 4.61	5.12/ 4.24/ 4.66	1.51/ 1.49/ 1.46	1.47/ 1.47/ 1.39	1.47/ 1.46/ 1.43
C1(SDAP)-N3(SDAP)		1.31/ 1.31/ 1.28	1.31/ 1.30/ 1.28	1.32/ 1.31/ 1.30	1.32/ 1.31/ 1.29	1.34/ 1.33/ 1.33	1.37/ 1.37/ 1.40	1.49/ 1.50/ 1.50	1.56/ 1.53/ 1.49	1.66/ 1.69/ 1.67
C1(SDAP)-O5(WAT)		3.88/ 3.86/ 3.89	3.89/ 3.85/ 3.90	3.43/ 3.35/ 3.31	2.38/ 2.40/ 2.42	2.15/ 2.16/ 2.19	1.67/ 1.66/ 1.64	1.39/ 1.38/ 1.38	1.38/ 1.37/ 1.40	1.37/ 1.37/ 1.36
C1(SDAP)-O7(SDAP)		1.28/ 1.27/ 1.29	1.28/ 1.28/ 1.29	1.27/ 1.27/ 1.27	1.28/ 1.27/ 1.28	1.28/ 1.27/ 1.26	1.35/ 1.36/ 1.34	1.41/ 1.40/ 1.39	1.37/ 1.38/ 1.38	1.29/ 1.27/ 1.27
H1(WAT)-N3(SDAP)		4.37/ 4.34/ 4.37	4.38/ 4.18/ 4.36	3.98/ 4.09/ 4.86	3.54/ 3.55/ 3.31	3.43/ 3.54/ 3.41	2.37/ 3.45/ 3.67	1.96/ 1.56/ 1.54	1.23/ 1.30/ 1.25	1.08/ 1.05/ 1.03
Zn2-O8(SDAP)		1.98/ 1.97/ 2.02	1.99/ 1.99/ 2.02	2.00/ 1.99/ 2.00	2.04/ 2.03/ 2.04	1.96/ 1.94/ 2.05	2.06/ 2.03/ 2.06	2.11/ 2.10/ 2.10	2.11/ 2.09/ 2.11	2.10/ 2.09/ 2.11
Zn2-O7(SDAP)		2.36/ 2.25/ 2.15	2.34/ 2.19/ 2.15	2.18/ 2.14/ 2.11	2.04/ 2.03/ 2.07	1.91/ 1.89/ 1.93	2.01/ 2.03/ 2.00	1.99/ 1.98/ 1.98	2.03/ 1.99/ 1.95	2.09/ 2.05/ 2.09
Zn1-O7(SDAP)		2.06/ 2.14/ 2.08	2.07/ 2.13/ 2.07	2.32/ 2.17/ 2.16	2.26/ 2.24/ 2.17	3.42/ 3.40/ 3.19	2.18/ 2.00/ 2.20	1.94/ 1.93/ 1.95	1.96/ 1.93/ 2.00	1.99/ 1.97/ 1.99

Table S7: Geometric characterization of the active site of DapE during its enzymatic action on SDAP. The important bond distances in the active site of DapE in the critical points during the hydrolysis of SDAP by DapE are given in Å. The reactant state, the tetrahedral intermediate, and the product states are referred as R, TD, and P, respectively. TS1 through TS4 represent four transition states while IN1 and IN2 represent two intermediates observed during the (B3LYP/CAM-B3LYP/M06-2X)//Amber study of the reaction. The coordination number (CN) of both the Zn atoms are shown for the crystal structure, all intermediates, and transition states (model 2).

Bond	**R**	**TS1**	**IN1**	**TS2**	**IN2**	**TS3**	**TD**	**TS4**	**P**
Zn1-Zn2	3.73/3.67/3.55	3.63/3.65/3.56	3.98/3.95/3.47	4.66/4.10/ 4.19	4.86/4.87/4.48	3.66/3.54/3.54	3.47/3.46/3.49	3.54/3.49/3.53	3.65/3.55/3.52
Zn2-O2(E135)	1.99/1.98/2.00	1.94/1.98/2.00	1.97/1.95/1.96	2.71/1.93/ 2.41	2.10/2.11/2.17	1.97/1.95/1.98	1.92/1.93/1.94	1.96/1.94/1.94	1.95/1.93/1.95
Zn1-O1(E163)	2.00/1.99/2.10	1.96/1.99/2.09	2.05/2.02/2.08	2.04/1.95/ 2.08	2.06/2.02/2.06	2.06/1.99/2.01	1.94/1.96/1.96	2.01/1.99/1.99	2.03/2.03/2.02
Zn2-O4(D100)	1.99/1.99/2.03	2.00/2.01/2.04	2.08/2.05/2.01	3.63/2.11/ 3.30	3.87/3.85/3.58	2.10/2.08/2.08	2.08/2.08/2.09	2.08/2.08/2.10	2.08/2.05/2.06
Zn1-O3(D100)	2.01/1.99/2.03	2.01/1.99/2.03	1.93/1.91/2.09	1.95/2.04/ 2.01	1.97/1.93/2.00	1.98/1.94/1.99	1.96/1.96/1.97	1.98/1.95/1.96	1.98/1.97/1.99
Zn2-N2(H349)	2.08/2.07/2.11	2.10/2.08/2.12	2.11/2.09/2.12	2.08/2.00/ 2.12	2.04/2.02/2.08	2.11/2.13/2.13	2.14/2.13/2.15	2.16/2.10/2.11	2.14/2.12/2.14
Zn1-N1(H67)	2.21/2.18/2.19	2.18/2.14/2.16	2.07/2.05/2.15	2.06/2.04/ 2.10	2.07/2.05/2.08	2.11/2.06/2.09	2.09/2.10/2.11	2.10/2.09/2.12	2.04/2.02/2.03
Zn2-O5(WAT)	3.77/3.72/3.72	3.64/3.70/3.70	3.50/3.51/3.96	3.92/4.45/ 3.67	3.91/3.88/3.69	4.13/4.29/4.15	4.12/4.11/4.13	4.17/4.12/4.15	4.43/4.22/4.45
Zn1-O5(WAT)	2.03/2.01/2.06	1.95/2.02/2.06	1.90/1.88/1.99	2.00/2.08/ 1.95	1.81/1.83/1.82	2.30/2.71/2.51	2.59/2.57/2.59	2.62/2.56/2.57	3.01/3.02/3.05
H1(WAT)-O5(WAT)	1.01/1.01/1.01	1.1/1.23/1.18	1.39/1.37/1.32	1.46/1.53/ 1.49	1.63/1.58/1.66	1.95/1.85/1.93	3.06/3.12/3.06	2.88/2.89/2.85	3.06/3.04/3.05
H2(WAT)-O5(WAT)	0.97/0.97/0.97	0.97/0.97/0.97	0.96/0.96/0.96	0.96/0.96/ 0.96	0.96/0.96/0.96	0.96/0.96/0.96	1.03/1.03/1.03	1.06/1.06/1.07	1.04/1.05/0.98
H1(WAT)-O6(E134)	1.55/1.53/1.49	1.28/1.34/1.25	1.03/1.05/1.04	1.04/1.02/ 1.04	1.01/1.04/1.04	1.02/1.00/1.07	1.04/1.04/1.07	1.30/1.20/1.29	2.80/2.72/2.68
H2(WAT)-O9(SDAP)	6.85/6.79/6.84	6.73/6.68/6.79	5.56/5.49/5.86	4.45/5.27/ 4.36	4.46/4.43/4.48	4.16/3.85/4.08	1.49/1.40/1.47	1.41/1.39/1.37	1.50/1.51/1.52
C1(SDAP)-N3(SDAP)	1.30/1.29/1.28	1.30/1.29/1.28	1.32/1.31/1.29	1.32/1.29/ 1.32	1.33/1.33/1.33	1.36/1.36/1.37	1.49/1.49/1.51	1.57/1.52/1.55	2.74/2.59/2.65
C1(SDAP)-O5(WAT)	3.93/3.90/3.97	3.85/3.84/3.92	3.67/3.66/3.40	2.37/2.51/ 2.32	2.21/2.18/2.04	1.65/1.72/1.73	1.38/1.38/1.36	1.37/1.37/1.36	1.35/1.23/1.26
C1(SDAP)-O7(SDAP)	1.28/1.28/1.30	1.27/1.28/1.30	1.26/1.25/1.28	1.27/1.28/ 1.26	1.27/1.27/1.27	1.37/1.37/1.35	1.39/1.39/1.40	1.39/1.39/1.34	1.28/1.30/1.28
H1(WAT)-N3(SDAP)	4.38/4.34/4.44	4.17/4.22/4.36	5.00/5.00/4.79	3.49/3.69/ 3.54	3.46/3.43/3.43	3.23/3.24/3.30	1.59/1.66/1.56	1.24/1.27/1.18	1.01/1.01/1.02
Zn2-O8(SDAP)	1.96/1.94/1.99	1.99/1.96/1.99	2.01/2.00/2.00	1.92/1.99/ 1.96	1.98/1.96/1.97	2.03/1.99/2.03	2.09/2.09/2.10	2.11/2.07/2.09	2.01/2.02/2.00
Zn2-O7(SDAP)	2.42/2.32/2.17	2.19/2.22/2.13	2.03/2.02/2.11	1.91/2.17/ 1.91	1.91/1.90/1.92	2.03/2.07/2.03	1.97/1.97/1.98	2.02/1.98/2.00	2.26/2.15/2.25
Zn1-O7(SDAP)	2.06/2.06/2.03	2.13/2.07/2.04	3.37/3.30/2.07	3.34/2.33/ 3.10	3.47/3.46/3.14	2.01/1.94/1.96	1.93/1.91/1.93	1.94/1.92/1.93	2.01/1.98/2.01

