The role of H_2O in the electron transfer–activation of substrates using SmI_2: A theoretical study

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Supporting Information

Computation details

All calculations conducted at M06 level of theory by using GAUSSIAN09 code.[1] The equilibrium and transition structures were fully optimized the meta-GGA functional M06.[2] Two different Stuttgart-Dresden effective core potentials were used for samarium atoms; the small core ECP was used in combination with its adapted basis set to study the change of oxidation state from +II to +III,[3] while the 4f-in-large-core ECP (augmented by a *f* polarization function, α = 1.0) was used for the reactions involving dinuclear complexes, in which the samarium's oxidation state is +III or +II.[4] Iodine atoms were represented by means of a Stuttgart-Dresden effective core potentials in association with its basis set[5], augmented by a d-polarization function (α = 0,730).[6] For the rest of non-metal atoms the 6-31G(d,p) basis set was used[7]. When specified, optimization in THF as a bulk solvent has been achieved by means of the SMD implicit solvation model implemented in Gaussian 09.[8]

The thermal stability of the SmI_2-$(H_2O)_{24}$ structure has been tested using a Born-Oppenheimer molecular dynamics (BO-MD) simulation at the B3PW91/6-311G** level. This simulation was carried out *in vacuo* with the Geraldyn2.1 code based on the method developed by Raynaud *et al.* [9], which uses the velocity-Verlet integration scheme [10]. For the integration of the equations of motion a time step of 0.5 fs was used. A Nosé–Hoover chain of four thermostats [11,12] was used to control the temperature at 300K during the 10 ps of the simulation.

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$[Sm(H_2O)n]I_3$	Sm-O(bond)	Sm-I(bond)
1	1	1
2	2	1
3	3	1
4	4	1
5	5	0
6	6	0
7	6	1
8	7	0
9	7	0
10	7	0
11	8	0
12	9	0
13	9	0
14	10	0
15	10	0
16	9	0
17	**9**	**0**
18	**9**	**0**
19	**9**	**0**
20	**9**	**0**

Table S1 Number of Sm-I and Sm-O(water) interactions in the stepwise construction of the SmI_3 solvation shell in water.

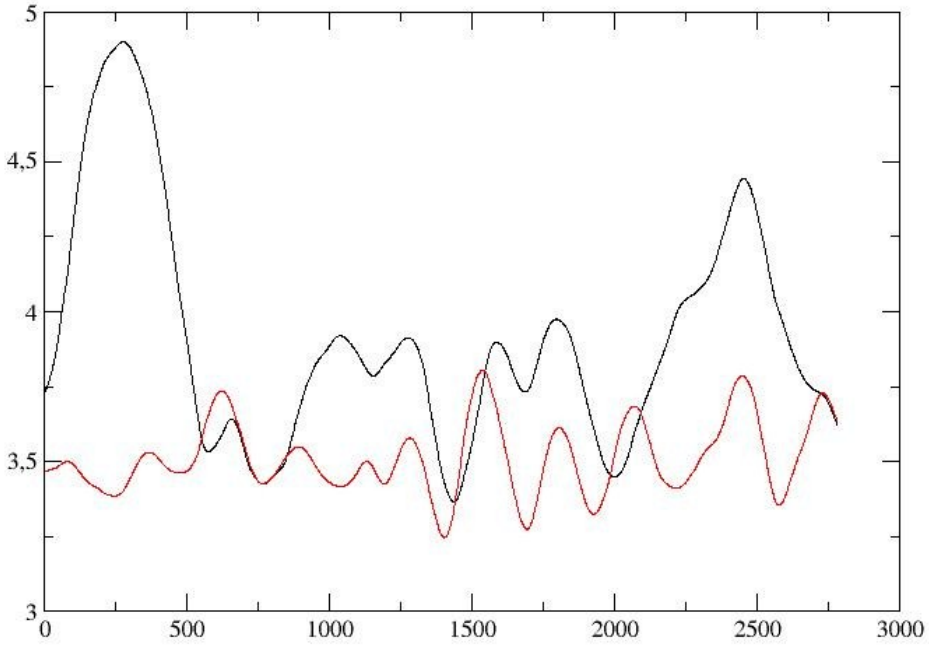


Figure S1: Sm-I bond variation during the dynamical process at 300K

Table S2. The coordination numbers of H_2O for complex and reaction energies for Alkyl Halide (kcal/mol)

Water number (n)	H_1(kcal/mol)	E_2(kcal/mol)	E_3(kcal/mol)	E(kcal/mol)
17	3.4	1.8	6.7	11.8
18	1.4	5.8	8.7	15.8
19	-1.6	1.0	11.2	10.6
20	-4.4	4.0	11.4	11.1

Table S3. The coordination numbers of H_2O for complex and reaction energies for Ketone (kcal/mol)

Water number (n)	H_1(kcal/mol)	E_2(kcal/mol)	E(kcal/mol)
9	3.7	28.4	32.2
17	-10.3	32.3	22.0
18	-4.2	23.2	19.0
19	-12.1	27.3	15.2
20	-10.4	22.8	12.4
22	-11.7	22.2	10.5
24	-12.6	20.1	7.5

Table S4. The coordination numbers of H_2O for complex and reaction energies for Lactone (kcal/mol)

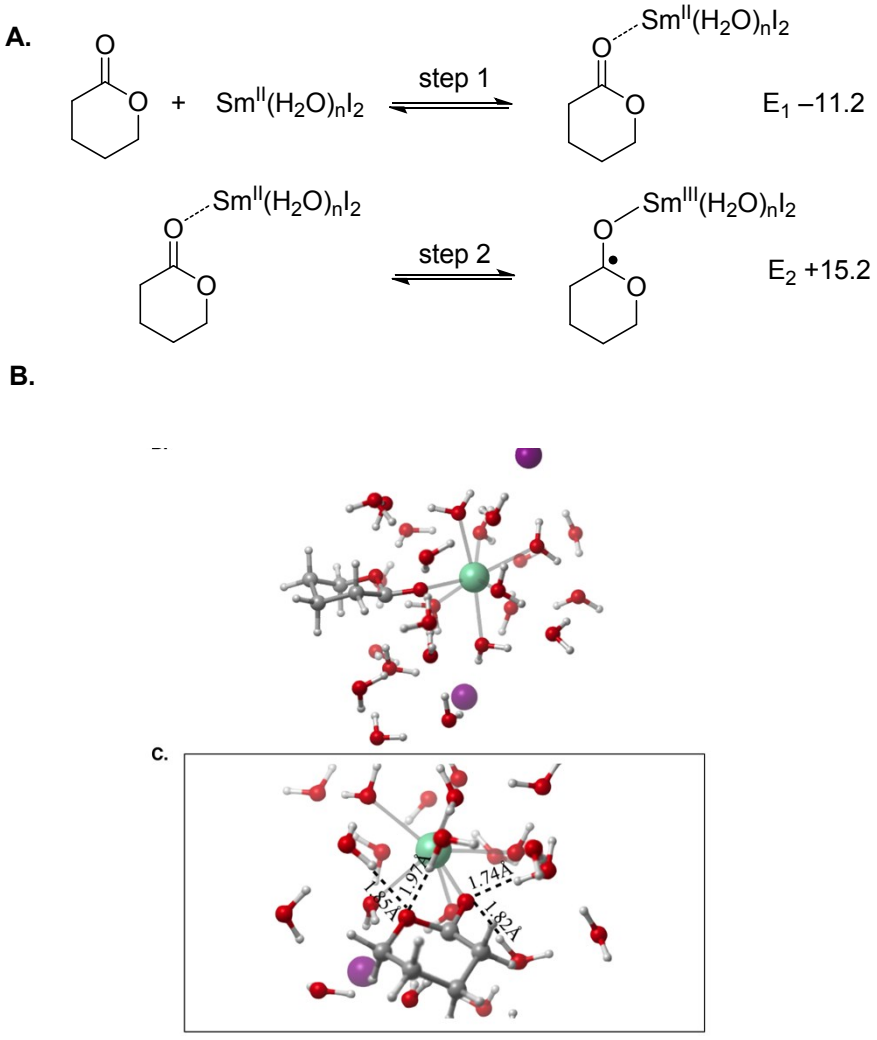
Water number (n)	H_1(kcal/mol)	E_2(kcal/mol)	E(kcal/mol)
24	-13.0	15.2	2.2

Table S5. The coordination numbers of H_2O for complex and reaction energies for Ester (kcal/mol)

Water number (n)	H_1(kcal/mol)	E_2(kcal/mol)	E(kcal/mol)
19	-11.5	32.5	21.0
24	-13.5	27.5	14.0

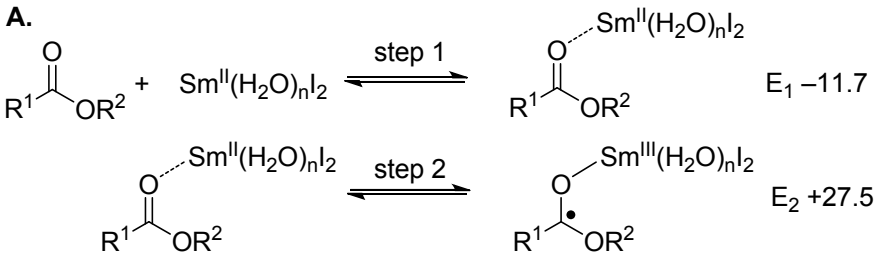
Table S6. The coordination numbers of H_2O for complex and reaction energies for Benzophenone (kcal/mol)

Water number (n)	H_1(kcal/mol)	E_2(kcal/mol)	E(kcal/mol)
24	-11.7	15.7	4.0

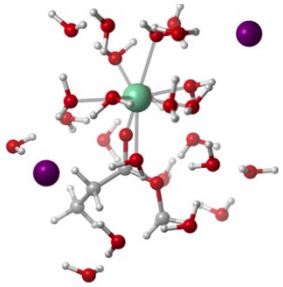


Scheme S1. Reduction of lactones with SmI_2–H_2O. **B** and **C**. Molecular structure of the ketyl-radical bound to Sm(III)–H_2O formed upon lactone reduction. E_1 and E_2 in kcal/mol (24 H_2O molecules). The color code is the same for all schemes: Green atom is Sm, the purple ones the iodine, the red the oxygen, the grey are the carbon and the white are the hydrogens.

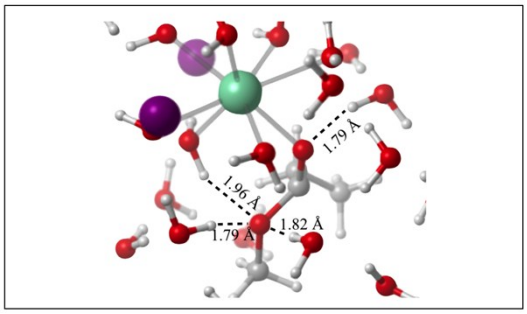
A.



B.



C.



Scheme S2. Reduction of esters with SmI_2–H_2O. **B** and **C**. Molecular structure of the acyl-radical bound to Sm(III)–H_2O formed upon lactone reduction. R^1 = Et, R^2= Me, E_1 and E_2 in kcal/mol (24 H_2O molecules). The color code is the same for all schemes: Green atom is Sm, the purple ones the iodine, the red the oxygen, the grey are the carbon and the white are the hydrogens.

Optimized Structures

Cartesian Coordinates.

