Supporting Information for "A Theoretical Study of Phosphoryl Transfers of Tyrosyl DNA-phosphodiesterase (Tdp1) and the Possibility of a 'Dead-End' Phosphohistidine Intermediate"

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SI TOC

Table S1. Energies and free energies (absolute energies in Hartrees, relative energies in kcal mol^{-1}).

	E	E_0	$G_{(gas)}$	$E_{(soln)}$	$\Delta G_{(gas)}$	$\Delta G_{(soln)}$
H_2O	-76.403471	-76.382356	-76.400008	-76.411791		
CH_3OH	-115.694897	-115.643437	-115.666178	-115.701645		
p-Ph(OH)(CH_3)	-346.712022	-346.578548	-346.610473	-346.721092		
$[P(O)_2(OCH_3)(OPhCH_3)]^-$	-953.171559	-952.996664	-953.039167	-953.240731		
$[P(O)_2(OCH_3)(OH)]^-$	-682.859018	-682.793599	-682.824598	-682.937466		
$[V(O)_2(OCH_3)(OPhCH_3)]^-$ (all electron)	-1555.855425	-1555.684346	-1555.729319	-1555.923188		
$[V(O)_2(OCH_3)(OPhCH_3)]^-$ (ECP)	-683.225891	-683.054823	-683.100331	-683.294990		
1RFF model without substrate	-4717.610701	-4715.827485	-4715.964288	-4717.737703		
VA-1 (all electron)	-6120.738648	-6118.835064	-6118.993341	-6120.847637		
VA-3 (all electron)	-6120.763915	-6118.857644	-6119.008931	-6120.858542		
VA-1 (ECP)	-5248.108803	-5246.205566	-5246.364446	-5248.218534		
VA-3 (ECP)	-5248.135428	-5246.229077	-5246.380149	-5248.230303		
A-1	-5518.066714	-5516.159099	-5516.315358	-5518.173507	0.00	0.00
A-2	-5518.068237	-5516.159745	-5516.314192	-5518.164800	0.73	7.15
A-TS-2-3	-5518.062726	-5516.154351	-5516.304168	-5518.156408	7.02	15.25
A-3	-5518.062797	-5516.154302	-5516.305328	-5518.156131	6.29	14.74
A-TS-3-4	-5518.061513	-5516.154233	-5516.303507	-5518.155359	7.44	15.56
A-4	-5518.080389	-5516.171752	-5516.324064	-5518.172874	-5.46	3.52
B-1	-5247.772218	-5245.973938	-5246.115614	-5247.865101	-6.73	1.53
B-TS-1-2	-5247.759119	-5245.964058	-5246.104623	-5247.852967	0.17	7.82
B-2	-5247.764630	-5245.965192	-5246.106892	-5247.859506	-1.25	5.75
B-TS-2-3	-5247.764599	-5245.965310	-5246.105746	-5247.859980	-0.54	6.15
B-3	-5247.770880	-5245.971503	-5246.115907	-5247.869718	-6.91	-2.39

Table S1 (continued). Energies and free energies (absolute energies in Hartrees, relative energies in kcal mol^{-1}).

C-1	-5247.799064	-5245.999970	-5246.142290	-5247.893177	-23.47	-15.98
C-TS-1-2	-5247.762106	-5245.963084	-5246.104448	-5247.859061	0.28	5.98
C-2	-5247.764112	-5245.964542	-5246.105840	-5247.859655	-0.59	5.99
C-TS-2-3	-5247.764009	-5245.964840	-5246.104179	-5247.859026	0.45	7.37
C-3	-5247.764251	-5245.964858	-5246.105658	-5247.858908	-0.48	6.66
C-TS-3-4	-5247.761935	-5245.965652	-5246.106217	-5247.855687	-0.83	6.88
C-4	-5247.787192	-5245.988355	-5246.129351	-5247.876193	-15.35	-4.65
C-TS-4-5	-5247.780977	-5245.987937	-5246.128667	-5247.869512	-14.92	-3.93
C-5	-5247.796282	-5245.996167	-5246.138702	-5247.890749	-21.22	-13.95

Table S2. List of residues included in fully QM model derived from 1RFF. Overall charge of total model is neutral.

Species/residue label	R group is protonated?	Species/residue charge	trim N-side	trim R	trim C-side
$[PO_2(OR^1)(OR^2)]^-$	N	-1	-	-	-
$[VO_2(OR^1)(OR^2)]^-$	N	-1	-	-	-
N203	N	0	H	-	-
Y204	N/A	0	-	CH_3	-
C205	N/A	0	-	H	H
H263	-	0, +1[a]	H	-	C(O)H
K265	Y	+1	H	-	H
T281	Y	0	H	-	-
S282	N/A	0	-	H	-
N283	Y	0	-	-	H
D288	N	-1	H	-	C(O)H
Q294	Y	0	H	-	H
F398	N/A	0	H	H	-
S399	Y	0	-	-	H
H493	-	0, +1[a]	H	-	C(O)H
K495	Y	+1	H	-	H
S514	Y	0	H	-	H
N516	Y	0	H	-	H
E538	N	-1	H	-	H
wat633	-	0	-	-	-
wat730	-	0	-	-	-

[a]Histidine residue charges will be altered by substrate binding and reactivity during the progress of the proposed chemical mechanism.

Cartesian coordinates and absolute energies of pertinent computed structures. For structures containing the enzyme, the Cartesian coordinates of the first 15 atoms are held frozen.

H_2O

O	0.000000	0.000000	0.110812
H	0.000000	0.783976	-0.443248
H	0.000000	-0.783976	-0.443248
O	0.000000	0.000000	0.110812
H	0.000000	0.783976	-0.443248
H	0.000000	-0.783976	-0.443248

CH_3OH

C	0.050461	0.673359	0.000000
H	1.059265	1.030025	0.000000
H	-0.455621	1.030026	0.872680
H	-0.455621	1.030026	-0.872680
O	0.050461	-0.756641	0.000000
H	-0.854475	-1.077096	0.000000
C	0.050461	0.673359	0.000000
H	1.059265	1.030025	0.000000
H	-0.455621	1.030026	0.872680
H	-0.455621	1.030026	-0.872680
O	0.050461	-0.756641	0.000000
H	-0.854475	-1.077096	0.000000

***p*-Ph(OH)(CH_3)**

C	-2.542690	1.388077	0.000000
C	-1.213369	0.665339	0.000000
C	-1.156274	-0.741902	0.000000
C	0.000000	1.368439	0.000000
C	0.060841	-1.421643	0.000000
C	1.230276	0.700368	0.000000
C	1.261738	-0.698318	0.000000
O	2.436467	-1.423526	0.000000
H	-3.142636	1.130722	0.882686
H	-3.142636	1.130722	-0.882686
H	-2.080886	-1.312824	0.000000
H	-0.012065	2.454704	0.000000
H	0.102331	-2.504929	0.000000
H	2.157458	1.268687	0.000000
H	-2.404367	2.474248	0.000000
H	3.187936	-0.815283	0.000000

el energy= -346.712022048
zpe= -346.578548
th energy= -346.571283
th enthalpy= -346.570339
free energy= -346.610473

$[P(O)_2(OCH_3)(OPhCH_3)]^-$

C	-2.480201	1.535955	-1.461495
O	-2.117066	0.157234	-1.286353
C	4.741269	-0.172814	-0.467370
C	3.269821	-0.032661	-0.136052
C	2.785968	1.066630	0.591882
C	2.338573	-1.011524	-0.527328
C	1.431707	1.182993	0.913052
C	0.981797	-0.915885	-0.211959
C	0.510291	0.196637	0.514756
O	-0.789424	0.392547	0.885461
P	-2.155636	-0.449140	0.263976
O	-3.299696	0.139556	1.020419
O	-1.834927	-1.904601	0.152723
H	-3.424285	1.759495	-0.953156
H	5.239257	-0.917822	0.171468
H	5.271716	0.777450	-0.330554
H	3.478513	1.844386	0.909223
H	2.684185	-1.875619	-1.092559
H	1.059086	2.035054	1.472119
H	0.273532	-1.683854	-0.497754
H	4.894420	-0.491964	-1.506873
H	-1.704111	2.204753	-1.064428
H	-2.584223	1.711335	-2.538036

el energy= -953.171558935
zpe= -952.996664
th energy= -952.983383
th enthalpy= -952.982438
free energy= -953.039167

$[P(O)_2(OCH_3)(OH)]^-$

P	-0.405363	0.121995	-0.425437
O	-1.708815	-0.836203	-0.660997
O	-0.548501	1.707869	0.018142
O	1.097257	-0.681741	-0.275328
O	-0.655476	-0.477917	1.426629
C	2.333413	-0.013790	0.024180
H	3.140797	-0.744919	0.065205
H	2.547186	0.720366	-0.752618
H	2.250144	0.489965	0.987195
H	-1.333886	0.091337	1.869133
P	-0.405363	0.121995	-0.425437
O	-1.708815	-0.836203	-0.660997
O	-0.548501	1.707869	0.018142
O	1.097257	-0.681741	-0.275328
O	-0.655476	-0.477917	1.426629
C	2.333413	-0.013790	0.024180
H	3.140797	-0.744919	0.065205
H	2.547186	0.720366	-0.752618
H	2.250144	0.489965	0.987195
H	-1.333886	0.091337	1.869133

$[V(O)_2(OCH_3)(OPhCH_3)]^-$ (all electron)

