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Geometries (Å) and Energies (kcal/mol)

1a-Ti

gas phase E = -8095.10
solvation E = -7.2086

Atom	X	Y	Z
Ti	-0.24640	0.11440	-0.08530
C	1.72340	-0.34060	0.09600
C	-1.47720	2.10110	-0.00860
C	-0.09650	2.42690	0.03510
C	0.45260	1.89410	1.23280
C	-0.58910	1.22400	1.92170
C	-1.78340	1.36410	1.16080
C	-0.44430	0.35410	-2.10300
H	-2.17830	2.36750	-0.80090
H	0.44690	3.00010	-0.71770
H	1.48040	2.00800	1.57480
H	-0.50010	0.69310	2.87310
H	-2.76410	0.96320	1.43780
H	-1.45290	0.49640	-2.53060
H	-0.06690	-0.65280	-2.40170
H	0.23690	1.13250	-2.49300
H	-1.32470	-1.11510	1.11870
H	-1.88720	-0.86240	-0.66920
H	-0.80920	-2.28600	-0.22740
C	-1.60180	-1.59600	0.13610
H	1.75560	-1.38460	-0.28810
H	2.12000	0.32670	-0.70380
H	2.35290	-0.24650	0.99230
B	-2.98500	-2.39490	0.51430
C	-4.13250	-1.29630	0.83000
C	-4.96800	-1.28450	1.93320
C	-5.95400	-0.33350	2.12180
C	-6.14750	0.65210	1.18140
C	-5.35680	0.66680	0.05430
C	-4.39440	-0.30440	-0.09990
C	-3.55530	-3.22800	-0.73060
C	-4.63550	-4.06360	-0.50730
C	-5.22830	-4.80900	-1.49780
C	-4.77030	-4.69210	-2.79180
C	-3.71740	-3.85100	-3.06830
C	-3.13250	-3.14140	-2.03830
C	-2.56840	-3.29770	1.78050
C	-2.44490	-4.67560	1.80330
C	-2.02920	-5.37350	2.92120
C	-1.69210	-4.69550	4.06860
C	-1.77150	-3.32040	4.08470
C	-2.19710	-2.66730	2.95310
F	-4.86740	-2.20370	2.88880
F	-6.71970	-0.36380	3.20370
F	-7.08770	1.56900	1.34990
F	-5.52820	1.60930	-0.86780
F	-3.67830	-0.23430	-1.23960
F	-5.12260	-4.18670	0.72650
F	-6.23000	-5.63750	-1.23440
F	-5.35380	-5.38510	-3.75640
F	-3.27130	-3.72810	-4.31390
F	-2.10930	-2.33980	-2.38890
F	-2.71050	-5.42460	0.73440
F	-1.93830	-6.69670	2.89150
F	-1.28010	-5.35430	5.14130
F	-1.43010	-2.64750	5.17880
F	-2.23920	-1.32120	3.02260

1b-Ti

gas phase E = -8809.28
solvation E = -14.9028

Atom	X	Y	Z
Ti	0.09040	0.16800	-0.03300
C	2.05950	0.30080	0.26070
H	1.83590	1.40060	0.37540
H	2.10850	-0.17430	1.26670
H	3.00380	0.18230	-0.28550
C	-0.29820	-1.64720	0.74860
H	-0.05300	-1.34000	1.79960
H	-1.36890	-1.92800	0.67470
H	0.33960	-2.50420	0.46890
C	0.75520	0.73640	-2.20160
C	0.57350	-0.67080	-2.12970
C	-0.79380	-0.92990	-1.85070
C	-1.45050	0.32100	-1.72340
C	-0.49220	1.34770	-1.94770
H	1.69360	1.24900	-2.41650
H	1.35320	-1.42230	-2.27140
H	-1.27270	-1.90710	-1.77620
H	-2.51480	0.45860	-1.51460
H	-0.69640	2.41970	-1.94340
C	-0.44320	2.21210	1.29830
C	-1.63030	1.64190	1.04620
H	-2.31140	2.02170	0.27700
H	-2.02400	0.81350	1.66010
H	-0.10020	3.07770	0.71460
H	0.17420	1.91600	2.15910
F	-7.28900	-4.03890	-0.01030
F	-7.84470	-5.38720	2.18920
F	-6.76040	-4.67080	4.56230
F	-5.05830	-2.56940	4.67790
F	-4.46230	-1.20190	2.49170
F	-8.13010	-1.32560	0.07630
F	-9.40100	0.97050	0.55150
F	-8.01670	3.28870	0.69860
F	-5.32330	3.26800	0.33320
F	-4.05370	1.02820	-0.16110
F	-4.80300	-4.45580	-0.91020
F	-6.63390	-1.46080	-4.99920
F	-5.86170	-4.01750	-5.42120
F	-4.96450	-5.50650	-3.34630
F	-6.49370	-0.38500	-2.60440
C	-5.79560	-2.58770	1.10760
C	-6.67980	-3.64940	1.10810
C	-7.00120	-4.36030	2.24650
C	-6.45280	-4.00180	3.45720
C	-5.58750	-2.93410	3.50970
C	-5.28910	-2.25300	2.35040
C	-6.02660	-0.28540	0.00300
C	-7.40020	-0.21630	0.17090
C	-8.08190	0.95830	0.40260
C	-7.38330	2.14510	0.46870
C	-6.02160	2.13000	0.28540
C	-5.38970	0.92920	0.05170
C	-5.68670	-2.38530	-1.60900
C	-5.29890	-3.68500	-1.88540
C	-6.20240	-2.19940	-3.97920
C	-5.80930	-3.49720	-4.19980
C	-5.35590	-4.25050	-3.13920
C	-6.13340	-1.67000	-2.70500
C	-3.70540	-1.70500	-0.20310
B	-5.33090	-1.73120	-0.18090
H	-3.34650	-2.74900	-0.11040
H	-3.26680	-1.10880	0.61710
H	-3.35040	-1.31550	-1.17230

1c-Ti

gas phase E = -3067.40
solvation E = -33.8666

Atom	X	Y	Z
Ti	0.13950	-0.09600	-0.07280
C	2.08410	-0.40810	-0.08020
H	2.02710	0.72490	-0.14040
H	2.12780	-0.73150	0.98530
H	2.95940	-0.74190	-0.65350
C	-0.45760	-1.76030	0.89950
H	-0.12370	-1.39230	1.90650
H	-1.53270	-2.00540	0.92550
H	0.12470	-2.67220	0.66770
C	0.42060	0.50100	-2.31930
C	0.32890	-0.91400	-2.21530
C	-0.96670	-1.23390	-1.72580
C	-1.66270	-0.01350	-1.51310
C	-0.80690	1.05420	-1.89030
H	1.28390	1.05690	-2.69010
H	1.09710	-1.62920	-2.51140
H	-1.37750	-2.23600	-1.60490
H	-2.69370	0.07850	-1.16270
H	-1.06130	2.11650	-1.89280
C	-1.00920	1.66700	1.21280
C	0.27060	2.06790	1.19260
H	0.98440	1.75720	1.97030
H	0.62740	2.80440	0.45850
H	-1.37670	0.99340	2.00270
H	-1.75400	2.08100	0.52480

1d-Ti

gas phase E = -2307.71
solvation E = -35.6702

Atom	X	Y	Z
Ti	0.02530	0.01380	-0.01290
C	1.99100	-0.17360	-0.04460
H	2.00560	0.94300	0.13540
H	2.12780	-0.69710	0.92930
H	2.80190	-0.41520	-0.74510
C	-0.56940	-1.63320	0.94890
H	-0.22370	-1.18330	1.92440
H	-1.64070	-1.88780	1.01290
H	0.03010	-2.54510	0.77020
C	0.25780	0.70900	-2.23180
C	0.20920	-0.70960	-2.17810
C	-1.06630	-1.08990	-1.66950
C	-1.78860	0.10310	-1.39060
C	-0.97260	1.20950	-1.74690
H	1.10270	1.30540	-2.58430
H	0.99160	-1.38700	-2.52250
H	-1.44900	-2.10730	-1.58870
H	-2.81180	0.15920	-1.00800
H	-1.25360	2.26540	-1.67440

1e-Ti

gas phase E = -8803.86
solvation E = -17.8082

Atom	X	Y	Z
B	-0.88300	-0.09890	-1.36510
C	0.73720	-0.10760	-1.35370
C	1.45150	0.25640	-2.48540
C	2.83230	0.21480	-2.59240
C	3.53360	-0.17860	-1.48460
C	2.86980	-0.51560	-0.34090
C	1.50240	-0.48550	-0.26460
F	0.82450	0.72460	-3.55400
F	3.46280	0.54990	-3.70920
F	4.89950	-0.29010	-1.45980
F	3.65770	-0.90570	0.71820
F	0.98210	-0.81340	0.91200
C	-1.37820	-0.86430	-2.71640
C	-1.44060	1.41150	-1.42030
C	-1.46790	-0.97190	-0.13610
C	-0.67830	2.56240	-1.39320
C	-2.37800	-0.55130	0.81560

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C	-1.20600	3.83220	-1.52200
C	-2.97600	-1.40770	1.72070
C	-2.56260	3.99070	-1.66120
C	-2.64850	-2.74230	1.72190
C	-3.37030	2.87620	-1.67000
C	-1.70490	-3.19950	0.82960
C	-2.80230	1.62620	-1.56810
C	-1.14220	-2.31510	-0.05990
F	0.65390	2.52140	-1.22310
F	-2.72990	0.72980	0.93480
F	-0.41400	4.90170	-1.49930
F	-3.86010	-0.94940	2.60080
F	-3.09510	5.20140	-1.77530
F	-3.21600	-3.57590	2.58520
F	-4.68630	3.03150	-1.76240
F	-1.34090	-4.48170	0.84930
F	-3.64620	0.59260	-1.56620
F	-0.18370	-2.82080	-0.85810
H	-0.85900	-1.82970	-2.85470
H	-2.45880	-1.07960	-2.63880
H	-1.22610	-0.25610	-3.62380
Ti	5.45440	-1.91830	-0.00510
C	7.36890	-1.33250	-0.36970
H	7.48450	-0.99260	-1.41820
H	7.41360	-0.44960	0.30820
H	8.19260	-2.02210	-0.12140
C	5.70130	-2.08020	2.00850
H	5.87680	-0.99720	2.21160
H	4.80620	-2.40740	2.56670
H	6.58150	-2.66050	2.33460
C	6.09040	-3.55910	-1.52270
C	6.11920	-4.13350	-0.22630
C	4.80030	-4.12730	0.29640
C	3.95060	-3.53930	-0.67680
C	4.74880	-3.19040	-1.80100
H	6.94400	-3.43840	-2.19070
H	7.00600	-4.50940	0.28600
H	4.49000	-4.52620	1.26220
H	2.86840	-3.39080	-0.58720
H	4.38770	-2.72130	-2.72050

1f-Ti

gas phase E = -10223.90
solvation E = -8.6190

Atom	X	Y	Z
Ti	1.95840	1.98630	-0.59370
C	3.83850	1.33100	-0.30870
C	0.80430	4.01780	-0.42920
C	2.19880	4.28520	-0.42370
C	2.76050	3.70330	0.74650
C	1.71320	3.06650	1.45500
C	0.50330	3.26810	0.73450
H	0.09220	4.32380	-1.19680
H	2.73930	4.84440	-1.18870
C	1.83040	2.25330	-2.61410
H	3.81020	3.72100	1.04580
H	1.81490	2.50500	2.38740
H	-0.48440	2.90250	1.03310
H	0.82560	2.44390	-3.03400
H	2.16680	1.24140	-2.93940
H	2.53900	3.01130	-2.99430
H	0.93960	0.77290	0.64360
H	0.35050	0.96120	-1.14580
C	0.67550	0.25940	-0.32650
H	1.50530	-0.38770	-0.68220
B	-0.66560	-0.58480	0.06580
C	-1.82540	0.50090	0.37930
C	-2.63450	0.52430	1.50100
C	-3.59020	1.49810	1.71900
C	-3.77610	2.49810	0.79210
C	-3.01760	2.49730	-0.35600
C	-2.08800	1.50020	-0.54160
C	-1.20590	-1.43270	-1.18230
C	-2.30510	-2.24750	-0.97830
C	-2.91290	-2.95710	-1.98610
C	-2.43220	-2.84420	-3.27290
C	-1.35190	-2.03440	-3.52790
C	-0.76290	-1.34890	-2.48460
C	-0.21840	-1.44990	1.34800
C	-0.06500	-2.82330	1.39530
C	0.38320	-3.49120	2.51930
C	0.71870	-2.78590	3.65030
C	0.60180	-1.41380	3.64430
C	0.14900	-0.78990	2.50650
F	-2.53220	-0.40470	2.44690
F	-4.33410	1.47880	2.81550
F	-4.68390	3.44110	0.99450
F	-3.18300	3.45160	-1.26700
F	-1.40540	1.56080	-1.70290
F	-2.80660	-2.36710	0.25030
F	-3.95350	-3.74430	-1.74960
F	-3.01820	-3.51230	-4.25340
F	-0.88840	-1.91450	-4.76790
F	0.28270	-0.57170	-2.82250
F	-0.33160	-3.59590	0.34420
F	0.51230	-4.81190	2.50920
F	1.16350	-3.41500	4.72740
F	0.93280	-0.71410	4.72460
F	0.07290	0.55500	2.55800
H	3.81480	0.32240	-0.77790
H	4.38170	2.02060	-0.99540
H	4.36900	1.29960	0.65580
C	5.84280	5.42010	1.32330
C	6.17190	3.97660	1.22790
C	6.60080	3.42560	0.02620
C	6.93750	2.08960	-0.06410
C	6.84920	1.27380	1.04970
C	6.07850	3.14560	2.33500
C	6.41510	1.80470	2.24960
H	6.67760	4.07060	-0.85820
H	7.26350	1.67290	-1.02250
H	7.10630	0.21250	0.97640
H	5.75060	3.56900	3.29230
H	6.34140	1.16840	3.13730
H	5.58280	5.70670	2.35470
H	6.70230	6.03760	1.00670
H	4.98890	5.69270	0.67660