Full optimization $SmI_2(H_2O)$

E: -128.279537 ; H: -128.245649 ; G: -128.295878 ;

Sm	0.283996	-0.851548	0.005686
I	-1.749560	0.339804	-2.893370
I	0.731727	1.942940	2.427822
O	1.160365	1.547262	-1.144934
H	1.019117	2.057402	-0.329428
H	0.345146	1.626485	-1.669155

$SmI_2(H_2O)_2$

E: -204.706105 ; H: -204.645018 ; G: -204.701958 ;

Sm	1.061760	-0.562469	-0.418619
I	-0.600377	1.521129	2.315850
I	1.217115	2.004431	-3.096425
O	-1.605401	-0.982825	-0.059631
O	2.389454	1.849300	0.323175
H	1.635213	2.029503	0.911700
H	2.139238	2.192439	-0.552381
H	-1.800198	-0.484330	0.750742
H	-2.074620	-1.824968	0.009458

$SmI_2(H_2O)_3$

E: -281.135418 ; H: -281.045967 ; G: -281.108024 ;

Sm	-0.119402	2.200933	-0.009310
I	-1.241122	0.822459	3.223628
I	1.064517	0.723635	-3.284158
O	-1.752995	-0.146423	-0.298526
O	2.676587	2.074639	-0.306040
O	0.971378	-0.465711	0.059176
H	-2.137381	-0.042137	0.585929
H	-0.889760	-0.577207	-0.155445
H	3.164812	2.892842	-0.470531
H	2.595809	1.629737	-1.167474
H	1.648504	-0.686351	0.713573
H	1.414930	-0.402543	-0.803673

$SmI_2(H_2O)_4$

E: -357.563261 ; H: -357.446451 ; G: -357.514779 ;

Sm	-0.120176	2.201694	-0.010951
I	-1.243407	0.815134	3.229690
I	1.049813	0.730367	-3.280189
O	-1.736969	-0.153281	-0.309239
O	-2.808415	2.631482	0.465986
O	2.686650	2.073367	-0.306903
O	0.977925	-0.469184	0.069222
H	-2.174989	-0.030602	0.547127
H	-0.884817	-0.584235	-0.110865
H	-3.280668	2.052959	-0.148668
H	-2.796926	2.162890	1.317962
H	3.173355	2.891358	-0.476422
H	2.594504	1.630393	-1.168169
H	1.672424	-0.684231	0.706978
H	1.401563	-0.396908	-0.803132

$SmI_2(H_2O)_5$

E: -433.994637 ; H: -433.850038 ; G: -433.924331 ;

Sm	0.487497	2.362593	0.623900
I	-1.430866	0.240553	2.966760
I	1.125358	1.689449	-2.979409
O	-1.637001	0.150465	-0.701636
O	-2.205880	3.066636	0.625442
O	3.178016	1.957148	0.002468
O	1.003450	-0.290746	0.112281
H	-2.011086	0.178126	0.193493
H	-0.698405	-0.084908	-0.566975
H	-2.348246	2.945119	-0.337421
H	-2.576222	2.292623	1.075140
H	3.696404	2.769234	-0.078815

H	2.916431	1.714885	-0.903200
H	1.036571	-0.975944	0.795321
H	1.649783	-0.532195	-0.567133
O	-2.255020	2.874227	-2.124670
H	-1.407910	2.458143	-2.364453
H	-2.253663	3.743949	-2.547151

$SmI_2(H_2O)_6$

E: -510.421667 ; H: -510.249275 ; G: -510.330672 ;

Sm	-0.070538	1.621384	0.660195
I	-2.365514	2.169144	3.533854
I	1.311199	1.448602	-2.750739
O	-2.028151	3.496382	0.109055
O	2.667652	2.346542	0.484142
O	2.399811	-0.425550	0.364735
H	-2.741634	3.209837	-0.477444
H	-2.386961	3.446615	1.012174
H	2.989192	3.135945	0.941975
H	2.769695	2.510272	-0.467207
H	2.660443	0.472128	0.639444
H	2.083581	-0.313648	-0.546147
O	1.161759	1.374893	3.076959
H	1.543905	0.506067	3.262622
H	0.347487	1.437671	3.604972
O	0.423353	4.141764	1.736300
H	0.692945	4.409040	0.830837
H	1.233300	4.058931	2.257167
O	0.941601	4.584503	-0.919955
H	0.990203	3.728878	-1.384659
H	0.171814	5.043657	-1.283648

$SmI_2(H_2O)_7$

E: -586.852134 ; H: -586.652074 ; G: -586.738817 ;

Sm	0.356289	2.672472	0.347496
I	-1.930001	1.672112	3.130722
I	1.105767	1.174804	-2.971934
O	-1.637639	0.206142	-0.220982
O	-2.234252	3.573951	-0.038079
O	3.051681	2.306630	-0.089987
O	1.107869	-0.026269	0.410477
H	-1.992022	0.615066	0.586189
H	-0.721334	-0.039483	0.000828
H	-2.375675	3.109232	-0.891458
H	-2.652757	3.039354	0.654225
H	3.575057	3.105008	-0.245071
H	2.921297	1.896730	-0.962378
H	1.765084	-0.119586	1.115120
H	1.591620	-0.023729	-0.432273
O	-2.359136	2.300951	-2.468937
H	-1.469019	1.934703	-2.619921
H	-2.528562	2.908329	-3.202083
O	1.637683	2.143382	2.765834
H	2.459482	1.636355	2.703877
H	0.978628	1.565459	3.182796
O	0.276410	4.599473	2.477214
H	0.888834	3.958366	2.879143
H	-0.607086	4.326144	2.769005

$SmI_2(H_2O)_8$

E: -663.281092 ; H: -663.054636 ; G: -663.146675 ;

Sm	0.220725	2.315466	0.765064
I	-2.211119	0.822404	3.076739
I	1.558981	1.373552	-2.596115
O	-1.616322	-0.005045	-0.476514
O	-2.310232	3.309656	0.300942
O	2.903557	2.727917	0.428857
O	1.005500	-0.380613	0.501397
H	-2.021715	0.345401	0.334434
H	-0.725397	-0.295574	-0.204031

H	-2.250264	3.089836	-0.654180
H	-2.819402	2.606879	0.732735
H	3.111153	3.664306	0.556610
H	2.919875	2.572184	-0.530755
H	1.443423	-0.842265	1.230438
H	1.655982	-0.289320	-0.213725
O	-1.783761	2.824591	-2.343688
H	-0.924015	2.368604	-2.393573
H	-1.660896	3.673252	-2.791824
O	1.387511	1.587309	3.159380
H	1.893276	0.775774	3.012168
H	0.539505	1.303600	3.541357
O	0.969312	4.757797	1.889496
H	1.129172	5.023510	0.967053
H	1.834809	4.675941	2.311925
O	0.736909	4.557336	-0.918783
H	1.176122	3.947098	-1.537142
H	-0.099656	4.804688	-1.338829

$SmI_2(H_2O)_9$

E: -739.714512 ; H: -739.459103 ; G: -739.557326 ;

Sm	0.286619	2.871725	0.463855
I	-1.995542	1.943250	3.195412
I	1.058316	0.618402	-3.099114
O	-1.706427	0.387042	-0.156876
O	-2.365188	3.547595	-0.107885
O	2.808168	2.572991	-0.571276
O	1.022130	0.176604	0.431359
H	-2.029150	0.805533	0.658660
H	-0.775192	0.162926	0.026631
H	-2.461268	3.063468	-0.950230
H	-2.800699	3.023005	0.581177
H	3.083087	3.427827	-0.932300
H	2.573932	2.018912	-1.337509
H	1.597011	-0.103076	1.157706
H	1.493203	0.000133	-0.399692
O	-2.119861	2.459336	-2.648670
H	-1.620534	1.641883	-2.815767
H	-2.618409	2.652954	-3.454793
O	1.675522	2.018145	2.771481
H	2.528633	1.605670	2.575433
H	1.092567	1.320146	3.106886
O	0.733771	4.567912	3.238721
H	1.145188	3.680820	3.207411
H	-0.222016	4.404841	3.226802
O	0.056928	4.087573	-1.967887
H	0.810454	3.812863	-2.509837
H	-0.716182	3.601593	-2.319750
O	1.539196	5.303213	0.712570
H	2.499796	5.263518	0.615761
H	1.341200	5.224472	1.670584

$SmI_2(H_2O)_{10}$

E: -816.154651 ; H: -815.870098 ; G: -815.967658 ;

Sm	-0.031368	2.800261	0.301413
I	-1.721109	2.954300	3.549328
I	0.738822	0.692249	-2.741028
O	-1.861187	0.240587	0.883965
O	-2.560931	2.416306	-0.710860
O	2.658886	2.820151	-0.432400
O	0.845732	-0.281004	0.729510
H	-1.947880	0.754710	1.704150
H	-0.909059	0.004888	0.809758
H	-2.476405	2.423711	-1.682735
H	-2.476083	1.497355	-0.389806
H	2.574766	3.791127	-0.503866
H	2.528593	2.444963	-1.317865
H	1.208843	0.344243	1.391120

H	1.087425	0.051599	-0.151884
O	-2.005360	2.847287	-3.406298
H	-1.474885	2.107949	-3.745965
H	-2.594179	3.132977	-4.118484
O	1.494982	1.491687	2.744531
H	2.130289	1.090045	3.355284
H	0.642806	1.529119	3.215858
O	1.673551	4.261103	2.629121
H	1.746784	3.284043	2.617864
H	0.780564	4.445219	2.962089
O	-0.060010	4.284654	-1.988793
H	0.781057	4.144207	-2.445988
H	-0.743868	3.862302	-2.547158
O	1.874263	5.409915	0.197934
H	2.464241	6.174544	0.156980
H	1.920799	5.048819	1.116020
O	-0.888987	5.412184	0.713228
H	0.017501	5.701117	0.489486
H	-0.971254	5.464630	1.676482

$SmI_2(H_2O)_{11}$

E: -892.586252 ; H: -892.272202 ; G: -892.374487 ;

Sm	-0.162781	2.597399	0.754346
I	-0.865063	3.416570	4.328797
I	0.718608	0.164065	-1.920360
O	-2.395661	0.230987	0.981058
O	-2.441361	2.294651	-0.931649
O	2.486306	2.833273	-0.190330
O	0.222292	-0.509434	1.625406
H	-2.692631	1.040550	1.439384
H	-1.495088	0.021091	1.300765
H	-2.099264	2.392803	-1.842162
H	-2.386689	1.354842	-0.679129
H	2.442245	3.777499	-0.424358
H	2.311270	2.329841	-1.001920
H	0.796856	0.162513	2.040558
H	0.518363	-0.577312	0.701442
O	-1.247118	2.664427	-3.462416
H	-0.751610	1.832853	-3.547943
H	-1.736172	2.794074	-4.286699
O	1.768218	1.639932	2.657894
H	2.639050	1.252204	2.831381
H	1.344615	1.780750	3.522182
O	2.050724	4.444187	2.433956
H	2.128256	3.472016	2.371230
H	1.275451	4.593538	3.000579
O	-0.150583	4.179514	-1.440681
H	0.640806	4.738843	-1.386435
H	-0.247229	3.810327	-2.335224
O	1.772279	5.570592	0.015104
H	2.292777	6.372625	-0.125298
H	1.953315	5.253053	0.933229
O	-0.916849	5.228181	1.164461
H	-0.129911	5.620941	0.746495
H	-0.796566	5.298335	2.124327
O	-3.299706	2.832390	1.663242
H	-2.634105	3.260748	2.228465
H	-3.056667	3.013938	0.736564

$SmI_2(H_2O)_{12}$

E: -969.021627; H: -968.679999 ; G: -968.787205 ;

Sm	-0.165703	2.368322	0.615537
I	-0.168610	3.953271	5.161886
I	0.777024	0.090141	-2.150651
O	-2.134150	-0.245513	0.631075
O	-2.535181	1.958852	-0.955122
O	2.363576	2.849911	-0.423923
O	0.486949	-0.674019	1.465597

