

Testing the Ability of DFT to Predict the Stereoselectivity of Group 4 Metallocenes for Propylene Polymerization

Naeimeh Bahri-Laleh,¹ Laura Falivene,² Luigi Cavallo^{2*}

¹Department of Polymerization Engineering, Iran Polymer and Petrochemical Institute, P.O. Box 14965/115, Tehran, Iran. ²Department of Chemistry and Biology, University of Salerno, Via Papa Giovanni Paolo II, Fisciano I-84084, Italy. **Email:** lcavallo@unisa.it

Computational details

DFT calculations were performed with the Gaussian03 package [1] using the BP86 level of theory [2-4]. In all cases the electronic configuration of the molecular systems was described with the standard triple- ζ basis set augmented with one polarization functions of Ahlrichs and coworkers (TZVP keyword in Gaussian 03) for H, C, P, Si and Cl [5]. For Zr we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated valence basis set (SDD keywords in Gaussian03) [6].

Characterization of the located stationary points as minima or transition state was performed by frequency calculations. Total energies and optimized xyz **coordinates** are provided below.

71	C	-2.308808	1.041065	0.923274
1-re SCF Done: -1101.07723648 A.U.	C	-2.866487	0.022399	0.077753
Zr -0.246918 -0.197824 0.115314	C	-2.521518	-1.228346	0.685020
C -1.821944 -1.001060 1.918489	C	0.183397	-2.669329	0.223245
C 0.829529 -2.067790 1.352184	C	0.872910	-2.284369	-0.964365
C -1.686147 0.415246 2.063098	C	2.001285	-1.474504	-0.593732

C	1.943167	-1.321034	0.841029	H	2.164767	-0.439852	-3.252588
H	-2.807413	-2.217928	0.303752	C	-3.585635	-0.784966	-2.226053
H	-2.407206	2.123721	0.776202	H	-3.596011	-1.842365	-1.888905
H	-1.232464	0.938561	2.915834	H	-4.355062	-0.684229	-3.021049
H	0.626205	-2.625948	-1.977037	H	-2.590287	-0.586720	-2.672682
H	-0.694677	-3.325153	0.256635	C	4.193295	-2.439732	-1.216508
H	2.665086	-0.771740	1.461224	H	3.699370	-3.408423	-1.437537
C	0.316027	-2.118357	2.777954	H	5.104081	-2.363351	-1.849427
C	-1.236593	-2.068214	2.824776	H	4.512821	-2.458696	-0.153989
H	0.737374	-1.260173	3.344766	C	0.896266	2.006457	0.980396
H	0.674658	-3.035558	3.299866	H	0.163196	2.795463	1.235884
H	-1.647959	-3.054160	2.520953	H	0.755005	1.199981	1.736631
H	-1.571079	-1.910407	3.873480	C	2.349525	2.491858	1.123443
C	-3.884070	0.184660	-1.058510	H	3.006343	1.784557	0.571939
C	3.230657	-1.247794	-1.490865	C	2.623991	3.903333	0.569059
C	-5.282979	-0.156291	-0.470421	H	1.988719	4.661393	1.078636
H	-5.321458	-1.201724	-0.100726	H	3.682555	4.192337	0.742035
H	-5.530335	0.511893	0.380637	H	2.438082	3.984709	-0.520351
H	-6.072343	-0.036269	-1.243717	C	2.781836	2.437349	2.607315
C	2.862372	-1.261748	-2.991138	H	3.844281	2.741118	2.733619
H	3.776226	-1.135081	-3.608882	H	2.161587	3.121337	3.227183
H	2.391770	-2.219486	-3.293709	H	2.671208	1.415310	3.028417

