

# What Can Quantum Chemistry Tell Us about Pa(V) Hydration and Hydrolysis?

## Supporting information

	SCF	ZPE	Entropy
	a.u.	a.u.	$\text{kJ}\cdot\text{mol}^{-1}\text{K}^{-1}$
$\text{PaO}_2^+/5/10/6$	-835.0752	0.5157	1318.2
$\text{PaO}(\text{OH})_2^+/3/6/8$	-783.3833	0.4577	1179.6
$\text{PaO}(\text{OH})_2^+/4/8/4$	-835.0611	0.5360	1286.5
$\text{PaOOH}^{2+}/5/10/6$	-835.3802	0.5458	1335.1
$\text{Pa}(\text{OH})_4^+/2/4/13$	-835.0493	0.5348	1287.8
$\text{Pa}(\text{OH})_3^{2+}/4/8/8$	-835.3606	0.5428	1361.4
$\text{Pa}(\text{OH})_2^{3+}/5/10/4$	-801.1384	0.5033	1276.1
$\text{PaO}^{3+}/6/14$	-801.1289	0.5068	1216.1

Table Sup.Inf 1 : SCF energy, zero point energy and entropy of clusters used to model reactions.

### 5 $\text{PaO}_2^+/5/10/6$

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scf done: -835.075229

	Pa	0.000000	0.000000	0.196929
	O	0.000000	1.893731	0.145956
10	O	0.000000	-1.893731	0.145956
	O	1.451046	-0.392612	2.211480
	O	2.368306	0.229777	-0.639129
	O	0.000000	0.000000	-2.394701
	O	-2.368306	-0.229777	-0.639129
15	O	-1.451046	0.392612	2.211480
	H	1.323743	-1.269827	2.647570
	H	1.573396	0.287886	2.930725
	H	2.743919	-0.535168	-1.152153
	H	2.585496	1.068264	-1.111419
20	H	-0.189031	-0.776691	-2.971607
	H	0.189031	0.776691	-2.971607
	H	-2.585496	-1.068264	-1.111419
	H	-2.743919	0.535168	-1.152153
	H	-1.573396	-0.287886	2.930725
25	H	-1.323743	1.269827	2.647570
	O	0.802127	-2.844467	3.528745
	O	1.582469	1.510396	4.141572
	O	3.281361	-2.020168	-1.944637
	O	2.682131	2.764395	-1.984667
30	O	-0.567497	-2.381996	-3.821161
	O	0.567497	2.381996	-3.821161
	O	-2.682131	-2.764395	-1.984667
	O	-3.281361	2.020168	-1.944637
	O	-1.582469	-1.510396	4.141572
35	O	-0.802127	2.844467	3.528745
	H	0.668156	-3.651533	2.956247
	H	1.411035	-3.113602	4.239844
	H	0.784672	2.083054	4.022865
	H	2.349452	2.103078	4.219042
40	H	2.592530	-2.707365	-2.103732

H	3.990102	-2.462011	-1.445019
H	2.080940	2.672889	-2.763013
H	3.562034	2.986553	-2.338293
H	0.141310	-3.015494	-3.516019
5 H	-0.591678	-2.428071	-4.793723
H	-0.141310	3.015494	-3.516019
H	0.591678	2.428071	-4.793723
H	-2.080940	-2.672889	-2.763013
H	-3.562034	-2.986553	-2.338293
10 H	-2.592530	2.707365	-2.103732
H	-3.990102	2.462011	-1.445019
H	-0.784672	-2.083054	4.022865
H	-2.349452	-2.103078	4.219042
H	-0.668156	3.651533	2.956247
15 H	-1.411035	3.113602	4.239844
O	0.388992	-5.097697	2.011678
O	-0.388992	5.097697	2.011678
H	0.013080	-4.977164	1.103893
H	-0.002529	-5.910265	2.375232
20 H	-0.013080	4.977164	1.103893
H	0.002529	5.910265	2.375232
O	1.250598	-4.002447	-2.581988
O	-1.250598	4.002447	-2.581988
H	0.655506	-4.255270	-1.808190
25 H	1.595471	-4.832666	-2.957658
H	-0.655506	4.255270	-1.808190
H	-1.595471	4.832666	-2.957658
H	-0.303720	-3.367728	-0.231307
O	-0.462987	-4.327231	-0.543461
30 H	-1.382275	-4.299975	-0.879838
H	0.303720	3.367728	-0.231307
O	0.462987	4.327231	-0.543461
H	1.382275	4.299975	-0.879838