H	-2.569580	0.194338	1.377359	E:-1045.452653; H:-1045.084751 ; G: -1045.198838 ;			
H	-1.209298	-0.396904	0.925630	Sm	-0.285040	2.467846	0.903269
H	-2.180013	2.111259	-1.852238	I	0.185725	3.578110	5.031657
H	-2.378538	1.030873	-0.687849	I	0.855438	-0.035967	-1.713974
H	2.245662	3.800937	-0.592685	O	-2.152513	-0.293821	0.504554
H	2.233900	2.384985	-1.265830	O	-2.909410	2.008142	-0.793514
H	0.839477	0.032193	2.043668	O	2.196904	2.982805	-0.285190
H	0.953699	-0.599001	0.616890	O	0.212733	-0.676909	1.877833
O	-1.295738	2.689949	-3.375748	H	-1.380131	-0.291173	1.110161
H	-0.670197	1.952434	-3.482930	H	-1.885303	-0.856219	-0.237466
H	-1.753424	2.805241	-4.219912	H	-2.332038	2.142959	-1.569936
O	1.492850	1.526287	2.900382	H	-2.642798	1.176371	-0.343994
H	2.337286	1.220324	3.264597	H	2.101839	3.874295	-0.656701
H	0.966701	1.829835	3.662519	H	2.139826	2.357729	-1.025727
O	2.281219	4.216851	2.429124	H	0.764847	0.068341	2.188944
H	2.046367	3.268925	2.397390	H	0.641760	-0.984763	1.063193
H	1.793344	4.566083	3.193397	O	-1.232388	2.556912	-3.010315
O	-0.583112	4.271938	-1.225145	H	-0.610737	1.808670	-3.027748
H	0.223228	4.807085	-1.142768	H	-1.660420	2.593554	-3.876857
H	-0.647409	3.907862	-2.126416	O	1.911256	1.487536	2.345392
O	1.505250	5.480116	0.187842	H	2.642169	1.077479	1.824576
H	1.926907	6.335173	0.028391	H	2.161718	1.475192	3.280866
H	1.891559	5.104772	1.017539	O	2.428057	4.277312	2.248087
O	-0.853612	4.916676	1.694225	H	2.304143	3.329019	2.042585
H	-0.167477	5.342593	1.145840	H	1.940655	4.421578	3.076186
H	-0.524552	4.895959	2.609623	O	-0.751683	4.341554	-0.979702
O	-3.168714	3.404076	1.318383	H	0.049172	4.885309	-0.873795
H	-2.451231	4.063736	1.385153	H	-0.739845	3.902852	-1.849450
H	-3.042663	2.955370	0.457431	O	1.350746	5.679942	0.225503
O	-1.662211	1.614905	2.807598	H	1.704814	6.572406	0.114965
H	-1.339038	2.024279	3.627354	H	1.846603	5.245388	0.963064
H	-2.342818	2.228325	2.450130	O	-0.873688	5.103922	1.881929
$SmI_2(H_2O)_{13}$				H	-0.174781	5.505582	1.329549

H	-0.504681	4.972566	2.772622
O	-3.267839	3.857205	1.172608
H	-3.101105	3.288180	0.387989
H	-2.470877	4.403341	1.311753
O	-2.208262	1.891264	2.834679
H	-1.783262	2.324163	3.594305
H	-2.761927	2.573568	2.399618
O	3.656804	0.324534	0.623258
H	4.223355	1.018529	0.257833
H	3.021251	0.103900	-0.080698

$SmI_2(H_2O)_{14}$

E: -1121.889877 ; H: -1121.492569 ; G: -1121.606594 ;

Sm	-0.721487	2.769558	1.177864
I	-1.186705	4.392967	5.050690
I	2.056216	-0.384492	-2.269272
O	-2.627273	0.148575	1.326192
O	-2.899483	1.845766	-0.857951
O	1.546554	2.640435	-0.242350
O	0.150791	0.127114	0.841686
H	-2.825434	0.855781	1.976854
H	-1.660711	0.012325	1.320647
H	-2.092093	1.833571	-1.409109
H	-2.805993	1.154623	-0.166946
H	1.861058	3.483369	-0.601866
H	1.815044	1.940835	-0.863160
H	0.943357	0.348085	1.380198
H	0.477615	-0.072214	-0.051868
O	-0.647820	1.998980	-2.502268
H	0.091301	1.379081	-2.357951
H	-0.912707	1.893959	-3.427013
O	2.348130	1.035575	2.267248
H	3.090866	1.003307	1.619348
H	2.604419	0.504919	3.034008
O	1.473956	3.613232	2.633652
H	1.857479	2.707384	2.615894
H	1.052129	3.748491	3.498460
O	-0.930194	4.399901	-1.140469
H	-0.111838	4.797252	-0.793204
H	-0.674773	3.658549	-1.722592
O	1.103117	5.380490	0.564040
H	1.608213	6.204451	0.586019
H	1.412314	4.822412	1.310126
O	-1.505582	5.519761	1.597255
H	-0.609468	5.672626	1.233484
H	-1.417795	5.479008	2.564993
O	-3.676151	4.023640	0.640341
H	-2.939356	4.639963	0.818998
H	-3.355740	3.352729	-0.002672
O	-3.379073	2.359090	2.824446
H	-2.774842	2.804003	3.443759
H	-3.561952	3.001684	2.101668
O	4.232119	0.985998	0.304164
H	4.388215	1.906729	0.051256
H	3.741035	0.586543	-0.436324
O	-0.449750	1.213522	3.521319
H	-1.123344	0.522083	3.592086
H	-0.700926	1.899989	4.163929

$SmI_2(H_2O)_{15}$

E: -1198.319646 ; H: -1197.894662 ; G: -1198.017100 ;

Sm	-0.504809	2.757209	1.255665
I	-0.206144	5.186647	4.771777
I	1.660094	-0.722431	-2.397461
O	-2.425516	0.040186	1.051665
O	-2.289462	2.031466	-0.851745
O	1.435624	2.416524	-0.530325
O	0.319607	0.015994	0.945124

H	-2.708980	0.756807	1.661542
H	-1.454533	-0.037401	1.134728
H	-1.675519	1.932971	-1.606429
H	-2.374841	1.174901	-0.384871
H	1.726896	3.096441	-1.154857
H	1.544761	1.564255	-0.988217
H	1.114165	0.260080	1.469263
H	0.637120	-0.253239	0.066395
O	-0.466815	2.176687	-2.941570
H	0.182985	1.451024	-2.910337
H	-0.870184	2.150085	-3.820587
O	2.570368	0.972828	2.181091
H	3.216474	0.830007	1.448620
H	2.913547	0.527460	2.967862
O	1.998721	3.618285	2.349724
H	2.269813	2.672086	2.379212
H	1.665615	3.870678	3.226758
O	-0.631955	4.572519	-1.466348
H	0.136675	4.778785	-0.902941
H	-0.424514	3.761835	-1.965314
O	1.228439	5.366658	0.427803
H	1.743706	6.184017	0.402352
H	1.637269	4.771913	1.094697
O	-1.356869	5.843101	1.368868
H	-0.456112	5.707150	1.006945
H	-1.256676	5.824681	2.335594
O	-3.370777	4.142614	0.587342
H	-2.645890	4.765756	0.809557
H	-3.014414	3.510277	-0.068631
O	-3.274825	2.176923	2.510221
H	-2.994872	2.396602	3.418970
H	-3.358921	2.994582	1.974014
O	4.109999	0.627988	-0.021825
H	4.361743	1.502993	-0.348606
H	3.494939	0.262543	-0.682926
O	-0.172924	1.483936	3.622326
H	-0.903592	1.721447	4.228779
H	0.630593	1.870637	3.999414
O	-2.347095	2.369260	5.113578
H	-2.815353	1.947429	5.847300
H	-2.037341	3.236729	5.423702

$SmI_2(H_2O)_{16}$

E: -1274.747075 ; H: -1274.295497 ; G: -1274.424664 ;

Sm	-0.530941	2.721636	1.266529
I	0.267127	5.274832	4.811855
I	1.776244	-0.708985	-2.413579
O	-2.461726	0.021761	1.129488
O	-2.288090	1.951347	-0.854009
O	1.448143	2.406799	-0.496664
O	0.275455	0.008753	0.858621
H	-2.730874	0.764222	1.714098
H	-1.490371	-0.061166	1.193454
H	-1.653703	1.852882	-1.592010
H	-2.378199	1.103372	-0.374491
H	1.849625	3.115019	-1.020434
H	1.637981	1.576106	-0.967445
H	1.118255	0.190768	1.331796
H	0.519665	-0.235155	-0.050458
O	-0.429123	2.136554	-2.892206
H	0.235353	1.423978	-2.875687
H	-0.819135	2.131790	-3.777606
O	2.615135	0.779786	2.035841
H	3.273045	0.740279	1.300200
H	2.980384	0.289552	2.785082
O	2.064496	3.421183	2.351732
H	2.302954	2.466840	2.328637

H	1.759030	3.646481	3.245894	O	-2.729049	0.485492	0.842459
O	-0.560756	4.537247	-1.409740	O	-3.322187	2.732235	-0.761313
H	0.166891	4.756074	-0.798356	O	1.570400	3.078351	-0.853363
H	-0.325988	3.707467	-1.862920	O	0.128104	-0.059887	0.621388
O	1.253825	5.305527	0.590862	H	-2.794470	1.009288	1.669635
H	1.745444	6.136409	0.639261	H	-1.832799	0.103580	0.809345
H	1.687519	4.663765	1.195862	H	-2.572373	2.887697	-1.354951
O	-1.393303	5.852038	1.302732	H	-3.119180	1.898587	-0.283674
H	-0.441130	5.649859	1.212826	H	2.345244	3.503223	-0.445949
H	-1.671021	5.709786	2.227916	H	1.894228	2.273478	-1.293361
O	-3.363729	4.101059	0.488862	H	0.858175	-0.118194	1.268366
H	-2.632209	4.735994	0.644335	H	0.521899	-0.272038	-0.241255
H	-3.022519	3.424241	-0.131096	O	-0.869884	1.568767	-1.703011
O	-3.316273	2.215499	2.515344	H	-0.021273	1.137387	-1.919032
H	-2.994860	2.484782	3.396691	H	-1.535777	0.865717	-1.747044
H	-3.380967	3.007524	1.938815	O	2.208460	0.416459	2.448369
O	4.229344	0.770881	-0.140213	H	2.883890	0.674825	1.770786
H	4.346549	1.696020	-0.398182	H	2.639982	-0.184322	3.071621
H	3.669852	0.368858	-0.828677	O	1.633103	3.159688	2.583026
O	-0.181165	1.437005	3.624600	H	1.888277	2.242923	2.804738
H	-0.848019	1.804645	4.241107	H	1.170759	3.517962	3.360661
H	0.686780	1.661176	3.988182	O	-0.673535	3.791609	-3.320619
O	-2.206472	2.665897	5.036447	H	0.235057	3.833683	-3.647833
H	-2.589560	2.345530	5.864990	H	-0.777899	2.914333	-2.899270
H	-1.816662	3.539833	5.216135	O	1.381329	5.989131	0.493760
O	-3.048355	5.224176	3.398251	H	1.600578	6.928845	0.433199
H	-3.035171	5.683184	4.249576	H	2.222439	5.495022	0.567974
H	-3.914771	5.398333	3.003429	O	-0.689833	5.171074	2.106480

$SmI_2(H_2O)_{17}$

H	0.125458	5.557261	1.724279				
H	-0.569895	5.082460	3.066910				
O	-3.239922	4.648318	1.212184				
H	-2.319837	4.966821	1.302173				
H	-3.277959	4.069416	0.418191				

E: -1351.185188 ; H: -1350.702886 ; G: -1350.830914 ;

Sm	-0.530701	2.693995	0.855487
I	-0.714607	3.841432	5.439040
I	2.270857	-0.158107	-2.376758