H	-1.125171	1.165872	-2.347237	C	-0.958271	-2.633840	0.396194
C	-0.131939	0.966171	-1.909353	C	-1.771961	-1.794036	1.210174
C	0.484739	2.055360	-1.185559	C	-2.557865	-0.943451	0.365873
H	0.521248	0.358735	-2.558540	C	-2.161679	-1.231949	-0.991741
H	1.577271	2.146268	-1.318799	C	1.636967	-0.569965	-1.958171
C	-0.244276	3.388883	-1.206081	C	2.349104	0.286636	-1.048874
H	-1.323814	3.257352	-0.992730	C	2.743311	-0.462648	0.102755
H	0.156672	4.139956	-0.499874	C	2.207932	-1.781338	-0.069303
H	-0.166718	3.816919	-2.230694	H	-2.596204	-0.793844	-1.901324
C	3.981606	0.061317	-1.175598	H	-1.816435	-1.835700	2.305529
H	3.361246	0.951666	-1.403178	H	-0.277014	-3.409077	0.769369
H	4.286987	0.115690	-0.110405	H	2.606047	1.331939	-1.246056
H	4.906336	0.130124	-1.786802	H	1.295524	-0.297425	-2.966315
C	-3.930078	1.634191	-1.586547	H	2.351248	-2.626360	0.617579
H	-4.197298	2.352510	-0.783692	C	0.955226	-3.121174	-1.953197
H	-2.959576	1.949067	-2.018800	C	-0.557744	-2.936559	-2.190162
H	-4.698265	1.727150	-2.382741	H	1.126157	-3.969536	-1.256617
<hr/>				H	1.468395	-3.397481	-2.901507
71				H	-0.726443	-2.281435	-3.071804
1-si SCF Done: -1101.08546703 A.U.				H	-1.040332	-3.910950	-2.434982
Zr	0.065678	-0.383275	-0.038081	C	-3.871095	-0.261366	0.784163
C	-1.205080	-2.301165	-0.980133	C	3.810978	-0.062533	1.129848
C	1.570293	-1.873806	-1.356194				

C	-3.920848	-0.003370	2.306129	H	-4.080033	0.915887	-1.074902
H	-3.877620	-0.950816	2.881456	H	-5.167305	1.423381	0.252146
H	-3.081015	0.635339	2.646745	C	-0.613851	1.981274	-0.877240
H	-4.868546	0.506022	2.580301	H	-1.710926	1.921923	-0.759619
C	3.830295	1.459684	1.393836	H	-0.343962	1.306786	-1.726767
H	4.655680	1.716686	2.090727	C	-0.199397	3.411087	-1.269201
H	3.999830	2.033508	0.459227	C	-1.150236	3.953870	-2.360726
H	2.884021	1.815345	1.847881	H	-2.208897	3.930007	-2.026874
C	-5.008839	-1.264758	0.433256	H	-0.902449	5.004508	-2.627105
H	-4.851202	-2.238252	0.942088	H	-1.079659	3.346452	-3.289607
H	-5.995478	-0.862975	0.751407	H	1.302116	0.636446	2.333082
H	-5.051530	-1.457551	-0.658539	C	0.267963	0.785533	1.986610
C	5.181229	-0.462614	0.508951	C	-0.016751	1.992126	1.245460
H	5.357165	0.069644	-0.448741	H	-0.493541	0.463727	2.719453
H	6.012779	-0.210780	1.202360	H	0.869615	2.588729	0.965040
H	5.222757	-1.551934	0.301784	C	-1.186766	2.832327	1.730785
C	3.647801	-0.826278	2.463763	C	1.260646	3.551766	-1.731111
H	2.677281	-0.610693	2.955073	H	-0.318330	4.083550	-0.387779
H	3.713113	-1.923601	2.313494	H	1.479693	4.600315	-2.024102
H	4.457290	-0.542756	3.169006	H	1.979421	3.279569	-0.931239
C	-4.144651	1.054852	0.024130	H	1.469688	2.909434	-2.614489
H	-3.431052	1.851199	0.310522	H	-1.564822	3.578240	1.004873