Table S8: Relative Energies of the stationary points in kcal/mol obtained from B3LYP, CAM-B3LYP, and M06-2X functionals for model 1 and model 2. The RMSD (in Å) of the optimized structures of the stationary points obtained from CAM-B3LYP and M06-2X functionals with reference to the optimized geometries obtained from B3LYP functional.

Point	B3LYP	CAM-B3LYP	M06-2X	RMSD(CAM-B3LYP)	RMSD(M06-2X)
Model 1					
R	0.00	0.00	0.00	0.059	0.060
TS1	2.39	4.17	5.00	0.441	0.190
IN1	-7.63	-9.47	-13.29	0.308	0.137
TS2	28.77	18.10	13.36	0.369	0.370
IN2	-4.19	-6.72	-3.40	0.092	0.234
TS3	20.63	0.90	9.10	0.376	0.511
TD	-7.39	-11.21	-20.04	0.079	0.111
TS4	3.52	-2.22	-15.27	0.909	0.451
P	-1.59	-5.12	-18.98	0.051	0.133
Model 2					
R	0	0	0	0.041	0.043
TS1	2.74	2.87	2.25	0.180	0.192
IN1	-10.59	-12.58	-13.70	0.060	0.081
TS2	13.09	9.65	6.18	0.401	0.235
IN2	-3.87	-2.27	-5.92	0.075	0.071
TS3	14.64	8.35	4.12	0.293	0.313
TD	-10.28	-15.94	-20.34	0.055	0.062
TS4	-4.30	-9.67	-13.37	0.392	0.408
PDT	-12.92	-19.98	-28.39	0.059	0.084

Table S9: RMSD (in Å) between the optimized structures of the stationary points obtained from Model 1 and Model 2, for the B3LYP, CAM-B3LYP, and M06-2X functionals.

	R	TS1	IN1	TS2	IN2	TS3	TD	TS4	PDT
RMSD (B3LYP)	0.097	0.445	0.320	0.720	0.351	0.244	0.072	0.048	0.434
RMSD (CAM-B3LYP)	0.109	0.312	0.301	0.798	0.378	0.328	0.202	0.172	0.501
RMSD (M06-2X)	0.072	0.299	0.207	0.801	0.323	0.246	0.175	0.079	0.477

Table S10: Comparison of relative energies (kcal/mol) between the iterative self-consistent mechanical embedding (SC-ME) optimized geometries and the single point energy calculations on the SC-ME optimized geometries using electronic embedding and 6-311+G(d,p) basis set and B3LYP functional.

	model 1		model 2	
Point	SC-ME	EE	SC-ME	EE
R	0.00	0.00	0.00	0.00
TS1	2.39	2.41	2.74	2.74
IN1	-7.63	-7.56	-10.59	-10.54
TS2	28.77	26.00	13.09	12.41
IN2	-4.19	-3.90	-3.87	-2.66
TS3	20.63	20.19	14.64	13.90
TD	-7.39	-7.62	-10.28	-10.69
TS	3.52	3.43	-4.30	-5.89
P	-1.59	-1.94	-12.92	-13.09

Table S11: Comparison of energies of the optimized geometries obtained from iterative self-consistent mechanical embedding (SC-ME) optimization and full electronic embedding optimization.

Point	SC-ME	EE	ΔE (kcal/mol)	ΔRMSD (Å)
R	-6807.864347	-6807.864017	0.21	0.041
TS2	-6807.820519	-6807.824963	2.78	0.056
TD	-6807.880731	-6807.881958	0.75	0.050
P	-6807.884942	-6807.883143	1.12	0.075

Table S12: Comparison of the atomic charges obtained from NBO calculations in the optimized structures obtained from iterative self-consistent mechanical embedding (SC-ME) and full electronic embedding schemes.

	R		TS2		TD		P	
Atom	SC-ME	EE	SC-ME	EE	SC-ME	EE	SC-ME	EE
Zn1	1.313	1.297	1.305	1.304	1.303	1.308	1.314	1.314
Zn2	1.323	1.332	1.307	1.310	1.307	1.310	1.310	1.321
O1	-0.765	-0.755	-0.840	-0.839	-0.795	-0.782	-0.797	-0.797
O2	-0.814	-0.802	-0.744	-0.750	-0.766	-0.755	-0.756	-0.760
O3	-0.776	-0.789	-0.725	-0.722	-0.737	-0.749	-0.757	-0.781
O4	-0.772	-0.775	-0.801	-0.805	-0.784	-0.784	-0.787	-0.781
O5	-1.059	-1.055	-1.048	-1.043	-0.829	-0.822	-0.729	-0.739
O6	-0.742	-0.736	-0.723	-0.720	-0.694	-0.689	-0.679	-0.665
O7	-0.811	-0.787	-0.774	-0.763	-0.983	-0.970	-0.838	-0.813
O8	-0.838	-0.828	-0.840	-0.830	-0.786	-0.771	-0.834	-0.825
H1	0.538	0.538	0.546	0.544	0.521	0.521	0.406	0.435
N1	-0.562	-0.617	-0.620	-0.623	-0.599	-0.617	-0.608	-0.621
N2	-0.620	-0.595	-0.609	-0.620	-0.590	-0.603	-0.611	-0.617
N3	-0.603	-0.554	-0.660	-0.657	-0.772	-0.770	-0.934	-0.938
C1	0.722	0.692	0.752	0.764	0.785	0.786	0.871	0.882