O	-3.090382	2.402233	2.810911	H	0.791974	-0.009414	1.385563
H	-2.528234	2.616923	3.573137	H	0.590630	-0.241281	-0.144160
H	-3.199653	3.234980	2.302867	O	-0.870347	1.580002	-1.694196
O	3.917869	1.327460	0.576098	H	-0.029967	1.120944	-1.881469
H	3.874374	2.302681	0.587023	H	-1.559792	0.905328	-1.788670
H	3.609937	1.036494	-0.299525	O	2.146135	0.509926	2.516526
O	-0.485102	0.981049	3.231095	H	2.845520	0.719206	1.848354
H	-0.480271	1.620263	3.963575	H	2.536266	-0.098045	3.159926
H	0.429775	0.665280	3.146499	O	1.659316	3.240479	2.541600
O	-3.594510	5.599038	3.867434	H	1.861987	2.318185	2.796404
H	-2.804661	5.135380	4.193578	H	1.284755	3.676231	3.327475
H	-3.703082	5.315911	2.943638	O	-0.680670	3.772879	-3.334278
O	3.461024	4.145558	0.915804	H	0.232218	3.835213	-3.646002
H	2.949909	3.891913	1.719037	H	-0.766849	2.902187	-2.893130
H	4.287569	4.562535	1.196190	O	1.422587	5.999080	0.403088
O	-0.886144	4.963442	-0.796211	H	1.646870	6.936718	0.329890
H	-0.746846	4.655075	-1.714204	H	2.260663	5.502998	0.498487
H	-0.048085	5.363875	-0.494679	O	-0.643621	5.302441	2.085307

$SmI_2(H_2O)_{18}$

H	0.169044	5.625634	1.642856				

E: -1427.615624 ; H: -1427.106771 ; G: -1427.243479 ;

H	-0.457885	5.237560	3.037682				
Sm	-0.586203	2.716979	0.903843	O	-3.203617	4.678503	1.275290
I	0.017156	4.527525	5.565565	H	-2.294418	5.026691	1.370317
I	2.259384	-0.205411	-2.308308	H	-3.228451	4.125930	0.462622
O	-2.740862	0.380841	0.581842	O	-3.324198	2.195254	2.529958
O	-3.320758	2.816370	-0.772414	H	-3.054954	2.192547	3.469343
O	1.542757	3.038700	-0.805391	H	-3.271333	3.115339	2.203347
O	0.115984	-0.028386	0.676892	O	3.911160	1.310888	0.626587
H	-2.888481	0.906340	1.399469	H	3.886408	2.286150	0.594868
H	-1.806957	0.098945	0.588891	H	3.598895	0.990266	-0.237056
H	-2.588971	3.006634	-1.378070	O	-0.584596	1.197689	3.183076
H	-3.120276	1.939426	-0.380815	H	-1.080287	1.356243	4.006921
H	2.323452	3.472912	-0.420537	H	0.302756	0.888521	3.418779
H	1.861670	2.212204	-1.207739	O	-2.410738	1.964875	5.140468

H	-2.993016	1.563467	5.800170	H	2.478772	-0.188727	3.245642
H	-2.030916	2.768369	5.536551	O	1.684693	3.129909	2.497509
O	-3.375991	5.077427	4.127877	H	1.869596	2.211417	2.778755
H	-2.461099	4.809175	4.317162	H	1.341792	3.598960	3.277995
H	-3.489267	4.999890	3.165522	O	-0.707174	3.742127	-3.403761
O	3.495002	4.152052	0.866698	H	0.199915	3.803215	-3.732292
H	2.980900	3.910981	1.674101	H	-0.786573	2.871898	-2.960780
H	4.325767	4.565543	1.139244	O	1.495869	5.952279	0.233913
O	-0.885162	4.966503	-0.813610	H	1.728573	6.877406	0.392880
H	-0.769862	4.643022	-1.729713	H	2.300150	5.420270	0.401188
H	-0.033833	5.358635	-0.540903	O	-0.509345	5.264238	2.031723

$SmI_2(H_2O)_{19}$

H	0.291781	5.579091	1.563247
H	-0.301374	5.205951	2.979789
O	-3.093134	4.625380	1.352077
H	-2.181461	4.969530	1.442655
H	-3.139866	4.120113	0.510165
O	-3.590230	2.139586	2.599645
H	-3.269230	2.108770	3.521672
H	-3.388202	3.030700	2.252852
O	3.752369	1.160023	0.599761
H	3.773501	2.135052	0.565043
H	3.383050	0.853813	-0.247132
O	-0.690318	1.185387	3.106311
H	-1.177957	1.358323	3.933234
H	0.197054	0.872351	3.339738
O	-2.451606	1.933094	5.129766
H	-2.859247	1.443528	5.857523
H	-2.051275	2.733650	5.509800
O	-3.310883	5.105533	4.167344
H	-2.398988	4.829413	4.359035
H	-3.425950	5.012478	3.206591
O	3.488818	4.036321	0.789200
H	2.964150	3.803180	1.592805

E: -1504.044066 ; H: -1503.508287 ; G: -1503.653771 ;

Sm	-0.483803	2.708612	0.773828
I	0.081772	4.453026	5.535754
I	2.208863	-0.259216	-2.437405
O	-2.691194	0.500864	0.618805
O	-3.284714	2.864322	-0.768837
O	1.570846	3.022452	-0.972312
O	0.164127	-0.023621	0.619593
H	-2.906457	0.948444	1.466641
H	-1.780886	0.157557	0.676980
H	-2.562339	3.025605	-1.394182
H	-3.091747	1.992983	-0.357945
H	2.366121	3.421260	-0.577462
H	1.864276	2.211299	-1.422006
H	0.790087	-0.075208	1.369785
H	0.678923	-0.218163	-0.182447
O	-0.883726	1.544563	-1.761604
H	-0.069965	1.050004	-1.975684
H	-1.601667	0.895063	-1.805938
O	2.087446	0.399993	2.585640
H	2.776299	0.579537	1.898275

H	4.311110	4.458337	1.074209	O	-0.644721	3.691024	-3.381924
O	-0.855353	4.959509	-0.890831	H	0.267927	3.740296	-3.696734
H	-0.758420	4.633019	-1.808238	H	-0.737757	2.827810	-2.927943
H	-0.002863	5.362695	-0.639712	O	1.508551	5.907094	0.265769
O	2.455243	6.083314	3.233621	H	1.721458	6.839719	0.407260
H	2.692354	6.991749	3.464953	H	2.324381	5.395710	0.441790
H	1.812556	5.797757	3.904839	O	-0.502283	5.220444	2.053413

$SmI_2(H_2O)_{20}$

H	0.302691	5.517470	1.579509

E: -1580.475534 ; H: -1579.910802 ; G: -1580.060708 ;

H	-0.280689	5.139784	2.996743
Sm	-0.517201	2.627064	0.852304	O	-3.095581	4.585727	1.403113
I	-0.001482	4.510882	5.568586	H	-2.181656	4.922342	1.500001
I	2.212945	-0.346961	-2.270083	H	-3.144995	4.100559	0.548587
O	-2.786345	0.567570	0.596477	O	-3.738943	2.125679	2.616947
O	-3.257147	2.932601	-0.794636	H	-3.484953	2.081141	3.557038
O	1.601784	2.923291	-0.828587	H	-3.488041	3.014781	2.296970
O	-0.071658	-0.241882	0.689502	O	4.136202	1.288506	0.459765
H	-3.040927	0.966791	1.457139	H	4.067259	2.261989	0.509081
H	-1.912946	0.144257	0.699692	H	3.845654	1.026772	-0.430178
H	-2.487464	3.114666	-1.354400	O	-0.710183	1.322735	3.222182
H	-3.093512	2.050698	-0.394128	H	-1.412054	1.526245	3.869700
H	2.387640	3.348639	-0.445772	H	0.108508	1.230193	3.749680
H	1.902994	2.078785	-1.206809	O	-2.632353	2.014387	5.169585
H	0.710931	-0.064093	1.257897	H	-2.655949	1.350577	5.872970
H	0.287005	-0.476194	-0.181515	H	-2.169116	2.790299	5.529031
O	-0.860961	1.531510	-1.699688	O	-3.396390	5.137781	4.187253
H	-0.042359	1.031366	-1.880381	H	-2.486393	4.886152	4.417350
H	-1.580149	0.884189	-1.753732	H	-3.477457	5.010882	3.226731
O	2.156543	0.459671	2.112345	O	3.557626	4.063350	0.850389
H	2.935571	0.632873	1.530024	H	3.034848	3.816128	1.649737
H	2.433106	-0.156246	2.804731	H	4.341788	4.551051	1.139200
O	1.717919	3.108633	2.508030	O	-0.826790	4.872613	-0.858404
H	1.874418	2.141240	2.585950	H	-0.715301	4.574100	-1.783716
H	1.368101	3.419035	3.360690	H	0.018347	5.281002	-0.591727

O	2.515065	6.004350	3.275042
H	2.578600	6.936170	3.525326
H	1.856778	5.615866	3.875768
O	1.442439	1.236527	5.046454
H	1.289584	2.140513	5.371818
H	2.341834	1.228342	4.690464

$SmI_3(H_2O)$

E: -145.608610 ; H: -145.571384 ; G: -145.627164 ;

Sm	0.152047	-0.685881	-0.054096
I	-1.238513	-0.319690	-3.364798
I	1.500061	1.501426	2.542731
O	0.737175	1.588457	-0.904050
H	0.684000	2.275535	-0.220519
H	0.158415	1.850447	-1.637778
I	-2.902725	0.755995	0.912249

$SmI_3(H_2O)_2$

E: -222.041640 ; H: -221.976854 ; G: -222.037650 ;

Sm	-0.364599	-0.171309	0.102185
I	-1.454104	0.367805	-3.221530
I	1.456186	1.904323	2.504375
O	1.292922	1.448573	-1.075129
H	1.507989	2.135220	-0.422695
H	0.796509	1.874177	-1.792656
I	-3.659173	-0.095142	1.669739
O	-1.333305	2.204965	0.157587
H	-0.774747	2.685483	0.792675
H	-2.199852	2.092911	0.585934

$SmI_3(H_2O)_3$

E: -298.474986 ; H: -298.382282 ; G: -298.448073 ;

Sm	-0.453058	-0.043789	0.103095
I	-1.675743	0.185254	-3.229863
I	1.199661	1.790793	2.729629
O	1.293576	1.395894	-1.040910
H	1.621839	2.102832	-0.464002
H	0.983663	1.815908	-1.857262
I	-3.516980	0.143922	2.042532
O	-1.392989	2.342546	0.103374
H	-0.816177	2.840920	0.706257
H	-2.250144	2.264315	0.555635
O	-1.876765	-2.064583	-0.336200
H	-2.118523	-2.043109	-1.276796
H	-2.701824	-1.947961	0.164138

$SmI_3(H_2O)_4$

E: -374.905883 ; H: -374.786037 ; G: -374.860255 ;

Sm	-0.472941	-0.012414	-0.000805
I	-1.085346	0.628260	-3.487656
I	1.122405	1.838625	2.686162
O	1.343153	1.510066	-0.972719
H	1.560356	2.221225	-0.349323
H	0.980920	1.920737	-1.774325
I	-3.403510	0.239292	2.171682
O	-1.412534	2.375725	0.027771
H	-0.808326	2.874025	0.603009
H	-2.245107	2.298225	0.523570
O	-2.141912	-1.939363	-0.320967
H	-1.784963	-2.838720	-0.303722
H	-2.763430	-1.862850	0.423180
O	0.160058	-1.540721	1.948460
H	0.629926	-2.370170	1.781067
H	0.690748	-1.033338	2.583615

$SmI_3(H_2O)_5$

E: -451.340125 ; H: -451.192353 ; G: -451.270589 ;

Sm	-0.584757	0.108849	0.031904
I	-0.791201	0.752541	-3.521187
I	0.803856	2.086696	2.801845
O	1.404188	1.538823	-0.707449