1g-Ti

gas phase E = -10214.86
solvation E = -18.1607

Atom	X	Y	Z
Ti	-0.83239	-0.36971	0.22975
C	2.77323	-0.19054	-0.47164
C	1.49342	0.50584	-0.34268
C	1.12536	1.13439	0.84958
C	-0.05004	1.86142	0.94434
C	-0.86619	2.02157	-0.17514
C	0.64989	0.65874	-1.44924
C	-0.47657	1.46528	-1.38540
H	1.77451	1.02477	1.72853
H	-0.33012	2.33312	1.89231
H	-1.77834	2.62157	-0.10696
H	0.93062	0.17519	-2.39254
H	-1.08719	1.61739	-2.28141
H	2.76450	-0.95313	-1.26718
H	3.52475	0.58343	-0.75707
H	3.11037	-0.63743	0.48072
C	-3.12622	-0.89063	0.27922
C	-2.41408	-2.11401	0.28293
C	-2.84119	-0.22804	-0.93837
C	-1.69776	-2.22118	-0.93273
C	-1.95371	-1.05331	-1.68967
H	-3.78671	-0.52817	1.06701
H	-2.41005	-2.84625	1.09116
H	-3.27468	0.71818	-1.26361
H	-1.07057	-3.05856	-1.23834
H	-1.58112	-0.85415	-2.69520
C	-1.37111	-0.13074	2.27510
C	0.55123	-1.91603	0.64196
H	1.14675	-2.27141	-0.22042
H	-1.86020	-1.05376	2.63032
H	-0.41870	0.01011	2.82409
H	-2.03622	0.72240	2.51262
H	1.25073	-1.50372	1.39646
H	0.01212	-2.77729	1.07460
B	4.95001	3.97410	-1.56862
C	6.26201	4.89921	-1.78499
C	6.12544	6.12403	-2.41898
C	7.18619	6.94006	-2.74056
C	8.46782	6.53189	-2.45370
C	8.65868	5.33430	-1.81340
C	7.56572	4.55703	-1.47828
F	4.90694	6.59443	-2.71329
F	7.00645	8.12590	-3.31393
F	9.49918	7.30192	-2.78252
F	9.89327	4.93875	-1.51131
F	7.86583	3.43305	-0.81499
C	4.28693	3.75685	-3.04432
C	3.82914	4.70887	-0.65369
C	5.35826	2.52470	-0.97772
C	4.01949	5.88193	0.05404
C	5.03767	2.02527	0.26909
C	2.99688	6.57655	0.67381
C	5.42712	0.77445	0.70983
C	1.71394	6.09240	0.61706
C	6.15665	-0.04748	-0.11261
C	1.47862	4.91456	-0.05273
C	6.50669	0.40566	-1.36510
C	2.52506	4.24896	-0.65001
C	6.11202	1.66459	-1.76200
F	5.22645	6.42808	0.18258
F	4.27203	2.71113	1.13200
F	3.23620	7.70961	1.32508
F	4.98521	0.30386	1.88249
F	0.71010	6.74604	1.19715
F	6.47978	-1.27817	0.27749
F	0.21949	4.45188	-0.12328
F	7.22820	-0.37151	-2.16776
F	2.20857	3.08476	-1.24952
F	6.55322	2.05833	-2.95550
H	5.06350	3.61724	-3.81569
H	3.62434	2.87209	-3.07315
H	3.68387	4.63621	-3.33469

1h-Ti

gas phase E = -4471.14
solvation E = -33.3266

Atom	X	Y	Z
Ti	0.19180	0.06770	0.36600
C	3.89150	0.36750	-0.01080
C	2.56540	1.00400	-0.03800
C	2.03760	1.62490	1.09840
C	0.84380	2.33390	1.04960
C	0.15030	2.44970	-0.15420
C	1.83330	1.10240	-1.22920
C	0.67280	1.85800	-1.29950

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H	2.57750	1.54240	2.05000
H	0.46740	2.83100	1.94720
H	-0.77650	3.03070	-0.20150
H	2.21740	0.60750	-2.12930
H	0.15180	1.97010	-2.25680
H	4.21000	0.04110	-1.01230
H	4.63740	1.08600	0.37340
H	3.91070	-0.50900	0.66070
C	-2.09920	-0.47090	0.34410
C	-1.36250	-1.68000	0.34020
C	-1.79220	0.22380	-0.84890
C	-0.61560	-1.74910	-0.86160
C	-0.87520	-0.57030	-1.59860
H	-2.79410	-0.13860	1.11510
H	-1.36880	-2.43530	1.12740
H	-2.24510	1.16300	-1.16970
H	0.01450	-2.57840	-1.18170
H	-0.50010	-0.35500	-2.60050
C	-0.35890	0.25700	2.40120
C	1.59100	-1.49050	0.75240
H	2.15920	-1.93300	-0.08460
H	-1.04730	-0.53130	2.73870
H	0.66480	0.03450	2.77910
H	-0.66370	1.21360	2.85510
H	2.29270	-1.07350	1.49910
H	1.01120	-2.29690	1.23590

1a-Zr

gas phase E = -8121.22
solvation E = -7.5337

Atom	X	Y	Z
Zr	-0.17510	0.13470	-0.11070
C	1.93140	-0.37510	0.13430
C	-1.47210	2.25300	0.04920
C	-0.10000	2.59850	0.08940
C	0.46070	2.07100	1.28770
C	-0.57130	1.38930	1.97850
C	-1.76460	1.50260	1.21680
H	-2.18220	2.52700	-0.73110
H	0.42390	3.20480	-0.65170
C	-0.45920	0.43290	-2.26290
H	1.48060	2.21520	1.63990
H	-0.48250	0.88860	2.94590
H	-2.74580	1.11200	1.50470
H	-1.48600	0.58530	-2.63990
H	-0.11100	-0.56440	-2.62710
H	0.19690	1.20790	-2.70090
H	-1.42590	-1.14340	1.12000
H	-1.93660	-0.97220	-0.69010
C	-1.66070	-1.66070	0.14890
H	-0.85530	-2.36540	-0.15870
B	-3.04180	-2.45740	0.52550
C	-4.16970	-1.34010	0.83380
C	-4.99930	-1.30680	1.94010
C	-5.96110	-0.33270	2.12980
C	-6.13100	0.65760	1.18950
C	-5.34320	0.65290	0.06030
C	-4.40770	-0.34360	-0.09720
C	-3.59950	-3.28260	-0.72940
C	-4.68790	-4.11160	-0.52800
C	-5.28160	-4.83720	-1.53460
C	-4.80360	-4.71670	-2.82200
C	-3.74560	-3.87650	-3.07580
C	-3.16630	-3.18220	-2.03390
C	-2.61830	-3.34130	1.80060
C	-2.47000	-4.71520	1.83060
C	-2.01680	-5.39700	2.94440
C	-1.67520	-4.70530	4.08260
C	-1.78230	-3.33170	4.09110
C	-2.23730	-2.69490	2.96160
F	-4.91370	-2.22700	2.89640
F	-6.72790	-0.34340	3.21130
F	-7.05010	1.59560	1.36060
F	-5.49150	1.59930	-0.86150
F	-3.70310	-0.29950	-1.24500
F	-5.18620	-4.24250	0.70080
F	-6.29760	-5.65220	-1.28710
F	-5.36000	-5.40430	-3.80590
F	-3.28870	-3.74280	-4.31610
F	-2.13690	-2.38400	-2.37440
F	-2.74200	-5.47250	0.76950
F	-1.89170	-6.71750	2.91860
F	-1.23240	-5.34850	5.15260
F	-1.43780	-2.64320	5.17420
F	-2.29170	-1.34830	3.02000
H	1.94150	-1.43250	-0.22030
H	2.39650	0.23460	-0.67330
H	2.55710	-0.29660	1.03440

1b-Zr

gas phase E = -8837.17
solvation E = -16.3527

Atom	X	Y	Z
Zr	0.08500	0.15390	0.03650
C	2.21330	0.34530	0.34950
H	2.07810	1.42960	0.60260
H	2.32420	-0.22460	1.30020
H	3.12520	0.24310	-0.25580
C	-0.33860	-1.84850	0.73870
H	-0.10550	-1.67120	1.82060
H	-1.41140	-2.10870	0.63940
H	0.27220	-2.69950	0.38950
C	0.77200	0.74670	-2.27130
C	0.55420	-0.65410	-2.24360
C	-0.82440	-0.88660	-1.99070
C	-1.45670	0.37620	-1.85350
C	-0.47110	1.38360	-2.02950
H	1.71740	1.24120	-2.48700
H	1.31050	-1.42010	-2.42560
H	-1.32740	-1.85240	-1.95720
H	-2.52340	0.53660	-1.67610
H	-0.65320	2.45990	-2.03900
C	-0.48880	2.35730	1.29150
C	-1.70140	1.83110	1.08140
H	-2.34310	2.15400	0.25500
H	-2.15220	1.09960	1.77190
H	-0.08980	3.14030	0.63140
H	0.10060	2.11280	2.18860
F	-7.27300	-4.02540	-0.06280
F	-7.84550	-5.38400	2.11850
F	-6.78260	-4.68770	4.50330
F	-5.10410	-2.56440	4.65640
F	-4.48380	-1.18480	2.48180
F	-8.12210	-1.29200	0.03930
F	-9.36880	1.00440	0.59090
F	-7.95980	3.30300	0.79830
F	-5.27210	3.26880	0.40610
F	-4.02820	1.03080	-0.17410
F	-4.73110	-4.42820	-0.88740
F	-6.72150	-1.56060	-5.00060
F	-5.92890	-4.14260	-5.36310
F	-4.92320	-5.53260	-3.30170
F	-6.53700	-0.42870	-2.63020
C	-5.79560	-2.57110	1.07810
C	-6.67730	-3.63470	1.06280
C	-7.00710	-4.35480	2.19200
C	-6.47150	-4.00260	3.40890
C	-5.61660	-2.92680	3.48040
C	-5.30590	-2.23980	2.32790
C	-6.01100	-0.26840	-0.01850
C	-7.38270	-0.19160	0.15680
C	-8.05110	0.98300	0.42810
C	-7.34080	2.16020	0.52970
C	-5.98100	2.13730	0.33400
C	-5.36160	0.93880	0.05520
C	-5.66650	-2.38970	-1.61910
C	-5.25960	-3.68850	-1.87000
C	-6.25520	-2.27180	-3.97660
C	-5.85310	-3.57280	-4.16770
C	-5.34400	-4.28530	-3.10490
C	-6.15570	-1.70880	-2.71740
C	-3.69270	-1.68070	-0.21440
B	-5.31650	-1.71330	-0.20310
H	-3.32260	-2.72280	-0.13800
H	-3.26180	-1.09550	0.61680
H	-3.33120	-1.27180	-1.17250

1c-Zr

gas phase E = -3093.16
solvation E = -34.6135

Atom	X	Y	Z
Zr	-0.02730	-0.05620	-0.00260
C	2.12690	0.12390	0.08990
H	2.28850	1.22280	0.15860
H	2.24860	-0.32000	1.10910
H	2.89390	-0.30000	-0.57520
C	-0.38890	-2.02170	0.85240
H	-0.11070	-1.85490	1.92130
H	-1.40870	-2.44400	0.81860
H	0.30300	-2.79140	0.45960
C	0.44850	0.41780	-2.39500
C	0.35050	-0.99010	-2.25380
C	-0.98410	-1.31120	-1.88170
C	-1.71070	-0.09690	-1.79780
C	-0.82310	0.97120	-2.11000
H	1.33000	0.96770	-2.72100
H	1.15270	-1.70740	-2.44630
H	-1.39200	-2.31510	-1.77260
H	-2.78560	-0.00990	-1.62950
H	-1.09380	2.02410	-2.20030
C	-1.19330	1.24300	1.85800
C	-2.23340	0.96270	1.06090
H	-2.69810	1.72700	0.42890
H	-2.70560	-0.03350	1.07790
H	-0.77610	2.25700	1.92540
H	-0.82060	0.49690	2.58350