35

### **PaO(OH)<sub>2</sub><sup>+</sup>/3/6/8**

57

scf done: -783.383333

O	-1.893212	0.149686	-0.088146
40 Pa	-0.020983	-0.044182	-0.012366
O	0.184410	2.251829	-0.828025
O	-0.076401	0.559318	2.382263
O	2.018921	0.029352	-0.021612
O	0.077044	-2.075152	0.762343
45 O	-0.044670	-1.172921	-2.205388
O	2.719512	2.895758	-1.041531
O	2.631652	-2.632324	1.012798
O	-4.137307	1.459112	-0.596958
O	4.684431	-0.001059	0.011890
50 O	-2.536446	-0.476150	3.014590
O	-2.496372	-2.383113	-2.016385
O	-2.532232	-2.868409	1.041091
O	-4.473167	-0.541870	-2.548950
O	-4.500612	1.267916	2.176923
55 O	3.769414	2.069627	1.666320
O	3.784758	0.519186	-2.591676
O	2.612349	-2.173414	-1.936411

O	2.567922	-0.368079	2.901305
O	-2.144675	3.877091	-1.039218
H	-0.761977	-2.579199	0.947411
H	0.749464	-1.751800	-2.307074
5 H	-0.881381	-1.716133	-2.293736
H	1.116632	2.639714	-0.956376
H	-0.528289	2.915168	-0.986941
H	0.713927	0.192772	2.849014
H	-0.915829	0.203763	2.796129
10 H	3.027889	-2.948388	-2.357007
H	2.735355	-2.302998	-0.960719
H	-4.517683	0.221389	-1.920625
H	-5.390573	-0.782235	-2.765534
H	2.704046	-1.114540	2.260160
15 H	2.953434	-0.673185	3.743007
H	-4.536982	1.391716	1.194632
H	-5.421121	1.202501	2.485213
H	1.623288	-2.633327	0.995618
H	2.914825	-3.503920	1.342722
20 H	-3.271416	0.984918	-0.419291
H	-3.862306	2.344778	-0.906605
H	-2.238901	4.433162	-0.242726
H	-2.227743	4.488821	-1.794886
H	3.074418	2.183494	-1.619716
25 H	3.071178	2.700909	-0.143607
H	4.854820	0.258710	-0.918402
H	4.847509	0.794546	0.561771
H	3.027014	-0.051783	0.021767
H	4.086348	2.708969	2.329213
30 H	3.306597	1.353441	2.162088
H	4.098205	0.577128	-3.512065
H	3.323899	-0.347871	-2.504727
H	-2.747196	-2.638509	0.112409
H	-2.760929	-2.078863	1.575411
35 H	-3.217461	-1.725815	-2.231614
H	-2.728279	-3.200056	-2.494056
H	-3.253829	0.160214	2.734326
H	-2.780051	-0.778002	3.908358

40 **PaO(OH)<sub>2</sub><sup>+</sup>/4/8/4**

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scf done: -835.061067

Pa	0.436559	-0.373324	-0.188298
O	-1.592376	0.022596	-0.016937
45 O	2.278992	-0.583964	-0.495266
O	-0.111245	-2.538255	0.040331
O	-0.076261	-1.093521	-2.549114
O	0.457218	1.648746	-1.755562
O	0.568512	1.637485	1.241626
50 O	1.028622	-0.956384	2.209569
H	-1.015373	-2.789752	0.320590
H	0.412027	-1.936129	-2.792690
H	-1.035693	-1.234106	-2.710384
H	0.928428	2.498473	-1.562215
55 H	-0.388037	1.861868	-2.214741
H	1.314587	1.814962	1.886636
H	0.085389	2.500522	1.084677