H	1.540907	2.252814	-0.063573
H	1.201466	1.949904	-1.563099
I	-3.449980	0.092350	2.224809
O	-1.549362	2.499689	0.053402
H	-0.953389	2.957732	0.670820
H	-2.398637	2.424330	0.518826
O	-2.010742	-1.903940	-0.386485
H	-1.585749	-2.755587	-0.562122
H	-2.655416	-2.039514	0.325937
O	0.597196	-1.334064	1.744545
H	1.291898	-1.909895	1.392749
H	1.018346	-0.735576	2.384052
O	0.809484	-1.554535	-1.287112
H	1.739673	-1.599168	-1.020908
H	0.795761	-1.240872	-2.207463

$SmI_3(H_2O)_6$

E: -527.772572 ; H: -527.596047 ; G: -527.678421 ;

Sm	-0.503014	0.259588	0.016203
I	-0.591702	1.062275	-3.533118
I	1.055552	1.973724	2.802234
O	1.640227	1.548265	-0.667240
H	1.833718	2.215344	0.010805
H	1.513569	2.010785	-1.510137
I	-3.089556	0.043600	2.599310
O	-1.676683	2.531162	0.023586
H	-1.820394	2.840464	0.930383
H	-2.536106	2.199908	-0.316601
O	-2.355295	-1.538449	-0.381922
H	-2.140936	-2.374074	-0.820919
H	-2.738836	-1.743177	0.487426
O	0.394082	-1.549867	1.569952
H	1.107660	-2.101469	1.218001
H	0.733836	-1.137260	2.379780
O	0.692422	-1.471693	-1.408596
H	1.556402	-1.777477	-1.095925
H	0.820545	-1.110187	-2.301092
O	-3.480523	0.946756	-1.326170
H	-2.948668	1.039541	-2.135428
H	-3.291455	0.048995	-0.997328

$SmI_3(H_2O)_7$

E: -604.208262 ; H: -604.005690 ; G: -604.091121 ;

Sm	-0.740342	0.051607	0.331197
I	-0.634769	0.873509	-3.219824
I	3.059392	1.546569	3.187818
O	1.469022	1.251923	-0.112863
H	1.938822	1.575941	0.677394
H	1.467511	1.967498	-0.765146
I	-3.403211	-0.590372	2.547728
O	-2.176720	2.063764	-0.036481
H	-2.510566	2.404440	0.806526
H	-2.959337	1.808257	-0.580554
O	-2.524534	-1.264520	-1.012818
H	-2.185707	-1.629600	-1.845211
H	-2.952326	-1.988218	-0.529958
O	0.864438	-1.079756	1.988616
H	1.392422	-1.790218	1.596049
H	1.495526	-0.460461	2.401619
O	0.577515	-1.656663	-0.985726
H	1.528605	-1.633051	-0.803951
H	0.467090	-1.387519	-1.913871
O	-4.129279	0.953709	-1.549989
H	-3.988006	1.238287	-2.463914
H	-3.673907	0.092546	-1.455574
O	-0.421612	1.648708	2.293693
H	-1.005995	1.364998	3.014409
H	0.487754	1.655683	2.648570

$SmI_3(H_2O)_8$

E: -680.640901 ; H: -680.409615 ; G: -680.502408 ;

Sm	-0.120986	0.751347	0.533717
I	1.818664	-0.563888	-4.145224
I	0.739973	-1.245400	5.029606
I	-4.834691	0.795826	2.048487
O	-2.075183	2.398292	0.307644
H	-2.731970	2.192308	0.996277
H	-2.521227	2.204617	-0.544841
O	-2.252784	-0.587671	-0.072757
H	-2.145902	-1.451939	0.353189
H	-3.019268	-0.165773	0.360800
O	0.064971	-1.607042	1.480844
H	0.806437	-2.111469	1.114950
H	0.189375	-1.604825	2.449358
O	1.900392	-0.249974	-0.559756
H	2.457922	-0.900866	-0.110962
H	1.942159	-0.436545	-1.517111
O	-3.054264	1.490267	-2.095980
H	-3.592300	1.984389	-2.729758
H	-3.504729	0.647817	-1.938148
O	-1.256870	0.783446	2.795123
H	-2.228701	0.700857	2.788735
H	-0.912903	0.197322	3.493863
O	-0.324626	1.341305	-1.920912
H	0.197007	0.819074	-2.556643
H	-1.259312	1.335202	-2.213816
O	1.763476	0.923724	2.269212
H	2.565062	0.485982	1.946627
H	1.508566	0.452649	3.085359

$SmI_3(H_2O)_9$

E: -757.067531 ; H: -756.808135 ; G: -756.907460 ;

Sm	-0.123015	0.754919	0.543128
I	1.730147	-0.565114	-4.165338
I	0.753525	-1.242258	5.034035
O	-1.349441	1.278383	-5.082602
H	-1.620351	1.859038	-4.358459
H	-0.538067	0.834954	-4.781414
I	-4.833867	0.777318	2.059288
O	-2.083499	2.394619	0.320443
H	-2.742264	2.179093	1.004462
H	-2.529799	2.222220	-0.535163
O	-2.254443	-0.585096	-0.079678
H	-2.143635	-1.456761	0.329735
H	-3.019456	-0.172821	0.365590
O	0.069025	-1.603062	1.488618
H	0.809064	-2.107167	1.119460
H	0.197348	-1.601294	2.456628
O	1.894259	-0.250614	-0.560750
H	2.454517	-0.900028	-0.113186
H	1.920414	-0.448189	-1.515841
O	-3.041318	1.503471	-2.106965
H	-3.500102	1.955601	-2.828913
H	-3.485608	0.652953	-1.976231
O	-1.255795	0.783575	2.805286
H	-2.227001	0.694022	2.800099
H	-0.906940	0.199044	3.502984
O	-0.325246	1.361871	-1.901634
H	0.180366	0.821903	-2.535211
H	-1.269405	1.340544	-2.166443
O	1.768160	0.926835	2.270677
H	2.567199	0.486877	1.944776
H	1.515658	0.456571	3.088026

$SmI_3(H_2O)_{10}$

E: -833.500992 ; H: -833.213743 ; G: -833.315871 ;

Sm	-0.302139	0.528260	-0.061160

I	-2.230277	2.345371	-4.731046
I	2.534045	1.124477	4.285005
O	0.864331	0.294427	-3.692104
H	0.678466	1.113173	-3.192522
H	0.057493	0.104083	-4.192758
I	-4.965241	-0.524284	-0.220637
O	-2.257832	1.281295	1.377433
H	-1.991249	0.892225	2.242716
H	-3.084498	0.845068	1.102422
O	-1.573595	-1.619728	0.493278
H	-1.491692	-1.899853	1.416950
H	-2.526825	-1.495379	0.324932
O	1.028229	-0.758722	1.648660
H	1.272363	-1.683643	1.496894
H	1.719882	-0.353986	2.206294
O	1.008516	-1.147364	-1.408455
H	1.917111	-1.317727	-1.125134
H	1.042127	-0.780030	-2.323618
O	-3.315324	2.631901	-1.252416
H	-3.713598	1.783811	-0.991922
H	-3.063606	2.527833	-2.186497
O	-1.020219	0.040586	3.448205
H	-0.368394	-0.401042	2.871275
H	-0.502316	0.637982	4.009220
O	-1.807685	-0.054738	-2.021273
H	-2.724689	-0.224723	-1.735404
H	-1.860949	0.568529	-2.770213
O	0.644316	2.323896	1.470968
H	1.204834	2.002980	2.203959
H	-0.044177	2.871708	1.876155
O	0.035298	2.327289	-1.911637
H	0.538657	3.124398	-1.689757
H	-0.727249	2.610542	-2.449024

$SmI_3(H_2O)_{11}$

E: -909.933501 ; H: -909.617697 ; G: -909.725834 ;

Sm	-0.133930	0.829236	0.586431
I	2.010087	-0.276986	-4.083235
I	0.290828	-1.566191	5.026722
O	-1.359255	0.980119	-4.981137
H	-1.610604	1.713681	-4.403552
H	-0.468825	0.709713	-4.699771
I	-4.862914	0.919736	2.074687
O	-2.089892	2.482677	0.287397
H	-2.754828	2.281445	0.970789
H	-2.514444	2.248438	-0.561840
O	-2.303746	-0.487203	-0.046924
H	-2.068021	-1.367104	0.289497
H	-3.030841	-0.163392	0.521131
O	-0.191360	-1.611989	1.434550
H	0.578837	-2.118752	1.137559
H	-0.158916	-1.629062	2.410055
O	1.884090	-0.242383	-0.479494
H	2.290115	-1.035986	-0.102912
H	1.964530	-0.313083	-1.449308
O	-2.904441	1.245601	-2.080206
H	-3.436365	1.251314	-2.887852
H	-2.975515	0.363761	-1.672652
O	-1.309870	0.864601	2.838048
H	-2.283814	0.823482	2.800577
H	-1.019235	0.229718	3.518969
O	-0.224582	1.489409	-1.854921
H	0.371347	1.059494	-2.495991
H	-1.149590	1.384795	-2.175351
O	1.696814	0.536693	2.419752
H	2.447227	0.029611	2.076319
H	1.360169	0.033936	3.185476

O	0.202896	4.163234	-1.219716
H	0.024401	3.267378	-1.573831
H	-0.642096	4.632987	-1.217374
O	0.654894	3.136945	1.253302
H	1.580553	3.179644	1.529764
H	0.563130	3.672085	0.430118

$SmI_3(H_2O)_{12}$

E: -986.377264 ; H: -986.033143 ; G: -986.144474 ;

Sm	-0.229723	0.660722	0.506221
I	2.097205	-0.087552	-4.028072
I	0.100141	-1.662108	5.031466
O	-1.519202	-0.805931	-3.490701
H	-2.088197	-0.042304	-3.278270
H	-0.764902	-0.463945	-3.998047
I	-4.980877	1.394052	2.116604
O	-2.058374	2.494538	0.233538
H	-2.720141	2.364994	0.937471
H	-2.534165	2.327581	-0.600749
O	-2.606857	-0.376846	0.023629
H	-2.570755	-1.338273	0.138707
H	-3.255279	-0.036074	0.670406
O	-0.328519	-1.729657	1.459299
H	0.092005	-2.353784	0.850575
H	-0.013021	-1.918380	2.360460
O	2.163689	0.692801	-0.460806
H	2.732739	-0.006359	-0.107027
H	2.232242	0.624482	-1.431285
O	-2.970016	1.211624	-2.158085
H	-3.845286	1.437830	-2.501632
H	-3.077555	0.515822	-1.475337
O	-1.468897	0.780985	2.759796
H	-2.443200	0.801553	2.732900
H	-1.212690	0.086843	3.394962
O	-0.240519	1.677938	-1.898890
H	0.285000	1.179087	-2.553056
H	-1.166670	1.665342	-2.210059
O	1.494368	0.461091	2.449574
H	2.342568	0.063911	2.204230
H	1.161061	-0.057733	3.206147
O	0.778578	4.123862	-1.153364
H	0.385076	3.326781	-1.566315
H	0.128495	4.834366	-1.236809
O	0.657205	2.925279	1.273148
H	1.527323	2.773414	1.668695
H	0.785836	3.477933	0.467092
O	-0.029384	-1.258498	-1.220732
H	-0.652150	-1.133387	-1.974115
H	0.852193	-1.240817	-1.626900

$SmI_3(H_2O)_{13}$

E: -1062.807856 ; H: -1062.434323 ; G: -1062.547633 ;

Sm	-0.070121	0.720601	0.380652
I	2.530812	0.320866	-3.559771
I	0.356255	-1.622668	4.933643
O	-1.324570	-0.558942	-3.813373
H	-2.031324	0.047589	-3.521347
H	-0.652779	-0.017781	-4.254713
I	-4.896337	1.165166	2.163150
O	-2.068003	2.377517	0.184794
H	-2.661776	2.242574	0.944268
H	-2.594422	2.131764	-0.597641
O	-2.452258	-0.468581	0.025254
H	-2.231521	-1.362319	0.332454
H	-3.104133	-0.107430	0.656293
O	-0.178425	-1.680850	1.356425
H	0.291695	-2.364473	0.858793
H	0.088070	-1.771969	2.290021