1d-Zr

gas phase E = -2334.38
solvation E = -37.3246

Atom	X	Y	Z
Zr	0.00110	0.03710	0.07580
C	2.13440	-0.03950	-0.07090
H	2.31960	1.06110	0.00810
H	2.38550	-0.50410	0.91310
H	2.81480	-0.43170	-0.84190
C	-0.50170	-1.87800	0.91630
H	-0.27040	-1.60050	1.98060
H	-1.53630	-2.25770	0.87650
H	0.18160	-2.70770	0.64480
C	0.28150	0.61970	-2.31660
C	0.12900	-0.78730	-2.22320
C	-1.18450	-1.06300	-1.74740
C	-1.83070	0.18190	-1.52360
C	-0.92340	1.21910	-1.87800
H	1.16020	1.14290	-2.69350
H	0.86800	-1.53010	-2.53000

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H	-1.63830	-2.04930	-1.66200
H	-2.87130	0.31690	-1.22010
H	-1.14330	2.28900	-1.88560

1f-Zr

gas phase E = -10252.53
solvation E = -8.2853

Atom	X	Y	Z
Zr	2.08430	1.75290	-0.51250
C	4.17110	1.12780	-0.20370
C	0.87470	3.91970	-0.26370
C	2.26030	4.20820	-0.24540
C	2.82320	3.62540	0.92460
C	1.78040	2.96360	1.61780
C	0.57580	3.14970	0.88790
H	0.15980	4.24450	-1.01920
H	2.79160	4.81410	-0.97900
C	1.82420	2.22000	-2.63730
H	3.85440	3.72120	1.26000
H	1.86820	2.43470	2.57000
H	-0.41520	2.79530	1.18830
H	0.79230	2.46880	-2.94620
H	2.09540	1.24650	-3.11000
H	2.50270	3.00080	-3.02420
H	0.66160	0.62660	0.63340
H	0.25890	0.74670	-1.19230
C	0.48300	0.07310	-0.32830
H	1.29400	-0.65230	-0.58390
B	-0.89990	-0.72420	0.03090
C	-2.02690	0.38900	0.34050
C	-2.85290	0.39590	1.45020
C	-3.76150	1.40590	1.70510
C	-3.88010	2.45830	0.82570
C	-3.10190	2.47690	-0.30990
C	-2.22050	1.44280	-0.53450
C	-1.39890	-1.58050	-1.22780
C	-2.46560	-2.44310	-1.05300
C	-3.00110	-3.20140	-2.06830
C	-2.47570	-3.08750	-3.33670
C	-1.44090	-2.21550	-3.56830
C	-0.92860	-1.47710	-2.52130
C	-0.45830	-1.55600	1.34200
C	-0.26090	-2.92060	1.43650
C	0.34120	-3.51950	2.52860
C	0.76780	-2.75870	3.59200
C	0.55800	-1.39830	3.56110
C	-0.04080	-0.84550	2.45400
F	-2.79930	-0.57900	2.35500
F	-4.52310	1.37420	2.79150
F	-4.74500	3.43420	1.06230
F	-3.21220	3.47960	-1.17630
F	-1.51670	1.51210	-1.68090
F	-3.00930	-2.56470	0.15740
F	-4.01710	-4.03100	-1.85730
F	-2.97050	-3.82210	-4.32220
F	-0.92500	-2.11010	-4.79020
F	0.07060	-0.63860	-2.84540
F	-0.61770	-3.75050	0.45940
F	0.53480	-4.83350	2.54920
F	1.37270	-3.32000	4.62930
F	0.94650	-0.63350	4.57630
F	-0.17290	0.49670	2.47770
H	4.16720	0.06400	-0.53540
H	4.78640	1.69240	-0.93870
H	4.67070	1.17870	0.77700
C	3.57210	-1.12040	-3.49490
C	2.71870	-2.17580	-2.89510
C	1.82700	-2.88710	-3.68820
C	1.05220	-3.89860	-3.15270
C	1.14380	-4.20940	-1.80640
C	2.80500	-2.49890	-1.54720
C	2.01890	-3.50300	-1.00210
H	1.72890	-2.63030	-4.74980
H	0.35840	-4.44710	-3.79760
H	0.52390	-5.00100	-1.37930
H	3.52790	-1.96900	-0.91490
H	2.10040	-3.74510	0.06160
H	4.02210	-0.46920	-2.72850
H	4.40170	-1.57260	-4.07030
H	2.99670	-0.49180	-4.19500

1g-Zr

gas phase E = -10249.12
solvation E = -17.9484

Atom	X	Y	Z
Zr	-0.81410	-0.39750	0.25390
C	2.81800	-0.19450	-0.53060
C	1.56220	0.54690	-0.38160
C	1.21720	1.18090	0.81920
C	0.05590	1.93640	0.92610
C	-0.76710	2.11220	-0.18650
C	0.71380	0.72770	-1.48090
C	-0.40730	1.54080	-1.39900
H	1.88110	1.06920	1.68910
H	-0.19940	2.42400	1.87180
H	-1.66500	2.73350	-0.11150
H	0.98460	0.26100	-2.43570
H	-1.02640	1.70310	-2.28530
H	2.73830	-0.99890	-1.27750
H	3.58180	0.52810	-0.89220
H	3.17400	-0.60800	0.42800
C	-3.23510	-0.98780	0.25290
C	-2.52220	-2.21330	0.25660
C	-2.95820	-0.33110	-0.97210
C	-1.81560	-2.32480	-0.96700
C	-2.07990	-1.15760	-1.72620
H	-3.90350	-0.63190	1.03520
H	-2.53410	-2.95720	1.05570
H	-3.40560	0.60400	-1.30940
H	-1.20410	-3.16910	-1.28090
H	-1.73210	-0.96520	-2.74130
C	-1.42550	-0.04430	2.39990
C	0.67890	-2.04160	0.60970
H	1.27350	-2.42650	-0.23550
H	-1.89000	-0.98770	2.74300
H	-0.48260	0.11220	2.96140
H	-2.11200	0.78230	2.64900
H	1.38370	-1.63650	1.36470
H	0.12180	-2.88630	1.05640
B	4.94650	3.97980	-1.56900
C	6.26140	4.90130	-1.78050
C	6.12400	6.13090	-2.40540
C	7.18460	6.94660	-2.72550
C	8.46560	6.52600	-2.45800
C	8.65820	5.32470	-1.82470
C	7.56490	4.55130	-1.48260
F	4.90490	6.60320	-2.69500
F	7.01220	8.14080	-3.28460
F	9.49440	7.29020	-2.80320
F	9.89420	4.92210	-1.53700
F	7.86310	3.42330	-0.82490
C	4.29260	3.76700	-3.04960
C	3.82940	4.72380	-0.65590
C	5.34680	2.52870	-0.97370
C	4.02930	5.88460	0.06920
C	5.02930	2.03860	0.27760
C	3.01140	6.58170	0.69610
C	5.41610	0.79020	0.72590
C	1.72350	6.11370	0.62380
C	6.14340	-0.03900	-0.09120
C	1.47630	4.95490	-0.07400
C	6.48980	0.40310	-1.34840
C	2.51800	4.28320	-0.67310
C	6.09300	1.65870	-1.75510
F	5.24090	6.41920	0.20850
F	4.26840	2.73210	1.13890
F	3.26040	7.70390	1.36300
F	4.96750	0.32340	1.89800
F	0.71940	6.76770	1.20310
F	6.45800	-1.26990	0.30510
F	0.20660	4.53010	-0.17990
F	7.20630	-0.38130	-2.14950
F	2.18960	3.14180	-1.30440
F	6.52480	2.03560	-2.95720
H	5.07550	3.63930	-3.81680
H	3.63690	2.87800	-3.09080
H	3.68520	4.64430	-3.33750

1h-Zr

gas phase E = -4506.28
solvation E = -32.9577

Atom	X	Y	Z
Zr	0.16410	0.04720	0.33500
C	3.92420	0.41990	-0.04250
C	2.60370	1.07090	-0.07740
C	2.07480	1.69340	1.06160
C	0.89510	2.42980	1.00460
C	0.21030	2.55160	-0.20480
C	1.88000	1.17830	-1.27160
C	0.71980	1.93840	-1.34500
H	2.60760	1.60380	2.01880
H	0.52000	2.93560	1.89820
H	-0.70400	3.15070	-0.26210
H	2.27180	0.68900	-2.17130
H	0.19730	2.04430	-2.29970
H	4.15960	-0.08800	-0.98820
H	4.69940	1.18800	0.13450
H	4.00150	-0.31270	0.77900
C	-2.24000	-0.58630	0.23140
C	-1.49460	-1.79310	0.25010
C	-1.92880	0.09730	-0.96850
C	-0.74560	-1.87430	-0.95130
C	-1.00650	-0.70230	-1.70170
H	-2.95960	-0.25950	0.97970
H	-1.53440	-2.55360	1.03280
H	-2.40070	1.01740	-1.31550
H	-0.12060	-2.70950	-1.26410
H	-0.64260	-0.50350	-2.70910
C	-0.50620	0.35990	2.44600
C	1.67920	-1.59340	0.57900
H	2.26140	-1.93880	-0.29110
H	-1.30150	-0.32900	2.76860
H	0.47350	-0.03700	2.82030
H	-0.67320	1.32780	2.94170
H	2.38800	-1.25170	1.35870
H	1.12680	-2.46450	0.97710

2a-Ti

gas phase E = -8130.46
solvation E = -7.5728

Atom	X	Y	Z
Ti	-0.14490	0.19200	-0.05750
N	1.65160	-0.28170	0.30060
C	-1.28110	2.28490	0.04380
C	0.12320	2.48020	0.06590
C	0.65770	1.88080	1.25290

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C	-0.45170	1.29640	1.94110
C	-1.63980	1.55610	1.20560
H	-1.96750	2.62790	-0.73190
H	0.70160	2.99260	-0.70460
C	-0.15520	0.47300	-2.08990
H	2.16130	-1.10290	-0.04850
Si	2.30790	1.01130	1.28360
H	-0.39400	0.71800	2.86830
H	-2.65230	1.25130	1.49490
H	-1.13530	0.76760	-2.50790
H	0.07710	-0.56350	-2.42610
H	0.62850	1.15330	-2.45960
H	2.70460	0.58980	2.66710
H	3.40160	1.78330	0.61040
H	-1.30760	-0.97150	1.04840
H	-1.92420	-0.62600	-0.69570
C	-1.59550	-1.40830	0.04310
H	-0.78690	-2.04570	-0.38330
B	-2.88330	-2.30810	0.48670
C	-4.00550	-1.31810	1.09360
C	-3.60130	-3.03540	-0.74300
C	-2.21160	-3.32790	1.53080
C	-4.70530	-1.50690	2.27190
C	-5.73530	-0.67960	2.67500
C	-6.11040	0.38300	1.88720
C	-5.44910	0.60800	0.70100
C	-4.42850	-0.24060	0.33370
C	-4.69830	-3.83140	-0.46600
C	-5.43000	-4.47200	-1.43880
C	-5.06220	-4.32590	-2.75910
C	-3.97630	-3.54490	-3.08090
C	-3.27330	-2.91360	-2.07440
C	-1.87360	-4.63570	1.23320
C	-1.14310	-5.43170	2.09320
C	-0.71170	-4.92600	3.29710
C	-1.00920	-3.62250	3.62960
C	-1.72920	-2.86090	2.73810
F	-4.43240	-2.52490	3.08320
F	-6.37770	-0.90740	3.81260
F	-7.10380	1.17550	2.25890
F	-5.80190	1.62800	-0.07610
F	-3.84990	0.02970	-0.85200
F	-5.06760	-4.01670	0.80150
F	-6.47340	-5.22910	-1.12560
F	-5.75300	-4.93550	-3.71160
F	-3.62280	-3.40440	-4.35350
F	-2.22700	-2.16070	-2.46120
F	-2.19730	-5.19240	0.06610
F	-0.82960	-6.67580	1.75650
F	0.00110	-5.68310	4.11390
F	-0.58320	-3.11100	4.77930
F	-1.91790	-1.56960	3.06880