H	1.594692	-1.783317	2.206422
H	0.225875	-1.156796	2.746398
O	1.354485	-3.341148	-3.022699
O	-2.938808	-0.631093	-2.823158
5 O	1.744443	4.040112	-1.073702
O	-2.179605	2.100584	-2.800778
O	2.714376	2.278930	2.723148
O	-0.584981	4.010382	0.673007
O	2.613803	-3.175816	2.044360
10 O	-1.575931	-1.457671	3.366469
H	2.171747	-3.236082	-3.539805
H	1.619841	-3.745305	-2.156262
H	-3.343927	-0.829871	-3.686995
H	-2.723884	0.337487	-2.835586
15 H	2.047641	4.635830	-1.782040
H	2.558027	3.805293	-0.547923
H	-2.608993	2.631728	-2.074343
H	-2.283950	2.615046	-3.621812
H	3.298403	2.633185	2.011051
20 H	3.184155	1.528696	3.127287
H	-1.441605	3.953946	0.196278
H	0.085638	4.347413	0.042180
H	2.458635	-3.620858	1.173308
H	3.569113	-2.996726	2.089080
25 H	-1.605183	-2.016921	4.164173
H	-2.037956	-1.972021	2.652582
H	0.900456	-3.723533	-0.199181
O	1.721997	-4.295533	-0.403434
H	1.461572	-5.228339	-0.303142
30 O	3.976037	3.198504	0.353930
H	4.758016	3.771289	0.451961
H	4.298835	2.323692	-0.030825
O	4.644864	0.762970	-0.490409
H	3.818310	0.202607	-0.515661
35 H	5.137334	0.565483	-1.305518
O	-3.157722	3.436280	-0.596152
H	-3.825508	4.145737	-0.606485
H	-3.503740	2.727944	0.018253
O	-3.823797	1.303908	0.931960
40 H	-3.730016	1.184865	1.921428
H	-4.353870	0.551823	0.585786
H	-2.311794	0.570740	0.392752
O	-3.301883	0.788561	3.529973
O	-4.425950	-1.148798	-0.459370
45 H	-2.630090	0.064022	3.565774
H	-2.983366	1.498412	4.114572
H	-3.886889	-0.996935	-1.280421
H	-5.288373	-1.489112	-0.759397
O	-2.827802	-2.783566	1.233460
50 H	-3.396941	-2.213257	0.655706
H	-3.316352	-3.616006	1.363680

### **PaOOH<sup>2+</sup>/5/10/6**

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55 scf done:	-835.380243		
Pa	0.021961	-0.037890	-0.335140
O	1.586471	-0.896529	0.201694

O	-1.788228	0.698819	-0.961483
H	-2.652889	1.170274	-0.648311
O	0.025146	-1.397291	-2.394546
O	-1.161501	-2.176398	0.182312
5 O	-0.687897	-0.011975	2.041587
O	0.663861	2.096590	0.729624
O	1.319778	1.217045	-1.962211
H	-0.787936	-1.401987	-2.949454
H	0.403345	-2.330641	-2.373956
10 H	-2.008071	-2.467779	-0.239233
H	-0.610815	-2.965947	0.423066
H	-1.558158	-0.397580	2.350877
H	0.009449	-0.287024	2.693558
H	0.037308	2.686126	1.238237
15 H	1.509948	2.593869	0.582767
H	1.339450	2.210201	-2.097386
H	2.232195	0.877429	-2.202882
O	-2.659107	-0.868432	-3.156178
O	0.917062	-3.887947	-2.126095
20 O	-3.639635	-2.468414	-1.114330
O	0.741196	-4.152347	0.701586
O	-3.083664	-1.011434	2.838489
O	1.402194	-0.872077	3.702155
O	-1.015375	3.802795	2.008005
25 O	3.129891	3.362268	0.284632
O	1.629724	3.877386	-2.065916
O	3.847621	0.373718	-2.314734
H	-2.522943	-0.050423	-2.622137
H	-3.063694	-0.602285	-4.003085
30 H	-3.440985	-1.988673	-1.961732
H	-4.015349	-3.333425	-1.364563
H	-3.841374	-0.969137	2.207379
H	-3.450999	-0.915879	3.734669
H	-1.932959	4.004830	1.716657
35 H	-0.975945	3.982899	2.963466
H	1.873787	4.409940	-2.843701
H	2.334234	3.992782	-1.390500
H	1.068667	-4.094408	-1.174775
H	1.665969	-4.252833	-2.630125
40 H	1.447568	-3.807589	1.306885
H	0.505592	-5.037996	1.035291
H	1.673214	-1.802639	3.517418
H	1.322602	-0.794394	4.670615
H	3.857754	2.686067	0.264716
45 H	3.411890	4.053442	0.911815
H	4.413131	0.650039	-1.556450
H	4.390935	0.418016	-3.121151
O	3.766345	-0.692416	1.750824
H	2.991657	-0.740310	1.122956
50 H	3.386642	-0.294963	2.560909
O	-4.047803	1.699672	-0.258094
H	-4.074949	2.516378	0.287575
H	-4.543504	0.981823	0.200347
O	-3.718537	4.286331	1.018616
55 O	-4.981556	-0.795732	0.741206
H	-4.636064	-1.425752	0.058631
H	-5.928371	-1.001636	0.852710
H	-3.697418	4.923927	0.278497
H	-4.379423	4.643385	1.642786