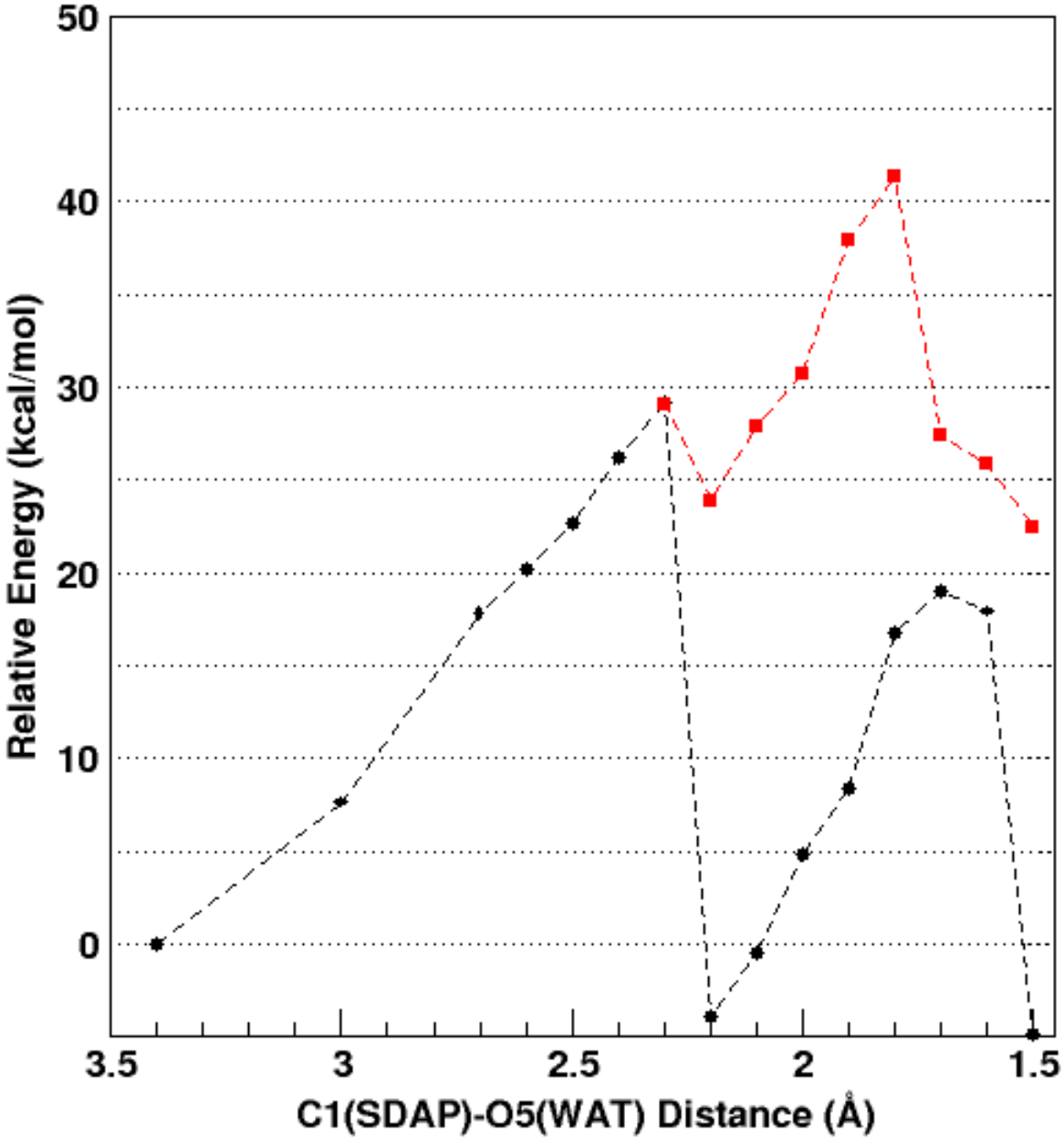

Figure S1: The potential energy profiles from linear transit scan along the C1-O5 distance representing the nucleophilic attack, with (red) and without (black) keeping the carboxylate group of Asp100 rigid. Upon, restricting the conformational change of Asp100, the intermediate at 2.2 Å(black line) disappears and the activation energy increases from 28 kcal/mol to 41 kcal/mol.

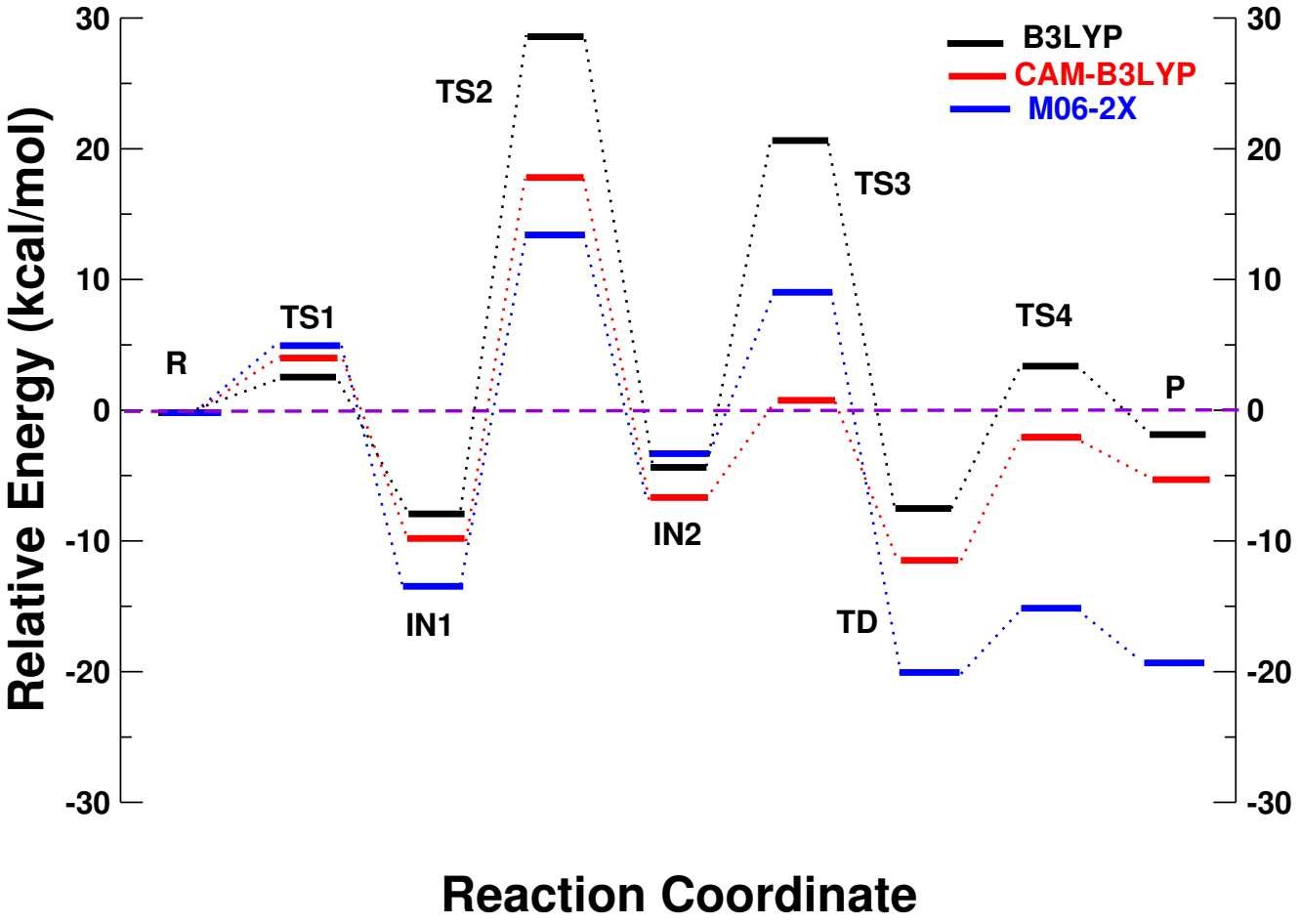

Figure S2: Relative energy (kcal/mol) profile diagram when the QM region contains only one water molecule (the catalytic water), i.e., model 1, for B3LYP, CAM-B3LYP, and M06-2X functionals.

Cartesian coordinates of the atoms described by QM method for the reactant, intermediates, transition states, and the product of the DapE catalyzed hydrolysis of SDAP.

Atom	X	Y	Z
		R	
C	13.437667	12.738253	-0.182361
H	14.325080	12.593281	-0.804860
H	13.436908	13.794406	0.100667
N	11.001911	13.052126	-0.861263
H	10.867022	13.960080	-0.420513
C	12.219660	12.396401	-0.976911
C	10.125424	12.463305	-1.723143
H	9.114618	12.816046	-1.863258
N	10.696042	11.462260	-2.362411
C	11.993527	11.411300	-1.897469
H	12.695806	10.693248	-2.280721
C	5.886420	10.687880	-3.727692
H	5.383108	11.609148	-3.413661
H	5.210112	10.178878	-4.420007
C	7.129645	11.089510	-4.511211
O	6.906050	11.467697	-5.702124
O	8.252897	11.021749	-3.933996
C	14.647977	13.574306	-3.959176
H	14.490210	12.601473	-3.480302
H	15.704058	13.822119	-3.827523
C	14.371077	13.371908	-5.453364
O	13.198681	13.338900	-5.904459

Atom	X	Y	Z
O	15.399756	13.168793	-6.182631
C	8.932635	15.384474	-3.433753
H	8.334878	15.393222	-2.524862
H	9.902545	14.925016	-3.232100
C	8.179021	14.545328	-4.460315
O	8.816224	14.223093	-5.537913
O	7.009831	14.190762	-4.233005
C	13.012637	7.946593	-4.928104
H	13.741907	8.200576	-5.703214
H	13.587659	7.688319	-4.032619
C	12.227023	9.229581	-4.671140
O	12.904803	10.274464	-4.466757
O	10.952797	9.225408	-4.710398
C	2.321275	14.073417	-7.926097
H	2.011038	15.125138	-7.976926
H	1.995281	13.612653	-8.868511
N	4.605940	14.852141	-8.605778
H	4.269359	15.592664	-9.211682
C	3.820763	14.025486	-7.807395
C	5.914669	14.584966	-8.370783
H	6.731478	15.108840	-8.860825
N	6.018590	13.631590	-7.459760
C	4.731801	13.280803	-7.100955
H	4.568087	12.528934	-6.347098
Zn	7.832621	12.933053	-6.696589
Zn	10.186369	11.066116	-4.486923
C	9.636267	10.579646	-7.515462
O	9.608139	11.306714	-6.454858