O	2.381548	-0.766082	0.020501	H	-1.563189	0.849408	-4.429831
H	2.353600	-1.733275	-0.007137	H	-0.256196	0.020183	-4.335540
H	2.822980	-0.489079	-0.800282	I	-4.855205	1.177676	2.311476
O	-2.998531	1.016196	-2.209603	O	-2.046047	2.325723	0.243728
H	-3.903517	1.185612	-2.506081	H	-2.604063	2.238402	1.035245
H	-3.025572	0.291962	-1.551593	H	-2.609049	2.051167	-0.503205
O	-1.319166	0.704716	2.653184	O	-2.442158	-0.523886	0.148172
H	-2.293197	0.704422	2.665414	H	-2.222197	-1.378247	0.553686
H	-1.025627	0.037789	3.300285	H	-3.115252	-0.111211	0.721742
O	-0.373761	1.876181	-1.991393	O	-0.158846	-1.717894	1.525422
H	0.263078	1.457010	-2.599359	H	0.250127	-2.469482	1.074191
H	-1.270823	1.657111	-2.307949	H	0.099727	-1.773205	2.464478
O	1.639225	0.597681	2.336261	O	2.195413	-0.675040	-0.094769
H	2.295027	0.037670	1.883977	H	2.093597	-1.630773	0.019513
H	1.320640	0.087652	3.103382	H	2.454932	-0.547079	-1.025093
O	0.456909	4.230184	-0.881717	O	-2.956276	1.007618	-2.066237
H	0.001329	3.575603	-1.449734	H	-3.422222	0.870073	-2.902753
H	0.443425	5.085810	-1.330431	H	-2.897837	0.142248	-1.618776
O	0.238445	3.072887	1.606896	O	-1.279684	0.695279	2.728604
H	1.133011	3.011746	1.971737	H	-2.253150	0.654996	2.728670
H	0.278445	3.699123	0.856667	H	-0.967168	0.076964	3.413383
O	-0.078063	-1.079996	-1.426933	O	-0.366405	1.804590	-1.917975
H	-0.581365	-0.902259	-2.254649	H	0.296342	1.424115	-2.521937
H	0.848633	-1.158784	-1.706091	H	-1.253018	1.492245	-2.204604
O	2.097607	2.035669	-0.362841	O	1.677279	0.708218	2.402819
H	2.385951	1.681086	-1.223504	H	2.421524	0.212189	2.025631
H	1.791464	2.945587	-0.544513	H	1.377057	0.198281	3.178842

$SmI_3(H_2O)_{14}$

E: -1139.237527 ; H: -1138.836802 ; G: -1138.955055 ;

Sm	-0.035910	0.656229	0.454751	O	0.400010	4.202746	-0.885452
I	2.373076	0.165998	-3.610953	H	-0.052677	3.529208	-1.433944
I	0.538515	-1.460309	5.074339	H	0.362494	5.050638	-1.347245
O	-1.194369	-0.030578	-4.592252	O	0.258065	3.048652	1.620265
H	-1.563189	0.849408	-4.429831	H	1.167632	2.999813	1.948295
H	-0.256196	0.020183	-4.335540	H	0.259067	3.665801	0.861988

O	-0.277587	-1.182449	-1.364737
H	-1.127645	-1.383652	-1.815501
H	0.406953	-1.131081	-2.053048
O	2.089285	2.042458	-0.378807
H	2.361049	1.676666	-1.239222
H	1.756866	2.940588	-0.569964
O	-2.505046	-1.718785	-2.866563
H	-2.478558	-2.647520	-3.134739
H	-2.121914	-1.192736	-3.602963

$SmI_3(H_2O)_{15}$

E: -1215.674698 ; H: -1215.245861 ; G: -1215.368831 ;

Sm	-0.017306	0.722839	0.372214
I	2.507503	0.096246	-3.549789
I	0.349392	-1.230816	5.133093
O	-0.988843	-0.117032	-4.641048
H	-1.238746	0.811666	-4.529683
H	-0.059823	-0.176916	-4.354502
I	-4.838334	0.926280	2.395503
O	-2.140450	2.273502	0.197447
H	-2.742620	2.166989	0.953430
H	-2.642848	1.978856	-0.590737
O	-2.228873	-0.675280	0.315151
H	-2.269128	-1.170636	1.163596
H	-3.012220	-0.102139	0.331966
O	0.320769	-1.635970	1.551419
H	-0.332288	-2.316064	1.332103
H	0.342574	-1.578433	2.524543
O	2.347640	-0.601194	0.056428
H	1.994708	-1.465246	0.325094
H	2.571488	-0.662326	-0.888705
O	-3.093446	1.214809	-2.137985
H	-3.694179	1.631929	-2.770202
H	-3.109980	0.246757	-2.303569
O	-1.227327	0.883349	2.673311
H	-2.186023	0.711800	2.634629
H	-0.872000	0.311107	3.377784
O	-0.410760	1.802761	-2.012279
H	0.206504	1.366551	-2.626068
H	-1.325683	1.573103	-2.284533
O	1.710358	0.872403	2.329370
H	2.424064	0.339783	1.940762
H	1.437678	0.413388	3.143879
O	0.458319	4.220150	-1.106846
H	-0.024097	3.537370	-1.616525
H	0.393621	5.060180	-1.579883
O	0.295333	3.180433	1.448189
H	1.198958	3.085638	1.783060
H	0.336448	3.765217	0.666129
O	-0.119207	-1.149729	-1.373922
H	-1.014270	-1.273873	-1.756192
H	0.492901	-0.999903	-2.115975
O	2.114336	2.087057	-0.469834
H	2.452695	1.635379	-1.262500
H	1.803915	2.963222	-0.767968
O	-2.493493	-1.345326	-2.762104
H	-2.972906	-2.168441	-2.925515
H	-2.034091	-1.077140	-3.589814
O	-2.541444	-1.942837	2.778030
H	-1.810224	-1.765125	3.394668
H	-3.265644	-1.350821	3.044701

$SmI_3(H_2O)_{16}$

E: -1292.109524 ; H: -1291.652222 ; G: -1291.780798 ;

Sm	-0.090745	0.872623	0.440453
I	2.592807	0.260969	-3.653359
I	0.670140	-1.374035	4.989439
O	-0.926073	-0.054613	-4.681625

H	-1.251128	0.845223	-4.532811	O	0.208413	-0.984342	-1.332544
H	0.018655	-0.040775	-4.444940	H	-0.651427	-1.201454	-1.757207
I	-4.677023	0.839898	2.760841	H	0.821773	-0.736557	-2.047983
O	-2.060406	2.405653	0.133151	O	2.087635	1.974208	-0.508273
H	-2.482346	2.814253	0.913011	H	2.390292	1.563737	-1.338160
H	-2.735136	2.057128	-0.478870	H	1.827545	2.887280	-0.739226
O	-2.210374	-0.569915	0.400829	O	-2.153200	-1.389821	-2.681178
H	-2.184607	-1.125073	1.213676	H	-2.522964	-2.275008	-2.800832
H	-3.001375	-0.015775	0.504419	H	-1.781852	-1.086610	-3.540703
O	0.421061	-1.574691	1.408531	O	-2.338154	-1.977797	2.785905
H	-0.218373	-2.260868	1.168555	H	-1.563043	-1.848525	3.359796
H	0.529389	-1.618566	2.376695	H	-3.035160	-1.399452	3.141518
O	2.800508	-0.930583	0.103651	O	-2.281753	3.724331	2.562689
H	1.904625	-1.294877	0.229975	H	-1.326550	3.555712	2.439028
H	2.850602	-0.634275	-0.819305	H	-2.621016	3.013113	3.126976
O	-3.064805	1.104107	-2.065672	$SmI_3(H_2O)_{17}$			
H	-3.640951	1.414426	-2.777653	E: -1368.542215 ; H: -1368.056762 ; G: -1368.187334 ;			
H	-2.946383	0.138342	-2.194258	Sm	-0.100146	0.924878	0.423720
O	-1.069092	0.909215	2.807931	I	2.567402	0.411290	-3.704277
H	-2.030415	0.739020	2.828157	I	0.592088	-1.605728	4.765055
H	-0.655755	0.270232	3.418148	O	-1.072235	-0.114187	-4.427499
O	-0.416423	1.885817	-2.045780	H	-1.448246	0.776012	-4.383169
H	0.196480	1.458452	-2.668889	H	-0.116368	-0.010629	-4.273892
H	-1.331268	1.610412	-2.273445	I	-4.672354	0.999508	2.801655
O	1.886164	0.796161	2.129073	O	-2.062796	2.553260	0.158245
H	2.472178	0.228276	1.588175	H	-2.433814	2.971919	0.960290
H	1.689363	0.304021	2.945123	H	-2.785299	2.230455	-0.404089
O	0.527891	4.217867	-1.031324	O	-2.350209	-0.404252	0.347950
H	0.017766	3.569506	-1.560299	H	-2.291390	-1.125102	1.014460
H	0.490814	5.074109	-1.477492	H	-3.025441	0.195305	0.717582
O	0.270394	3.269502	1.511351	O	0.296121	-1.494201	1.199546
H	1.141533	3.243680	1.933509	H	-0.319852	-2.147964	0.793752
H	0.351723	3.834510	0.712147	H	0.355247	-1.676275	2.154117

O	2.789469	-0.927306	0.067009	O	-1.475097	-3.148869	-0.054412
H	1.880941	-1.263282	0.191949	H	-1.026376	-3.922886	-0.422039
H	2.844033	-0.624474	-0.853297	H	-1.852338	-2.670639	-0.813108
O	-2.897248	0.909480	-2.004126	O	-2.221626	3.815284	2.606641
H	-3.276017	0.624205	-2.847428	H	-1.269345	3.627946	2.487266
H	-2.765511	0.106787	-1.466587	H	-2.580533	3.109486	3.165680
O	-1.065930	0.944309	2.799972	$SmI_3(H_2O)_{18}$			
H	-2.037157	0.843812	2.819777	E: -1444.965635 ; H: -1444.454632 ; G: -1444.597111 ;			
H	-0.700017	0.247835	3.376906	Sm	0.069610	0.803777	0.425763
O	-0.409577	2.005315	-2.021299	I	2.313938	0.240487	-3.713960
H	0.216392	1.599568	-2.645590	I	0.303149	-1.589924	4.930354
H	-1.304460	1.638675	-2.205943	O	-1.290009	0.112807	-4.580041
O	1.861245	0.772252	2.120065	H	-1.622930	0.984481	-4.323365
H	2.456956	0.249625	1.544547	H	-0.345947	0.106314	-4.342154
H	1.620121	0.194508	2.866367	I	-4.901819	1.177340	2.438115
O	0.602104	4.285411	-0.988808	O	-1.934723	2.418221	0.298308
H	0.067077	3.653797	-1.514078	H	-2.273509	2.827287	1.118976
H	0.565085	5.150230	-1.418052	H	-2.683905	2.155911	-0.260407
O	0.294462	3.298843	1.522688	O	-2.780409	-0.789298	0.216632
H	1.160387	3.247396	1.953142	H	-2.034828	-1.210397	0.688251
H	0.396426	3.876881	0.734560	H	-3.298001	-0.312899	0.889723
O	0.212569	-0.866745	-1.408511	O	-0.321676	-1.567791	1.376751
H	-0.588214	-1.287317	-1.782335	H	0.027661	-2.365133	0.922168
H	0.766354	-0.588933	-2.160305	H	-0.203824	-1.679801	2.337295
O	2.094106	1.974141	-0.488951	O	2.175527	-0.605890	-0.196734
H	2.364710	1.569777	-1.333194	H	2.051951	-1.540192	0.027895
H	1.870631	2.901839	-0.697990	H	2.346635	-0.578856	-1.155945
O	-2.072191	-1.916737	-2.616940	O	-2.882527	1.007081	-1.855864
H	-1.977455	-2.788768	-3.026884	H	-3.329348	0.717183	-2.662965
H	-1.856798	-1.259472	-3.318682	H	-2.841064	0.228611	-1.258229
O	-2.496261	-1.942874	2.656205	O	-1.250931	0.870773	2.657082
H	-1.682638	-1.901999	3.188291	H	-2.223093	0.940660	2.644112
H	-3.094846	-1.275613	3.035414	H	-1.006826	0.253494	3.369474