C	-3.821551	1.428663	-1.011829
O	-2.827334	0.432298	-1.160323
C	5.222700	-0.156760	-0.406695
C	3.736921	0.028203	-0.177327
C	3.221344	1.227604	0.342697
C	2.821566	-1.004354	-0.454171
C	1.855469	1.390583	0.583535
C	1.453770	-0.858459	-0.222446
C	0.941886	0.348995	0.306165
O	-0.362926	0.541460	0.554773
V	-1.949892	-0.404187	0.204928
O	-2.880932	-0.347263	1.511481
O	-1.631188	-1.926735	-0.202572
H	-4.363449	1.322491	-0.059892
H	5.714392	-0.660960	0.439735
H	5.728657	0.807060	-0.544376
H	3.902295	2.048631	0.562452
H	3.189596	-1.943685	-0.864257
H	1.464354	2.320072	0.984921
H	0.752005	-1.656423	-0.442233
H	5.419602	-0.766159	-1.298220
H	-3.383194	2.440466	-1.041916
H	-4.550344	1.359882	-1.835995

el energy= -1555.85542474
zpe= -1555.684346
th energy= -1555.669868
th enthalpy= -1555.668924
free energy= -1555.729319

$[V(O)_2(OCH_3)(OPhCH_3)]^-$ (ECP)

C	-3.821551	1.428663	-1.011829
O	-2.827334	0.432298	-1.160323
C	5.222700	-0.156760	-0.406695
C	3.736921	0.028203	-0.177327
C	3.221344	1.227604	0.342697
C	2.821566	-1.004354	-0.454171
C	1.855469	1.390583	0.583535
C	1.453770	-0.858459	-0.222446
C	0.941886	0.348995	0.306165
O	-0.362926	0.541460	0.554773
V	-1.949892	-0.404187	0.204928
O	-2.880932	-0.347263	1.511481
O	-1.631188	-1.926735	-0.202572
H	-4.363449	1.322491	-0.059892
H	5.714392	-0.660960	0.439735
H	5.728657	0.807060	-0.544376
H	3.902295	2.048631	0.562452
H	3.189596	-1.943685	-0.864257
H	1.464354	2.320072	0.984921
H	0.752005	-1.656423	-0.442233
H	5.419602	-0.766159	-1.298220

```
H    -3.383194  2.440466 -1.041916
H    -4.550344  1.359882 -1.835995
    el energy= -1555.85542474
          zpe= -1555.684346
    th energy= -1555.669868
  th enthalpy= -1555.668924
  free energy= -1555.729319
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1RFF model without substrate

```
C     1.616290 -6.265635  0.003390
C    -3.439847  5.220213 -0.336010
C    -2.684942 -8.002099  3.938390
C    -3.063297 -8.263872  2.494151
C     3.802002  7.429860 -2.016934
C     4.051731  5.971970 -1.641045
C     3.619874 -1.153089  4.172578
C    -6.451607  0.194545  3.333493
C     0.404546  1.855333  4.159438
C     0.277206  7.180031  3.636179
C    -7.536006 -3.308273 -0.038174
C    -8.878431  2.142819 -1.078789
C    -2.367135 -2.646375  3.895218
C     7.493204 -2.392783  0.967555
C     7.180659 -1.506334 -4.460071
C     0.198813 -6.456703 -0.628046
C    -2.184650  5.085401 -1.266703
C     3.565410 -1.153810  2.648893
C    -6.070629  0.296060  1.854157
C    -1.043089  2.390971  4.034970
C     5.437906  2.055414 -0.553503
C     4.971563  1.910935 -2.024266
C    -0.028723  7.280391  2.128539
C    -7.728188 -2.692698 -1.437955
N    -7.924445  1.686734 -1.956351
C    -1.125827 -3.123344  3.129843
C     6.644239 -3.677728  1.196464
C     3.832245 -3.917500 -2.815420
C     1.592541 -5.216271  1.078115
O     2.146953 -4.125864  0.959043
C    -0.459595 -5.175126 -1.060260
N    -1.552211 -4.677257 -0.373038
C    -0.192373 -4.246927 -2.049963
C    -1.906996 -3.506832 -0.935967
N    -1.101931 -3.196697 -1.966900
C    -3.368287  4.474931  0.973312
O    -3.526005  3.257001  1.040604
C    -1.619232  3.704460 -1.371837
N    -0.821196  3.170452 -0.369837
C    -1.709731  2.732551 -2.342059
C    -0.430537  1.940392 -0.698918
N    -0.965980  1.647940 -1.896651
C    -3.221186 -7.005331  1.619061
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O	-4.196392	-6.948158	0.831146
O	-2.297705	-6.096198	1.701349
C	3.328224	8.367431	-0.950109
O	2.874856	8.058104	0.145927
C	2.784154	5.119975	-1.953299
O	2.595793	4.068563	-1.193758
O	2.029993	5.470796	-2.866621
C	2.133515	-1.205357	2.089256
C	2.078632	-0.885455	0.593033
N	3.054460	-1.728774	-0.189421
C	-4.555697	0.117284	1.649906
C	-4.139758	-0.015140	0.186043
N	-4.536078	1.181853	-0.635043
C	1.283533	2.296365	2.992723
O	0.913873	2.162803	1.810484
O	-1.063381	3.826031	4.108316
C	-1.925884	1.866847	5.166811
N	2.486779	2.850301	3.301202
C	3.335456	3.500693	2.302128
C	4.382845	2.595880	1.628323
O	5.134541	1.885773	2.326344
N	4.429279	2.711147	0.288912
C	3.814447	0.936544	-2.217670
O	4.008441	-0.294395	-2.388062
N	2.577307	1.462742	-2.181081
C	0.173230	5.955510	1.420013
O	-0.640572	4.995886	1.597601
N	1.227035	5.839525	0.617084
C	-6.470812	-2.073637	-2.026516
O	-6.472590	-0.861434	-2.394423
N	-5.384103	-2.850749	-2.137132
O	-0.789363	-4.495034	3.364512
O	-9.370570	3.263026	-1.109382
C	-7.631663	2.450175	-3.177438
C	-6.575583	3.544540	-2.989727
O	-5.280041	3.036509	-2.591395
C	5.942696	-4.340885	-0.004337
O	5.691131	-5.545527	0.028412
C	6.674004	-1.127062	1.022745
O	5.710473	-0.976386	0.228209
N	6.998620	-0.192976	1.925688
N	5.606927	-3.538811	-1.065928
C	5.299832	-4.113861	-2.387175
C	6.272817	-3.539326	-3.432164
O	6.989663	-4.271606	-4.111614
N	6.295054	-2.172202	-3.513664
O	-5.017479	-5.437968	-1.193394
O	-4.271798	0.470862	-3.266362
H	1.926339	-7.224310	0.439624
H	2.353795	-5.985677	-0.754055
H	0.300039	-7.145257	-1.474009
H	-0.454317	-6.938629	0.106420

H	-2.010354	-5.189095	0.459263
H	0.578896	-4.270707	-2.804183
H	-2.754315	-2.925818	-0.609409
H	1.002634	-5.423342	1.985951
H	-3.616525	6.283882	-0.151398
H	-4.295245	4.814795	-0.891514
H	-2.482103	5.424536	-2.262565
H	-1.397601	5.762904	-0.924653
H	-0.575684	3.683489	0.507386
H	-2.236058	2.730484	-3.279852
H	0.203320	1.321470	-0.091583
H	-0.759391	0.753648	-2.382117
H	-3.170587	5.045126	1.889662
H	-1.762697	-7.415477	4.007665
H	-2.530890	-8.942200	4.480012
H	-3.470456	-7.444513	4.462828
H	-2.286774	-8.880564	2.015078
H	-3.999867	-8.824731	2.422126
H	4.690835	7.898260	-2.465023
H	3.041100	7.434516	-2.819606
H	4.877118	5.573654	-2.245038
H	4.331896	5.856250	-0.589297
H	3.397087	9.438752	-1.217386
H	3.118128	-2.031391	4.597136
H	3.134478	-0.258531	4.582320
H	4.655675	-1.154665	4.529243
H	4.077992	-0.260565	2.278605
H	4.121743	-2.025498	2.280567
H	1.698023	-2.190259	2.277232
H	1.506278	-0.461897	2.593277
H	1.087965	-1.075810	0.170322
H	2.349513	0.157824	0.412398
H	3.077171	-1.450285	-1.185389
H	4.027689	-1.555020	0.127811
H	2.842199	-2.733538	-0.070050
H	-5.926001	0.951227	3.928237
H	-6.191823	-0.790140	3.739673
H	-7.526175	0.344344	3.480879
H	-6.614362	-0.467606	1.279105
H	-6.393707	1.273395	1.466497
H	-4.020487	0.955693	2.112541
H	-4.228190	-0.794178	2.166317
H	-3.053455	-0.108308	0.090725
H	-4.603611	-0.885862	-0.284364
H	-4.246610	1.043939	-1.634179
H	-5.552664	1.314622	-0.680202
H	-4.132258	2.053268	-0.242493
H	0.818555	2.191708	5.116454
H	0.379422	0.757708	4.174501
H	-1.444576	2.059241	3.066132
H	-0.904494	4.201247	3.223242
H	-2.944688	2.246955	5.047473