H	-0.858374	3.391921	2.634821	C	-1.590009	-3.092355	1.455590
H	-2.034052	2.191756	2.042422	H	0.294679	-2.785055	2.524301
<hr/>							
65							
2-re SCF Done: -1022.53054779 A.U.							
Zr	-0.266435	-0.303982	-0.054857	H	0.226154	-4.322257	1.631947
C	-1.982809	-1.667442	1.120585	H	-1.973139	-3.763513	0.657772
C	0.637123	-2.560220	0.416148	H	-2.084393	-3.424897	2.395616
C	-1.757271	-0.502464	1.932398	C	-3.719164	0.993268	-0.982185
C	-2.293917	0.630948	1.225229	C	3.316287	-0.442167	-1.277258
C	-2.870000	0.188480	-0.006642	H	3.380626	0.499642	-0.687401
C	-2.630063	-1.223531	-0.085493	C	-5.084316	0.305131	-1.210901
C	0.221690	-2.609134	-0.957727	H	-4.969418	-0.725032	-1.604539
C	1.090354	-1.779524	-1.722018	H	-5.659834	0.240635	-0.262795
C	2.065415	-1.199566	-0.847842	H	-5.693165	0.877867	-1.942210
C	1.766349	-1.675061	0.486258	C	3.307761	-0.052258	-2.765161
H	-2.965508	-1.883648	-0.897229	H	4.213340	0.537296	-3.017999
H	-2.305286	1.661674	1.601734	H	3.306106	-0.951457	-3.417558
H	-1.337064	-0.488269	2.947427	H	2.422449	0.560836	-3.031682
H	1.026314	-1.629170	-2.806758	C	4.581384	-1.267444	-0.945468
H	-0.614139	-3.194716	-1.362133	H	4.580213	-2.227643	-1.504340
H	2.352608	-1.472713	1.393343	H	5.501793	-0.710464	-1.222553
C	-0.055167	-3.245429	1.575310	H	4.642938	-1.509611	0.135055
				C	0.847686	1.669342	1.229161
				H	0.243034	2.548136	1.522283

H	0.470117	0.825694	1.855844
C	2.332405	1.859817	1.584732
H	2.925844	1.079348	1.056680
C	2.921900	3.226813	1.189632
H	2.385489	4.055386	1.702562
H	3.990218	3.294621	1.486444
H	2.872132	3.417834	0.098704
C	2.546352	1.623385	3.098075
H	3.618276	1.719744	3.378716
H	1.973690	2.362820	3.699692
H	2.206937	0.610619	3.403003
H	-1.232936	1.630553	-2.081567
C	-0.230614	1.263032	-1.794247
C	0.541734	2.118670	-0.919825
H	0.310949	0.779551	-2.625187
H	1.635280	2.069470	-1.070302
C	0.032154	3.532478	-0.694607
H	-1.035617	3.532647	-0.393827
H	0.602485	4.103616	0.061904
H	0.097395	4.086490	-1.657524
H	-3.196226	1.013130	-1.966448
C	-3.927430	2.447682	-0.530832

H	-4.465890	2.491923	0.439891
H	-2.966102	2.986301	-0.408182
H	-4.529977	3.007158	-1.275865

65

2-si Done: -1022.53783009 A.U.

Zr	0.031111	-0.482466	0.127044
C	-1.323000	-2.497616	-0.341782
C	1.437617	-2.276996	-0.863138
C	-1.270059	-2.350045	1.092343
C	-2.071916	-1.212456	1.436955
C	-2.629483	-0.649510	0.246324
C	-2.131879	-1.423939	-0.853748
C	1.341189	-1.265306	-1.879780
C	2.076772	-0.125803	-1.435587
C	2.640641	-0.400365	-0.146327
C	2.215083	-1.727359	0.213930
H	-2.391264	-1.285220	-1.911506
H	-2.262022	-0.861278	2.459719
H	-0.777050	-3.025677	1.803768
H	2.213102	0.798075	-2.010411
H	0.827026	-1.359479	-2.845899
H	2.504104	-2.273915	1.120221