2b-Ti

gas phase E = -8848.02
solvation E = -13.1362

Atom	X	Y	Z
F	-0.73650	1.34800	-1.65420
F	0.68960	1.80600	-3.82310
F	3.38400	1.62290	-3.77350
F	4.63810	0.92790	-1.47590
F	3.24810	0.43230	0.71640
F	-1.04740	-1.28280	-0.35690
F	-1.12850	-3.92390	0.16660
F	0.37130	-4.96110	2.10860
F	1.90640	-3.33400	3.65990
F	1.96410	-0.75810	3.24470
F	-0.12050	3.36870	0.26140
F	-4.51550	0.87930	2.12900
F	-4.62470	3.48200	1.35610
F	-2.39410	4.69760	0.45120
F	-2.27190	-0.47660	1.97420
C	1.17890	0.91780	-0.32860
C	0.58610	1.23640	-1.53890
C	1.30540	1.47480	-2.69340
C	2.67780	1.38270	-2.67610
C	3.31100	1.03330	-1.50540
C	2.55640	0.79490	-0.37730
C	0.44200	-0.87950	1.40790
C	-0.30240	-1.75980	0.64050
C	-0.35720	-3.11420	0.87990
C	0.40050	-3.65350	1.89300
C	1.17430	-2.82730	2.66810
C	1.18040	-1.47000	2.41550
C	-1.07370	1.35140	1.05520
C	-1.19310	2.68580	0.70160
C	-3.43120	1.47630	1.64570
C	-3.49370	2.79600	1.26420
C	-2.35570	3.41060	0.79400
C	-2.23710	0.78460	1.54070
C	1.11320	1.54000	2.27420
B	0.40070	0.69680	1.06810
H	0.91510	2.61190	2.12100
H	2.19470	1.35480	2.32850
H	0.64510	1.20250	3.20910
Ti	2.69980	3.88150	4.41600
N	3.50260	4.75530	5.90070
H	3.74320	4.28410	6.78420
Si	4.35790	6.14960	5.24990
C	3.97760	2.33780	4.37730
H	3.62550	1.99400	5.38560
H	3.55440	1.66770	3.59940
H	5.07640	2.31900	4.35690
C	2.21760	5.89150	3.39340
C	3.63430	5.78040	3.58180
C	4.07620	4.70690	2.73860
C	2.95960	4.19840	2.03630
C	1.80790	4.92090	2.44580
H	1.56570	6.61410	3.89100
H	5.10350	4.35650	2.63550
H	2.97160	3.37790	1.31350
H	0.80030	4.78630	2.04080
C	0.80910	3.67300	6.07530
C	0.50920	2.83070	5.07740
H	-0.13800	3.11560	4.23680
H	0.84530	1.78340	5.09050
H	0.40970	4.69290	6.11460
H	1.36450	3.32810	6.95690
H	5.84670	5.97570	5.30500
H	3.92950	7.46670	5.82040

2c-Ti

gas phase E = -3103.33
solvation E = -33.6241

Atom	X	Y	Z
Ti	0.14210	0.07170	0.09470
N	1.98550	0.32540	0.34760
H	2.46010	1.22430	0.16270
Si	2.47720	-0.78400	1.64690
C	-0.48960	1.75260	1.01950
H	-0.11340	2.43390	0.21240
H	-1.59240	1.82920	1.09120
H	-0.03670	2.07500	1.97220
C	0.33170	-2.18810	0.42310
C	0.75880	-1.50820	1.60820
C	-0.40290	-0.86000	2.14520
C	-1.51290	-1.16410	1.31970
C	-1.06160	-1.97910	0.25070
H	0.97430	-2.78490	-0.23060
H	-0.43920	-0.25980	3.05610
H	-2.54250	-0.83850	1.48530
H	-1.69340	-2.43050	-0.51680
C	0.93560	0.23940	-2.28890
C	-0.35050	-0.14600	-2.25110
H	-0.63840	-1.18810	-2.42660
H	-1.16400	0.60000	-2.21090
H	1.75220	-0.47700	-2.43390
H	1.21940	1.30110	-2.25330
H	2.76470	-0.00980	2.89570
H	3.55420	-1.74500	1.26490

2d-Ti

gas phase E = -2343.96
solvation E = -35.0248

Atom	X	Y	Z
Ti	-0.02380	0.21520	-0.00050
C	1.91230	-0.18420	0.00380
H	2.06700	0.93710	0.02790
H	2.02060	-0.57960	1.04000
H	2.67190	-0.61580	-0.66190
N	-0.85380	-1.23700	0.82980
H	-0.51500	-1.69740	1.68890
C	0.33400	0.67330	-2.30900
C	-0.07540	-0.67090	-2.10970
C	-1.40430	-0.67150	-1.56680
C	-1.77200	0.69880	-1.39510
C	-0.70600	1.52130	-1.85540
H	1.28260	0.99840	-2.74230
H	0.51890	-1.55460	-2.35280
Si	-1.99680	-1.94070	-0.32730
H	-2.72450	1.05450	-0.98930
H	-0.70920	2.61480	-1.89540
H	-3.42330	-1.70710	0.05200
H	-1.66580	-3.35670	-0.66420

2f-Ti

gas phase E = -10265.27
solvation E = -7.3023

Atom	X	Y	Z
Ti	1.70890	2.03150	-0.32210
N	3.49530	1.55210	0.05720
C	0.58690	4.13060	-0.22040
C	1.99040	4.32660	-0.20440
C	2.53020	3.72810	0.97820
C	1.42360	3.14300	1.67270
C	0.23270	3.40570	0.94510
H	-0.10210	4.47540	-0.99330
H	2.56440	4.83970	-0.97630
C	1.70550	2.31760	-2.35640
H	3.88330	0.63510	-0.22190
Si	4.17650	2.84620	1.01000
H	1.48550	2.56430	2.59870
H	-0.77640	3.09810	1.23880
H	0.72420	2.63540	-2.75770
H	1.90600	1.26630	-2.66680
H	2.50010	2.97280	-2.75000
H	4.59850	2.45000	2.39360
H	5.26520	3.60590	0.31130
H	0.59020	0.83760	0.82170
H	-0.08070	1.19760	-0.89810
C	0.27370	0.41060	-0.17690
H	1.07260	-0.22460	-0.63320
B	-1.02010	-0.48760	0.26110
C	-2.14760	0.49690	0.87170
C	-1.70910	-1.20670	-0.99270
C	-0.36830	-1.51020	1.31580
C	-2.83810	0.29440	2.05310

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C	-3.83990	1.13870	2.49300
C	-4.19500	2.23350	1.73930
C	-3.54700	2.46820	0.54750
C	-2.55850	1.59880	0.14160
C	-2.77660	-2.04930	-0.74310
C	-3.47160	-2.70090	-1.73470
C	-3.09450	-2.51960	-3.04650
C	-2.04720	-1.68100	-3.34310
C	-1.38580	-1.03490	-2.32020
C	-0.09880	-2.84340	1.07650
C	0.63190	-3.62880	1.94490
C	1.11880	-3.09120	3.11320
C	0.87190	-1.76520	3.39590
C	0.15140	-1.01620	2.49660
F	-2.56980	-0.74670	2.83650
F	-4.47150	0.90510	3.63530
F	-5.15780	3.04580	2.15060
F	-3.88520	3.51650	-0.19720
F	-1.98970	1.87630	-1.04700
F	-3.14630	-2.27650	0.51690
F	-4.49080	-3.50090	-1.45650
F	-3.74460	-3.14400	-4.01710
F	-1.68650	-1.49760	-4.61060
F	-0.38710	-0.21800	-2.69990
F	-0.49230	-3.45030	-0.04560
F	0.89600	-4.89490	1.63870
F	1.82570	-3.83570	3.95230
F	1.34030	-1.22360	4.51430
F	-0.01070	0.28560	2.79830
C	4.46040	0.27090	-3.03510
C	3.69940	-0.78350	-2.32320
C	2.50570	-1.27810	-2.82880
C	1.82490	-2.29740	-2.18390
C	2.32770	-2.83880	-1.01530
C	4.18240	-1.32440	-1.13560
C	3.50530	-2.34120	-0.48490
H	2.10790	-0.86760	-3.76520
H	0.89090	-2.68590	-2.60590
H	1.80680	-3.67410	-0.53610
H	5.14270	-0.96810	-0.73860
H	3.91370	-2.76620	0.43820
H	5.39300	-0.14630	-3.45740
H	3.87850	0.69990	-3.86670
H	4.74140	1.09700	-2.35650

2g-Ti

gas phase E = -10247.24
solvation E = -16.5608

Atom	X	Y	Z
Ti	-0.91460	-0.35660	0.27480
C	2.82130	-0.15450	-0.14170
C	1.50520	0.49720	-0.16660
C	1.03150	1.17720	0.96160
C	-0.12980	1.92770	0.90420
C	-0.86310	2.00580	-0.28000
C	0.74460	0.55310	-1.33540
C	-0.39400	1.34480	-1.40880
H	1.61940	1.14360	1.88840
H	-0.47490	2.47950	1.78550
H	-1.75370	2.63970	-0.33390
H	1.10310	0.02650	-2.22770
H	-0.91980	1.46480	-2.36070
H	3.05290	-0.65320	-1.09430
H	3.59130	0.62570	0.02780
H	2.90230	-0.88690	0.67990
C	-3.13320	-1.07660	0.31060
C	-2.32020	-2.22840	0.11140
C	-2.95380	-0.24780	-0.83690
C	-1.67160	-2.12940	-1.14460
C	-2.08100	-0.91520	-1.74180
H	-2.20560	-3.04760	0.82130
H	-3.43590	0.71670	-1.00560
H	-1.00370	-2.86960	-1.58680
H	-1.80970	-0.58400	-2.74490
N	-1.60020	-0.08860	2.06550
C	0.48790	-1.93200	0.69080
H	1.10820	-2.20490	-0.18380
Si	-3.31130	-0.43600	2.04930
H	1.14340	-1.56350	1.50030
H	-0.04120	-2.83070	1.04410
H	-4.18440	0.78180	2.13440
H	-3.75350	-1.48980	3.02020
H	-1.12660	0.44660	2.80220
F	1.37320	7.14880	-0.07490
F	0.76450	7.56570	2.45200
F	1.34060	5.71910	4.34010
F	2.59530	3.41650	3.61950
F	3.28820	2.98890	1.12870
F	3.92000	7.18280	-1.04750
F	6.55850	7.63860	-1.00890
F	8.29320	5.58490	-1.30690
F	7.34870	3.07290	-1.65260
F	4.78650	2.58450	-1.69350
F	-0.20900	5.02900	-0.74640
F	1.33950	6.38090	-5.72310
F	-1.27920	6.49750	-5.01660
F	-2.00450	5.80340	-2.49750
F	3.15050	5.57940	-4.01540
C	2.31410	5.02250	0.35460
C	1.70960	6.19160	0.78600
C	1.37490	6.43770	2.10330
C	1.66190	5.50090	3.06870
C	2.29820	4.33930	2.69680
C	2.62640	4.13760	1.37230
C	4.20350	4.88180	-1.39080
C	4.74070	6.14510	-1.22250
C	6.09420	6.40520	-1.19160
C	6.98360	5.36330	-1.33790
C	6.49900	4.08990	-1.51310
C	5.13700	3.87180	-1.53580
C	1.61190	5.39370	-2.22960
C	0.25630	5.43280	-1.94560
C	0.97170	6.09510	-4.47700
C	-0.35500	6.15080	-4.12760
C	-0.71460	5.80450	-2.84570
C	1.91240	5.70440	-3.54320
C	2.18710	3.13270	-1.47700
B	2.62110	4.65430	-1.20130
H	1.10960	3.07190	-1.26360
H	2.71880	2.40400	-0.85460
H	2.34530	2.85400	-2.53720

2h-Ti

gas phase E = -4506.47
solvation E = -33.3576

Atom	X	Y	Z
Ti	0.16330	0.07090	0.42350
C	3.90750	0.34130	-0.01860
C	2.59380	0.99740	-0.04200
C	2.09100	1.62490	1.10380
C	0.90160	2.33630	1.06760
C	0.17370	2.43030	-0.11910
C	1.84680	1.08610	-1.21920
C	0.67210	1.82620	-1.26920
H	2.65840	1.55200	2.04010
H	0.52390	2.83100	1.96800
H	-0.75700	3.00530	-0.14920
H	2.21590	0.58570	-2.12200
H	0.13220	1.93210	-2.21490
H	4.17930	-0.07680	-0.99850
H	4.67980	1.08010	0.26510
H	3.94050	-0.46760	0.73260
C	-2.05050	-0.64190	0.49070
C	-1.24370	-1.79620	0.28180
C	-1.88570	0.18560	-0.65870
C	-0.61000	-1.70010	-0.98100
C	-1.02110	-0.48290	-1.57260
H	-1.13160	-2.61930	0.98850
H	-2.38580	1.14020	-0.83020
H	0.03770	-2.45110	-1.43510
H	-0.77020	-0.16030	-2.58390
N	-0.48920	0.30510	2.22420
C	1.57990	-1.48010	0.81160
H	2.19270	-1.75550	-0.06580
Si	-2.20990	-0.03460	2.24550
H	2.22900	-1.08690	1.61630
H	1.07420	-2.38250	1.18650
H	-3.04740	1.20150	2.36770
H	-2.62420	-1.10340	3.20680
H	0.02010	0.76190	2.98730