H	-1.955603	0.771385	5.180134
H	-1.548091	2.217511	6.133455
H	3.884194	4.301220	2.810328
H	2.755796	2.913427	4.271848
H	2.689291	3.952797	1.551933
H	6.367287	2.641821	-0.548054
H	3.753146	3.336071	-0.190738
H	5.653945	1.066620	-0.150299
H	4.704496	2.890019	-2.431681
H	5.818010	1.523917	-2.598999
H	1.798355	0.825919	-2.304435
H	2.416671	2.458061	-1.940940
H	-0.312161	6.391048	4.113626
H	0.045741	8.128851	4.129394
H	1.338218	6.965115	3.805508
H	-1.076773	7.570757	1.988888
H	0.597743	8.050281	1.667596
H	1.875123	6.619988	0.487996
H	1.433827	4.984780	0.090965
H	-8.082466	-3.469051	-2.129622
H	-8.491652	-1.910206	-1.416690
H	-4.565013	-2.484657	-2.623414
H	-5.341845	-3.824935	-1.784331
H	-8.493231	-3.683775	0.336866
H	-6.831414	-4.144854	-0.062351
H	-7.168821	-2.564864	0.678258
H	-1.256197	-2.923887	2.051589
H	-0.254821	-2.546346	3.459247
H	-1.438216	-5.082826	2.919159
H	-2.528046	-1.570161	3.747533
H	-3.263593	-3.182546	3.560070
H	-2.245584	-2.834254	4.966893
H	-9.144809	1.392884	-0.311881
H	-7.304403	1.737007	-3.942690
H	-7.707330	0.691082	-1.978240
H	-8.554232	2.927564	-3.529262
H	-6.491986	4.122774	-3.921148
H	-6.890121	4.222902	-2.194269
H	-4.973176	2.382167	-3.243804
H	7.295046	-4.462623	1.592637
H	5.889647	-3.496681	1.973864
H	8.290806	-2.364828	1.717658
H	7.986833	-2.444722	-0.011434
H	6.399112	0.637834	2.040345
H	7.765123	-0.343487	2.564597
H	5.860027	-2.557340	-1.011247
H	5.513545	-5.181685	-2.316672
H	3.161778	-4.334776	-2.057627
H	3.591123	-2.858782	-2.964345
H	5.569420	-1.610721	-3.075684
H	8.018545	-2.172314	-4.671785
H	6.677998	-1.279114	-5.409264

```
H     7.556063 -0.572694 -4.029307
H     3.652081 -4.438870 -3.762439
H    -5.438001 -6.172036 -1.657671
H    -4.629995 -5.853805 -0.370831
H    -5.110790 -0.037119 -3.120285
H    -3.622240 -0.205809 -3.550403
O    -2.931213 -1.906118 -3.699831
O     0.077148 -0.734446 -2.676506
H    -2.214563 -2.358417 -3.187504
H    -3.052255 -2.401492 -4.520902
H    -0.349440 -1.582841 -2.375698
H     0.421850 -0.897143 -3.564663
    el energy= -4717.61070132
          zpe= -4715.827485
    th energy= -4715.727756
  th enthalpy= -4715.726812
  free energy= -4715.964288
```

VA-1 (all electron)

```
C     2.676168  5.993963  0.156797
C    -4.046614 -4.482927 -1.468571
C    -0.820049  8.827630 -3.935508
C    -1.323342  8.987706 -2.514710
C     2.532284 -8.012406  0.632466
C     3.040191 -6.582323  0.471236
C     4.371315  1.111256 -4.406093
C    -5.816101  1.336940 -4.753307
C     0.763202 -1.316886 -5.095175
C    -0.220825 -6.574714 -5.266487
C    -6.755506  4.578980 -1.089859
C    -9.012421 -0.661620 -0.887795
C    -1.314941  3.519500 -4.540161
C     7.979443  1.345511 -0.699586
C     6.897185 -0.067235  4.513412
C     1.178068  6.112270  0.607596
C    -2.882515 -4.828971 -0.480865
C     4.092032  0.997513 -2.906079
C    -5.490552  0.981172 -3.297776
C    -0.723363 -1.700851 -5.300543
C     5.125427 -2.707074  0.140459
C     4.576202 -2.661454  1.582191
C    -0.549896 -6.859144 -3.792520
C    -6.975819  3.793392  0.221584
N    -8.128602 -0.422510  0.121592
C     0.055578  3.848825 -3.926487
C     7.441868  2.802172 -0.822843
C     4.324148  3.150981  2.942746
C     2.782496  5.213542 -1.124227
O     3.260052  4.083837 -1.184365
C     0.401758  4.822934  0.542142
N    -0.631362  4.675102 -0.361579
C     0.501654  3.590537  1.178280
```

```
C    -1.098614  3.403609 -0.248770
N    -0.438279  2.706462  0.671968
C    -3.629875 -3.761903 -2.723021
O    -3.483005 -2.542561 -2.771682
C    -2.072965 -3.656910 -0.027034
N    -1.125118 -3.038512 -0.833599
C    -2.042046 -2.978674  1.170458
C    -0.531927 -2.047871 -0.155198
N    -1.085663 -1.987158  1.059328
C    -1.804870  7.684779 -1.853511
O    -2.772063  7.768108 -1.052053
O    -1.154674  6.605571 -2.118637
C     2.147110 -8.764751 -0.599446
O     1.864199 -8.277768 -1.689518
C     1.894110 -5.581588  0.843527
O     1.980544 -4.387165  0.334512
O     0.974384 -5.980901  1.571726
C     2.628395  1.264664 -2.507386
C     2.310115  0.834805 -1.067913
N     3.296651  1.421028 -0.082627
C    -3.973868  0.840850 -3.070817
C    -3.571687  0.722032 -1.600093
N    -4.166430 -0.492031 -0.943665
C     1.340769 -1.978757 -3.849825
O     0.773022 -1.884159 -2.747941
O    -0.850501 -3.113595 -5.535679
C    -1.323027 -0.982040 -6.507817
N     2.487570 -2.696621 -4.009224
C     3.036108 -3.540172 -2.951527
C     4.181881 -2.911993 -2.143062
O     5.110390 -2.319335 -2.733872
N     4.092230 -3.116022 -0.819452
C     3.557627 -1.547655  1.843365
O     3.932036 -0.361310  2.036995
N     2.268424 -1.911469  1.856157
C    -0.317398 -5.645297 -2.910523
O    -0.941479 -4.565501 -3.119565
N     0.546998 -5.784366 -1.904247
C    -5.817847  2.887945  0.623926
O    -5.989060  1.638102  0.723772
N    -4.636199  3.472134  0.865111
O     0.396618  5.238251 -3.973281
O    -9.714748 -1.664515 -0.986313
C    -7.987798 -1.353898  1.241326
C    -7.144939 -2.590865  0.903396
O    -5.802762 -2.263031  0.491617
C     6.892327  3.469542  0.450711
O     7.098117  4.666917  0.651799
C     6.932190  0.302104 -0.990758
O     5.859048  0.304006 -0.340121
N     7.188557 -0.610763 -1.938934
N     6.156999  2.676398  1.292909
```

```
C     5.837314  3.108255  2.664303
C     6.576825  2.216580  3.678745
O     7.383555  2.691124  4.480007
N     6.287419  0.882390  3.594871
O    -4.140590  6.131817  0.470731
O    -4.332458 -0.332261  1.742233
C    -1.139361  3.198330  4.396689
O    -0.388033  1.996612  4.208863
C    -3.818092 -2.479292  9.966652
C    -3.019797 -1.985849  8.779276
C    -3.645359 -1.343977  7.697406
C    -1.621628 -2.133983  8.733881
C    -2.912720 -0.856821  6.611649
C    -0.874694 -1.655721  7.656728
C    -1.516756 -1.009808  6.585724
O    -0.751118 -0.557650  5.551308
V    -0.918793  0.321687  3.985894
O    -2.470446  0.307952  3.536467
O    -0.002099 -0.456130  2.847866
H     3.078037  7.005074  0.011716
H     3.272355  5.490994  0.923262
H     1.174188  6.526486  1.622716
H     0.673964  6.841521 -0.035652
H    -0.974475  5.421541 -1.021203
H     1.157798  3.295644  1.983638
H    -1.915564  3.035714 -0.849155
H     2.355335  5.672569 -2.033039
H    -4.544384 -5.420318 -1.741363
H    -4.759456 -3.848206 -0.926002
H    -3.338986 -5.293879  0.398034
H    -2.224346 -5.580616 -0.926133
H    -0.883113 -3.342937 -1.791286
H    -2.604738 -3.133811  2.074262
H     0.258527 -1.431858 -0.538914
H    -0.736981 -1.323592  1.830619
H    -3.451623 -4.360888 -3.626485
H    -0.009178  8.094763 -3.989526
H    -0.447782  9.779541 -4.333418
H    -1.617271  8.478834 -4.603323
H    -0.519171  9.386928 -1.876038
H    -2.147453  9.706197 -2.456957
H     3.238689 -8.648751  1.183958
H     1.633267 -7.947793  1.278850
H     3.878929 -6.398405  1.154143
H     3.397897 -6.375247 -0.542928
H     2.098397 -9.864108 -0.477645
H     4.105933  2.102802 -4.793723
H     3.798058  0.365342 -4.971267
H     5.432761  0.939947 -4.617600
H     4.386455 -0.002818 -2.573639
H     4.735616  1.715088 -2.381651
H     2.396313  2.325816 -2.638951
```

```
H     1.950610  0.698157 -3.156630
H     1.316171  1.162449 -0.750217
H     2.384642 -0.251138 -0.963068
H     3.129902  1.067004  0.874090
H     4.258232  1.102532 -0.298955
H     3.281274  2.453599 -0.119833
H    -5.431284  0.573898 -5.440834
H    -5.364647  2.296419 -5.032408
H    -6.896917  1.414973 -4.913337
H    -5.890391  1.757180 -2.629456
H    -6.004170  0.044800 -3.033959
H    -3.592882 -0.022237 -3.631907
H    -3.468974  1.727873 -3.473341
H    -2.487172  0.637390 -1.487843
H    -3.912242  1.587703 -1.027822
H    -3.950562 -0.516503  0.087376
H    -5.191480 -0.497691 -0.965586
H    -3.860065 -1.358698 -1.425697
H     1.324902 -1.596628 -5.993729
H     0.839474 -0.228604 -4.974511
H    -1.271838 -1.422753 -4.389783
H    -0.892225 -3.580262 -4.681190
H    -2.375180 -1.260710 -6.618782
H    -1.254959  0.106626 -6.401067
H    -0.797545 -1.277199 -7.423078
H     3.421081 -4.456416 -3.414729
H     2.939183 -2.699805 -4.911311
H     2.218153 -3.809671 -2.287720
H     5.967933 -3.412646  0.105948
H     3.291941 -3.665122 -0.443708
H     5.493499 -1.718820 -0.130405
H     4.144150 -3.629896  1.850647
H     5.423493 -2.474581  2.250358
H     1.557539 -1.259541  2.209952
H     1.995165 -2.854527  1.563096
H    -0.779740 -5.714608 -5.645373
H    -0.467193 -7.445043 -5.883196
H     0.846887 -6.364799 -5.396731
H    -1.612290 -7.123281 -3.701683
H     0.031861 -7.709662 -3.425216
H     1.074652 -6.652223 -1.794463
H     0.754316 -5.028101 -1.250589
H    -7.154110  4.505170  1.038534
H    -7.861722  3.156367  0.146484
H    -3.862694  2.896305  1.177337
H    -4.462382  4.491604  0.739526
H    -7.661796  5.140001 -1.340971
H    -5.930993  5.290196 -0.985566
H    -6.538322  3.905341 -1.926773
H     0.091724  3.464419 -2.894447
H     0.841407  3.333464 -4.491583
H    -0.212202  5.753166 -3.400118
```

```
H    -1.488767  2.435389 -4.543689
H    -2.117730  4.004448 -3.970551
H    -1.367538  3.883849 -5.571793
H    -9.037139  0.156460 -1.631832
H    -7.535462 -0.803745  2.073436
H    -7.584927  0.437901  0.148771
H    -8.984489 -1.688579  1.552098
H    -7.132164 -3.264052  1.773807
H    -7.602735 -3.122224  0.066600
H    -5.347178 -1.771323  1.207898
H     8.254138  3.457633 -1.146522
H     6.671414  2.855424 -1.603946
H     8.835637  1.224951 -1.372559
H     8.355080  1.179085  0.318493
H     6.467372 -1.301319 -2.201946
H     8.052218 -0.573665 -2.458692
H     6.079096  1.690338  1.057634
H     6.260681  4.108127  2.770809
H     3.830266  3.813574  2.225267
H     3.865339  2.157951  2.883918
H     5.513732  0.547931  3.023578
H     7.709017  0.444518  5.032730
H     6.178126 -0.430331  5.258734
H     7.300663 -0.929642  3.969698
H     4.139778  3.539107  3.950359
H    -4.413783  6.805351  1.103954
H    -3.546251  6.611391 -0.181947
H    -4.906860  0.456859  1.625924
H    -3.654158 -0.140940  2.444620
H    -0.814451  3.941416  3.660800
H    -3.436220 -3.437310 10.338786
H    -4.873719 -2.617079  9.708378
H    -4.725531 -1.220593  7.705001
H    -1.110991 -2.632303  9.553963
H    -3.405621 -0.365535  5.780030
H     0.202626 -1.773487  7.622574
H    -3.777606 -1.768962 10.804408
H    -2.214277  3.016688  4.271356
H    -0.958861  3.587783  5.405775
    el energy= -6120.73864767
          zpe= -6118.835064
    th energy= -6118.723726
  th enthalpy= -6118.722782
  free energy= -6118.993341
```