Atom	X	Y	Z
N	10.217043	10.980432	-8.615197
H	10.073615	10.317955	-9.493813
C	8.957344	9.221136	-7.562866
H	9.730025	8.444775	-7.509120
H	8.361865	9.145846	-6.650194
C	8.044560	9.003907	-8.791324
H	7.369183	8.172281	-8.590595
H	7.417093	9.897399	-8.909947
C	8.690316	8.698786	-10.171718
O	8.104611	7.878595	-10.900181
O	9.755194	9.335374	-10.496136
C	10.889151	12.263857	-8.719428
H	11.489066	12.419949	-7.814845
C	13.626184	8.786411	-12.066428
O	13.222910	7.843096	-11.429200
O	13.314343	8.888160	-13.379515
C	11.826421	12.275056	-9.936619
H	12.436085	13.179634	-9.867064
H	11.223110	12.360078	-10.849597
C	12.723574	11.034097	-10.030183
H	13.299893	10.910268	-9.104919
H	12.114406	10.133661	-10.155334
C	13.676058	11.172778	-11.216563
H	14.380785	11.992476	-11.021358
H	13.120751	11.452781	-12.121890
C	14.505590	9.920109	-11.547811
H	15.024716	9.564184	-10.650973
C	9.883754	13.437659	-8.791448

Atom	X	Y	Z
O	8.664723	13.224631	-8.448389
O	10.313475	14.523218	-9.227811
N	15.402609	10.266958	-12.657011
H	16.134927	9.556505	-12.789105
H	13.868758	9.627828	-13.739714
H	15.929288	11.107475	-12.396956
O	5.051576	13.959659	-2.420762
H	5.828881	14.061953	-3.019886
H	5.411156	13.312880	-1.781382
O	11.002525	12.919270	-4.659437
H	10.361952	13.516366	-5.098732
H	11.889278	13.039694	-5.129722
O	5.648485	12.957208	-11.410879
H	4.785830	12.634738	-11.751229
H	6.231427	12.196610	-11.594039
O	17.385827	11.737037	-4.736340
H	16.798332	12.243956	-5.334520
H	16.736655	11.422954	-4.076831
O	8.227445	16.125199	-9.882587
H	8.385811	16.924858	-9.339262
H	8.957053	15.525874	-9.574556
O	15.359290	10.054200	-3.221686
H	14.467082	10.218500	-3.610637
H	15.760795	9.573847	-3.982849
O	14.563128	10.529642	-7.083197
H	14.912176	11.444309	-7.070948
H	13.899140	10.584674	-6.371687
O	14.153946	14.456845	-8.462877

Atom	X	Y	Z
H	14.879583	14.038255	-7.962516
H	13.437310	14.282655	-7.825888
O	17.405345	14.834321	-7.043532
H	16.676955	14.460401	-6.504085
H	17.448449	14.100467	-7.710492
	TS1		
C	13.596246	12.800870	-0.393603
H	14.452780	12.602848	-1.042885
H	13.637316	13.868014	-0.161267
N	11.188330	13.236099	-1.047818
H	11.133626	14.178720	-0.669747
C	12.337874	12.472292	-1.121240
C	10.249786	12.651493	-1.833667
H	9.271183	13.081331	-1.991581
N	10.716736	11.556859	-2.380673
C	12.012984	11.438156	-1.942203
H	12.647655	10.646955	-2.298036
C	5.946737	10.539218	-3.717991
H	5.239764	11.337981	-3.488309
H	5.445671	9.885351	-4.435687
C	7.141635	11.148790	-4.434142
O	6.850486	11.675515	-5.543802
O	8.277179	11.062743	-3.907170
C	14.534345	13.401061	-4.069770
H	14.201043	12.505932	-3.536503
H	15.609903	13.519627	-3.921856
C	14.312795	13.161265	-5.566378
O	13.121669	12.998397	-6.009005

Atom	X	Y	Z
O	15.315666	13.066005	-6.279145
C	9.277332	15.602757	-3.684199
H	8.833292	15.718917	-2.698319
H	10.244853	15.106933	-3.593717
C	8.340100	14.733112	-4.509099
O	8.864452	14.253027	-5.592963
O	7.188588	14.544979	-4.119817
C	12.908888	7.886839	-4.722934
H	13.752690	8.042871	-5.396485
H	13.345904	7.642680	-3.749436
C	12.206466	9.241678	-4.613836
O	12.945611	10.223757	-4.474081
O	10.924750	9.298477	-4.698194
C	2.501686	14.053641	-8.109832
H	2.225204	15.106257	-8.244812
H	2.161669	13.531418	-9.012099
N	4.808620	14.655606	-8.872537
H	4.501399	15.338315	-9.554875
C	3.996404	13.963085	-7.985910
C	6.103567	14.379600	-8.587608
H	6.940433	14.802528	-9.137580
N	6.169146	13.548234	-7.571218
C	4.873738	13.286061	-7.187396
H	4.687227	12.630773	-6.353262
Zn	7.954023	12.911994	-6.665367
Zn	10.212060	11.117052	-4.458828
C	9.547693	10.503022	-7.427808
O	9.368252	11.255328	-6.412681

Atom	X	Y	Z
N	10.281651	10.864293	-8.443047
H	10.214457	10.196118	-9.291498
C	8.868737	9.155670	-7.505000
H	9.632399	8.375640	-7.428527
H	8.244086	9.089191	-6.612937
C	8.009040	8.960686	-8.763354
H	7.277028	8.174085	-8.585475
H	7.443748	9.882347	-8.949750
C	8.734230	8.585280	-10.071919
O	8.153417	7.793797	-10.829204
O	9.862350	9.131298	-10.299610
C	10.976927	12.141394	-8.461448
H	11.247500	12.368516	-7.426068
C	13.796489	8.917322	-12.136662
O	13.781237	8.014841	-11.338742
O	13.449852	8.711331	-13.417040
C	12.280841	12.094612	-9.280279
H	13.075548	12.465675	-8.626429
H	12.198224	12.799995	-10.113096
C	12.680967	10.708729	-9.798239
H	12.612956	9.976605	-8.993341
H	11.965758	10.347214	-10.545361
C	14.109643	10.711714	-10.364831
H	14.754646	10.022441	-9.816735
H	14.547774	11.706027	-10.239405
C	14.213478	10.355101	-11.840122
H	15.269363	10.407274	-12.144477
C	10.005848	13.263973	-8.872492

Atom	X	Y	Z
O	8.806596	13.179479	−8.447528
O	10.431878	14.199152	−9.575989
N	13.478087	11.219880	−12.768712
H	13.999885	12.082612	−12.919985
H	13.443296	9.617497	−13.821248
H	12.571539	11.482296	−12.397626
O	5.227921	13.823523	−2.548183
H	5.956261	14.024276	−3.172410
H	5.636457	13.153906	−1.975530
O	11.072227	12.842889	−4.772816
H	10.454403	13.470440	−5.189021
H	12.074709	12.920785	−5.278617
O	5.611705	12.713113	−11.658378
H	4.787544	12.363928	−12.048773
H	6.253584	12.002607	−11.826471
O	17.415715	11.628757	−5.287746
H	16.765437	12.271853	−5.628244
H	16.877103	10.818376	−5.214733
O	8.363638	15.762334	−10.331456
H	8.520562	16.575085	−9.814265
H	9.083689	15.163918	−10.001758
O	15.258491	9.986823	−2.914760
H	14.382787	10.249130	−3.230401
H	15.645587	9.581154	−3.715334
O	14.320249	10.361883	−6.929145
H	14.637709	11.261400	−7.106767
H	13.720987	10.507380	−6.175951
O	14.554194	14.797404	−8.218630

Atom	X	Y	Z
H	14.895198	14.027854	-7.727252
H	14.013128	15.233962	-7.531343
O	17.479270	14.694177	-7.011933
H	16.694540	14.553821	-6.465437
H	17.435662	13.911773	-7.611399
	IN1		
C	13.777971	12.730832	-0.377339
H	14.651078	12.580331	-1.019311
H	13.806994	13.779102	-0.067326
N	11.430739	13.295264	-1.157045
H	11.414022	14.236021	-0.763029
C	12.530313	12.455005	-1.151672
C	10.489116	12.768244	-1.979840
H	9.542486	13.249012	-2.171107
N	10.914658	11.623546	-2.486121
C	12.178040	11.418449	-1.967983
H	12.765379	10.570615	-2.269060
C	6.101092	10.316029	-3.709432
H	5.407972	11.125112	-3.472422
H	5.645355	9.693248	-4.486206
C	7.367047	10.934350	-4.293323
O	7.196643	11.974111	-4.961109
O	8.467228	10.312895	-4.083801
C	14.866844	13.966754	-3.963488
H	15.195465	13.128863	-3.335174
H	15.737526	14.296327	-4.536322
C	13.855810	13.373669	-4.923500
O	12.603376	13.452953	-4.616851