2a-Zr

gas phase E = -8155.01
solvation E = -8.0953

Atom	X	Y	Z
Zr	-0.08540	0.19840	-0.08630
N	1.87690	-0.19810	0.37570
C	-1.16810	2.47810	0.11970
C	0.24060	2.62390	0.12280
C	0.77100	1.99210	1.29730
C	-0.35020	1.45440	2.00270
C	-1.53630	1.75130	1.28330
H	-1.85670	2.87810	-0.62560
H	0.82180	3.14060	-0.64240
C	-0.14460	0.55750	-2.25290
H	2.45680	-0.99450	0.08660
Si	2.43420	1.13620	1.35990
H	-0.30460	0.89960	2.94410
H	-2.55710	1.51310	1.59860
H	-1.13640	0.86810	-2.63090
H	0.05220	-0.46970	-2.64090
H	0.62220	1.23350	-2.66890
H	2.79510	0.74590	2.76090
H	3.52780	1.94220	0.72290
H	-1.40850	-1.06780	1.05210
H	-2.03180	-0.73020	-0.68640
C	-1.68790	-1.50090	0.05030
H	-0.88430	-2.14560	-0.37980
B	-2.97560	-2.40960	0.48380
C	-4.09010	-1.40230	1.07170
C	-3.66490	-3.13210	-0.76470
C	-2.29930	-3.40120	1.55340
C	-4.78260	-1.57280	2.25590
C	-5.75900	-0.69610	2.68740
C	-6.08760	0.39800	1.91860
C	-5.43740	0.59980	0.72230
C	-4.47470	-0.30100	0.32630
C	-4.74790	-3.95360	-0.51200
C	-5.47890	-4.56520	-1.50430
C	-5.12040	-4.36460	-2.82090
C	-4.04800	-3.55570	-3.11820
C	-3.34920	-2.95240	-2.09300
C	-1.94120	-4.71020	1.29150
C	-1.14470	-5.45210	2.14350
C	-0.69110	-4.89620	3.31640
C	-1.02200	-3.59400	3.61820
C	-1.79760	-2.88470	2.73230
F	-4.53890	-2.60990	3.05150

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F	-6.38520	-0.89510	3.83920
F	-7.02100	1.24580	2.32240
F	-5.74460	1.64580	-0.03920
F	-3.91110	-0.05210	-0.87170
F	-5.10930	-4.18240	0.75070
F	-6.51470	-5.34130	-1.21500
F	-5.80510	-4.94740	-3.79370
F	-3.69820	-3.36150	-4.38570
F	-2.32450	-2.16330	-2.46730
F	-2.31170	-5.31450	0.16330
F	-0.79040	-6.69130	1.83480
F	0.07830	-5.59890	4.13420
F	-0.56290	-3.02990	4.72930
F	-2.00890	-1.58870	3.03040

2b-Zr

gas phase E = -8874.84
solvation E = -15.6970

Atom	X	Y	Z
Zr	0.04000	0.00520	0.04410
N	2.04920	0.43370	0.19640
H	2.67840	0.25900	0.99060
Si	2.63710	0.73780	-1.43390
C	-0.24160	-1.99900	0.78880
H	-0.00270	-1.78330	1.86260
H	-1.34060	-2.16260	0.70490
H	0.27760	-2.92340	0.49610
C	0.95790	0.41140	-2.17180
C	0.45780	-0.93510	-2.18410
C	-0.95040	-0.90290	-2.08200
C	-1.35060	0.45720	-1.99270
C	-0.18200	1.26210	-2.06190
H	1.06670	-1.83740	-2.27130
H	-1.61910	-1.76390	-2.08900
H	-2.38370	0.81140	-1.93660
H	-0.16010	2.35430	-2.03510
C	-0.41770	2.20780	1.39240
C	-1.64190	1.77370	1.06860
H	-2.21490	2.20080	0.23830
H	-2.18010	1.02800	1.67840
H	0.07690	3.00630	0.82680
H	0.10380	1.85590	2.29470
F	-7.21550	-4.02420	-0.07100
F	-7.79960	-5.39730	2.10290
F	-6.77220	-4.69520	4.49910
F	-5.12570	-2.55050	4.67730
F	-4.48910	-1.16170	2.51480
F	-8.07320	-1.30080	0.11420
F	-9.34850	0.98140	0.63350
F	-7.97880	3.30990	0.74750
F	-5.29720	3.31190	0.30470
F	-4.01810	1.08450	-0.22800
F	-4.67190	-4.39220	-0.90270
F	-6.74400	-1.52840	-4.96990
F	-5.93350	-4.08790	-5.36800
F	-4.90480	-5.49870	-3.30760
F	-6.54350	-0.40540	-2.60400
C	-5.75840	-2.56390	1.08820
C	-6.63060	-3.63650	1.06080
C	-6.96910	-4.36290	2.18520
C	-6.45340	-4.00650	3.40890
C	-5.61200	-2.92140	3.49320
C	-5.29160	-2.22920	2.34640
C	-5.97930	-0.24730	-0.00420
C	-7.34820	-0.18720	0.19470
C	-8.03330	0.98130	0.44620
C	-7.34180	2.17220	0.49780
C	-5.98530	2.16690	0.27540
C	-5.34630	0.97230	0.02280
C	-5.62360	-2.35530	-1.61010
C	-5.21410	-3.65020	-1.87650
C	-6.25340	-2.23800	-3.95640
C	-5.84120	-3.53310	-4.16520
C	-5.31630	-4.24810	-3.11170
C	-6.14000	-1.67710	-2.69830
C	-3.65790	-1.61450	-0.18890
B	-5.28050	-1.68930	-0.18370
H	-3.24660	-2.64330	-0.18160
H	-3.25280	-1.06920	0.68550
H	-3.32530	-1.11430	-1.11120
H	3.14270	2.13150	-1.64120
H	3.63720	-0.28130	-1.89440

2c-Zr

gas phase E = -3128.70
solvation E = -34.3735

Atom	X	Y	Z
Zr	0.12860	0.14570	0.06620
N	2.11460	0.31400	0.47320
H	2.66230	1.17750	0.33290
Si	2.52210	-0.88600	1.70920
C	-0.64440	1.92040	1.03190
H	-0.25060	2.63250	0.25750
H	-1.74840	1.99630	1.03880
H	-0.27140	2.27550	2.00630
C	0.33490	-2.27010	0.47380
C	0.78670	-1.57250	1.63440
C	-0.37060	-0.94410	2.21040
C	-1.49530	-1.25500	1.40970
C	-1.06160	-2.06730	0.33010
H	0.96030	-2.88850	-0.17630
H	-0.39290	-0.36030	3.13310
H	-2.52740	-0.96690	1.61910
H	-1.70910	-2.54610	-0.40550
C	0.90500	0.22910	-2.47350
C	-0.37330	-0.16900	-2.46280
H	-0.64730	-1.22130	-2.58920
H	-1.19550	0.56590	-2.46110
H	1.73200	-0.48230	-2.57690
H	1.17490	1.29740	-2.46260
H	2.84050	-0.22290	3.01160
H	3.55880	-1.86570	1.26740

2d-Zr

gas phase E = -2369.20
solvation E = -36.6689

Atom	X	Y	Z
Zr	0.01720	0.27100	0.07410
C	2.09280	-0.20540	0.00060
H	2.36940	0.88720	0.02200
H	2.22510	-0.60780	1.03470
H	2.80170	-0.70700	-0.67250
N	-0.93140	-1.35160	0.82380
H	-0.66160	-1.85300	1.68380
C	0.27370	0.63300	-2.39860
C	-0.13540	-0.70200	-2.15060
C	-1.45890	-0.67770	-1.58900
C	-1.82810	0.69530	-1.47420
C	-0.76450	1.49830	-1.96720
H	1.20220	0.93790	-2.88460
H	0.43870	-1.59580	-2.39720
Si	-2.04640	-1.98890	-0.38860
H	-2.78820	1.06590	-1.10410
H	-0.78120	2.58400	-2.08760
H	-3.47950	-1.79750	-0.01640
H	-1.71220	-3.37810	-0.82060

2f-Zr

gas phase E = -10290.73
solvation E = -7.8992

Atom	X	Y	Z
Zr	1.78150	2.02620	-0.36030
N	3.73690	1.64660	0.14480
C	0.71020	4.30870	-0.18570
C	2.11830	4.45730	-0.17390
C	2.63940	3.84420	1.01230
C	1.51400	3.31170	1.71550
C	0.33320	3.59980	0.98460
H	0.02660	4.69730	-0.94100
H	2.70490	4.96570	-0.94040
C	1.72060	2.40850	-2.52940
H	4.21300	0.75370	-0.04310
Si	4.29700	2.98400	1.11190
H	1.55160	2.77160	2.66520
H	-0.68890	3.36220	1.29520
H	0.73370	2.77140	-2.87560
H	1.85450	1.37220	-2.91470
H	2.50540	3.04840	-2.96730
H	4.64070	2.62080	2.52550
H	5.40650	3.77070	0.47650
H	0.45990	0.79130	0.83610
H	-0.16730	1.08430	-0.90320
C	0.18470	0.33290	-0.15380
H	0.99670	-0.31300	-0.57580
B	-1.10480	-0.57290	0.27150
C	-2.21900	0.42930	0.86620
C	-1.77030	-1.28700	-0.99830
C	-0.45000	-1.57720	1.34360
C	-2.89480	0.26180	2.06110
C	-3.85500	1.14710	2.50950
C	-4.17960	2.24790	1.74870
C	-3.54420	2.44800	0.54490
C	-2.60030	1.53640	0.12920
C	-2.82790	-2.15130	-0.77810
C	-3.50570	-2.79210	-1.79030
C	-3.12130	-2.57190	-3.09550
C	-2.08670	-1.70830	-3.36230
C	-1.44260	-1.07610	-2.32010
C	-0.15970	-2.90770	1.11640
C	0.62160	-3.66370	1.96820
C	1.14200	-3.09970	3.10860
C	0.86810	-1.77800	3.38560
C	0.09340	-1.06030	2.50470
F	-2.64770	-0.78040	2.84980
F	-4.47170	0.94970	3.66760
F	-5.10230	3.10310	2.16350
F	-3.85200	3.50290	-0.20310
F	-2.05140	1.77840	-1.07650
F	-3.20290	-2.40540	0.47510
F	-4.51540	-3.61380	-1.53650
F	-3.75250	-3.17440	-4.09200
F	-1.72500	-1.48090	-4.62160
F	-0.46000	-0.23100	-2.68180
F	-0.56360	-3.53540	0.00980
F	0.91690	-4.92300	1.66160
F	1.91170	-3.81010	3.92110
F	1.37030	-1.21000	4.47580
F	-0.08380	0.24200	2.79590
C	4.39090	0.28830	-3.03290
C	3.62340	-0.74750	-2.29880
C	2.40930	-1.22500	-2.77480
C	1.73760	-2.24670	-2.12290
C	2.26920	-2.80600	-0.97620
C	4.13340	-1.30750	-1.13010
C	3.46690	-2.32540	-0.47330
H	1.98800	-0.80370	-3.69610

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H	0.78720	-2.62120	-2.52130
H	1.75610	-3.64120	-0.48940
H	5.11240	-0.97120	-0.76050
H	3.89630	-2.76760	0.43200
H	5.32720	-0.14030	-3.43420
H	3.81880	0.69060	-3.88390
H	4.66540	1.13230	-2.37400

2g-Zr

gas phase E = -10282.42
solvation E = -16.1761

Atom	X	Y	Z
Zr	-0.93480	-0.36820	0.35060
C	2.85080	-0.17290	-0.14440
C	1.54970	0.51020	-0.17230
C	1.09450	1.22460	0.94660
C	-0.03310	2.02970	0.86860
C	-0.76620	2.10510	-0.31710
C	0.79590	0.58310	-1.34530
C	-0.33450	1.38800	-1.42570
H	1.67350	1.18590	1.88000
H	-0.35050	2.61500	1.73910
H	-1.63100	2.77220	-0.38830
H	1.14430	0.04630	-2.23500
H	-0.86780	1.48560	-2.37510
H	3.02910	-0.75390	-1.06170
H	3.64230	0.60240	-0.07430
H	2.95250	-0.83380	0.73290
C	-3.26850	-1.12400	0.40920
C	-2.48720	-2.29770	0.18400
C	-3.12650	-0.31300	-0.75790
C	-1.88940	-2.21900	-1.09700
C	-2.29080	-0.99270	-1.68410
H	-2.36940	-3.12410	0.88680
H	-3.61340	0.64810	-0.92930
H	-1.27030	-2.98540	-1.56460
H	-2.06780	-0.66970	-2.70140
N	-1.77540	0.02760	2.21690
C	0.54070	-2.04870	0.74980
H	1.15020	-2.32750	-0.13020
Si	-3.45770	-0.42840	2.13190
H	1.22860	-1.71590	1.54970
H	0.00770	-2.94850	1.09570
H	-4.39790	0.74080	2.14760
H	-3.87970	-1.46610	3.13020
H	-1.38320	0.60680	2.96650
F	1.46510	7.12510	-0.09250
F	0.87560	7.49740	2.43800
F	1.33210	5.55710	4.26960
F	2.49420	3.22590	3.48210
F	3.25100	2.87930	0.99260
F	3.89350	7.22610	-1.04610
F	6.49300	7.74220	-0.85680
F	8.30910	5.75200	-1.15190
F	7.45770	3.23320	-1.64640
F	4.91270	2.67480	-1.80550
F	-0.16500	5.01340	-0.76870
F	1.30400	6.32310	-5.77280
F	-1.27340	6.45910	-5.03690
F	-1.97880	5.79580	-2.49490
F	3.20350	5.70000	-4.00250
C	2.34940	4.96200	0.27840
C	1.77670	6.13660	0.73980
C	1.44090	6.35560	2.06100
C	1.67080	5.37370	2.99680
C	2.26340	4.19980	2.59190
C	2.61740	4.03630	1.26860
C	4.25030	4.94240	-1.44610
C	4.74410	6.21370	-1.22230
C	6.08470	6.50700	-1.11900
C	7.01100	5.49790	-1.26090
C	6.57300	4.22010	-1.50810
C	5.21880	3.96510	-1.59270
C	1.64260	5.42530	-2.25950
C	0.29030	5.43910	-1.96460
C	0.98190	6.08020	-4.50660
C	-0.34390	6.12800	-4.14520
C	-0.69270	5.80200	-2.85590
C	1.94360	5.75800	-3.56610
C	2.29650	3.14360	-1.68270
B	2.67440	4.65570	-1.28420
H	1.21020	3.03720	-1.54500
H	2.81570	2.37070	-1.09960
H	2.51910	2.96540	-2.75280