C	0.834090	-3.663997	-0.894955	H	-4.517039	-0.033717	-1.797107
C	-0.678974	-3.584346	-1.176214	H	-4.807859	1.650203	-1.263560
H	1.009125	-4.147889	0.089684	C	-0.526951	1.981700	-0.472881
H	1.344401	-4.306680	-1.648293	H	-1.619903	2.007165	-0.309933
H	-0.850864	-3.351501	-2.249052	H	-0.349367	1.352506	-1.383581
H	-1.167105	-4.569516	-0.995710	C	-0.005709	3.397341	-0.771289
C	-3.691542	0.440137	0.182236	C	-0.933924	4.122644	-1.769942
C	3.639333	0.474397	0.606073	H	-1.976052	4.177745	-1.390865
C	-4.950606	0.008150	0.968823	H	-0.588167	5.161887	-1.961008
H	-4.715093	-0.224850	2.027042	H	-0.961170	3.593507	-2.747589
H	-5.716574	0.812603	0.959360	H	1.609523	0.394992	2.362658
H	-5.403036	-0.901052	0.518571	C	0.534117	0.548152	2.180192
C	4.745852	0.988982	-0.340830	C	0.145280	1.801855	1.580381
H	4.331286	1.576083	-1.185193	H	-0.108118	0.160508	2.990391
H	5.457078	1.644484	0.205090	H	0.981887	2.472626	1.316336
H	5.321153	0.142047	-0.771712	C	-1.038813	2.526428	2.201735
C	4.264495	-0.253029	1.809929	C	1.445633	3.428131	-1.277689
H	3.499957	-0.589942	2.539795	H	-0.032570	3.992795	0.172971
H	4.832799	-1.148905	1.480682	H	1.802918	4.472089	-1.401847
H	4.967949	0.415452	2.348231	H	2.140585	2.916761	-0.580092
C	-4.064371	0.826368	-1.259229	H	1.532473	2.929800	-2.268115
H	-3.182012	1.163264	-1.840986	H	-1.431408	3.366576	1.594874

H	-0.718933	2.947398	3.180495	C	-0.280554	3.985934	-0.517086
H	-1.873803	1.825962	2.409806	C	-3.163377	-1.761961	2.256003
H	3.106003	1.370950	1.001987	H	-3.637141	-1.211124	3.095854
H	-3.293640	1.351660	0.685842	H	-3.832575	-2.605584	1.982998
<hr/>				H	-2.213047	-2.195197	2.626578
62				C	-4.653064	-0.164651	0.106947
3-re SCF Done: -1234.63438237 A.U.				H	-5.263316	0.248239	0.938528
Zr	0.056161	0.216085	-0.328876	H	-4.626774	0.596389	-0.698151
C	-1.775135	-1.421150	-0.516780	H	-5.177126	-1.060282	-0.289154
C	-1.867900	0.906725	1.049212	Si	-2.933617	-0.629523	0.754016
C	-1.509900	-0.972704	-1.878501	H	1.941371	-3.409630	-0.296747
C	-0.242347	-1.518120	-2.266163	H	2.303149	-2.763239	-1.933806
C	0.305980	-2.282510	-1.196337	H	1.209903	-4.161190	-1.740501
C	-0.619010	-2.195921	-0.102439	H	0.804081	4.214350	-0.502699
C	-0.701171	1.075015	1.898384	H	-0.799506	4.852052	-0.049975
C	0.054770	2.179213	1.363403	H	-0.608280	3.940381	-1.576029
C	-0.613983	2.720503	0.224462	C	-0.406580	0.405095	3.217689
C	-1.765322	1.907008	0.000508	H	0.683197	0.382038	3.426255
H	-0.508227	-2.726604	0.854342	H	-0.885767	0.956619	4.058646
H	0.215926	-1.402590	-3.258952	H	-0.780188	-0.636360	3.260882
H	0.978744	2.579065	1.805694	C	-2.449858	-0.271319	-2.827834
H	-2.503069	2.082546	-0.795607	H	-3.129598	0.434856	-2.313556
C	1.505127	-3.187385	-1.290003				