VA-3 (all electron)

```
C    -2.305333 -6.050804 -0.386741
C     3.978405  4.817221 -0.426883
C     1.775546 -8.381601 -4.248614
C     2.124537 -8.633456 -2.795213
C    -2.976096  7.862747  1.158278
C    -3.384408  6.428958  0.831848
```

```
C    -3.741718 -0.895634 -4.733636
C     6.417645 -0.630561 -3.914356
C    -0.216316  1.741371 -4.814816
C     0.493878  7.034926 -4.473532
C     7.115766 -4.113438 -0.421985
C     9.048202  1.190375  0.435098
C     2.046098 -3.024929 -4.389435
C    -7.723928 -1.593288 -1.498326
C    -7.310193 -0.560846  3.896609
C    -0.952278 -6.389477  0.312472
C     2.705966  5.220765  0.387018
C    -3.632700 -0.879942 -3.209746
C     5.512145 -0.857622 -2.696853
C     1.226520  2.301340 -4.905892
C    -5.236324  2.513797  0.133439
C    -4.795455  2.301542  1.603643
C     0.612012  7.214512 -2.951030
C     7.047684 -3.274288  0.874187
N     7.992915  0.907058  1.243742
C     0.666076 -3.432979 -3.853661
C    -7.099585 -3.009261 -1.669629
C    -4.430697 -3.545257  2.400614
C    -2.112382 -5.135728 -1.564377
O    -2.560779 -3.993259 -1.598666
C    -0.153922 -5.158479  0.618922
N     0.891464 -4.772633 -0.200827
C    -0.297933 -4.145480  1.547226
C     1.344417 -3.580169  0.227785
N     0.643639 -3.164522  1.286356
C     3.676920  4.117633 -1.725065
O     3.543371  2.902547 -1.804945
C     1.927132  4.022848  0.814952
N     1.085411  3.310755 -0.029944
C     1.986029  3.301500  1.981454
C     0.650637  2.204767  0.589966
N     1.189118  2.187824  1.816907
C     2.368796 -7.363183 -1.965577
O     3.278224 -7.391463 -1.100330
O     1.577790 -6.361074 -2.173625
C    -2.595958  8.771771  0.033288
O    -2.219310  8.432067 -1.083555
C    -2.277912  5.444015  1.347006
O    -2.204692  4.294265  0.737611
O    -1.538931  5.813267  2.267589
C    -2.198252 -1.078917 -2.687773
C    -2.045376 -0.732839 -1.203202
N    -3.064981 -1.466574 -0.358817
C     4.253183  0.021949 -2.771346
C     3.275558 -0.143094 -1.608028
N     3.828702  0.346777 -0.295886
C    -0.888169  2.184016 -3.518903
O    -0.361104  1.978104 -2.411226
```

```
O     1.207833  3.738606 -4.899808
C     1.917152  1.860338 -6.194806
N    -2.076359  2.841971 -3.652355
C    -2.711534  3.541268 -2.544476
C    -3.991977  2.885626 -2.001534
O    -4.801834  2.333196 -2.775116
N    -4.121237  3.020602 -0.672189
C    -3.742976  1.205048  1.764260
O    -4.074500 -0.004964  1.843329
N    -2.460953  1.602917  1.787905
C     0.269098  5.951405 -2.178485
O     0.928335  4.886844 -2.337695
N    -0.734218  6.036458 -1.300950
C     5.798107 -2.413383  0.999259
O     5.890452 -1.144969  1.006250
N     4.616246 -3.022015  1.112472
O     0.336276 -4.807563 -4.086235
O     9.760766  2.189836  0.512545
C     7.560199  1.831699  2.288552
C     6.579392  2.904567  1.794718
O     5.338694  2.364139  1.299999
C    -6.677380 -3.760378 -0.393897
O    -6.853653 -4.976822 -0.312036
C    -6.702438 -0.483035 -1.552566
O    -5.711116 -0.507696 -0.782774
N    -6.900252  0.516675 -2.424264
N    -6.083510 -3.013552  0.589175
C    -5.903641 -3.540053  1.951516
C    -6.794616 -2.758818  2.936343
O    -7.671718 -3.322344  3.593009
N    -6.550367 -1.414429  2.995545
O     4.184173 -5.731933  0.762637
O     4.321339  0.528367  2.974065
C     1.305886 -3.085185  4.590761
O     0.492403 -2.252574  3.768097
C     0.128421  1.380483  8.905436
C     0.512329  1.030330  7.483866
C     1.859421  0.952738  7.091681
C    -0.469265  0.792833  6.505796
C     2.217482  0.654990  5.774182
C    -0.127601  0.494906  5.184764
C     1.223990  0.424773  4.806463
O     1.603145  0.174480  3.506773
V     0.922780 -1.300855  2.297130
O     2.314217 -1.131643  1.408154
O    -0.333466 -0.509387  1.642850
H    -2.765740 -6.986998 -0.733553
H    -2.993841 -5.575142  0.317215
H    -1.172846 -6.955546  1.223556
H    -0.360127 -7.039552 -0.339993
H     1.293507 -5.369142 -0.990970
H    -0.982480 -4.055023  2.374098
```