2h-Zr

gas phase E = -4541.04
solvation E = -33.5381

Atom	X	Y	Z
Zr	0.18830	0.07180	0.43330
C	3.97440	0.36450	-0.02910
C	2.67160	1.04760	-0.05510
C	2.17300	1.69230	1.08890
C	1.00560	2.44370	1.03960
C	0.28920	2.55270	-0.15310
C	1.93560	1.16420	-1.23900
C	0.77240	1.92360	-1.29540
H	2.73000	1.60940	2.03180
H	0.63830	2.95250	1.93610
H	-0.62390	3.15310	-0.19500
H	2.30260	0.66570	-2.14400
H	0.23310	2.02500	-2.24130
H	4.21320	-0.10300	-0.99580
H	4.76630	1.10120	0.20150
H	4.00960	-0.41150	0.75530
C	-2.12140	-0.72060	0.51210
C	-1.32480	-1.87850	0.26310
C	-2.01170	0.10400	-0.64730
C	-0.74410	-1.77630	-1.02380
C	-1.17330	-0.54980	-1.59160
H	-1.19610	-2.71510	0.95220
H	-2.53400	1.04910	-0.80510
H	-0.12710	-2.53120	-1.51230
H	-0.97470	-0.22160	-2.61290
N	-0.61380	0.35660	2.32910
C	1.70090	-1.57380	0.79890
H	2.32200	-1.84310	-0.07450
Si	-2.31000	-0.08680	2.25860
H	2.36310	-1.22720	1.61520
H	1.18190	-2.48250	1.14240
H	-3.22120	1.10170	2.32410
H	-2.70970	-1.15180	3.23110
H	-0.20820	0.87630	3.11560

3a-Ti

gas phase E = -9065.44
solvation E = -9.0669

Atom	X	Y	Z
Ti	0.04190	-0.01280	0.04300
C	2.39140	-0.13110	0.09560
C	2.04160	1.24430	0.12310
C	1.36730	1.54780	-1.07770
C	1.31280	0.35640	-1.86150
C	1.95980	-0.67260	-1.13750
H	2.91000	-0.68170	0.88130
H	2.23140	1.94260	0.94300
C	-2.25700	-0.62330	-0.05700
C	-1.78670	-0.39320	-1.37720
C	-1.43910	0.97550	-1.48240
C	-1.62430	1.57840	-0.21430
C	-2.16520	0.58880	0.65640
H	-2.64460	-1.56500	0.33040
H	-1.73850	-1.13210	-2.17850
C	0.07090	-2.16370	0.07020
H	0.98420	2.52850	-1.36040
H	0.90170	0.26010	-2.86600
H	2.11670	-1.69460	-1.47750
H	-1.10120	1.48230	-2.38640
H	-1.45370	2.62590	0.04300
H	-2.46630	0.75330	1.69590
H	-0.75140	-2.52900	0.71150
H	1.03060	-2.50170	0.49940
H	-0.05710	-2.61560	-0.92980
H	-0.03780	1.07530	1.77230
H	-0.27730	-0.77460	1.98740
C	0.28370	0.13630	2.31600
H	1.36900	-0.00610	2.27770
B	-0.07740	0.45040	3.88490
C	-1.66750	0.38920	4.13200
C	-2.42500	1.33790	4.79300
C	-3.78190	1.18950	4.99890
C	-4.43180	0.06820	4.54760
C	-3.71730	-0.91560	3.90400
C	-2.36300	-0.73980	3.73050
C	0.54570	-0.68720	4.83840
C	0.52920	-0.47680	6.20600
C	1.04030	-1.37570	7.11270
C	1.53480	-2.57950	6.66570
C	1.54810	-2.84660	5.31880
C	1.06240	-1.90050	4.43690
C	0.58390	1.91240	4.09870
C	1.73870	2.19740	4.80560
C	2.29510	3.46170	4.86360
C	1.71880	4.50490	4.17430
C	0.58280	4.26610	3.43290
C	0.05450	2.99300	3.41500
F	-1.87960	2.45360	5.27240
F	-4.48810	2.10620	5.64010
F	-5.73200	-0.05180	4.75970
F	-4.33280	-2.00770	3.46240
F	-1.71780	-1.74350	3.10810
F	0.03740	0.66690	6.68180
F	1.07740	-1.11800	8.41130
F	1.98870	-3.46190	7.54240
F	2.02630	-4.00470	4.87590
F	1.12870	-2.23920	3.13730
F	2.40840	1.25740	5.47020
F	3.39610	3.67320	5.57290
F	2.24770	5.71810	4.22920
F	0.00590	5.25250	2.75360
F	-1.04470	2.81560	2.65410

3b-Ti

gas phase E = -9791.67
solvation E = -14.0749

Atom	X	Y	Z
Ti	-0.00067	0.06384	0.06772
C	2.07147	0.08093	0.34331
H	2.66699	1.00328	0.40482
H	2.68075	-0.77186	0.00729
H	1.67113	-0.14443	1.38365
C	0.13869	-2.15457	-0.75720
C	0.44646	-2.20016	0.61298
C	-0.68453	-1.73603	1.33964
C	-1.72473	-1.47751	0.40046
C	-1.21537	-1.71636	-0.88988
H	0.81030	-2.43207	-1.56947

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H	1.39441	-2.51533	1.05035
H	-0.76973	-1.68633	2.42619
H	-2.74329	-1.16630	0.63283
H	-1.77936	-1.62326	-1.81902
C	-1.37378	1.12757	1.63476
C	-0.05632	1.59713	1.84831
C	0.35560	2.30178	0.68492
C	-0.71703	2.27486	-0.23584
C	-1.78014	1.53143	0.33277
H	-1.98332	0.58687	2.36027
H	0.53087	1.46931	2.76025
H	1.29096	2.85074	0.55742
H	-0.74749	2.79268	-1.19709
H	-2.75501	1.36013	-0.13209
C	0.05058	0.30279	-2.37338
C	1.28293	0.74661	-2.04307
H	1.46109	1.77066	-1.69554
H	2.17847	0.15365	-2.26494
H	-0.06504	-0.64669	-2.90535
H	-0.82767	0.96577	-2.35597
B	-0.86806	3.74539	-4.18321
H	-0.69958	2.27583	-5.89151
H	-2.26076	2.18935	-5.04996
H	-0.80821	1.44248	-4.33259
C	-1.17662	2.31971	-4.89709
C	-1.03141	4.83638	-5.36551
C	-0.02830	5.61389	-5.91031
C	-0.21701	6.43162	-7.00725
C	-1.45749	6.50784	-7.59448
C	-2.49426	5.76499	-7.07678
C	-2.26243	4.95433	-5.98816
C	-1.99356	4.08085	-3.05713
C	-2.26030	5.39174	-2.69505
C	-3.27123	5.76039	-1.83474
C	-4.06715	4.79039	-1.26509
C	-3.82529	3.47307	-1.56800
C	-2.81167	3.15248	-2.44948
C	0.62183	3.73121	-3.53428
C	1.66947	3.14463	-4.23012
C	2.23376	4.02303	-1.71851
C	3.22149	3.39297	-2.43528
C	2.93820	2.96180	-3.71160
C	0.97666	4.19679	-2.28037
F	1.20872	5.61539	-5.40003
F	0.78872	7.15021	-7.50076
F	-1.65739	7.29129	-8.64802
F	-3.69919	5.82712	-7.63947
F	-3.31188	4.25216	-5.54380
F	-1.49845	6.37765	-3.16153
F	-3.48087	7.03521	-1.52816
F	-5.03985	5.12372	-0.42687
F	-4.55397	2.50795	-0.99401
F	-2.63571	1.82162	-2.63181
F	1.50271	2.73746	-5.48478
F	2.48311	4.43365	-0.47079
F	4.41976	3.18186	-1.89932
F	3.88648	2.35878	-4.42306
F	0.10789	4.83047	-1.48433

3c-Ti

gas phase E = -4045.65
solvtion E = -33.5852

Atom	X	Y	Z
Ti	0.01320	-0.01420	-0.00650
C	2.07110	-0.10310	0.24600
H	2.74830	0.75040	0.39600
H	2.62590	-1.00650	-0.05020
H	1.56340	-0.31020	1.25500
C	0.11070	-2.22320	-0.78860
C	0.25610	-2.28500	0.60880
C	-0.91960	-1.76160	1.20710
C	-1.83230	-1.44760	0.16100
C	-1.20080	-1.72040	-1.06740
H	0.84220	-2.56070	-1.52470
H	1.12840	-2.66010	1.14710
H	-1.12230	-1.71860	2.27850
H	-2.85830	-1.10120	0.28680
H	-1.67560	-1.65070	-2.04590
C	-1.40320	1.10620	1.49300
C	-0.06980	1.46980	1.79570
C	0.45990	2.16970	0.67650
C	-0.55740	2.24720	-0.30390
C	-1.69940	1.56770	0.18380
H	-2.10040	0.61080	2.16940
H	0.44100	1.28840	2.74400
H	1.44030	2.64200	0.62460
H	-0.49320	2.78440	-1.25220
H	-2.66030	1.47930	-0.32560
C	0.10240	0.29430	-2.47130
C	1.33090	0.72000	-2.10660
H	1.52130	1.74800	-1.78370
H	2.21650	0.10780	-2.30500
H	-0.00300	-0.65690	-2.99860
H	-0.75890	0.97330	-2.50880

3d-Ti

gas phase E = -3293.86
solvation E = -32.9703

Atom	X	Y	Z
Ti	0.01430	-0.00740	0.03730
C	2.05330	0.01000	-0.03930
H	2.64510	0.93620	0.00570
H	2.65970	-0.82220	-0.42670
H	1.77060	-0.26640	1.04080
C	0.30680	-1.94480	-1.15070
C	0.21160	-2.29780	0.21990
C	-1.09100	-1.95260	0.67880
C	-1.80760	-1.40870	-0.41380
C	-0.94180	-1.37820	-1.53860
H	1.15790	-2.12570	-1.80730
H	0.99230	-2.78090	0.81240
H	-1.48700	-2.12850	1.68220
H	-2.85520	-1.10830	-0.40690
H	-1.20820	-1.04120	-2.54390
C	-1.81190	1.41610	0.34900
C	-1.02120	1.46470	1.52100
C	0.25240	1.99560	1.16910
C	0.25440	2.25770	-0.22360
C	-1.02380	1.88250	-0.73740
H	-2.85930	1.12000	0.30000
H	-1.34660	1.18930	2.52760
H	1.07680	2.19160	1.85840
H	1.06830	2.70780	-0.79330
H	-1.36210	2.00180	-1.76980