Atom	X	Y	Z
O	14.296645	12.781956	-5.929145
C	9.493848	15.642128	-3.479945
H	9.151433	15.736770	-2.447628
H	10.460406	15.135321	-3.511013
C	8.447986	14.839716	-4.269213
O	8.888880	14.314138	-5.348480
O	7.279883	14.827853	-3.824643
C	13.046374	7.500791	-4.838662
H	13.815247	7.796467	-5.554831
H	13.576289	7.106118	-3.964511
C	12.317603	8.781304	-4.445539
O	13.063210	9.777434	-4.203081
O	11.052972	8.831989	-4.425705
C	2.402102	13.982047	-7.823269
H	2.076383	15.029012	-7.896474
H	2.097645	13.506102	-8.765686
N	4.674665	14.782926	-8.483662
H	4.332297	15.531838	-9.075780
C	3.897589	13.959455	-7.676374
C	5.983505	14.556941	-8.214690
H	6.791516	15.070046	-8.718624
N	6.097934	13.633265	-7.276199
C	4.815674	13.254273	-6.936624
H	4.656440	12.514177	-6.170168
Zn	8.003469	13.037437	-6.564644
Zn	10.338017	10.753307	-4.284189
C	8.824308	10.565369	-8.189149
O	8.530453	11.150227	-7.111256

Atom	X	Y	Z
N	9.566212	11.075805	-9.162770
H	9.706947	10.409629	-9.985236
C	8.352832	9.130203	-8.359875
H	9.210438	8.477137	-8.148783
H	7.628284	8.973578	-7.556920
C	7.734002	8.755105	-9.716000
H	7.135533	7.849931	-9.590552
H	7.052423	9.558746	-10.025831
C	8.701644	8.466484	-10.893615
O	8.357897	7.561970	-11.678644
O	9.750999	9.186499	-10.995134
C	10.408373	12.269895	-9.007847
H	10.783635	12.261836	-7.978120
C	13.660143	8.953844	-12.144388
O	12.883145	8.057407	-11.917581
O	13.894881	9.355567	-13.414166
C	11.576221	12.220317	-10.002196
H	12.251130	13.044455	-9.740082
H	11.193562	12.457811	-11.000661
C	12.347244	10.889871	-10.041749
H	12.545968	10.523692	-9.028967
H	11.745705	10.121563	-10.536193
C	13.677294	11.069176	-10.781012
H	14.339911	11.710684	-10.183037
H	13.518495	11.599265	-11.729748
C	14.427615	9.760674	-11.094308
H	14.494415	9.144036	-10.191472
C	9.605636	13.588424	-9.148602

Atom	X	Y	Z
O	8.721718	13.841971	−8.268520
O	9.873565	14.359091	−10.098294
N	15.717613	10.096010	−11.699061
H	16.320362	9.281166	−11.834669
H	14.656635	9.988708	−13.358041
H	16.247300	10.769138	−11.140361
O	5.301969	13.453717	−2.543639
H	6.040839	13.774870	−3.108181
H	5.774078	12.819717	−1.968393
O	11.152445	11.816229	−5.634806
H	11.746386	11.173422	−5.219424
H	11.992864	12.805422	−5.135381
O	5.855082	12.143258	−10.968818
H	5.018021	11.933049	−11.437403
H	6.506430	11.646766	−11.504302
O	17.157677	11.763606	−5.532738
H	16.474604	11.612832	−4.843270
H	16.596381	11.716891	−6.338445
O	7.897086	16.240313	−10.224462
H	8.091999	16.885835	−9.511953
H	8.636727	15.585539	−10.100155
O	15.634920	10.403918	−3.505477
H	14.677379	10.242212	−3.681048
H	16.014187	9.772874	−4.157275
O	13.471354	10.290794	−6.917851
H	13.694667	11.235879	−6.962399
H	13.498720	10.158145	−5.948306
O	14.724849	13.959294	−8.306067

Atom	X	Y	Z
H	15.350015	13.186039	-8.343203
H	14.277928	13.678049	-7.473995
O	17.144309	14.623721	-6.676597
H	16.289371	14.594567	-7.147510
H	17.145106	13.758320	-6.223619
	TS2		
C	13.632331	12.409656	-0.194507
H	14.540197	12.257382	-0.785902
H	13.633853	13.463825	0.097385
N	11.300625	12.911950	-1.060343
H	11.199822	13.806397	-0.582049
C	12.439996	12.119056	-1.048261
C	10.462089	12.453454	-2.024661
H	9.502019	12.883569	-2.263887
N	10.991885	11.396843	-2.618948
C	12.212068	11.173415	-2.009872
H	12.865270	10.387729	-2.345609
C	6.321390	10.362596	-3.618348
H	5.690287	11.243742	-3.495476
H	5.959156	9.756214	-4.451415
C	7.765649	10.768048	-3.877785
O	8.127959	11.949730	-3.706625
O	8.552637	9.810939	-4.219952
C	13.820545	13.248960	-4.263411
H	13.258798	12.371756	-3.946536
H	14.882525	13.049479	-4.086998
C	13.689752	13.457650	-5.755936
O	12.747917	12.900230	-6.457234

Atom	X	Y	Z
O	14.570621	14.103487	-6.349166
C	9.140946	15.607031	-3.701853
H	8.226500	15.478138	-3.119052
H	10.004177	15.283438	-3.114687
C	9.032114	14.764463	-4.974403
O	10.022287	14.398202	-5.616794
O	7.806990	14.528226	-5.342639
C	13.315870	7.485081	-5.020439
H	13.975996	7.751351	-5.850719
H	13.962077	7.184767	-4.189561
C	12.579527	8.762053	-4.632196
O	13.298418	9.799311	-4.470459
O	11.320623	8.746857	-4.514229
C	2.141888	14.052779	-7.776822
H	1.799768	15.095469	-7.807709
H	1.751221	13.577631	-8.686805
N	4.315676	14.878761	-8.680303
H	3.901808	15.596425	-9.263627
C	3.640235	14.057414	-7.785926
C	5.649202	14.693707	-8.529934
H	6.398614	15.235566	-9.093152
N	5.873356	13.796636	-7.584810
C	4.638125	13.393124	-7.119792
H	4.550583	12.674652	-6.320896
Zn	7.846232	13.503538	-6.981236
Zn	10.355375	10.550554	-4.390235
C	9.128436	11.001608	-7.672774
O	8.404000	11.674703	-6.870143

Atom	X	Y	Z
N	9.781124	11.453678	-8.738665
H	9.878754	10.692613	-9.492308
C	8.979127	9.487895	-7.625864
H	9.959588	9.007912	-7.706127
H	8.554830	9.248869	-6.649343
C	8.063787	8.957703	-8.754614
H	7.651646	7.985836	-8.474496
H	7.207253	9.635982	-8.858999
C	8.707140	8.768274	-10.158418
O	8.193491	7.903934	-10.894006
O	9.699247	9.510431	-10.468979
C	10.370685	12.772152	-8.968521
H	10.731069	13.131081	-7.999796
C	13.520813	8.946325	-11.458015
O	12.474610	8.475471	-11.085265
O	14.047900	8.565505	-12.650154
C	11.547733	12.650091	-9.962080
H	12.165896	13.549775	-9.851946
H	11.138346	12.680607	-10.976035
C	12.405181	11.392799	-9.788911
H	12.750143	11.310849	-8.751286
H	11.805034	10.503786	-9.992110
C	13.631147	11.371981	-10.710690
H	14.342858	12.141014	-10.382570
H	13.345205	11.616795	-11.742337
C	14.335129	9.997347	-10.682541
H	14.367984	9.668518	-9.636463
C	9.356560	13.830640	-9.470703

Atom	X	Y	Z
O	8.501641	14.277160	−8.618353
O	9.407210	14.250837	−10.640136
N	15.663547	10.071362	−11.304659
H	16.240182	9.274606	−11.022086
H	14.895314	9.065430	−12.747998
H	16.197089	10.892899	−10.984911
O	5.962513	14.068646	−3.253586
H	6.510192	14.228575	−4.056239
H	6.492750	13.340983	−2.870450
O	10.947660	11.252610	−6.172630
H	11.462123	10.530581	−6.557574
H	11.973292	12.286811	−6.130759
O	6.920771	12.220403	−10.040792
H	6.405617	11.724929	−10.712333
H	7.775000	11.745054	−10.046428
O	16.869287	11.416901	−5.662887
H	16.734893	12.373145	−5.796423
H	16.084286	11.025953	−6.097702
O	7.830918	16.366124	−10.502689
H	8.154696	16.808515	−9.689072
H	8.426914	15.574088	−10.522089
O	15.485823	9.071738	−3.116466
H	14.677920	9.465676	−3.507849
H	15.937193	8.816330	−3.956364
O	14.683076	10.586519	−6.821809
H	14.189989	11.388502	−7.053985
H	14.258624	10.300519	−5.981649
O	15.037573	13.680284	−8.897359