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H     2.170681 -3.052090 -0.210668
H    -1.511083 -5.506661 -2.411538
H     4.553577  5.727808 -0.635225
H     4.573420  4.138155  0.193754
H     3.041394  5.758687  1.278912
H     2.082145  5.910756 -0.185707
H     0.852223  3.595405 -0.993994
H     2.538169  3.481898  2.886546
H     0.002742  1.456982  0.172651
H     1.173882  1.387033  2.502910
H     3.563407  4.741918 -2.625476
H     0.898248 -7.733441 -4.339195
H     1.561672 -9.321068 -4.772218
H     2.600822 -7.889168 -4.777363
H     1.301270 -9.176347 -2.304137
H     3.014595 -9.263040 -2.697638
H    -3.746794  8.390499  1.737861
H    -2.112077  7.793291  1.849805
H    -4.321310  6.171873  1.341405
H    -3.550321  6.275467 -0.239648
H    -2.646439  9.851468  0.273301
H    -3.365150 -1.834929 -5.158014
H    -3.164839 -0.073709 -5.176254
H    -4.783076 -0.776524 -5.053967
H    -4.031504  0.070357 -2.841827
H    -4.271001 -1.676690 -2.805848
H    -1.881722 -2.110646 -2.864411
H    -1.506469 -0.427526 -3.232410
H    -1.062442 -0.995391 -0.808825
H    -2.209781  0.332866 -1.028551
H    -2.982054 -1.208840  0.637985
H    -4.025670 -1.183092 -0.620212
H    -2.975743 -2.487149 -0.494643
H     6.742530  0.415452 -3.973087
H     5.891426 -0.870199 -4.846580
H     7.315970 -1.256283 -3.868978
H     5.218428 -1.916049 -2.642394
H     6.077763 -0.643639 -1.779186
H     4.533890  1.077042 -2.856870
H     3.704924 -0.223487 -3.691490
H     2.357940  0.423174 -1.787364
H     3.009355 -1.192948 -1.458441
H     3.163262  0.064716  0.464271
H     4.716325 -0.115953 -0.019309
H     3.988505  1.364140 -0.313494
H    -0.780901  2.077374 -5.691860
H    -0.177935  0.644903 -4.834081
H     1.788304  1.934650 -4.035696
H     1.142819  4.058835 -3.980741
H     2.937380  2.254157 -6.222139
H     1.958309  0.767958 -6.273733
H     1.379461  2.253433 -7.065071
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H	-2.960181	4.560041	-2.866911
H	-2.468285	2.950925	-4.575561
H	-1.975099	3.606495	-1.746675
H	-6.076784	3.221905	0.116690
H	-3.397454	3.573521	-0.167747
H	-5.573359	1.563816	-0.280059
H	-4.423463	3.242223	2.021025
H	-5.675857	1.998562	2.178427
H	-1.733719	0.889131	1.870050
H	-2.207467	2.582292	1.609557
H	1.107467	6.204957	-4.833555
H	0.814419	7.948860	-4.984165
H	-0.543555	6.836047	-4.765631
H	1.649524	7.470460	-2.696341
H	-0.020160	8.041996	-2.614041
H	-1.299055	6.884241	-1.232484
H	-1.005946	5.241898	-0.722017
H	7.091764	-3.948348	1.739518
H	7.905649	-2.599414	0.938985
H	3.788165	-2.437845	1.265529
H	4.501751	-4.047954	1.032792
H	8.071054	-4.646494	-0.468628
H	6.309934	-4.853103	-0.450925
H	7.042340	-3.476570	-1.310538
H	0.598767	-3.183880	-2.781209
H	-0.109904	-2.853152	-4.366065
H	0.889532	-5.384296	-3.516332
H	2.213033	-1.948556	-4.254724
H	2.842875	-3.568953	-3.867424
H	2.122166	-3.257901	-5.456822
H	9.220429	0.399989	-0.320136
H	7.095056	1.250180	3.092247
H	7.402698	0.100608	1.046711
H	8.450381	2.328171	2.688719
H	6.393848	3.615488	2.616224
H	7.033539	3.455581	0.966339
H	4.919957	1.817527	2.009667
H	-7.830155	-3.667767	-2.145841
H	-6.237528	-2.960019	-2.348607
H	-8.488096	-1.445941	-2.269474
H	-8.239707	-1.535147	-0.530637
H	-6.187197	1.255969	-2.529015
H	-7.690023	0.495733	-3.051275
H	-6.006330	-2.011276	0.433682
H	-6.289741	-4.560367	1.934799
H	-3.829105	-4.138289	1.704625
H	-4.014068	-2.533751	2.453914
H	-5.730537	-1.010435	2.546416
H	-8.183136	-1.122413	4.233326
H	-6.722403	-0.269890	4.776916
H	-7.639673	0.348894	3.381371
H	-4.345134	-3.993600	3.396699

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H     4.346655 -6.396147  1.442117
H     3.794644 -6.231968 -0.009585
H     4.706181 -0.239463  2.520902
H     3.370946  0.333670  3.147022
H     1.698995 -3.936962  4.017611
H    -0.083052  2.453604  9.014123
H     0.931942  1.135192  9.608490
H     2.640068  1.126095  7.828048
H    -1.519328  0.838663  6.782926
H     3.260175  0.599492  5.478103
H    -0.898412  0.300992  4.448206
H    -0.771294  0.840943  9.222768
H     2.145966 -2.520399  5.015625
H     0.698137 -3.469203  5.417448
    el energy= -6120.76391531
          zpe= -6118.857644
    th energy= -6118.747303
  th enthalpy= -6118.746359
  free energy= -6119.008931
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VA-1 (ECP)

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C     2.399113  6.053093 -0.382033
C    -3.787092 -4.849083 -1.072145
C    -1.149498  8.302211 -4.780783
C    -1.686625  8.574236 -3.389708
C     2.910883 -7.831501  1.456846
C     3.353334 -6.400565  1.163995
C     4.410069  0.840542 -4.421796
C    -5.768182  0.531499 -4.934274
C     0.934903 -1.816985 -4.921760
C     0.204839 -7.108605 -4.592862
C    -6.929520  4.063054 -1.618618
C    -8.938697 -1.237728 -0.937956
C    -1.380476  2.942618 -4.871241
C     7.932204  1.609348 -0.704920
C     6.819690  0.656670  4.605183
C     0.876799  6.132784 -0.016288
C    -2.626400 -5.032347 -0.038167
C     4.103190  0.857953 -2.922895
C    -5.467921  0.333513 -3.444019
C    -0.536749 -2.266062 -5.097355
C     5.250475 -2.484965  0.472131
C     4.666823 -2.332402  1.892813
C    -0.159331 -7.254157 -3.106493
C    -7.122648  3.473522 -0.203805
N    -8.085077 -0.850969  0.051778
C    -0.031837  3.402091 -4.293700
C     7.332102  3.020665 -0.976907
C     4.128723  3.573675  2.687695
C     2.607354  5.156795 -1.571604
O     3.142980  4.054340 -1.500144
C     0.178475  4.799103  0.034834
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N    -0.841805  4.510614 -0.849251
C     0.348563  3.636779  0.778535
C    -1.233062  3.228693 -0.622476
N    -0.535389  2.656945  0.355403
C    -3.389902 -4.221973 -2.382101
O    -3.315510 -3.005411 -2.540925
C    -1.886425 -3.779656  0.306197
N    -0.965543 -3.190098 -0.551722
C    -1.902448 -2.991079  1.434364
C    -0.433595 -2.108120  0.030825
N    -1.000682 -1.963481  1.232173
C    -2.127530  7.318825 -2.616222
O    -3.104964  7.437157 -1.831587
O    -1.436280  6.244894 -2.778855
C     2.562475 -8.711269  0.300530
O     2.278984 -8.342798 -0.834696
C     2.156150 -5.424260  1.419941
O     2.185623 -4.292131  0.778870
O     1.254538 -5.784486  2.189845
C     2.620747  1.097160 -2.577182
C     2.288630  0.787771 -1.110324
N     3.228490  1.504285 -0.166167
C    -3.953266  0.299891 -3.167090
C    -3.590994  0.339774 -1.682123
N    -4.150028 -0.834034 -0.928318
C     1.526524 -2.336760 -3.616544
O     0.943973 -2.169319 -2.531252
O    -0.618459 -3.697422 -5.206408
C    -1.150268 -1.677493 -6.366754
N     2.707178 -3.011266 -3.700997
C     3.282948 -3.723397 -2.564013
C     4.372749 -2.958180 -1.797626
O     5.282585 -2.374309 -2.425000
N     4.263157 -3.040651 -0.462346
C     3.600000 -1.242270  2.029136
O     3.922643 -0.029602  2.121918
N     2.324916 -1.654783  2.042730
C     0.004262 -5.949470 -2.346623
O    -0.666327 -4.926586 -2.668082
N     0.861155 -5.946852 -1.324324
C    -5.955005  2.629734  0.292703
O    -6.101555  1.388360  0.490967
N    -4.790662  3.258608  0.503924
O     0.232802  4.797792 -4.469037
O    -9.585396 -2.281913 -0.941392
C    -7.935871 -1.645002  1.272401
C    -7.039999 -2.878304  1.094421
O    -5.698604 -2.548936  0.681657
C     6.729311  3.780695  0.218238
O     6.876601  5.000263  0.305483
C     6.938411  0.494939 -0.908784
O     5.853968  0.509387 -0.277431
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N     7.254036 -0.491499 -1.760660
N     6.016738  3.037563  1.122588
C     5.648142  3.582012  2.440097
C     6.406885  2.828780  3.548096
O     7.168065  3.416067  4.318511
N     6.189867  1.478727  3.582942
O    -4.401745  5.883367 -0.161842
O    -4.382339 -0.391439  1.717827
C    -1.233022  3.647246  3.994909
O    -0.471102  2.443141  3.874701
C    -4.123337 -0.770067 10.146894
C    -3.287678 -0.560227  8.902669
C    -3.833699  0.028883  7.750038
C    -1.930147 -0.927625  8.870994
C    -3.061462  0.257129  6.607672
C    -1.145108 -0.710622  7.738224
C    -1.706622 -0.113514  6.595660
O    -0.899732  0.078672  5.512669
V    -1.000309  0.746349  3.835248
O    -2.555430  0.667683  3.339546
O    -0.026050 -0.183450  2.851170
H     2.756716  7.065083 -0.612227
H     2.980325  5.663904  0.458509
H     0.797545  6.661532  0.941181
H     0.366798  6.750312 -0.763464
H    -1.219801  5.172889 -1.575685
H     1.015270  3.455200  1.608268
H    -2.024322  2.760940 -1.186700
H     2.200407  5.502860 -2.538231
H    -4.223242 -5.835901 -1.264320
H    -4.548085 -4.212660 -0.601790
H    -3.075296 -5.430192  0.876766
H    -1.921442 -5.788372 -0.395875
H    -0.693117 -3.575946 -1.471307
H    -2.464178 -3.090036  2.346653
H     0.323560 -1.486249 -0.406945
H    -0.694990 -1.212001  1.935434
H    -3.159201 -4.888836 -3.223812
H    -0.310080  7.600876 -4.752428
H    -0.806589  9.226932 -5.260825
H    -1.919333  7.860552 -5.425352
H    -0.912071  9.064839 -2.778701
H    -2.540098  9.259664 -3.412633
H     3.645955 -8.382418  2.060874
H     2.010424 -7.751061  2.098854
H     4.168593 -6.111410  1.838934
H     3.721302 -6.276059  0.140242
H     2.546740 -9.794451  0.529461
H     4.108651  1.777206 -4.907107
H     3.883308  0.018482 -4.922929
H     5.482466  0.699765 -4.597237
H     4.432684 -0.091835 -2.490032
```