O	-0.321006	1.952111	-1.919948	$SmI_3(H_2O)_{19}$			
H	0.278351	1.545404	-2.570704	E: -1521.396394 ; H: -1520.856711 ; G: -1521.005461 ;			
H	-1.233835	1.627289	-2.100017	Sm	0.096014	0.798210	0.431310
O	1.635109	0.733931	2.446691	I	2.290621	0.164721	-3.772358
H	2.589263	0.816231	2.225686	I	0.284692	-1.637396	4.935013
H	1.517104	-0.010311	3.061921	O	-1.324806	0.116068	-4.580863
O	0.628979	4.301766	-0.935780	H	-1.589119	1.004409	-4.300902
H	0.109483	3.660901	-1.463984	H	-0.378237	0.040201	-4.365776
H	0.602728	5.160541	-1.377775	I	-4.858613	1.229524	2.431575
O	0.427939	3.187423	1.548210	O	-1.886232	2.441424	0.291626
H	1.297299	3.137050	1.972349	H	-2.218562	2.830179	1.124699
H	0.506940	3.797973	0.784632	H	-2.641401	2.168049	-0.253924
O	-0.345696	-1.022699	-1.471172	O	-2.771217	-0.774774	0.229093
H	-1.222948	-1.229251	-1.869532	H	-2.021348	-1.203043	0.687291
H	0.238628	-0.774833	-2.211019	H	-3.276647	-0.299471	0.911941
O	2.239883	2.113184	-0.485591	O	-0.308817	-1.570349	1.372899
H	2.424881	1.722826	-1.359531	H	0.027940	-2.370572	0.914442
H	1.944984	3.029895	-0.658066	H	-0.190721	-1.690554	2.332370
O	-2.576976	-1.669041	-2.934226	O	2.172017	-0.642295	-0.242539
H	-2.520543	-2.595914	-3.203148	H	2.019289	-1.574385	-0.025700
H	-2.202558	-1.131352	-3.665715	H	2.331504	-0.614355	-1.203645
O	-3.043913	-1.894267	3.315614	O	-2.902602	1.013823	-1.840260
H	-2.177955	-1.728322	3.724121	H	-3.351460	0.731471	-2.648902
H	-3.434049	-1.021016	3.140158	H	-2.862734	0.232528	-1.245997
O	0.390004	-3.460266	-0.435178	O	-1.202250	0.880882	2.672017
H	1.310544	-3.727825	-0.555227	H	-2.173824	0.959428	2.656227
H	0.231736	-2.682484	-1.010410	H	-0.968814	0.249856	3.375956
O	-1.988825	3.809752	2.702822	O	-0.327947	1.881014	-1.950988
H	-1.040036	3.700632	2.486615	H	0.253903	1.460305	-2.607614
H	-2.172440	4.758417	2.686076	H	-1.246528	1.552006	-2.094537
O	4.064950	1.366997	1.404653	O	1.684979	0.599652	2.413596
H	4.491464	2.106708	1.856953	H	2.633894	0.615253	2.164820
H	3.549034	1.743331	0.659622	H	1.529155	-0.139464	3.026781

O	0.612656	4.253877	-1.019628	I	2.114563	-0.031167	-3.956680
H	0.109614	3.584472	-1.528833	I	0.258647	-1.248531	5.045978
H	0.493529	5.114465	-1.442969	O	-1.521869	0.085523	-4.704913
O	0.490262	3.189849	1.505494	H	-1.747628	0.978578	-4.407419
H	1.401616	3.309323	1.847629	H	-0.554276	0.013089	-4.624029
H	0.426522	3.758937	0.709171	I	-4.852852	1.368080	2.217496
O	-0.362501	-1.042127	-1.462739	O	-1.860901	2.423014	0.145493
H	-1.247198	-1.232409	-1.851676	H	-2.165892	2.850809	0.969050
H	0.219728	-0.825157	-2.213534	H	-2.637377	2.119166	-0.352815
O	2.221487	2.040387	-0.551105	O	-2.743656	-0.776768	0.178530
H	2.364523	1.673141	-1.443070	H	-2.008137	-1.204337	0.658131
H	1.962457	2.972736	-0.686362	H	-3.242523	-0.263587	0.838432
O	-2.610106	-1.656080	-2.923118	O	-0.323688	-1.505667	1.446269
H	-2.548849	-2.578851	-3.204793	H	0.171994	-2.264328	1.071545
H	-2.241714	-1.106963	-3.649531	H	-0.224066	-1.526057	2.414895
O	-3.047495	-1.872272	3.313836	O	2.224385	-0.662622	-0.285001
H	-2.170011	-1.727728	3.706077	H	2.031250	-1.608234	-0.140428
H	-3.422280	-0.989859	3.151777	H	2.425427	-0.585903	-1.234459
O	0.339631	-3.499463	-0.430022	O	-3.047391	0.959931	-1.910267
H	1.255698	-3.774654	-0.566716	H	-3.513458	0.722251	-2.723639
H	0.174861	-2.729386	-1.013035	H	-2.969343	0.146309	-1.368558
O	-1.897907	3.828355	2.710716	O	-1.193499	0.979386	2.526990
H	-0.957420	3.690263	2.470299	H	-2.163226	1.072293	2.540599
H	-2.087655	4.764325	2.561581	H	-0.933458	0.470877	3.315404
O	4.119204	1.293645	1.365926	O	-0.468132	1.795443	-2.108208
H	4.030760	2.151126	1.825373	H	0.060150	1.321553	-2.773082
H	3.615790	1.427372	0.539581	H	-1.400804	1.487172	-2.187166
O	3.124604	3.730867	2.232841	O	1.661562	0.676792	2.331983
H	3.212196	4.135723	3.107368	H	2.597035	0.825945	2.076318
H	3.379431	4.411893	1.593548	H	1.607922	-0.106167	2.904492

$SmI_3(H_2O)_{20}$

E: -1597.832428 ; H: -1597.265519 ; G: -1597.418090 ;

Sm	0.126034	0.774709	0.309176	O	0.558035	4.163258	-1.269762
				H	-0.003108	3.516629	-1.746018
				H	0.595660	4.980468	-1.783842

O	0.562802	3.173099	1.296298
H	1.400407	3.318807	1.787717
H	0.573468	3.747939	0.504169
O	-0.314542	-1.144050	-1.496988
H	-1.195328	-1.325015	-1.899055
H	0.284560	-0.926204	-2.235716
O	2.174369	1.989476	-0.847690
H	2.370253	1.562931	-1.700667
H	1.846963	2.888243	-1.059846
O	-2.580727	-1.713249	-2.924732
H	-2.499286	-2.616789	-3.259212
H	-2.290909	-1.113708	-3.648351
O	-3.055060	-1.672698	3.391453
H	-2.194450	-1.454559	3.786565
H	-3.447244	-0.827825	3.113866
O	0.994427	-3.172665	-0.231081
H	0.962706	-4.130801	-0.352538
H	0.424468	-2.748736	-0.904665
O	-1.801210	3.935137	2.497530
H	-0.873246	3.747569	2.240699
H	-1.964798	4.862878	2.280983
O	3.945516	1.758599	1.293465
H	3.701022	2.522707	1.852390
H	3.452332	1.867016	0.455478
O	2.715456	3.558419	2.988638
H	2.186403	3.163259	3.719690
H	2.857392	4.489760	3.204618
O	0.967005	2.397764	4.712665
H	0.905660	1.437096	4.570481
H	0.965646	2.529641	5.670387

Scheme 2B

E: -1755.501106 ; H: -1754.806368 ; G: -1754.977435 ;

Sm	-0.409776	3.353632	0.236477
I	-1.263576	5.105518	4.890714
I	0.961416	-1.244190	-1.434088
O	-3.171149	1.424110	-1.111834
O	-2.143123	4.505955	-1.255499
O	1.724513	2.089518	-0.291899
O	-1.105812	0.917565	0.614059
H	-3.744340	2.186192	-0.910429
H	-2.645134	1.235466	-0.306544
H	-2.018716	4.396140	-2.210456
H	-3.092994	4.376261	-1.070580
H	2.419848	2.103991	0.388640
H	1.609550	1.161998	-0.569819
H	-1.017009	0.543968	1.519199
H	-0.616470	0.314454	0.021937
O	-0.662489	2.089613	-2.088040
H	-0.218696	1.222215	-2.086971
H	-1.623469	1.907804	-2.015910
O	-0.327693	0.095721	3.066310
H	0.563930	-0.253261	2.835251
H	-0.685711	-0.394730	3.818216
O	0.254167	2.702198	2.635596
H	-0.036270	1.815250	2.948693
H	-0.055530	3.350103	3.295833
O	0.668365	3.960620	-3.592645
H	1.432717	3.586037	-4.049783
H	0.158121	3.210702	-3.223177
O	2.853310	4.943242	0.897444
H	3.590253	5.552246	1.040858
H	3.076892	4.100297	1.341511
O	0.266636	5.470340	1.588694

H	1.247893	5.452651	1.521023	C	-6.637146	1.729510	3.617153
H	0.019822	5.512702	2.529363	H	-7.623461	1.281576	3.770475
O	-1.578550	6.875085	0.113824	H	-6.197297	1.921580	4.601260
H	-0.791894	6.533293	0.583933	H	-6.777064	2.691123	3.111596
H	-1.844214	6.149819	-0.482225	I	-5.557372	3.969928	-0.095130
O	-2.443072	-0.746271	-2.771133	C	-4.331748	1.290121	2.620158
H	-2.821216	0.003546	-2.280303	H	-3.902178	1.322474	1.620109
H	-1.529831	-0.836410	-2.451385	O	-5.903798	7.001861	1.991288
O	2.110957	-0.345281	1.994062	H	-6.090621	6.175292	1.519667
H	2.510922	0.544876	2.020079	H	-4.933911	6.996582	2.142711
H	1.900933	-0.533514	1.063001	O	-5.639844	0.068609	-0.824206
O	-2.393780	3.808378	1.654061	H	-4.719133	0.349713	-0.976212
H	-3.250361	4.143501	1.331598	H	-6.086936	0.860304	-0.489780
H	-2.235238	4.178266	2.541762	Scheme 3B			
O	-4.705991	4.399413	3.730800	E: -2124.454332 ; H: -2123.654091 ; G: -2123.828628 ;			
H	-4.632498	3.601718	3.179930	Sm	-0.724217	2.407519	0.570808
H	-3.820334	4.552873	4.101487	I	-1.156680	3.814555	5.261554
O	-3.183168	7.003344	2.325019	I	2.706750	-0.040994	-2.294018
H	-2.790272	6.394746	2.972201	O	-1.962173	-0.829776	0.292181
H	-2.654898	6.922509	1.498074	O	-3.687577	3.937229	-1.225987
O	2.926932	2.413256	2.170966	O	1.475665	2.922244	-0.682481
H	2.034524	2.589819	2.544267	O	0.640437	0.213181	0.642594
H	3.570617	2.441791	2.893068	H	-2.435687	0.031467	0.231552
O	0.925279	5.001526	-1.103618	H	-1.028508	-0.594219	0.452700
H	1.030139	4.695409	-2.032448	H	-2.824076	4.392014	-1.212965
H	1.798552	5.009999	-0.665511	H	-3.513531	3.097413	-0.744235
C	-3.392391	1.276748	3.786962	H	2.199642	3.384380	-0.225333
H	-3.040895	0.253883	4.003705	H	1.865935	2.158768	-1.146558
H	-2.503408	1.892994	3.605026	H	1.164453	0.104108	1.464335
H	-3.876161	1.639507	4.702446	H	1.259210	0.085470	-0.100604
C	-5.743343	0.799464	2.776707	O	-0.724551	1.316836	-1.757449
H	-5.730531	-0.192486	3.258369	H	-0.080097	0.603653	-1.903879
H	-6.201320	0.663689	1.791341	H	-1.609354	1.004326	-2.069408