Atom	X	Y	Z
H	15.840037	13.154013	-8.653387
H	14.619523	13.757368	-8.008894
O	17.206093	14.468511	-6.494702
H	16.246992	14.546986	-6.303987
H	17.190983	13.820996	-7.232144
	IN2		
C	13.90097	12.46140	-0.45176
H	14.80016	12.28889	-1.05120
H	13.91445	13.51992	-0.17592
N	11.54475	12.93623	-1.24855
H	11.48232	13.86593	-0.83281
C	12.69252	12.15852	-1.27384
C	10.64428	12.40447	-2.11393
H	9.66976	12.81946	-2.31665
N	11.13929	11.31191	-2.67030
C	12.40713	11.14891	-2.15108
H	13.04179	10.33979	-2.46459
C	6.41223	10.36848	-3.60276
H	5.86702	11.30426	-3.47033
H	5.97542	9.78577	-4.41542
C	7.88215	10.61378	-3.89332
O	8.39739	11.73794	-3.71910
O	8.56637	9.58062	-4.23428
C	14.10570	13.54185	-4.55315
H	14.24500	12.61131	-3.98800
H	15.04691	13.76355	-5.06212
C	13.03045	13.20835	-5.56444
O	11.79332	13.21291	-5.15277

Atom	X	Y	Z
O	13.33865	12.82733	-6.70628
C	9.05943	15.44896	-3.98679
H	8.33750	15.32367	-3.17855
H	10.00229	14.96790	-3.71159
C	8.50872	14.73243	-5.21179
O	9.15812	14.70235	-6.29854
O	7.38831	14.14164	-5.11882
C	13.35895	7.35450	-4.94552
H	14.11434	7.56886	-5.70310
H	13.89229	7.02317	-4.04667
C	12.62170	8.65972	-4.64929
O	13.30500	9.73323	-4.71984
O	11.39559	8.62210	-4.36505
C	2.11221	14.06982	-7.87603
H	1.70960	15.08790	-7.96805
H	1.75224	13.52444	-8.75875
N	4.26911	15.01311	-8.73163
H	3.84198	15.73324	-9.30076
C	3.60592	14.14981	-7.86734
C	5.60667	14.84988	-8.57744
H	6.35694	15.42056	-9.11462
N	5.83610	13.93208	-7.65723
C	4.61152	13.49360	-7.20762
H	4.53704	12.75286	-6.42765
Zn	7.74776	13.40619	-7.15981
Zn	10.35804	10.40544	-4.36021
C	9.14936	10.93554	-7.61899
O	8.31662	11.59519	-6.90667

Atom	X	Y	Z
N	9.85800	11.39098	-8.66029
H	10.00880	10.62524	-9.37376
C	8.99853	9.42024	-7.59145
H	9.98070	8.94377	-7.65536
H	8.55657	9.17516	-6.62478
C	8.10534	8.90637	-8.74185
H	7.62868	7.96455	-8.45964
H	7.29131	9.62500	-8.90332
C	8.81051	8.65277	-10.10280
O	8.30146	7.78524	-10.84345
O	9.84624	9.34484	-10.37631
C	10.46512	12.69200	-8.90049
H	10.93999	13.01846	-7.96584
C	13.67441	8.98011	-11.59018
O	12.70006	8.42773	-11.14583
O	14.11394	8.66208	-12.83697
C	11.56973	12.56072	-9.97838
H	12.16279	13.47894	-9.93498
H	11.09721	12.55332	-10.96841
C	12.46240	11.32021	-9.84617
H	12.83011	11.22301	-8.81899
H	11.88601	10.41800	-10.06085
C	13.66720	11.38737	-10.79339
H	14.34263	12.18649	-10.45693
H	13.34950	11.65640	-11.80989
C	14.47464	10.07258	-10.85787
H	14.62842	9.71589	-9.83032
C	9.50874	13.83903	-9.30294

Atom	X	Y	Z
O	8.26186	13.72366	-9.04832
O	10.01109	14.83877	-9.85969
N	15.72850	10.29774	-11.59845
H	16.37888	9.51632	-11.45229
H	14.89730	9.23391	-13.01265
H	16.23138	11.10882	-11.21595
O	5.78593	13.92381	-2.92898
H	6.39632	13.93607	-3.70840
H	6.25999	13.29885	-2.34697
O	10.66793	11.08060	-6.01520
H	11.48563	10.70679	-6.37169
H	11.24594	12.57012	-5.71765
O	5.62991	12.63444	-10.95030
H	4.83937	12.30095	-11.43225
H	6.30820	11.98029	-11.20186
O	17.16270	11.32963	-5.57242
H	16.49313	10.99879	-6.21874
H	16.65629	11.20878	-4.74064
O	7.91623	16.57834	-10.15552
H	8.09329	17.22220	-9.43582
H	8.65703	15.92794	-10.01175
O	15.70918	10.03326	-3.43259
H	14.79773	9.99530	-3.81172
H	16.13401	9.34982	-4.00124
O	14.76368	10.39743	-6.94605
H	14.42057	11.30640	-7.03389
H	14.28741	10.08849	-6.14129
O	15.09978	14.05629	-8.35687

Atom	X	Y	Z
H	15.70344	13.26367	-8.39812
H	14.41244	13.68634	-7.75181
O	17.00030	14.17254	-6.11672
H	16.36852	14.29790	-6.84853
H	16.99564	13.20317	-5.97289
		TS3	
C	13.50378	12.63648	-0.72063
H	14.37391	12.48042	-1.36592
H	13.54053	13.68780	-0.42106
N	11.14680	13.19950	-1.51037
H	11.09605	14.11049	-1.05417
C	12.25798	12.36792	-1.50992
C	10.25822	12.73367	-2.42749
H	9.31146	13.21466	-2.61527
N	10.72554	11.63966	-3.00395
C	11.95706	11.39888	-2.42544
H	12.56217	10.57645	-2.75781
C	5.85942	10.30122	-3.76589
H	5.27194	11.18283	-3.49740
H	5.26004	9.71535	-4.46891
C	7.10747	10.76607	-4.50949
O	6.89621	11.63841	-5.38706
O	8.21361	10.19846	-4.21095
C	14.35798	13.61507	-4.53465
H	14.56189	12.73882	-3.90587
H	15.30153	13.91392	-5.00073
C	13.44631	13.10410	-5.62020
O	12.15731	13.05474	-5.37094

Atom	X	Y	Z
O	13.92455	12.66555	-6.67038
C	9.20698	15.82794	-3.58279
H	8.80577	15.99615	-2.58536
H	10.18290	15.34700	-3.50368
C	8.23929	14.91511	-4.34591
O	8.74483	14.34117	-5.36895
O	7.06405	14.83901	-3.93187
C	13.00096	7.43199	-4.93256
H	13.73134	7.64504	-5.71863
H	13.57207	7.09025	-4.06211
C	12.33334	8.76802	-4.60375
O	13.14585	9.73841	-4.47938
O	11.07657	8.85639	-4.49503
C	2.39234	13.93381	-7.95617
H	2.06090	14.97238	-8.09355
H	2.11128	13.40430	-8.87614
N	4.66812	14.82079	-8.49887
H	4.33053	15.57621	-9.08308
C	3.88403	13.93339	-7.77256
C	5.97198	14.58000	-8.22939
H	6.78383	15.13275	-8.67970
N	6.07901	13.59060	-7.35707
C	4.79267	13.18504	-7.06545
H	4.62862	12.39953	-6.34647
Zn	7.96117	13.00395	-6.58883
Zn	10.07557	10.64483	-4.75279
C	9.93932	10.81106	-7.41618
O	9.40150	11.57400	-6.41332

Atom	X	Y	Z
N	10.05451	11.36732	-8.65642
H	9.97304	10.67971	-9.44160
C	9.42262	9.36191	-7.51159
H	10.25186	8.71193	-7.80789
H	9.11520	9.06597	-6.50630
C	8.24919	9.15985	-8.49688
H	7.56528	8.39812	-8.11912
H	7.67270	10.09182	-8.56273
C	8.67025	8.73752	-9.93811
O	8.00282	7.84616	-10.50516
O	9.66897	9.35270	-10.42284
C	10.72065	12.62453	-8.90301
H	11.35700	12.85635	-8.03635
C	13.81029	8.86239	-11.80319
O	13.16875	8.01093	-11.24002
O	13.89843	8.84567	-13.15781
C	11.64113	12.50648	-10.13591
H	12.25263	13.41243	-10.19172
H	11.02583	12.49729	-11.04297
C	12.52141	11.24676	-10.09179
H	12.95139	11.14308	-9.08798
H	11.90872	10.35486	-10.25197
C	13.66354	11.29535	-11.10923
H	14.30819	12.15361	-10.87904
H	13.27386	11.46552	-12.12131
C	14.54296	10.02667	-11.12873
H	14.75079	9.71451	-10.09818
C	9.72875	13.80096	-9.02482