3f-Ti

gas phase E = -11197.26
solvation E = -10.6258

Atom	X	Y	Z
Ti	1.24480	-0.90940	-2.75180
C	3.59270	-1.03830	-2.73210
C	3.24840	0.33880	-2.70440
C	2.55820	0.64080	-3.89770
C	2.49060	-0.55250	-4.67930
C	3.14510	-1.57870	-3.95940
H	4.11970	-1.58870	-1.95170
H	3.45700	1.03940	-1.89080
C	-1.05540	-1.50310	-2.77760
C	-0.61920	-1.29980	-4.11410
C	-0.26440	0.06400	-4.25420
C	-0.41740	0.69310	-2.99330
C	-0.94170	-0.27600	-2.09160
H	-1.43250	-2.43510	-2.35720
H	-0.56530	-2.05340	-4.90150
C	1.27130	-3.05940	-2.72200
H	2.17280	1.62140	-4.17790
H	2.06200	-0.66370	-5.67870
H	3.28500	-2.60140	-4.30530
H	0.05780	0.54790	-5.17630
H	-0.23270	1.74290	-2.75740
H	-1.21150	-0.08850	-1.04780
H	0.45440	-3.43950	-2.08310
H	2.23740	-3.40400	-2.31230
H	1.13970	-3.47480	-3.73930
H	1.23120	0.19010	-1.04000
H	0.98250	-1.66340	-0.82260
C	1.52700	-0.74570	-0.47700
H	2.61410	-0.89100	-0.49170
B	1.12580	-0.42110	1.07580
C	-0.46640	-0.48260	1.32020
C	-1.21700	0.45090	2.01180
C	-2.57320	0.30730	2.23710
C	-3.22920	-0.81050	1.77510
C	-2.51800	-1.78170	1.10720
C	-1.16810	-1.60390	0.91100
C	1.72870	-1.54230	2.05510
C	1.69170	-1.30610	3.41750
C	2.14410	-2.20510	4.35370
C	2.63340	-3.42310	3.93450
C	2.67230	-3.71140	2.59030
C	2.22110	-2.77430	1.68160
C	1.77280	1.04280	1.28540
C	2.92800	1.33770	1.98620
C	3.46180	2.61090	2.05280
C	2.85670	3.64550	1.38010
C	1.72150	3.39460	0.64050
C	1.21910	2.11470	0.60980
F	-0.66390	1.55660	2.50420
F	-3.24910	1.23710	2.89990
F	-4.52730	-0.96170	1.98300
F	-3.13600	-2.87380	0.66690
F	-0.53480	-2.59940	0.26450
F	1.21860	-0.14340	3.86580
F	2.11950	-1.92080	5.64980
F	3.05700	-4.30750	4.82580
F	3.14010	-4.88600	2.17530
F	2.29460	-3.13700	0.38900
F	3.61490	0.39910	2.63630
F	4.56450	2.84350	2.75370
F	3.36640	4.86760	1.43420
F	1.13530	4.38020	-0.03270
F	0.12250	1.92370	-0.14750
C	2.52040	-5.17340	-5.51850
C	2.22770	-3.98380	-6.35190
C	0.92450	-3.56660	-6.57850
C	0.65370	-2.48150	-7.39490
C	1.68980	-1.79140	-7.99630
C	3.25870	-3.27580	-6.95720
C	2.99640	-2.19250	-7.77230
H	0.10260	-4.13400	-6.12550
H	-0.38360	-2.18660	-7.58480
H	1.48110	-0.94730	-8.66120
H	4.29500	-3.59670	-6.79410
H	3.82570	-1.66010	-8.24940
H	2.94640	-5.98340	-6.13850
H	3.25990	-4.95310	-4.72870
H	1.61410	-5.56530	-5.03070

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3g-Ti

gas phase E = -11171.05
solvation E = -16.5094

Atom	X	Y	Z
B	-1.17730	0.19860	0.01690
C	-0.20960	0.42100	-1.24900
C	-0.57640	1.30890	-2.24740
C	0.04240	1.38890	-3.47260
C	1.10110	0.55290	-3.74810
C	1.52570	-0.32690	-2.78120
C	0.88280	-0.36790	-1.55820
F	-1.59770	2.16220	-2.05750
F	-0.37000	2.25930	-4.39480
F	1.70710	0.60590	-4.92950
F	2.55360	-1.13160	-3.03480
F	1.37610	-1.24230	-0.68100
C	-2.62210	-0.14590	-0.66190
C	-1.48550	1.53400	0.87670
C	-0.87650	-1.11420	0.89780
C	-0.89920	2.76910	0.66770
C	-0.77820	-1.14500	2.27490
C	-1.37330	3.94540	1.22210
C	-0.84520	-2.31070	3.01440
C	-2.47450	3.92040	2.04410
C	-0.99070	-3.51790	2.37480
C	-3.06710	2.70670	2.31490
C	-1.04200	-3.54400	0.99910
C	-2.55630	1.55700	1.75680
C	-0.96940	-2.36170	0.30030
F	0.16930	2.90500	-0.11470
F	-0.64170	-0.02100	2.98500
F	-0.78050	5.10600	0.95910
F	-0.77800	-2.27720	4.34390
F	-2.95420	5.04040	2.57810
F	-1.07240	-4.64770	3.07160
F	-4.14440	2.65800	3.11880
F	-1.17230	-4.70840	0.36360
F	-3.17690	0.42440	2.11620
F	-1.02290	-2.47300	-1.03290
H	-2.53010	-0.95220	-1.41200
H	-3.32400	-0.48050	0.12010
H	-3.02250	0.75070	-1.16590
Ti	-7.88690	1.76720	0.37210
C	-8.44280	0.14940	-1.20690
C	-7.92780	1.26250	-1.93840
C	-8.78950	2.35290	-1.73600
C	-9.84590	1.92610	-0.88060
C	-9.64890	0.55410	-0.59300
H	-7.99810	-0.84700	-1.15660
H	-7.03950	1.27230	-2.57080
C	-7.14480	3.04560	2.25060
C	-8.50160	3.35740	1.99280
C	-8.57280	3.95290	0.71050
C	-7.25500	3.99300	0.16780
C	-6.37660	3.45210	1.13500
H	-6.75180	2.59890	3.16520
H	-9.33720	3.19290	2.67240
C	-8.81510	0.62210	1.92590
H	-8.67920	3.34240	-2.17940
H	-10.70410	2.52130	-0.57080
H	-10.32200	-0.08120	-0.02150
H	-9.46530	4.37440	0.24950
H	-6.95720	4.43830	-0.78150
H	-5.28700	3.38690	1.05090
H	-8.22180	0.76180	2.84730
H	-8.78930	-0.44060	1.62650
H	-9.86240	0.89710	2.14840
C	-5.78480	0.46640	0.92370
C	-5.48360	0.76570	-0.40120
C	-5.38660	-0.25370	-1.35490
C	-5.63850	-1.55250	-0.95170
C	-6.08590	-0.84040	1.29110
C	-6.00000	-1.84640	0.35280
H	-5.15200	1.77690	-0.67910
H	-5.51060	-2.36730	-1.67500
C	-4.97090	0.02290	-2.74450
H	-6.31840	-1.06890	2.33600
H	-6.17140	-2.88640	0.64960
H	-5.60730	1.20380	1.71350
H	-5.75860	-0.25950	-3.46810
H	-4.69620	1.07930	-2.89520
H	-4.07540	-0.57580	-2.98990

3h-Ti

gas phase E = -5437.21
solvation E = -32.7363

Atom	X	Y	Z
Ti	0.56150	0.24160	-0.36200
C	2.42150	1.31810	0.51670
C	1.39280	2.30470	0.44600
C	1.05800	2.49020	-0.90650
C	1.88020	1.62530	-1.68510
C	2.74710	0.93360	-0.80490
H	2.91780	0.96790	1.42370
H	0.96440	2.85800	1.28380
C	-1.21220	-1.23670	-0.93200
C	-0.53610	-0.87540	-2.12070
C	-0.68690	0.52080	-2.29810
C	-1.45940	1.02460	-1.21040
C	-1.79480	-0.06870	-0.38210
H	-1.30250	-2.25050	-0.53920
H	-0.02460	-1.55820	-2.79850
C	1.72850	-1.50840	-0.72600
H	0.33020	3.20290	-1.29510
H	1.91220	1.57460	-2.77350
H	3.54920	0.26070	-1.10180
H	-0.35620	1.09430	-3.16330
H	-1.81260	2.04820	-1.08750
H	-2.43090	-0.02170	0.50510
H	1.07960	-2.38120	-0.52860
H	2.58450	-1.50970	-0.02860
H	2.12360	-1.61270	-1.75300
C	0.06070	-0.69950	1.96400
C	-0.12350	0.60260	2.42660
C	0.80470	1.18700	3.28620
C	1.91180	0.43880	3.65830
C	1.20540	-1.40920	2.31030
C	2.12220	-0.83890	3.16810
H	-1.04510	1.15170	2.18830
H	2.63630	0.87400	4.35790
C	0.61140	2.55120	3.82000
H	1.34140	-2.43230	1.94760
H	3.00490	-1.40600	3.48160
H	-0.76480	-1.23050	1.48420
H	1.54450	3.13880	3.77300
H	-0.18260	3.10080	3.29040
H	0.31910	2.50640	4.88570

3a-Zr

gas phase E = -9102.94
sovlation E = -8.8524

Atom	X	Y	Z
Zr	0.02050	-0.01200	0.01850
C	2.53410	-0.09940	0.03210
C	2.18180	1.27450	0.03730
C	1.51830	1.56000	-1.17590
C	1.46890	0.36170	-1.93890
C	2.10520	-0.66020	-1.19360
H	3.07400	-0.62880	0.82140
H	2.39890	1.99120	0.83350
C	-2.43130	-0.61060	-0.18200
C	-1.93180	-0.37470	-1.48740
C	-1.57370	0.99480	-1.57740
C	-1.81450	1.59740	-0.32030
C	-2.36100	0.60480	0.53810
H	-2.83370	-1.55340	0.19130
H	-1.89280	-1.10220	-2.29710
C	0.03830	-2.26420	0.02600
H	1.16030	2.53880	-1.48990
H	1.07860	0.26310	-2.95210
H	2.26990	-1.68670	-1.51780
H	-1.22270	1.50650	-2.47240
H	-1.67860	2.65050	-0.07000
H	-2.70690	0.76920	1.56520
H	-0.78210	-2.61740	0.68070
H	0.99780	-2.61420	0.44880
H	-0.09900	-2.73500	-0.96270
H	-0.21150	1.07120	1.90070
H	-0.30490	-0.78620	2.10030
C	0.21720	0.15630	2.39830
H	1.30860	0.07720	2.27490
B	-0.08770	0.44740	3.97810
C	-1.68230	0.38580	4.20920
C	-2.46240	1.34370	4.82910
C	-3.83210	1.22000	4.97390
C	-4.47420	0.09670	4.50300
C	-3.73370	-0.89940	3.90760
C	-2.37140	-0.73940	3.78880
C	0.55430	-0.69240	4.90480
C	0.55450	-0.49660	6.27460
C	1.08370	-1.40020	7.16520
C	1.59590	-2.58620	6.69260
C	1.60080	-2.83730	5.34070
C	1.08250	-1.89180	4.47760
C	0.57350	1.90660	4.17910
C	1.74090	2.19360	4.86440
C	2.31510	3.45220	4.88280
C	1.73480	4.48180	4.18050
C	0.58730	4.23700	3.46010
C	0.04430	2.97520	3.47900
F	-1.92270	2.45790	5.31970
F	-4.53630	2.17420	5.56680
F	-5.78610	-0.03200	4.64330
F	-4.33410	-1.99780	3.46080
F	-1.71180	-1.76190	3.21430
F	0.06030	0.63780	6.77030
F	1.12010	-1.15870	8.46810
F	2.08180	-3.46690	7.54910
F	2.10150	-3.97710	4.87470
F	1.12410	-2.21540	3.17130
F	2.41050	1.25810	5.53690
F	3.43530	3.66760	5.56020
F	2.27430	5.69270	4.17800
F	0.03100	5.21330	2.74870
F	-1.06050	2.79610	2.72880

3b-Zr

gas phase E = -9829.34
sovlation E = -11.6344

Atom	X	Y	Z
Zr	-0.17980	0.09510	-0.13240
C	2.11310	0.00830	-0.20390
H	2.67640	0.90150	-0.51950
H	2.51170	-0.88790	-0.70500
H	2.30150	-0.11540	0.88360
C	0.06390	-2.37710	-0.53480
C	0.44070	-2.14380	0.80750

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C	-0.70080	-1.67690	1.50580
C	-1.78500	-1.63010	0.59020
C	-1.31530	-2.07130	-0.66890
H	0.71290	-2.76570	-1.32040
H	1.42470	-2.32450	1.23310
H	-0.75950	-1.47120	2.57440
H	-2.81110	-1.34560	0.81480
H	-1.92300	-2.17670	-1.57280
C	-1.41080	1.48240	1.51200
C	-0.03380	1.48680	1.89150
C	0.69470	2.19280	0.90940
C	-0.21980	2.60790	-0.09420
C	-1.51780	2.17850	0.29080
H	-2.23770	1.07390	2.08450
H	0.36750	1.09120	2.82420
H	1.75730	2.42650	0.94600
H	0.00880	3.25350	-0.94620
H	-2.43990	2.40000	-0.25030
C	-0.21530	0.12880	-2.60530
C	1.01750	0.66050	-2.47010
H	1.16900	1.70630	-2.17980
H	1.91360	0.10370	-2.75770
H	-0.37640	-0.86820	-3.02770
H	-1.12230	0.75570	-2.46330
B	-3.95670	1.05020	-3.92380
C	-3.72750	-0.57200	-3.92770
H	-4.54390	-1.07820	-3.37960
H	-2.77030	-0.88490	-3.47500
H	-3.73480	-0.96680	-4.96080
C	-4.56610	1.45780	-2.47610
C	-5.65580	2.29050	-2.28280
C	-6.25540	2.47880	-1.05110
C	-5.76730	1.82940	0.06180
C	-4.66070	1.02090	-0.07830
C	-4.08960	0.87600	-1.32040
C	-2.52680	1.74880	-4.19630
C	-1.95680	2.75460	-3.43730
C	-0.69020	3.25700	-3.67150
C	0.07180	2.73590	-4.68940
C	-0.47420	1.76570	-5.50220
C	-1.74300	1.29920	-5.24260
C	-5.03410	1.35160	-5.08930
C	-6.27940	0.74840	-5.00620
C	-7.25600	0.85710	-5.97440
C	-6.99210	1.59520	-7.10860
C	-5.76480	2.20280	-7.24540
C	-4.81780	2.08370	-6.23980
F	-6.19180	2.97150	-3.29000
F	-7.30370	3.27860	-0.93180
F	-6.34340	1.98770	1.24900
F	-4.15210	0.39930	0.99490
F	-2.96100	0.12130	-1.35680
F	-2.59790	3.30480	-2.39660
F	-0.17310	4.20340	-2.87780
F	1.31850	3.15960	-4.88390
F	0.23510	1.27890	-6.51260
F	-2.21800	0.39160	-6.09640
F	-6.60540	0.03650	-3.92110
F	-8.44290	0.27440	-5.82440
F	-7.90580	1.70300	-8.06230
F	-5.50530	2.90370	-8.34510
F	-3.67520	2.74730	-6.45220