O	2.672462	-3.168433	2.563851
O	4.969948	1.241423	0.175289
H	3.317248	-2.502613	2.213067
H	3.199278	-3.833831	3.045432
5 H	4.694633	0.525110	0.812315
H	5.929739	1.368246	0.294288

### Pa(OH)<sub>4</sub><sup>+</sup>/2/4/13

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10 scf done:	-835.049279		
Pa	0.776950	-0.591873	-0.597835
O	-1.243198	-0.751409	0.021344
O	2.660787	-0.180332	-1.492783
O	1.617602	-2.345851	0.838017
15 O	1.233480	0.604412	1.023487
O	-3.073084	2.369404	1.822947
O	0.093760	1.543690	-1.521690
O	0.299243	-1.867365	-2.235238
H	2.107493	-1.954529	1.659599
20 H	1.104293	-3.114158	1.186456
H	1.171591	1.376914	1.632205
H	-3.188116	3.149693	2.394916
H	-4.002633	2.065140	1.566151
H	0.734826	2.257773	-1.241840
25 H	-0.814122	1.911059	-1.291031
H	0.963099	-1.994631	-2.971019
O	2.642447	-1.306196	2.979683
O	0.259944	-4.244215	2.439406
O	1.777788	2.981611	2.330110
30 O	-0.491540	5.050177	-1.098144
O	-5.376527	1.377647	0.948853
O	1.710932	3.530724	-0.485132
O	-2.203940	2.770472	-0.836607
O	2.467996	-1.713862	-3.905028
35 H	3.028398	-0.426500	2.779543
H	1.773435	-1.149694	3.433075
H	-0.457137	-4.839342	2.151672
H	0.892708	-4.809614	2.921433
H	1.478404	3.478080	3.112503
40 H	2.663175	2.588311	2.543254
H	-0.732776	5.813213	-1.651104
H	-1.245777	4.416072	-1.129616
H	-5.302915	1.421789	-0.030722
H	-5.349553	0.418474	1.171397
45 H	1.629293	3.510551	0.497923
H	1.131641	4.277578	-0.786456
H	-2.983020	2.377685	-1.303154
H	-2.417756	2.686989	0.129858
H	3.119551	-2.397855	-4.137128
50 H	2.886517	-1.136906	-3.227158
O	4.019741	1.392389	2.292991
O	-4.425670	1.279666	-1.770538
H	4.182504	1.536713	1.327738
H	4.883462	1.481675	2.735501
55 H	-4.170580	0.319440	-1.723279
H	-4.940087	1.398861	-2.588998
H	3.313503	0.513075	-1.228193

H	-2.106240	-0.948650	-0.445760
O	4.099288	2.083514	-0.499552
O	-3.634755	-1.283742	-1.150659
H	3.374691	2.748600	-0.629152
5 H	4.885103	2.440228	-0.952184
H	-4.122738	-1.611768	-0.360111
H	-3.325298	-2.056184	-1.700962
H	-2.449893	0.673721	2.537235
O	-2.253496	-0.292730	2.510912
10 H	-1.796418	-0.417672	1.634960
O	-4.620798	-1.326898	1.516401
O	0.013853	-1.478764	3.898532
H	-3.803573	-1.054260	2.021525
H	-5.129478	-1.922907	2.094782
15 H	-0.151249	-2.411627	3.661120
H	-0.772190	-0.983503	3.569704
H	-1.296821	-2.749863	-2.509409
O	-2.212330	-3.131213	-2.509706
H	-2.359942	-3.510550	-3.393147