```
H     4.703445  1.650400 -2.458643
H     2.347727  2.130575 -2.811553
H     1.981671  0.444864 -3.183942
H     1.275408  1.099576 -0.841282
H     2.406018 -0.279953 -0.905105
H     3.060584  1.230693  0.816363
H     4.207468  1.214548 -0.339533
H     3.167946  2.527704 -0.294671
H    -5.322505 -0.270459 -5.535337
H    -5.360952  1.484047 -5.293664
H    -6.846353  0.532797 -5.127816
H    -5.929110  1.144771 -2.862753
H    -5.938695 -0.601620 -3.105966
H    -3.510628 -0.589207 -3.634444
H    -3.484026  1.172469 -3.638689
H    -2.507842  0.318417 -1.533429
H    -3.987387  1.238108 -1.204085
H    -3.965562 -0.745839  0.106131
H    -5.172308 -0.890312 -0.979050
H    -3.788611 -1.726511 -1.315511
H     1.512111 -2.162656 -5.786933
H     0.975608 -0.720242 -4.905442
H    -1.100854 -1.925233 -4.217878
H    -0.647870 -4.087831 -4.314147
H    -2.192344 -1.998300 -6.456800
H    -1.116737 -0.582038 -6.357543
H    -0.609263 -2.036576 -7.249562
H     3.731590 -4.651154 -2.938247
H     3.171819 -3.072299 -4.594363
H     2.468814 -3.983294 -1.891655
H     6.129913 -3.142973  0.520343
H     3.480125 -3.588022 -0.049933
H     5.571770 -1.507915  0.114172
H     4.267391 -3.289412  2.240594
H     5.489980 -2.049919  2.557514
H     1.584437 -1.000895  2.321095
H     2.095247 -2.631916  1.837668
H    -0.372074 -6.313309 -5.073205
H     0.008545 -8.045828 -5.123434
H     1.268165 -6.872441 -4.714059
H    -1.213901 -7.547933 -3.017716
H     0.441138 -8.040291 -2.639402
H     1.424186 -6.774770 -1.122325
H     1.026677 -5.122006 -0.745176
H    -7.280800  4.296245  0.505046
H    -8.009815  2.834813 -0.169846
H    -4.010385  2.730623  0.878357
H    -4.640290  4.265466  0.283136
H    -7.842575  4.580507 -1.931168
H    -6.108118  4.785012 -1.628240
H    -6.723169  3.277536 -2.354569
H     0.022217  3.117149 -3.230603
```

```
H     0.782841  2.880625 -4.810435
H    -0.412402  5.329136 -3.953775
H    -1.496247  1.855321 -4.770935
H    -2.209952  3.435928 -4.349027
H    -1.449076  3.203783 -5.932769
H    -8.992248 -0.503001 -1.763003
H    -7.525056 -0.987111  2.045719
H    -7.607948  0.047450  0.008172
H    -8.926287 -1.983062  1.599890
H    -7.029218 -3.449634  2.034906
H    -7.454971 -3.516135  0.311368
H    -5.286424 -1.955695  1.344566
H     8.119959  3.679144 -1.350905
H     6.574370  2.963090 -1.770030
H     8.805294  1.464546 -1.350785
H     8.295661  1.559701  0.329780
H     6.571057 -1.237899 -1.967169
H     8.124723 -0.463105 -2.269145
H     5.987506  2.031032  0.982010
H     6.019894  4.607592  2.457350
H     3.618948  4.138713  1.901181
H     3.721254  2.557250  2.716721
H     5.441166  1.053672  3.039469
H     7.670861  1.209127  5.006452
H     6.133155  0.431065  5.431727
H     7.167979 -0.288336  4.173697
H     3.903137  4.045749  3.650139
H    -4.712548  6.602032  0.400549
H    -3.828495  6.326645 -0.857577
H    -5.000166  0.342067  1.497887
H    -3.713629 -0.056796  2.373143
H    -0.871064  4.367051  3.253343
H    -3.861186 -1.705831 10.654201
H    -5.192130 -0.805613  9.909152
H    -4.881980  0.317232  7.746095
H    -1.482338 -1.391655  9.745998
H    -3.497339  0.705695  5.721821
H    -0.099580 -0.997140  7.714109
H    -3.978102  0.042200 10.873012
H    -2.300358  3.461335  3.821610
H    -1.099436  4.062712  5.001040
    el energy= -5248.10880334
          zpe= -5246.205566
    th energy= -5246.094032
  th enthalpy= -5246.093088
  free energy= -5246.364446
```

VA-3 (ECP)