H -1.888756 0.302468 -3.593639
H -3.093518 -1.005315 -3.364570
C 2.372971 -0.109850 0.766534
H 1.517730 -0.675331 1.221525
C 2.509433 1.031471 -1.136119
C 1.371866 1.271882 -1.985651
H 1.058242 2.322186 -2.115192
H 1.289392 0.665424 -2.902608
H 3.185306 0.221546 -1.463919
H 2.589934 0.728329 1.456457
C 3.225280 2.249900 -0.576767
H 2.501167 2.999758 -0.201551
H 3.939183 2.026413 0.237397
H 3.795870 2.732703 -1.401672
C 3.556651 -1.088596 0.657611
H 3.456114 -1.658616 -0.294482
C 3.510227 -2.120457 1.807952
H 4.321422 -2.875138 1.712082
H 3.633182 -1.619170 2.792801
H 2.542583 -2.664826 1.834290
C 4.945240 -0.419597 0.638558
H 5.100481 0.201911 1.548103

H 5.747444 -1.187762 0.623478
H 5.100611 0.229437 -0.245782

62

3-si SCF Done: -1234.64229206 A.U.

Zr 0.068770 0.169562 0.248414
C -2.019955 1.146927 -0.606729
C -1.724279 -1.520829 0.202823
C -1.551320 2.040348 0.443429
C -0.370556 2.695675 -0.055783
C -0.084710 2.241356 -1.378212
C -1.073437 1.261690 -1.702675
C -0.633160 -2.122556 -0.545682
C 0.416977 -2.411315 0.389195
C 0.021622 -2.017319 1.702532
C -1.281593 -1.432311 1.585952
H -1.138009 0.734115 -2.665526
H 0.194201 3.469042 0.483438
H 1.363869 -2.910795 0.138047
H -1.881279 -1.070431 2.433225
C 0.969077 2.777188 -2.309425
C 0.757659 -2.309409 2.982258
C -3.846913 -0.891136 -2.111965

H	-4.265936	-1.918680	-2.067076	C	2.458810	0.082376	-0.716630
H	-4.675746	-0.196076	-2.365488	H	1.632799	-0.303110	-1.374827
H	-3.117391	-0.858000	-2.945332	H	2.819630	1.004493	-1.208873
C	-4.521719	-0.279550	0.811554	C	3.552384	-1.001993	-0.648874
H	-5.124122	-1.212064	0.767875	H	3.321982	-1.678510	0.210003
H	-4.175005	-0.156013	1.857006	C	3.554098	-1.872930	-1.924221
H	-5.194268	0.571039	0.571955	H	3.789261	-1.259490	-2.821157
Si	-3.103365	-0.396460	-0.440065	H	4.312916	-2.683187	-1.862451
H	1.338470	1.999451	-3.009101	H	2.566126	-2.348644	-2.096882
H	1.840636	3.189681	-1.762465	C	4.968740	-0.437263	-0.420200
H	0.552409	3.602401	-2.927950	H	5.721342	-1.253934	-0.406886
H	1.858116	-2.227720	2.865193	H	5.250268	0.260468	-1.239556
H	0.543032	-3.346151	3.324670	H	5.065399	0.112088	0.537633
H	0.447028	-1.628538	3.800640	H	3.132913	0.067319	1.555478
C	-0.646166	-2.566885	-1.988059	C	2.458763	0.905515	1.306398
H	0.382154	-2.751251	-2.360701	C	1.266842	0.981372	2.111296
H	-1.213219	-3.518014	-2.105649	H	1.158378	0.241127	2.919885
H	-1.117113	-1.826529	-2.664740	H	0.905785	1.989841	2.380765
C	-2.252299	2.420400	1.723633	C	3.183819	2.208721	1.011607
H	-2.868354	1.595999	2.130314	H	3.660800	2.565018	1.951735
H	-1.524790	2.714354	2.508497	H	3.977730	2.124941	0.244565
H	-2.933334	3.288055	1.564165	H	2.473535	2.997251	0.690585