20

### Pa(OH)<sub>3</sub><sup>2+</sup> 4/8/8

67

scf done: -835.360615

Pa	0.354106	-0.194959	0.189991
25 O	0.875959	1.760273	0.039387
O	0.057543	-2.216417	0.152008
O	-0.809122	-0.117800	-2.009416
O	-1.656151	0.364812	0.619469
O	0.110335	-0.246765	2.627722
30 O	2.610284	-0.258476	1.236452
O	1.896015	-0.685266	-1.630691
H	-0.923259	-0.917059	-2.578255
H	-1.590352	0.475531	-2.178110
H	-2.511061	0.001118	0.265410
35 H	-0.805437	-0.264639	3.022003
H	0.764197	-0.552428	3.309042
H	3.217753	-1.032897	1.309125
H	3.175108	0.536924	0.987635
H	2.548742	-1.441061	-1.634183
40 H	2.205941	0.025367	-2.271196
O	-1.701903	-2.483865	-3.317176
O	-3.063056	1.456735	-2.289988
O	-4.116824	-0.291975	-0.417176
O	-2.428837	-0.216911	3.718564
45 O	1.876638	-1.156745	4.574360
O	4.504874	-2.425696	1.265027
O	4.137153	1.820291	0.447898
O	3.606215	-2.780965	-1.448874
O	2.603854	1.324201	-3.239471
50 H	-2.653796	-2.499853	-3.057163
H	-1.666005	-2.615974	-4.282927
H	-3.537429	1.614549	-3.127132
H	-3.676450	0.951953	-1.697134
H	-4.630516	-0.124001	0.409510
55 H	-4.241643	-1.227865	-0.699815
H	-2.682528	-0.474459	4.622387
H	-3.266432	-0.056962	3.224599

H	1.579341	-1.829958	5.214098
H	2.354132	-0.488506	5.099781
H	4.328605	-3.177313	1.862871
H	5.419053	-2.143846	1.461389
5 H	3.747661	2.440122	-0.213892
H	4.662532	2.364893	1.060215
H	4.107552	-2.786798	-0.604634
H	4.199539	-3.121228	-2.141824
H	2.821768	2.166460	-2.771885
10 H	3.150510	1.284083	-4.043511
O	-3.948744	-2.881230	-1.616618
O	3.035562	3.583292	-1.598424
H	-3.321400	-3.499113	-1.172225
H	-4.755459	-3.396264	-1.806775
15 H	2.140646	3.957525	-1.401148
H	3.574891	4.321947	-1.937263
H	-0.432458	-3.027511	-0.147451
H	0.734427	2.751663	-0.047593
O	-1.456316	-4.178107	-1.098585
20 O	0.496255	4.324851	-0.583283
H	-1.224745	-5.123873	-1.040035
H	-1.255687	-3.884152	-2.018604
H	0.552095	5.089898	0.018482
H	-0.480864	4.237237	-0.834453
25 H	-2.249663	1.865412	1.339386
O	-2.845213	2.629436	1.578263
H	-2.487443	3.020582	2.396143
O	-4.723684	0.670876	2.140107
O	-2.104186	3.890303	-0.919169
30 H	-4.278771	1.545463	1.986989
H	-5.590734	0.859657	2.544652
H	-2.419870	3.180299	-1.519182
H	-2.479349	3.657487	-0.039610

35 **Pa(OH)<sub>2</sub><sup>3+</sup>/5/10/4**

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scf done: -801.138368

Pa	0.000000	0.000000	0.243838
O	1.839729	-0.804760	0.202592
40 O	-1.839729	0.804760	0.202592
O	0.500916	1.299106	-1.730247
O	0.876990	2.104853	0.987974
O	0.000000	0.000000	2.652780
O	-0.876990	-2.104853	0.987974
45 O	-0.500916	-1.299106	-1.730247
H	-0.233357	1.553353	-2.380421
H	1.183310	2.026298	-1.775271
H	0.452281	2.969050	0.723126
H	1.880000	2.278978	1.013788
50 H	0.068938	0.804344	3.248424
H	-0.068938	-0.804344	3.248424
H	-1.880000	-2.278978	1.013788
H	-0.452281	-2.969050	0.723126
H	-1.183310	-2.026298	-1.775271
55 H	0.233357	-1.553353	-2.380421
O	-1.496660	2.161129	-3.229025
O	2.148977	3.521084	-1.686408