Atom	X	Y	Z
O	8.65274	13.75762	-8.34765
O	10.03874	14.74396	-9.79294
N	15.75287	10.30220	-11.92408
H	16.37412	9.48284	-11.91890
H	14.54443	9.54212	-13.41058
H	16.30172	11.04358	-11.47064
O	5.15019	13.53436	-2.51249
H	5.86487	13.88612	-3.08685
H	5.64075	12.87473	-1.98327
O	11.39582	10.70123	-6.64314
H	12.04550	10.14647	-7.09909
H	11.74460	12.56068	-6.16615
O	5.53337	12.63111	-10.73540
H	4.91268	12.15201	-11.31984
H	6.29415	12.02800	-10.67791
O	17.00716	11.40901	-5.66176
H	16.37189	11.00147	-6.28584
H	16.47968	11.38548	-4.83486
O	7.94487	16.35727	-10.15501
H	8.11567	17.07076	-9.50374
H	8.70741	15.74522	-9.95610
O	15.50917	10.32972	-3.41814
H	14.56339	10.19486	-3.65735
H	15.88738	9.59050	-3.94436
O	14.54696	9.92055	-6.93107
H	14.41981	10.85805	-7.17638
H	14.11817	9.89893	-6.04500
O	14.85008	13.98919	-8.80127

Atom	X	Y	Z
H	15.41865	13.17138	-8.78745
H	14.21001	13.67476	-8.12796
O	16.89973	14.18889	-6.61793
H	16.18155	14.28050	-7.26918
H	16.84959	13.24261	-6.37341
	TD		
C	13.358880	12.710021	-0.639155
H	14.224036	12.555601	-1.289889
H	13.379446	13.770943	-0.378131
N	10.982269	13.184539	-1.397318
H	10.900272	14.089857	-0.939103
C	12.115656	12.389637	-1.406933
C	10.098791	12.676547	-2.289922
H	9.132617	13.125424	-2.471022
N	10.591087	11.597777	-2.856994
C	11.840226	11.409912	-2.310575
H	12.473382	10.617011	-2.663942
C	5.752952	10.121583	-3.593357
H	5.045960	10.934675	-3.436298
H	5.308736	9.426623	-4.309675
C	7.032469	10.663359	-4.208277
O	6.906686	11.670004	-4.939818
O	8.088430	10.012812	-3.955739
C	14.108549	13.485111	-4.367645
H	14.062042	12.601107	-3.724292
H	15.143977	13.630254	-4.678501
C	13.301559	13.135594	-5.604247
O	12.012719	13.025171	-5.433921

Atom	X	Y	Z
O	13.884844	12.881908	-6.650969
C	9.154960	15.902099	-3.433452
H	8.715977	16.133715	-2.466769
H	10.137698	15.455474	-3.277762
C	8.251043	14.893795	-4.137229
O	8.781676	14.347224	-5.164473
O	7.120035	14.689157	-3.679694
C	12.955644	7.556977	-4.675376
H	13.757655	7.787138	-5.377956
H	13.433792	7.269482	-3.732390
C	12.183233	8.859532	-4.474518
O	12.843218	9.905367	-4.586108
O	10.935019	8.798931	-4.204413
C	2.574629	13.741356	-7.834672
H	2.286910	14.780403	-8.036898
H	2.301154	13.173854	-8.732181
N	4.879348	14.463854	-8.437186
H	4.569461	15.187004	-9.076240
C	4.063568	13.696925	-7.620122
C	6.168740	14.228762	-8.110539
H	6.996703	14.716683	-8.603530
N	6.240002	13.346691	-7.138106
C	4.939713	13.012470	-6.821376
H	4.743887	12.318081	-6.021126
Zn	8.095557	12.858231	-6.181652
Zn	9.930563	10.447810	-4.477659
C	10.017395	10.860968	-7.229581
O	9.402805	11.376367	-6.087185

Atom	X	Y	Z
N	11.118128	11.814845	-7.584475
H	11.945536	11.234166	-7.664018
C	8.902278	10.543959	-8.248091
H	8.271474	9.842525	-7.691917
H	8.312826	11.450015	-8.394147
C	9.202983	9.960483	-9.629072
H	8.249963	9.787275	-10.136585
H	9.712611	10.706088	-10.243988
C	10.009220	8.656483	-9.817306
O	9.770001	8.039826	-10.867709
O	10.912456	8.350728	-8.967221
C	11.161750	12.860908	-8.606623
H	11.929024	13.554200	-8.236331
C	13.243288	8.688980	-12.042325
O	12.825978	7.735787	-11.451874
O	12.909001	8.870839	-13.345927
C	11.656890	12.428870	-10.007046
H	12.102716	13.315855	-10.466723
H	10.816058	12.165568	-10.653926
C	12.663034	11.281914	-9.980988
H	13.434023	11.489828	-9.229975
H	12.172055	10.345532	-9.688214
C	13.345812	11.104854	-11.330301
H	14.042074	11.936115	-11.499992
H	12.608718	11.163699	-12.139174
C	14.126451	9.787476	-11.470663
H	14.482846	9.445942	-10.492818
C	9.909254	13.730820	-8.736293

Atom	X	Y	Z
O	8.934501	13.608711	-7.949367
O	9.974886	14.568086	-9.669237
N	15.188314	9.998889	-12.447105
H	15.796067	9.176919	-12.545313
H	13.478393	9.595507	-13.693423
H	15.819396	10.729068	-12.098505
O	5.147769	13.560999	-2.358652
H	5.882487	13.911604	-2.904653
H	5.574723	12.819626	-1.897373
O	10.662940	9.700007	-6.849650
H	10.764864	9.089366	-7.676587
H	11.571542	12.563060	-6.254540
O	5.775681	11.848220	-11.062040
H	4.906876	11.745781	-11.496245
H	6.322440	11.197516	-11.521192
O	17.260348	11.345835	-4.544871
H	16.804206	11.691525	-3.767889
H	16.613769	10.710872	-4.916140
O	7.830381	16.013691	-10.109103
H	7.946306	16.740172	-9.465643
H	8.633823	15.448468	-9.905782
O	15.200916	10.028823	-3.116061
H	14.257942	10.087776	-3.327212
H	15.570370	9.717790	-3.965479
O	13.884644	10.275516	-6.987071
H	14.040545	11.236569	-7.004124
H	13.409068	10.163923	-6.136530
O	14.717131	13.937361	-8.816795

Atom	X	Y	Z
H	15.554873	13.422930	-8.773128
H	14.235127	13.589077	-8.042806
O	16.433579	14.169995	-7.013496
H	15.575295	14.159213	-6.578416
H	16.415565	13.350775	-7.549660
	TS4		
C	13.436659	12.647405	-0.618849
H	14.288808	12.430024	-1.271469
H	13.508293	13.709767	-0.367904
N	11.044996	13.184585	-1.348749
H	10.991083	14.101699	-0.906199
C	12.171624	12.370584	-1.370372
C	10.128557	12.687466	-2.226407
H	9.171779	13.158146	-2.396526
N	10.602482	11.589883	-2.799430
C	11.853915	11.380818	-2.260314
H	12.458854	10.559630	-2.592364
C	5.693308	10.223751	-3.507112
H	5.067409	11.089712	-3.280165
H	5.168616	9.591720	-4.230939
C	6.984725	10.709324	-4.153752
O	6.855157	11.679317	-4.945451
O	8.051683	10.066480	-3.868598
C	14.171177	13.495831	-4.508542
H	14.220000	12.593729	-3.882943
H	15.183642	13.682154	-4.875825
C	13.292082	13.143059	-5.702746
O	12.048813	12.974939	-5.556292