O	2.406109	0.456087	2.705954	O	2.989542	4.214629	1.234409
H	3.154922	0.739506	2.130198	H	2.386751	3.816399	1.902860
H	2.760053	-0.001559	3.479985	H	3.684235	4.704944	1.696064
O	1.065692	2.791213	2.457318	O	-0.973663	4.435884	-1.073160
H	1.502489	1.952238	2.733908	H	-0.612708	4.180142	-1.950341
H	0.627685	3.161978	3.244838	H	-0.343191	5.077940	-0.686637
O	0.002645	3.340084	-3.416597	C	-4.024957	1.747501	1.179716
H	0.963035	3.452563	-3.411024	O	-3.037548	1.691767	0.228985
H	-0.181384	2.507290	-2.928211	C	-3.943022	2.899224	2.140982
O	0.831440	5.884729	0.490949	H	-4.658403	2.784380	2.962199
H	0.968549	6.841649	0.510082	H	-4.169095	3.853426	1.628932
H	1.691475	5.459329	0.683131	C	-5.388596	1.292647	0.724017
O	-1.199434	4.632243	1.765729	H	-6.121342	1.519185	1.508348
H	-0.439134	5.207341	1.520489	H	-5.681040	1.889986	-0.161215
H	-1.212177	4.550252	2.737904	H	-2.937889	2.997350	2.564460
O	-3.255197	6.491272	1.489672	C	-5.459309	-0.197057	0.366608
H	-2.577362	5.789691	1.423826	H	-5.274113	-0.812945	1.252848
H	-4.013684	6.224911	0.925353	H	-6.442047	-0.461218	-0.035723
O	-3.076513	-1.843201	2.587355	H	-4.707981	-0.461826	-0.384552
H	-3.473703	-1.067461	3.014413	O	-3.303611	0.818935	-2.298324
H	-2.655055	-1.509933	1.764838	H	-3.420277	1.079962	-1.350420
O	4.051271	1.547595	0.860373	H	-3.531820	-0.117841	-2.369525
H	3.815315	2.492098	0.928827	O	-5.447513	5.579371	0.061394
H	3.715372	1.236985	0.001717	H	-4.919957	4.887639	-0.396879
O	-1.328737	1.084605	2.724341	H	-5.899290	5.166751	0.824821
H	-2.245265	0.863173	2.988042	O	-4.524920	2.598974	5.661547
H	-0.960673	1.552359	3.493315	H	-3.721305	3.150035	5.669154
O	-3.594516	0.417798	4.261116	H	-4.658018	2.301232	6.573159
H	-3.147523	-0.078518	4.962929	O	-6.565255	4.740116	2.489614
H	-3.931289	1.237695	4.689281	H	-7.294680	5.351145	2.665375
O	-4.354472	5.648831	3.850129	H	-5.801000	5.051404	3.030906
H	-3.771916	4.954069	4.195500	O	-6.935937	2.604170	4.257883
H	-3.900104	6.017632	3.056574	H	-6.119417	2.750029	4.774266

H	-6.909032	3.258912	3.531785	O	0.545265	-0.277975	3.594873
O	-6.372994	-0.071686	3.755336	H	0.654837	-0.526927	4.522693
H	-5.404672	-0.080490	3.855964	H	0.650420	0.693898	3.534399
H	-6.637562	0.868138	3.839904	O	1.502233	-1.414083	1.274525

Scheme 4B

E: -2237.767293 ; H: -2236.955094 ; G: -2237.134891 ;

Sm	-0.113260	-0.048276	-0.099321	O	0.246011	-4.161662	0.946637
I	4.874630	-1.087206	0.289922	H	-0.015021	-3.410139	0.371837
I	-3.141691	3.901820	-0.537156	H	-0.593752	-4.536925	1.292133
O	-0.107756	0.641403	-3.752945	O	2.541875	0.173806	-4.650718
O	-3.081834	-3.053439	-0.068381	H	2.955438	-0.536667	-4.120148
O	-1.297457	1.612002	1.507061	H	1.654393	0.342526	-4.278038
O	-0.121048	2.169115	-1.441272	O	0.185565	4.609553	1.240708
H	-0.211339	-0.265661	-3.412432	H	0.345261	3.899699	1.892236
H	-0.100063	1.228451	-2.969391	H	-0.695892	4.453820	0.861597
H	-3.481618	-2.318528	0.440217	O	1.816241	-0.441759	-1.668414
H	-2.188307	-2.737669	-0.351060	H	2.678944	-0.680198	-1.283116
H	-0.689106	1.975201	2.176148	H	1.569638	-1.146549	-2.291913
H	-1.723570	2.365888	1.060787	O	3.994864	-1.828390	-3.334124
H	0.627586	2.795706	-1.322850	H	4.603700	-1.346882	-2.753731
H	-0.940255	2.687630	-1.334521	H	3.493576	-2.426291	-2.739729
O	-2.461209	0.266278	-1.082796	O	2.880277	-4.197023	1.832793
H	-2.713024	1.194880	-1.232573	H	3.318248	-3.344524	1.684834
H	-2.615793	-0.232920	-1.928108	H	1.945087	-4.085994	1.559411
O	1.911532	3.772077	-0.654548	O	0.959116	2.405523	2.902247
H	1.383391	4.279531	0.005038	H	1.553537	2.090874	2.184594
H	2.504979	4.375639	-1.120513	H	1.499837	2.831573	3.582579
O	1.979738	1.377725	0.610164	O	-1.295201	-1.284650	1.826797
H	2.157564	2.188319	0.083878	H	-2.226403	-0.992311	1.857085
H	2.795653	0.846722	0.598735	H	-0.837055	-0.926633	2.614921
O	-3.861435	-0.651466	1.093130	O	-2.769826	-1.202775	-3.309539
H	-4.739665	-0.323228	1.327157	H	-1.896144	-1.609968	-3.441582
H	-3.558828	-0.181042	0.288011	H	-3.398284	-1.919971	-3.068042

O	-2.275705	-5.080901	1.566239	Sm	-0.294477	2.823980	0.837918
H	-2.677151	-4.397672	0.982166	I	-0.395872	3.247984	5.739919
H	-2.363910	-5.927692	1.108370	I	1.928331	0.419444	-2.936245
O	1.072409	-6.333983	-0.582049	O	-1.834403	-0.738032	0.556464
H	0.775245	-5.538671	-0.092539	O	-3.478251	4.298984	-1.500627
H	2.046352	-6.316726	-0.537475	O	1.600149	3.261278	-0.838115
O	3.831227	-5.702237	-0.296692	O	0.681291	0.465583	0.435385
H	3.613276	-5.290273	0.565735	H	-2.355252	0.041394	0.832185
H	3.622386	-4.997084	-0.937169	H	-0.910559	-0.425730	0.465367
O	-4.552930	-3.054706	-2.360103	H	-2.740036	4.474998	-0.890679
H	-4.062531	-3.160292	-1.512270	H	-3.620801	3.335784	-1.462499
H	-4.498251	-3.900790	-2.824370	H	2.420095	3.574525	-0.416139
O	2.697434	-3.421175	-1.460961	H	1.826370	2.530252	-1.442081
H	1.726170	-3.466061	-1.599370	H	1.340907	0.183870	1.106601
H	2.838255	-2.897883	-0.652178	H	1.106393	0.374767	-0.438222
H	0.611178	-1.948057	-5.040169	O	-1.118690	1.967131	-1.435405
C	0.565661	-2.728198	-4.277637	H	-0.606119	1.223015	-1.797542
C	-0.272439	-3.918028	-4.719727	H	-2.065698	1.702362	-1.408259
O	-0.018514	-2.082063	-3.106987	O	2.739023	0.191539	2.183988
C	-0.427327	-4.912555	-3.564302	H	3.417576	0.487137	1.534299
H	0.211392	-4.386627	-5.582118	H	3.123701	-0.481496	2.760941
C	-0.268481	-2.947951	-1.998788	O	1.621747	2.618608	2.582437
C	-1.039706	-4.196992	-2.354875	H	2.012682	1.716027	2.630115
H	0.558619	-5.312851	-3.293446	H	1.258159	2.824883	3.462296
O	-0.610709	-2.265842	-0.913926	O	-0.480159	4.107324	-3.056511
H	-1.080411	-4.847292	-1.473964	H	0.456492	4.016925	-3.280240
H	1.585856	-3.040147	-4.018405	H	-0.743694	3.257104	-2.647691
H	-1.259923	-3.564178	-5.043126	O	1.331275	6.065379	0.897280
H	-1.055368	-5.757055	-3.860842	H	1.653093	6.975317	0.954040
H	-2.079300	-3.906707	-2.594180	H	2.114793	5.478244	0.892247
Scheme 5B				O	-0.473102	4.772739	2.495718
E: -2199.650500 ; H: -2198.845950 ; G: -2199.030627 ;				H	0.224339	5.392917	2.197804
				H	-0.313977	4.556381	3.431106

O	-3.258439	5.765377	1.635684	C	-5.150298	3.535861	3.626858
H	-2.865478	4.883778	1.440510	H	-2.996679	3.723154	3.516953
H	-4.188726	5.668260	1.355531	H	-3.552448	2.114007	3.962994
O	-2.069313	-1.745099	3.244105	H	-5.213112	3.835463	4.678463
H	-2.222882	-1.010921	3.872015	H	-5.362197	4.415105	3.009038
H	-1.958031	-1.361578	2.355015	H	-5.934024	2.794666	3.431996
O	4.106825	1.427049	0.210433	O	-3.538217	1.118280	1.644397
H	3.944912	2.361322	0.440965	C	-4.628193	0.352517	2.196840
H	3.605587	1.248049	-0.602074	H	-4.556761	-0.647820	1.766049
O	-0.965449	1.273656	2.783616	H	-4.540131	0.285445	3.284768
H	-1.887963	0.977296	2.687001	H	-5.584022	0.808946	1.923699
H	-0.902399	1.749655	3.632987	O	-6.395069	2.288345	-0.274631
O	-2.526342	0.084649	5.300314	H	-5.543826	2.197978	-0.747882
H	-1.940398	0.848806	5.425113	H	-7.055584	2.540543	-0.935656
H	-3.436330	0.404291	5.478323	O	-6.462049	-0.590559	-0.482078
O	-2.736308	6.208623	4.317517	H	-5.542615	-0.831826	-0.702076
H	-2.129608	5.510830	4.609233	H	-6.465437	0.367325	-0.301427
H	-2.928854	6.029230	3.370181	O	-3.826642	-1.249366	-1.292349
O	3.348277	4.084860	1.099731	H	-3.749671	-1.970860	-1.930491
H	2.861359	3.653434	1.836900	H	-3.024948	-1.258187	-0.728399
H	4.155417	4.479756	1.458637	O	-5.061093	1.059085	5.887287
O	-0.843284	4.978339	-0.461196	H	-5.599949	1.153337	5.089100
H	-0.619785	4.841558	-1.408358	H	-4.898018	1.959451	6.202427
H	-0.155715	5.568630	-0.088971				
O	-3.835745	1.486280	-1.114964				
H	-3.747503	1.323576	-0.152592				
H	-3.958210	0.600548	-1.511228				
O	-5.564965	5.017472	0.190409				
H	-4.865913	4.842761	-0.476546				
H	-5.953480	4.141663	0.365253				
C	-3.582205	2.547374	1.856383				
O	-2.670281	3.137130	1.102058				
C	-3.763851	2.968467	3.304139				