```
C    -2.242444 -6.069458 -0.405169
C     3.947802  4.852160 -0.396884
C     1.883831 -8.362509 -4.241316
C     2.225328 -8.612340 -2.785788
```

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C    -3.042971  7.836772  1.143974
C    -3.436773  6.399750  0.813955
C    -3.694218 -0.923878 -4.758310
C     6.456835 -0.572113 -3.871463
C    -0.191146  1.743363 -4.814460
C     0.471256  7.042590 -4.465195
C     7.161686 -4.051225 -0.376692
C     9.042750  1.268408  0.496478
C     2.109271 -3.003617 -4.377024
C    -7.691652 -1.657894 -1.549931
C    -7.322585 -0.625583  3.848269
C    -0.889795 -6.395384  0.299946
C     2.665350  5.244185  0.406801
C    -3.589649 -0.905916 -3.234286
C     5.545907 -0.809710 -2.659580
C     1.249319  2.310966 -4.894622
C    -5.262351  2.476737  0.089825
C    -4.833960  2.266391  1.563843
C     0.583710  7.219485 -2.941954
C     7.091480 -3.200690  0.911397
N     7.980952  0.977063  1.293923
C     0.732856 -3.423789 -3.841435
C    -7.057023 -3.069991 -1.715712
C    -4.400510 -3.574934  2.366601
C    -2.052226 -5.152242 -1.581627
O    -2.512710 -4.014777 -1.618827
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A-1

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H    -2.979015 -1.083957  6.127695
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A-2

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C	-3.944132	6.032678	0.761696
C	-3.625843	-1.413589	-4.642287
C	6.465650	-0.171388	-3.884833
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C	-0.158824	6.885656	-4.576791
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C	-7.513067	-2.413172	-1.370892
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A-TS-2-3

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  th enthalpy= -5516.044211
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free energy= -5516.304168

A-3

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C	-0.253807	1.726144	-4.726183
C	-0.035385	7.060257	-4.349333
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A-TS-3-4

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  th enthalpy= -5516.060502
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B-1

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C    -2.451731 -8.509323  2.487662
C     3.149030  7.770643 -1.679391
C     3.513812  6.336407 -1.306710
C     3.524936 -0.858987  4.435975
C    -6.594273 -0.389007  3.280300
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C    -0.517635  7.154801  3.854034
C    -7.259602 -3.938130 -0.151248
C    -9.041495  1.384844 -1.193658
C    -2.296073 -2.867395  3.952957
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B-TS-1-2

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H     2.590408  2.944124  4.126218
H     2.283781  3.669609  1.287916
H     6.317333  2.667547 -0.451944
H     3.669588  3.300255 -0.286941
H     5.619457  1.092472 -0.013680
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H     5.854035  1.443165 -2.487777
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H     2.430396  2.297267 -2.132125
H    -0.818158  6.620497  4.007904
H    -0.084191  8.224645  4.183181
H     0.936696  6.781488  4.094474
H    -0.836704  7.873090  1.821368
H     0.914613  8.065170  1.892703
H     1.827415  6.745741  0.407567
H     1.315384  5.131852 -0.011683
H    -7.368076 -3.306124 -2.245135
H    -8.085047 -1.867181 -1.510229
H    -3.962069 -2.121058 -1.663524
H    -4.848382 -3.645226 -1.468412
H    -8.499847 -3.858017 -0.066307
H    -6.764734 -4.218209  0.003765
H    -7.408673 -2.759400  0.792851
H    -0.914969 -3.029638  2.481501
H    -0.285732 -2.726661  4.103547
H    -1.517068 -5.146933  3.245877
H    -2.458653 -1.543351  3.792411
H    -3.264722 -3.084274  3.407096
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H    -9.171077  1.323149 -0.361139
H    -6.928001  1.609782 -3.778883
H    -7.322420  0.750969 -1.593323
H    -8.126066  2.889397 -3.478976
H    -5.914343  3.896219 -3.532872
H    -6.546245  3.979445 -1.875102
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H     7.414539 -4.273178  1.968644
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H     8.237667 -2.099212  2.065442
H     8.015657 -2.206078  0.322309
H     6.177291  0.789105  2.218732
H     7.608986 -0.075361  2.761589
H     5.608924 -2.530532 -0.578087
H     5.691792 -5.106586 -2.090396
H     3.318078 -4.353899 -1.860187
H     3.715207 -2.783373 -2.599188
H     5.708179 -1.522719 -2.729775
H     6.739899 -1.081793 -5.070532
H     7.699692 -0.457488 -3.705734
H     8.096557 -2.035922 -4.440449
H     3.833974 -4.270564 -3.558533
H    -5.018968 -6.028866 -1.764455
H    -4.338131 -5.848744 -0.372718
H    -4.327423  0.011083 -3.201075
H    -3.012342  0.570277 -3.823828
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H    -2.893751 -1.762754 -4.673756
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  th enthalpy= -5245.860232
  free energy= -5246.104623
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B-2

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C    -3.058896 -8.248236  2.592658
C     3.736309  7.487451 -1.877898
C     3.993284  6.035047 -1.486101
C     3.508481 -1.053580  4.367825
C    -6.555639  0.178447  3.295538
C     0.262139  1.919440  4.261552
C     0.089318  7.238665  3.697117
C    -7.527022 -3.359458 -0.074050
C    -8.904420  2.069291 -1.183442
C    -2.454484 -2.613887  3.968298
C     7.465333 -2.273337  1.258570
C     7.264314 -1.428217 -4.180898
C     0.305861 -6.431325 -0.569988
C    -2.180359  5.505672 -1.095695
C     3.324083 -1.027308  2.841416
C    -5.644950 -0.199717  2.117517
C    -1.102353  2.655500  4.313773
C     5.435296  1.999253 -0.448721
C     5.008763  1.772189 -1.917560
C     0.131899  7.414509  2.175398
C    -7.300852 -2.640640 -1.424469
N    -7.836478  1.626702 -1.901363
C    -1.108090 -3.250424  3.590547
C     6.721454 -3.628350  1.443463
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C     1.461340 -5.305145  1.375263
O     1.844773 -4.139814  1.386928
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N    -1.383299 -4.640776 -0.097521
C    -0.084222 -4.130729 -1.803929
C    -1.699253 -3.404991 -0.533139
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C    -1.468939  3.489818 -2.573963
C    -0.304367  2.371256 -1.053584
N    -0.750579  2.340129 -2.315447
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O    -4.012396 -6.982340  0.795343
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C	1.850891	-1.145885	2.417288
C	1.536143	-0.735875	0.974116
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O	-1.016980	-4.642771	3.908145
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P	-1.027350	-1.197459	-2.623485

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H     7.986987 -2.150352 -4.564583
H     6.689554 -1.028061 -5.026889
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H     3.783907 -4.298585 -3.567512
H    -5.082430 -6.017028 -1.745110
H    -4.387288 -5.834678 -0.359684
H    -4.488844  0.087336 -3.179192
H    -3.110634  0.552263 -3.746422
H    -2.477578 -3.581642 -3.660795
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  th enthalpy= -5245.860955
  free energy= -5246.106892
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B-TS-2-3

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C     3.731780  7.484965 -1.859732
C     3.989302  6.031785 -1.471224
C     3.507419 -1.070246  4.366694
C    -6.557217  0.160277  3.297389
C     0.259912  1.901734  4.267188
C     0.085001  7.222140  3.714745
C    -7.527304 -3.370398 -0.080158
C    -8.906813  2.060312 -1.177268
C    -2.454943 -2.631971  3.963748
C     7.464667 -2.281432  1.254583
C     7.263203 -1.424094 -4.182955
C     0.290571 -6.445081 -0.550544
C    -2.185436  5.525624 -1.072854
C     3.320108 -1.037033  2.839707
C    -5.649972 -0.214737  2.115583
C    -1.106306  2.634279  4.321079
C     5.445482  1.997018 -0.434222
C     5.024418  1.774293 -1.905205
C     0.129812  7.404164  2.194068
C    -7.296434 -2.654514 -1.431844
N    -7.843375  1.621841 -1.904458
C    -1.106617 -3.262230  3.582189
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O     2.618262  4.026367 -1.280493
O     2.084395  5.532311 -2.874970
C     1.847187 -1.160822  2.414357
C     1.526169 -0.741118  0.974430
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C    -4.317689  0.551708  2.172546
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O    -0.908251 -2.134611 -3.953534
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P    -1.022177 -1.112408 -2.675380
O    -2.366162 -0.930232 -1.967477
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B-3

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C-1

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C     3.982312  0.912359 -1.937487
O     4.256294 -0.308172 -1.922668
N     2.725532  1.369062 -2.104326
C    -0.012746  6.055684  1.536686
O    -0.785871  5.076521  1.732726
N     1.023190  5.991866  0.697476
C    -5.920266 -1.971352 -1.431283
O    -5.881616 -0.715886 -1.605287
N    -4.798640 -2.687228 -1.302734
O    -1.134514 -4.752416  3.559715
O    -9.671513  2.750539 -1.504876
C    -7.347867  2.250828 -3.096732
C    -6.290446  3.256993 -2.619768
O    -5.125635  2.640898 -2.039738
C     6.380427 -4.169677  0.361398
O     6.601164 -5.377484  0.246455
C     6.481259 -0.895703  1.511825
O     5.492951 -0.888134  0.747169
N     6.728706  0.108452  2.377416
N     5.761634 -3.413770 -0.596362
C     5.542363 -3.925870 -1.954664
C     6.525695 -3.294461 -2.963234
O     7.243492 -3.996558 -3.678516
N     6.529901 -1.927931 -2.995120
O    -4.640407 -5.384262 -0.826026
O    -4.190050  0.612814 -3.541909
C     0.348983  0.218083 -5.137322
O    -0.573942  0.388357 -4.018990
H    -0.735351 -3.069263 -3.411908
O    -0.678641 -2.077426 -3.791673
P    -0.690176 -0.811116 -2.864074
O    -2.042157 -0.543120 -2.192316
O     0.534841 -0.659069 -1.962642
H     2.387595 -6.916252  0.877670
H     2.499042 -5.674948 -0.385826
H     1.187954 -7.694576 -1.123619
H     0.044280 -7.458548  0.202023
H    -1.831520 -5.825285 -0.050033
H     1.116045 -5.290733 -3.058334
H    -2.703777 -4.116599 -1.770010
H     0.542948 -5.569342  2.033058
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H    -1.834896  6.196912 -0.414356
H    -0.736516  3.791555  0.452193
H    -1.862943  3.966578 -3.626222
H     0.234178  1.710092 -0.720598
H    -0.537535  1.820633 -3.164976
H    -3.416481  5.052756  1.858760
H    -1.733904 -7.398027  4.155381
H    -2.344982 -9.008455  4.586061
H    -3.441387 -7.619994  4.549408
H    -2.036623 -8.915584  2.149209
H    -3.766276 -9.010972  2.501783
H     4.311081  8.037076 -2.297355
H     2.641864  7.545575 -2.451898
H     4.703946  5.795475 -1.815444
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H     3.255706  9.621008 -0.922015
H     3.031615 -1.906010  4.931367
H     2.832026 -0.145677  4.973759
H     4.448490 -0.846892  4.807858
H     3.651547  0.025280  2.616087
H     3.889509 -1.708816  2.538758
H     1.489098 -2.150320  2.661943
H     1.148588 -0.493282  3.129894
H     0.463523 -0.794888  0.836838
H     1.818813  0.333617  0.880647
H     1.735296 -1.377775 -0.886043
H     3.220733 -1.286830 -0.095720
H     2.153566 -2.547728  0.264433
H    -6.822087  1.012818  3.361644
H    -6.233485 -0.471627  4.131652
H    -7.658381 -0.522660  3.080210
H    -5.649445 -1.418801  1.861648
H    -6.246761  0.049629  1.091406
H    -4.468410  1.392491  2.285007
H    -3.937045 -0.060867  3.114283
H    -2.369962  0.406336  1.342439
H    -3.249193 -1.073927  0.908063
H    -2.969019  0.357560 -0.968179
H    -4.594138  0.259491 -0.651321
H    -3.771145  1.643175 -0.173343