3c-Zr

gas phase E = -4079.85
solvation E = -33.2858

Atom	X	Y	Z
Zr	0.12250	0.17760	-0.20990
C	2.11520	-0.09080	0.74740
H	2.68740	0.74150	1.18160
H	2.77070	-0.95300	0.55980
H	1.34870	-0.41590	1.52970
C	0.22670	-1.86370	-1.68180
C	0.37970	-2.31050	-0.35230
C	-0.82890	-2.02930	0.34650
C	-1.73370	-1.44150	-0.57150
C	-1.07530	-1.31010	-1.81700
H	0.95880	-1.98730	-2.48290
H	1.24450	-2.83930	0.05210
H	-1.06070	-2.32810	1.36930
H	-2.77590	-1.20020	-0.37290
H	-1.53060	-0.95200	-2.74020
C	-1.87200	1.50720	0.46490
C	-1.03220	1.38740	1.60040
C	0.15130	2.13870	1.34750
C	0.05270	2.68180	0.05020
C	-1.19280	2.27930	-0.50600
H	-2.88960	1.13090	0.38100
H	-1.29960	0.91420	2.54570
H	0.96130	2.31530	2.05750
H	0.77780	3.35250	-0.41570
H	-1.60450	2.60040	-1.46250
C	1.13160	1.04580	-2.37200
C	2.27630	0.78270	-1.69620
H	2.81840	1.57060	-1.16650
H	2.80310	-0.16820	-1.81460
H	0.73170	0.32350	-3.09150
H	0.74450	2.06760	-2.43430

3d-Zr

gas phase E = -3322.34
solvation E = -33.5845

Atom	X	Y	Z
Zr	0.03560	-0.00950	0.04390
C	2.21180	0.00430	-0.00800
H	2.79510	0.93800	-0.02350
H	2.80590	-0.81530	-0.44140
H	2.06790	-0.26110	1.08910
C	0.26540	-2.13520	-1.20660
C	0.18030	-2.48970	0.15820
C	-1.11450	-2.12780	0.63270
C	-1.83610	-1.57660	-0.45240
C	-0.98010	-1.54630	-1.58220
H	1.10600	-2.34090	-1.87130
H	0.95470	-3.00520	0.73280
H	-1.51620	-2.34530	1.62320
H	-2.88300	-1.27760	-0.43670
H	-1.26910	-1.25020	-2.59220
C	-1.84330	1.58990	0.38530
C	-1.04750	1.63780	1.55380
C	0.21930	2.18930	1.19930
C	0.21230	2.45310	-0.18740
C	-1.06010	2.05800	-0.70130
H	-2.89030	1.29530	0.33830
H	-1.38300	1.40570	2.56570
H	1.03460	2.42160	1.88930
H	1.01320	2.93470	-0.75180
H	-1.41710	2.21950	-1.71970

3f-Zr

gas phase E = -11234.13
solvation E = -10.4393

Atom	X	Y	Z
Zr	1.23310	-0.90100	-2.78360
C	3.73800	-1.00610	-2.79490
C	3.39680	0.37080	-2.76750
C	2.72670	0.68060	-3.97290
C	2.66210	-0.50590	-4.75510
C	3.29600	-1.54340	-4.02730
H	4.27790	-1.55010	-2.01680
H	3.62460	1.07380	-1.96310
C	-1.22370	-1.46540	-2.87670
C	-0.76900	-1.25780	-4.20380
C	-0.40200	0.10720	-4.33330
C	-0.59790	0.73680	-3.07910
C	-1.12240	-0.23480	-2.18380
H	-1.60840	-2.39890	-2.46440
H	-0.73270	-2.00400	-4.99770
C	1.23910	-3.15580	-2.76690
H	2.37150	1.66710	-4.26680
H	2.25750	-0.59750	-5.76640
H	3.44090	-2.56510	-4.37570
H	-0.06980	0.59450	-5.24840
H	-0.44720	1.79220	-2.84950
H	-1.42590	-0.04750	-1.14770
H	0.41800	-3.53250	-2.12790
H	2.20050	-3.52250	-2.35920
H	1.10650	-3.57800	-3.78070
H	1.09570	0.20770	-0.93330
H	0.93500	-1.65200	-0.72110
C	1.46610	-0.71820	-0.40760
H	2.56030	-0.82270	-0.48500
B	1.10030	-0.41240	1.15090
C	-0.49300	-0.47030	1.36910
C	-1.25630	0.46800	2.03760
C	-2.61540	0.32350	2.24010
C	-3.25750	-0.80160	1.77570
C	-2.53670	-1.76760	1.11310
C	-1.18460	-1.59070	0.94290
C	1.70310	-1.54730	2.10950
C	1.68140	-1.32940	3.47520
C	2.19140	-2.22280	4.38810
C	2.71740	-3.41710	3.94030
C	2.70980	-3.69880	2.59560
C	2.20800	-2.76580	1.71040
C	1.75170	1.04790	1.35950
C	2.90930	1.33770	2.05740
C	3.46720	2.60220	2.09840
C	2.87600	3.63420	1.40830
C	1.73700	3.38720	0.67460
C	1.21460	2.11630	0.66580
F	-0.71110	1.57750	2.53130
F	-3.30670	1.25730	2.88170
F	-4.55560	-0.96410	1.96730
F	-3.15170	-2.85370	0.65510
F	-0.53870	-2.59350	0.32130
F	1.18630	-0.18230	3.94120
F	2.19750	-1.95420	5.68780
F	3.22430	-4.28740	4.80350
F	3.19140	-4.85850	2.15790
F	2.24870	-3.11730	0.41270
F	3.58100	0.39780	2.72170
F	4.58020	2.82440	2.78500
F	3.40080	4.85040	1.42960
F	1.16940	4.36930	-0.01790
F	0.12150	1.93080	-0.09850
C	2.49710	-5.21860	-5.51200
C	2.22150	-4.02940	-6.35150
C	0.92470	-3.59500	-6.58290
C	0.67100	-2.51160	-7.40610
C	1.71760	-1.83950	-8.00910
C	3.26330	-3.33830	-6.95740
C	3.01780	-2.25550	-7.77860
H	0.09390	-4.14540	-6.12570
H	-0.36140	-2.20120	-7.59950
H	1.52100	-0.99570	-8.67890
H	4.29500	-3.67020	-6.78800
H	3.85470	-1.73170	-8.25080

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H	2.92270	-6.03370	-6.12570
H	3.23030	-5.00140	-4.71560
H	1.58380	-5.60300	-5.03150

3g-Zr

gas phase E = -11210.70
solvation E = -16.8643

Atom	X	Y	Z
B	-1.16350	0.18360	0.01800
C	-0.18830	0.42130	-1.23950
C	-0.56030	1.31870	-2.22720
C	0.04430	1.40090	-3.45840
C	1.09300	0.55800	-3.75010
C	1.53010	-0.32290	-2.79000
C	0.90080	-0.36570	-1.55950
F	-1.57850	2.17370	-2.02310
F	-0.37410	2.27560	-4.37460
F	1.67560	0.60630	-4.94320
F	2.55250	-1.13030	-3.05720
F	1.40040	-1.24390	-0.68880
C	-2.59730	-0.16920	-0.67890
C	-1.47590	1.51900	0.87570
C	-0.85900	-1.12420	0.90790
C	-0.89420	2.75710	0.67210
C	-0.76940	-1.14650	2.28620
C	-1.38300	3.93070	1.21950
C	-0.83620	-2.30790	3.03290
C	-2.48970	3.89780	2.03410
C	-0.96260	-3.52090	2.39950
C	-3.06950	2.67930	2.30940
C	-1.00220	-3.55550	1.02370
C	-2.54770	1.53420	1.75300
C	-0.93950	-2.37600	0.31800
F	0.18290	2.89950	-0.09690
F	-0.64280	-0.01840	2.99220
F	-0.79600	5.09510	0.96080
F	-0.78430	-2.26520	4.36300
F	-2.98830	5.01490	2.55760
F	-1.03560	-4.64720	3.10330
F	-4.14250	2.62080	3.11720
F	-1.11220	-4.72570	0.39510
F	-3.15580	0.39470	2.11320
F	-0.98770	-2.49560	-1.01480
H	-2.48230	-0.96440	-1.43870
H	-3.31180	-0.52420	0.08370
H	-3.00300	0.72720	-1.18040
Zr	-7.86660	1.74490	0.37520
C	-8.58620	0.09100	-1.33610
C	-8.07030	1.20360	-2.06220
C	-8.90870	2.30910	-1.82280
C	-9.95410	1.88700	-0.95480
C	-9.76690	0.51080	-0.67790
H	-8.17280	-0.92070	-1.33230
H	-7.20640	1.19890	-2.72680
C	-7.07760	3.17750	2.30870
C	-8.43860	3.48410	2.06690
C	-8.52850	4.07480	0.77980
C	-7.21990	4.12580	0.22530
C	-6.32570	3.58150	1.17800
H	-6.66630	2.75550	3.22810
H	-9.26010	3.33940	2.76640
C	-8.90040	0.61180	2.03030
H	-8.80410	3.29630	-2.26880
H	-10.80140	2.49210	-0.63310
H	-10.43160	-0.12070	-0.09190
H	-9.42650	4.49680	0.32990
H	-6.93880	4.58860	-0.71920
H	-5.23600	3.53950	1.08790
H	-8.28930	0.74420	2.94350
H	-8.89910	-0.45750	1.74510
H	-9.93850	0.89250	2.27830
C	-5.72090	0.44550	0.91920
C	-5.45600	0.76940	-0.40850
C	-5.41710	-0.22790	-1.38460
C	-5.69440	-1.53120	-1.00320
C	-6.06530	-0.85310	1.26550
C	-6.03380	-1.84220	0.29980
H	-5.10370	1.77710	-0.66790
H	-5.60820	-2.33220	-1.74800
C	-5.00830	0.06400	-2.77070
H	-6.28100	-1.09740	2.30970
H	-6.23180	-2.88290	0.57810
H	-5.54130	1.18240	1.71590
H	-5.77390	-0.26060	-3.49910
H	-4.77970	1.13020	-2.92410
H	-4.08360	-0.49760	-3.00020

3h-Zr

gas phase E = -5476.13
solvation E = -33.0060

Atom	X	Y	Z
Zr	0.39580	0.26130	-0.32950
C	2.39820	1.38450	0.64700
C	1.42620	2.40970	0.47590
C	1.16780	2.54900	-0.90280
C	2.00590	1.63090	-1.59630
C	2.77250	0.92250	-0.63980
H	2.85070	1.07710	1.59260
H	1.00620	3.03740	1.26100
C	-1.34360	-1.28530	-1.31340
C	-0.45810	-0.91930	-2.35600
C	-0.59580	0.47460	-2.57350
C	-1.55650	0.97530	-1.65210
C	-2.03050	-0.12140	-0.89180
H	-1.51300	-2.30080	-0.94980
H	0.16370	-1.60220	-2.93160
C	1.62090	-1.63060	-0.50140
H	0.51020	3.28660	-1.35880
H	2.11460	1.55560	-2.67800
H	3.55740	0.20200	-0.85920
H	-0.12950	1.04700	-3.37360
H	-1.94430	1.99230	-1.62130å
H	-2.84020	-0.09020	-0.15910
H	0.93510	-2.48770	-0.35940
H	2.38620	-1.62470	0.29720
H	2.14690	-1.79380	-1.45800
C	-0.62670	-0.46100	1.90470
C	-1.01460	0.87440	2.00230
C	-0.35970	1.73890	2.87460
C	0.69020	1.23660	3.63250
C	0.48610	-0.91870	2.59590
C	1.12570	-0.06540	3.48070
H	-1.90010	1.23580	1.46800
H	1.18550	1.89550	4.35620
C	-0.80740	3.13670	3.03120
H	0.79800	-1.96220	2.49780
H	1.96170	-0.43360	4.08480
H	-1.24250	-1.17020	1.33520
H	0.03700	3.82090	3.21820
H	-1.36920	3.49270	2.15370
H	-1.47890	3.22130	3.90680