80			H	-4.463732	3.428086	-1.391947	
4-re SCF Done: -1470.30912624 A.U.			C	3.865976	0.465737	-1.963929	
Zr	-0.116082	0.067351	-0.171347	H	4.941906	0.648239	-2.171686
C	-1.798858	-1.109330	1.208658	H	3.343369	0.411517	-2.941514
C	0.331507	-2.357890	-0.120682	H	3.470271	1.346999	-1.420456
C	-1.490712	0.099626	1.943296	C	-5.165967	1.143390	-0.134624
C	-2.046134	1.203859	1.195983	H	-5.190394	1.549183	0.898027
C	-2.740233	0.714356	0.043468	H	-5.991225	1.615062	-0.710949
C	-2.522950	-0.695682	0.023728	H	-5.364365	0.053721	-0.073686
C	0.110036	-2.052056	-1.527135	C	4.291424	-2.011987	-1.961387
C	1.248484	-1.321119	-1.987089	H	3.820538	-2.101896	-2.961847
C	2.198071	-1.169923	-0.931845	H	5.382674	-1.858983	-2.108259
C	1.605962	-1.764198	0.235813	H	4.146752	-2.976232	-1.431303
H	-2.931709	-1.377822	-0.732916	C	4.444273	-0.742293	0.188903
H	-2.011722	2.251963	1.524467	H	4.013316	0.022363	0.862834
H	1.395805	-1.001563	-3.028609	H	4.430475	-1.713272	0.725748
H	2.092973	-1.858981	1.215645	H	5.507359	-0.477309	0.009051
C	-3.794894	1.428373	-0.814204	C	-3.832747	0.865591	-2.253930
C	3.680451	-0.833671	-1.148716	H	-2.860460	0.998905	-2.770134
C	-3.602681	2.958099	-0.871634	H	-4.075158	-0.216889	-2.265204
H	-3.546462	3.406106	0.142254	H	-4.614643	1.382892	-2.849203
H	-2.686816	3.241766	-1.425849	C	-2.170641	-4.174508	0.688498

H	-1.625995	-5.119131	0.476605	H	1.755725	2.612089	-1.140863
H	-2.881146	-4.368712	1.520227	H	0.510211	2.555276	1.645485
H	-2.767393	-3.919093	-0.209619	C	2.678910	2.384179	1.296364
C	-0.119233	-3.318806	2.806922	H	3.315332	1.868030	0.542850
H	0.348669	-4.318666	2.682763	C	3.210103	1.971791	2.690102
H	0.674123	-2.613467	3.126260	H	4.275716	2.261319	2.822120
H	-0.860785	-3.392226	3.630203	H	2.624831	2.466640	3.495650
Si	-0.958744	-2.805487	1.187652	H	3.135394	0.875871	2.852852
C	-0.919694	0.210999	3.334177	C	2.909499	3.896687	1.108684
H	-0.356097	1.156363	3.474851	H	2.285858	4.489370	1.813945
H	-1.732993	0.202380	4.094952	H	3.970219	4.151546	1.317865
H	-0.239343	-0.628196	3.576779	H	2.689929	4.248776	0.081434
C	-0.947960	-2.607832	-2.449292	C	0.015707	3.839567	-0.543343
H	-1.117282	-1.939295	-3.317989	H	-1.033854	3.679359	-0.234123
H	-0.632613	-3.598526	-2.848841	H	0.535556	4.366849	0.276200
H	-1.923795	-2.763957	-1.950504	H	-0.002597	4.522994	-1.422285
C	1.228963	1.892007	1.126813	<hr/>			
H	1.169334	0.898163	1.634877	80			
H	0.515741	1.242440	-2.708486	4-si SCF Done: -1470.31731032 A.U.			
C	-0.054069	1.691798	-1.878305	Zr	-0.019526	-0.063705	-0.249589
C	0.669627	2.535145	-0.962432	C	-1.239106	-1.875625	0.891423
H	-1.069125	2.021279	-2.158093	C	1.270975	-2.162325	-0.293092
				C	-1.196445	-0.788663	1.852724