H     0.602243  2.192207  5.237472
H    -0.058327  0.811726  4.340167
H    -1.889024  2.222963  3.460547
H    -1.095728  4.294939  3.407885
H    -3.109356  2.650491  5.588142
H    -2.232817  1.105147  5.705355
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H     2.420212  2.904127  4.215723
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H     5.649092  1.236485  0.211309
H     4.775705  2.912133 -2.207496
H     5.971381  1.605158 -2.248970
H     1.970505  0.682921 -2.190143
H     2.510550  2.362781 -1.967024
H    -1.040235  6.496658  4.071655
H    -0.485862  8.172514  4.243665
H     0.688681  6.853939  4.137424
H    -1.212158  7.768527  1.890909
H     0.521542  8.104947  1.940586
H     1.664786  6.781119  0.608768
H     1.246144  5.144338  0.176944
H    -7.336980 -3.291099 -2.316082
H    -8.032682 -1.937665 -1.427898
H    -3.913689 -2.209792 -1.452302
H    -4.797420 -3.709181 -1.119925
H    -8.455044 -4.066012 -0.207017
H    -6.724772 -4.447705 -0.169927
H    -7.357904 -3.074850  0.763721
H    -1.143523 -3.066754  2.310884
H    -0.350010 -2.909198  3.880605
H    -1.631420 -5.226849  2.857717
H    -2.464322 -1.623145  3.915592
H    -3.393836 -3.072254  3.454330
H    -2.588765 -3.002219  5.031712
H    -9.219637  1.008599 -0.531384
H    -6.919690  1.605508 -3.872862
H    -7.322040  0.599804 -1.746406
H    -8.187896  2.801442 -3.532195
H    -6.010701  3.900194 -3.470084
H    -6.724203  3.893555 -1.842770
H    -4.715938  2.026845 -2.699217
H     7.455754 -4.119427  2.166047
H     5.886528 -3.334705  2.291964
H     8.214166 -1.925395  2.278580
H     8.002699 -2.019110  0.533546
H     6.070944  0.895227  2.457548
H     7.516758  0.058288  3.004070
H     5.628330 -2.422488 -0.397172
H     5.794593 -4.987008 -1.921811
H     3.403964 -4.256882 -1.733999
H     3.804102 -2.680839 -2.456245
H     5.804321 -1.400922 -2.512097
H     8.103267 -1.903484 -4.340365
H     6.767303 -0.825599 -4.797666
H     7.862234 -0.364231 -3.470244
H     3.953234 -4.161120 -3.419651
H    -4.787596 -6.030072 -1.527418
H    -4.469214 -5.927073  0.014671
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H    -3.312466  0.244566 -3.302180
H     1.379876  0.141836 -4.778079
H     0.080603 -0.680990 -5.692522
H     0.238685  1.102831 -5.766428
    el energy= -5247.79906417
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  th enthalpy= -5245.895984
  free energy= -5246.142290
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C-TS-1-2

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C    -2.718452 -8.512118  2.322628
C     3.282134  7.685318 -1.601483
C     3.611368  6.239901 -1.238819
C     3.393459 -1.011946  4.428112
C    -6.697470 -0.313422  3.146410
C    -0.011302  1.778061  4.316574
C    -0.469428  7.092167  3.877365
C    -7.392835 -3.812625 -0.330250
C    -9.046956  1.557858 -1.340385
C    -2.462138 -2.890063  3.848718
C     7.481310 -1.930329  1.385444
C     7.355491 -0.959016 -4.035149
C     0.515867 -6.381240 -0.550895
C    -2.549841  5.399592 -1.020874
C     3.213444 -0.959674  2.906541
C    -5.704118 -0.617342  2.011475
C    -1.429273  2.404340  4.355946
C     5.386317  2.311472 -0.240141
C     5.048178  2.092784 -1.733984
C    -0.479655  7.286594  2.354663
C    -7.150988 -3.059455 -1.658208
N    -7.920550  1.188526 -2.011919
C    -1.071118 -3.433613  3.486585
C     6.862084 -3.353344  1.509123
C     4.193322 -3.657293 -2.556599
C     1.824276 -5.277704  1.297758
O     2.280022 -4.139575  1.343173
C    -0.157496 -5.080398 -0.871318
N    -1.254840 -4.635359 -0.162122
C     0.172412 -4.046557 -1.730719
C    -1.548551 -3.384242 -0.597636
N    -0.701769 -2.996915 -1.546457
C    -3.640445  4.272991  1.020894
O    -3.556112  3.054807  1.117239
C    -1.733034  4.217813 -1.423095
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C    -1.669187  3.548491 -2.619895
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O    -2.199987 -6.221003  1.737188
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O     2.477757  8.320692  0.604578
C     2.475427  5.286219 -1.734014
O     2.382577  4.148871 -1.106159
O     1.734255  5.661911 -2.651968
C     1.771085 -1.241331  2.460781
C     1.464731 -0.862966  1.009589
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C    -4.428186  0.234420  2.139794
C    -3.351253 -0.010166  1.078493
N    -3.761131  0.436083 -0.305047
C     0.732136  2.204138  3.057855
O     0.237504  2.041268  1.926360
O    -1.349172  3.839734  4.338043
C    -2.180198  2.007154  5.625095
N     1.937383  2.807376  3.254190
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N     4.238479  2.894583  0.459955
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O     4.284564 -0.193592 -1.984713
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O    -0.908721  4.975506  1.771910
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O     6.828307 -5.254350  0.032785
C     6.444317 -0.827267  1.444740
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N     5.869547 -3.318259 -0.744419
C     5.661637 -3.801714 -2.113246
C     6.606176 -3.105333 -3.115035
O     7.321154 -3.758555 -3.878106
N     6.576177 -1.739332 -3.087237
O    -4.629537 -5.671885 -1.345245
O    -4.177660  0.447776 -3.532895
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O    -1.978058 -0.628982 -2.206433
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H     0.641893 -6.998030 -1.447851
H    -0.114110 -6.945595  0.145039
H    -1.769299 -5.207878  0.564668
H     0.951292 -4.001367 -2.474736
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H    -2.832791  5.952734 -1.921670
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H    -6.190877 -0.434706  1.043152
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H    -0.104000  0.685375  4.322491
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H    -3.183505  2.443118  5.615034
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H    -6.061136  3.690647 -3.447987
H    -6.779217  3.667005 -1.823301
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H     7.568000 -4.014749  2.016647
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H     8.227868 -1.793367  2.175562
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H     5.663313 -2.348435 -0.507503
H     5.954826 -4.852824 -2.111596
H     3.543508 -4.218110 -1.877407
H     3.874557 -2.609178 -2.563109
H     5.845851 -1.251570 -2.571402
H     8.099921 -1.620443 -4.481888
H     6.730734 -0.545628 -4.838666
H     7.864934 -0.130153 -3.529511
H     4.064974 -4.058773 -3.567995
H    -4.720242 -6.340461 -2.033691
H    -4.256841 -6.157929 -0.551435
H    -4.800313 -0.178158 -3.121304
H    -3.285171  0.118983 -3.291961
H     1.475917  0.119031 -4.423101
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H     0.595003  1.415769 -5.278237
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          zpe= -5245.963084
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  th enthalpy= -5245.859309
  free energy= -5246.104448
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C-2

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C    -2.688185 -8.443001  2.439520
C     3.327859  7.691912 -1.711916
C     3.655781  6.249657 -1.335723
C     3.461544 -0.937937  4.413332
C    -6.637086 -0.223913  3.202799
C     0.064029  1.860705  4.297265
C    -0.382286  7.170920  3.802358
C    -7.369741 -3.759557 -0.229046
C    -9.016327  1.604205 -1.286110
C    -2.403781 -2.805077  3.900710
C     7.522745 -1.902234  1.349257
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C     3.307404 -0.924399  2.887144
C    -5.669150 -0.553349  2.055791
C    -1.355381  2.485120  4.329129
C     5.325878  2.297606 -0.354943
C     4.930422  2.051178 -1.830515
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H     3.501099 -4.230431 -1.891100
H     3.830432 -2.631550 -2.599345
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H     8.101953 -1.712424 -4.508192
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H     7.847835 -0.194920 -3.603969
H     4.028045 -4.095972 -3.581872
H    -4.601366 -6.211420 -1.946733
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  th enthalpy= -5245.861645
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C-3

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C	3.469914	7.618113	-1.753141
C	3.774546	6.170883	-1.376652
C	3.491149	-1.002033	4.387121
C	-6.600917	-0.110258	3.242941
C	0.143319	1.856501	4.288635
C	-0.211681	7.172960	3.786799
C	-7.419710	-3.638200	-0.177246
C	-8.977881	1.752223	-1.233055
C	-2.409826	-2.765266	3.917403
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C	-5.663684	-0.444005	2.073097
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O	2.682893	8.286344	0.448027
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  free energy= -5246.105658
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C-TS-3-4

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H     3.115476  4.524325  2.549003
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H     2.096566  3.691138  1.364202
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H     3.516877  3.421246 -0.193050
H     5.556599  1.294458  0.066100
H     4.575644  2.972236 -2.309932
H     5.791345  1.685610 -2.402836
H     1.821949  0.696121 -2.280004
H     2.328550  2.382512 -2.037291
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H    -0.500420  8.121682  4.299203
H     0.621907  6.757046  4.197685
H    -1.228204  7.746401  1.939040
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H     1.538320  6.786449  0.548174
H     1.113878  5.157047  0.093929
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H    -3.860171 -2.234492 -1.754747
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H    -8.197524  2.531515 -3.531685
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H     5.891630 -4.878744 -2.097895
H     3.486725 -4.232123 -1.889189
H     3.823691 -2.635890 -2.602862
H     5.764689 -1.289226 -2.689428
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H     4.018624 -4.104059 -3.579688
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H    -4.197056 -0.114766 -3.372603
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C-4

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C     2.861198  7.875909 -1.488542
C     3.272869  6.448842 -1.137583
C     3.469659 -0.850438  4.468995
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C    -0.090158  1.739694  4.376814
C    -0.853415  7.022018  3.980992
C    -7.134366 -4.228155 -0.324266
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C    -2.267655 -3.057835  3.867623
C     7.605655 -1.506387  1.423384
C     7.427215 -0.499038 -3.989076
C     1.071844 -6.394470 -0.814728
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C    -5.586311 -0.943023  2.094513
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O	2.225022	-3.954632	1.264085
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N	-0.918351	-4.936930	-0.402085
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C-TS-4-5

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C	3.437015	-0.812827	2.938394
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C-5

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C     3.458386 -0.928063  4.446306
C    -6.652850 -0.578289  3.183712
C    -0.043464  1.739937  4.361863
C    -0.690829  7.037816  3.965947
C    -7.229410 -4.072083 -0.319891
C    -9.074984  1.244236 -1.284464
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C     7.571320 -1.676281  1.390847
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C     4.335062 -3.504479 -2.580452
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