Atom	X	Y	Z
O	13.906299	12.923233	-6.801601
C	9.085319	15.937982	-3.403567
H	8.631256	16.198114	-2.450718
H	10.068111	15.499181	-3.213099
C	8.199408	14.915877	-4.115348
O	8.723672	14.391328	-5.154427
O	7.053259	14.700412	-3.653245
C	12.941858	7.491047	-4.734065
H	13.727544	7.741971	-5.451758
H	13.440409	7.181382	-3.805934
C	12.154094	8.765523	-4.471913
O	12.809340	9.856792	-4.599153
O	10.929842	8.718046	-4.171279
C	2.487233	13.808343	-7.849867
H	2.197714	14.855406	-8.019809
H	2.200056	13.267264	-8.763253
N	4.808327	14.503873	-8.477934
H	4.502122	15.231588	-9.116819
C	3.981045	13.750766	-7.648536
C	6.102148	14.257933	-8.155702
H	6.930327	14.740230	-8.652487
N	6.167666	13.375842	-7.166305
C	4.856498	13.058937	-6.841635
H	4.651550	12.375579	-6.034076
Zn	8.033001	12.865666	-6.183239
Zn	9.918282	10.438911	-4.425672
C	9.948137	10.786941	-7.198872
O	9.390390	11.32941	-6.09563

Atom	X	Y	Z
N	11.124215	11.759601	-7.571023
H	11.925706	11.130465	-7.711716
C	8.827762	10.509368	-8.229107
H	8.188519	9.815249	-7.669284
H	8.245948	11.424687	-8.361875
C	9.131727	9.927343	-9.616699
H	8.163218	9.732062	-10.094520
H	9.610668	10.692231	-10.238856
C	9.975516	8.633891	-9.813075
O	9.820070	8.069855	-10.913513
O	10.825180	8.289688	-8.911059
C	11.157917	12.836077	-8.617378
H	11.914019	13.527051	-8.225584
C	13.370048	8.720881	-11.924113
O	12.880002	7.816523	-11.297156
O	13.075028	8.845667	-13.253846
C	11.680597	12.395014	-10.007766
H	12.119507	13.291065	-10.454754
H	10.851335	12.102478	-10.660974
C	12.720669	11.272403	-9.951767
H	13.455294	11.471557	-9.168989
H	12.251345	10.316402	-9.695335
C	13.494889	11.151351	-11.262590
H	14.206137	11.986419	-11.329189
H	12.834635	11.246300	-12.133943
C	14.277132	9.822699	-11.370412
H	14.613672	9.500850	-10.376738
C	9.888719	13.704473	-8.752584

Atom	X	Y	Z
O	8.902336	13.577225	-7.970976
O	9.959577	14.542272	-9.689855
N	15.350279	10.016717	-12.348417
H	15.952760	9.187049	-12.438616
H	13.675016	9.549836	-13.613872
H	15.984695	10.752322	-12.011568
O	5.080583	13.430474	-2.279323
H	5.843026	13.752277	-2.815076
H	5.539125	12.739005	-1.737118
O	10.579144	9.616559	-6.834042
H	10.675033	9.004763	-7.695646
H	11.484463	12.342426	-6.541907
O	5.492286	12.532890	-10.605803
H	4.696635	12.184999	-11.086332
H	6.185858	11.924761	-10.948095
O	17.388067	11.685480	-4.691597
H	16.826147	11.957393	-3.935663
H	16.723307	11.071970	-5.109584
O	7.776201	15.989896	-10.201081
H	7.869171	16.735378	-9.568398
H	8.575799	15.442009	-9.945860
O	15.181305	10.029779	-3.231602
H	14.224174	10.053415	-3.471331
H	15.513313	9.809946	-4.141937
O	13.866821	10.147641	-7.132657
H	14.030495	11.121965	-7.137902
H	13.428015	10.082425	-6.243304
O	14.683267	13.960223	-9.070016

Atom	X	Y	Z
H	15.517897	13.402034	-8.937709
H	14.250091	13.620026	-8.245860
O	16.822563	14.513691	-7.165521
H	15.949394	14.464013	-6.728414
H	16.757738	13.644144	-7.648604
	P		
C	13.473589	12.743814	-0.379960
H	14.359193	12.589482	-1.002305
H	13.483077	13.801037	-0.101360
N	11.099644	13.199350	-1.160304
H	11.020270	14.117339	-0.723769
C	12.254224	12.431820	-1.185444
C	10.216008	12.680547	-2.050577
H	9.236937	13.098121	-2.221183
N	10.732053	11.613532	-2.632842
C	11.992149	11.446023	-2.094656
H	12.634958	10.642469	-2.400709
C	5.717953	10.355918	-3.450778
H	5.132773	11.240913	-3.185797
H	5.123069	9.774528	-4.160130
C	6.978775	10.819650	-4.166761
O	6.784254	11.414493	-5.261025
O	8.097226	10.558995	-3.624282
C	14.572731	13.694216	-3.948956
H	14.445955	12.784186	-3.352018
H	15.643608	13.913064	-3.970018
C	14.064996	13.367476	-5.364750
O	12.860472	13.300316	-5.619435

Atom	X	Y	Z
O	15.015539	13.096923	-6.213776
C	9.183227	15.655774	-3.432248
H	8.750830	15.884929	-2.458737
H	10.169265	15.210673	-3.297969
C	8.253249	14.664959	-4.140129
O	8.819270	13.949338	-5.038312
O	7.049827	14.647542	-3.810363
C	12.766498	7.654821	-4.783514
H	13.441593	7.994976	-5.571490
H	13.373257	7.418311	-3.901536
C	11.840192	8.818254	-4.470029
O	12.276436	9.995344	-4.662114
O	10.663128	8.625233	-4.032487
C	2.513164	13.710548	-7.922722
H	2.216240	14.749233	-8.121638
H	2.228969	13.141965	-8.819018
N	4.830203	14.459182	-8.518551
H	4.523542	15.210966	-9.128125
C	4.007220	13.670880	-7.719290
C	6.124245	14.207778	-8.200524
H	6.948592	14.709056	-8.686547
N	6.191237	13.295813	-7.246472
C	4.884114	12.956895	-6.938514
H	4.684844	12.239791	-6.160065
Zn	8.035928	12.704059	-6.320248
Zn	9.996511	10.535580	-4.206645
C	9.464927	10.071506	-6.969727
O	9.337777	10.988091	-6.043083

Atom	X	Y	Z
N	11.278933	11.780345	-7.894631
H	12.207908	11.365432	-7.827260
C	8.499498	10.127356	-8.143531
H	7.704505	9.404320	-7.915056
H	8.039411	11.112120	-8.203314
C	9.128449	9.856129	-9.520499
H	8.427738	10.182741	-10.291772
H	10.015937	10.495334	-9.575164
C	9.539116	8.438972	-9.902611
O	9.321158	8.002463	-11.022899
O	10.201952	7.705355	-9.013932
C	11.333062	12.994807	-8.696555
H	11.997343	13.743558	-8.232896
C	13.152811	8.891388	-11.865133
O	12.445996	8.410105	-11.015655
O	12.998421	8.571358	-13.176954
C	11.867090	12.692214	-10.122252
H	12.285504	13.614883	-10.532369
H	11.030871	12.409387	-10.775028
C	12.914280	11.574396	-10.146930
H	13.729477	11.814762	-9.457597
H	12.460508	10.638800	-9.804441
C	13.520173	11.329786	-11.529598
H	14.258047	12.106814	-11.766340
H	12.757513	11.384168	-12.318262
C	14.218494	9.951898	-11.601333
H	14.688400	9.736512	-10.634417
C	9.948981	13.674922	-8.783852

Atom	X	Y	Z
O	8.998842	13.348421	-7.987444
O	9.847972	14.549995	-9.677803
N	15.153990	9.926557	-12.724208
H	15.803995	9.130259	-12.672603
H	13.668560	9.135213	-13.647695
H	15.773079	10.740791	-12.657531
O	5.050201	13.552899	-2.338791
H	5.808479	13.834434	-2.896376
H	5.485797	12.918278	-1.734696
O	10.234401	9.104741	-6.851722
H	10.251123	8.497164	-7.703932
H	11.065060	12.056604	-6.943301
O	10.234403	9.104741	-6.851723
H	10.259471	8.193435	-8.129948
H	11.065060	12.056604	-6.943301
O	5.976497	11.595074	-11.118222
H	5.040007	11.555697	-11.412567
H	6.398064	11.055911	-11.812261
O	17.094215	11.667606	-4.909868
H	16.454544	11.415703	-4.217497
H	16.507087	12.212208	-5.478880
O	7.725504	16.035941	-10.144615
H	7.827029	16.778287	-9.510187
H	8.517694	15.468823	-9.902692
O	14.880281	10.145234	-3.356772
H	14.029635	10.317849	-3.811332
H	15.313828	9.584500	-4.042265
O	14.078093	10.405916	-6.900720

Atom	X	Y	Z
H	14.454208	11.305709	-6.792475
H	13.407628	10.387569	-6.185836
O	14.729876	13.947538	-8.799973
H	15.600673	13.483481	-8.844590
H	14.508587	13.689168	-7.873827
O	17.214843	14.618439	-7.005881
H	16.400517	14.319079	-6.543305
H	17.256504	13.900316	-7.676280

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