C	-2.075388	0.238311	1.369198	H	-5.006743	0.478205	1.467168
C	-2.689336	-0.174303	0.144639	H	-6.097441	0.423361	0.038916
C	-2.124167	-1.450697	-0.178829	H	-5.211492	-1.053238	0.558361
C	1.282962	-1.638806	-1.649641	C	5.157517	-0.364870	-0.138473
C	2.149232	-0.485416	-1.644297	H	5.245110	-0.707986	-1.190132
C	2.694856	-0.286329	-0.336249	H	6.090350	0.178538	0.126320
C	2.098317	-1.277534	0.501478	H	5.087195	-1.265363	0.505617
H	-2.409905	-2.067232	-1.040235	C	3.863533	1.013409	1.523904
H	-2.297011	1.168685	1.910841	H	2.992166	1.670677	1.717843
H	2.409054	0.093821	-2.540915	H	3.801985	0.150278	2.218282
H	2.316029	-1.414372	1.569536	H	4.782943	1.578842	1.785209
C	-3.952025	0.438358	-0.479907	C	-4.242038	-0.145063	-1.881198
C	3.918279	0.557989	0.047450	H	-3.413347	0.040852	-2.594534
C	-3.887151	1.979918	-0.563359	H	-4.411301	-1.240725	-1.837912
H	-3.679679	2.434830	0.427287	H	-5.160421	0.314061	-2.303871
H	-3.102273	2.320722	-1.267246	C	-0.740904	-4.645084	-0.471565
H	-4.857518	2.388278	-0.917272	H	0.052551	-5.340765	-0.818169
C	4.098092	1.790320	-0.863106	H	-1.463887	-5.229539	0.136432
H	5.030137	2.331691	-0.595579	H	-1.277412	-4.273581	-1.367172
H	4.180464	1.502818	-1.931759	C	0.741783	-4.040898	2.145610
H	3.255611	2.502367	-0.765952	H	1.476471	-4.825694	1.865464
C	-5.135800	0.048850	0.452334	H	1.261559	-3.309799	2.796538

H -0.056401 -4.522447 2.749718
Si 0.006839 -3.260112 0.582167
C -0.542971 -0.792294 3.213430
H -0.449179 0.236272 3.617231
H -1.147442 -1.377410 3.943056
H 0.470818 -1.239179 3.202482
C 0.726328 -2.278525 -2.897159
H 0.516451 -1.519773 -3.678986
H 1.450471 -3.005884 -3.331749
H -0.215075 -2.829677 -2.707634
C 0.496850 2.347098 0.536247
H 0.683542 1.527602 1.280987
H 1.496078 2.740750 0.276808
C -0.379875 3.416680 1.217586
H -1.451607 3.163030 1.037090
C -0.167148 3.419963 2.747271
H 0.882589 3.684085 3.000581
H -0.830010 4.158500 3.248888
H -0.375248 2.424308 3.191967
C -0.151944 4.840164 0.671527
H 0.907076 5.150945 0.810536
H -0.390947 4.931241 -0.406813

H -0.786471 5.575129 1.210760
H -0.048925 0.783732 -3.050008
C -0.649873 1.116856 -2.185663
C -0.238686 2.329140 -1.530096
H -1.731563 0.948590 -2.304422
H -1.062306 2.956040 -1.146167
C 0.875267 3.127084 -2.185596
H 0.458282 3.617204 -3.093798
H 1.306027 3.923116 -1.547774
H 1.699139 2.467610 -2.522128

68

5-re SCF Done: -1313.19353240 A.U.

Zr 0.150301 0.271071 -0.255104
C -1.865456 0.719013 1.092547
C -1.566619 -1.443203 -0.702996
C -0.751532 0.653005 2.038104
C 0.050815 1.821060 1.827775
C -0.521061 2.624716 0.801705
C -1.687033 1.942601 0.312804
C -1.248600 -0.821959 -1.991687
C 0.062453 -1.263459 -2.358851
C 0.579081 -2.135270 -1.361091