	O	0.000000	4.492213	-0.109737
	O	3.429448	2.565094	0.663243
	O	0.100523	2.089475	4.386213
	O	-0.100523	-2.089475	4.386213
5	O	-3.429448	-2.565094	0.663243
	O	0.000000	-4.492213	-0.109737
	O	-2.148977	-3.521084	-1.686408
	O	1.496660	-2.161129	-3.229025
	H	-1.839830	3.020244	-2.889352
10	H	-1.536953	2.187739	-4.202820
	H	2.525474	3.916848	-2.496141
	H	1.501809	4.168275	-1.317221
	H	-0.874774	4.504704	-0.580420
	H	0.035176	5.307966	0.426527
15	H	4.088322	2.999912	1.236034
	H	3.409196	3.048790	-0.192271
	H	0.898566	2.315043	4.900091
	H	-0.652940	2.269776	4.979448
	H	-0.898566	-2.315043	4.900091
20	H	0.652940	-2.269776	4.979448
	H	-4.088322	-2.999912	1.236034
	H	-3.409196	-3.048790	-0.192271
	H	0.874774	-4.504704	-0.580420
	H	-0.035176	-5.307966	0.426527
25	H	-2.525474	-3.916848	-2.496141
	H	-1.501809	-4.168275	-1.317221
	H	1.839830	-3.020244	-2.889352
	H	1.536953	-2.187739	-4.202820
	O	-2.405931	4.285366	-1.566326
30	O	2.405931	-4.285366	-1.566326
	H	-3.119969	3.788679	-1.101291
	H	-2.811473	5.110195	-1.898883
	H	3.119969	-3.788679	-1.101291
	H	2.811473	-5.110195	-1.898883
35	H	-2.715405	1.268381	0.058776
	H	2.715405	-1.268381	0.058776
	O	-4.107769	2.310300	-0.293532
	O	4.107769	-2.310300	-0.293532
	H	-4.658406	2.543651	0.480846
40	H	-4.726698	1.909475	-0.936709
	H	4.658406	-2.543651	0.480846
	H	4.726698	-1.909475	-0.936709

45 **PaO<sup>3+</sup>/6/14**

62

scf done: -801.128865

	Pa	-0.017985	-0.167059	-0.082449
	O	1.139199	-1.512164	-0.527593
50	O	1.503473	1.619532	0.600891
	O	0.636952	-0.692876	2.138850
	O	-1.617995	-1.800354	0.595335
	O	-1.675992	-0.386344	-1.895821
	O	0.793937	0.870402	-2.073655
55	H	1.564709	2.012775	1.517047
	H	2.372345	1.818057	0.127413
	H	0.362444	-0.251347	3.013371

H	1.266069	-1.456755	2.311770
H	-2.617387	-1.801719	0.655434
H	-1.252455	-2.645910	1.037409
H	-1.515199	0.128841	-2.710890
5 H	-2.498792	-0.952170	-2.051457
H	1.054294	1.844650	-2.211255
H	1.432284	0.326152	-2.660057
O	3.809711	2.048125	-0.732028
O	2.185356	-2.906321	2.270914
10 O	-0.507744	-3.855787	1.775414
O	-4.024305	-1.610616	-2.274072
O	2.539047	-0.526831	-3.418441
O	1.327437	2.893134	3.045132
O	-0.087397	0.724715	4.206405
15 O	-4.333588	-1.615073	0.505917
O	-4.749532	1.170582	-2.300612
O	1.739002	3.307169	-2.300933
H	4.525029	2.569615	-0.319259
H	4.219897	1.184892	-1.009919
20 H	2.668480	-3.203577	3.066437
H	2.834700	-2.914425	1.521275
H	-0.756824	-4.797864	1.747434
H	0.457353	-3.800162	1.958019
H	-4.179304	-2.343377	-2.901939
25 H	-4.361609	-1.898132	-1.391880
H	2.665679	-0.551162	-4.385015
H	3.427984	-0.544036	-2.990462
H	0.615671	3.535636	2.821541
H	2.053982	3.404031	3.453034
30 H	-0.221204	0.435055	5.128629
H	0.486275	1.522059	4.216646
H	-4.525803	-0.651917	0.623113
H	-4.940310	-2.110852	1.090388
H	-5.429702	1.689801	-2.770413
35 H	-4.835420	0.238496	-2.596021
H	2.679942	3.188515	-2.048405
H	1.717252	3.870050	-3.097975
H	2.772645	-2.666768	-0.657990
O	3.633389	-2.755932	-0.191879
40 H	4.031248	-3.596845	-0.492338
H	4.508878	-1.253620	-1.010592
O	4.705168	-0.471959	-1.587032
H	5.641258	-0.556195	-1.855316
O	-1.578131	1.519360	0.615950
45 H	-2.591608	1.444983	0.492116
H	-1.382996	2.401812	1.045688
O	-4.193869	1.194525	0.290549
O	-1.073341	3.977997	1.870512
H	-0.970775	4.742741	1.268279
50 H	-1.740674	4.259591	2.528871
H	-4.795069	1.764349	0.809323
H	-4.472870	1.286850	-0.679573