C	-0.402783	-2.237127	-0.315563	H	-0.901371	4.748125	0.807304
H	0.944680	2.083130	2.412596	H	0.830207	4.326425	0.909079
H	0.571008	-1.013675	-3.301270	H	-0.043837	4.196589	-0.652787
C	-0.130945	4.032429	0.442416	H	2.299304	-3.225937	-0.552254
C	1.803176	-2.997179	-1.515487	H	2.552849	-2.534201	-2.189035
C	-4.546502	-0.391649	-0.322632	H	1.520264	-3.974170	-1.968742
H	-5.080457	-1.352486	-0.488054	C	-2.665051	2.602084	-0.628364
H	-5.172566	0.225507	0.356626	H	-3.481474	1.924721	-0.935308
H	-4.487065	0.121396	-1.300368	H	-3.148432	3.476186	-0.133969
C	-3.369487	-1.949453	1.921777	H	-2.175026	2.982143	-1.549346
H	-3.726974	-2.917714	1.511098	C	-0.312451	-3.247930	0.800650
H	-2.572988	-2.159086	2.658808	H	-0.622125	-4.256911	0.442880
H	-4.216675	-1.487041	2.473109	H	0.721664	-3.349039	1.190167
Si	-2.878285	-0.780720	0.504874	H	-0.968854	-3.003398	1.655470
C	-0.532592	-0.305388	3.185837	C	2.553865	0.033814	0.695201
H	0.452095	-0.116769	3.660361	H	1.765489	-0.619055	1.156618
H	-1.307501	-0.174388	3.973991	C	2.490554	1.377781	-1.070928
H	-0.549672	-1.372189	2.887162	C	1.277145	1.658044	-1.793955
C	-2.158290	-0.091220	-2.948937	H	1.158874	1.193220	-2.786609
H	-1.563612	0.467404	-3.700344	H	0.889969	2.690394	-1.736397
H	-2.807513	-0.806827	-3.503778	H	2.778644	0.817737	1.442754
H	-2.825119	0.636564	-2.454293	H	3.168272	0.650391	-1.552639

C	3.776235	-0.861155	0.416723	C	-1.254147	2.106804	-0.438161
H	3.620880	-1.373275	-0.559894	C	-1.440156	-1.383580	-1.565521
C	3.198486	2.554668	-0.421397	C	-0.221589	-2.130098	-1.677827
H	2.478300	3.209405	0.106028	C	0.171656	-2.611772	-0.396935
H	3.993809	2.271778	0.292454	C	-0.796961	-2.154433	0.559268
H	3.668401	3.167442	-1.223113	H	1.389747	2.431878	1.629529
C	5.122186	-0.114836	0.324172	H	0.297786	-2.343657	-2.622652
H	5.955548	-0.835561	0.183031	C	0.760921	3.705128	-0.958878
H	5.164976	0.599752	-0.521154	C	1.295040	-3.572165	-0.113999
H	5.330743	0.450808	1.259173	C	-4.531498	0.262440	-0.368453
C	3.893260	-1.964572	1.493465	H	-5.228281	-0.594575	-0.244622
H	2.964458	-2.568539	1.569875	H	-5.039159	1.167130	0.029199
H	4.732158	-2.660596	1.273510	H	-4.374291	0.404263	-1.453498
H	4.079475	-1.519908	2.495478	C	-3.666086	-0.547700	2.356480

68

5-si SCF Done: -1313.20196591 A.U.

Zr	0.168618	0.033600	-0.333908	H	-4.378604	0.249517	2.660107
C	-1.670887	1.298795	0.709871	Si	-2.965459	-0.096651	0.646914
C	-1.825038	-1.396457	-0.151131	C	-0.565976	0.858065	3.109506
C	-0.578911	1.346967	1.680132	H	0.430629	1.027067	3.565815
C	0.450611	2.167991	1.122188	H	-1.306193	1.414966	3.726098
C	0.048220	2.651590	-0.155099	H	-0.795865	-0.219219	3.220532

C	-2.236610	-0.937755	-2.768465	H	3.375805	1.562234	0.871295
H	-1.583055	-0.880827	-3.663067	C	3.608279	0.394008	2.666614
H	-3.050499	-1.662706	-2.999379	H	2.606865	0.635256	3.080034
H	-2.709612	0.054652	-2.648604	H	3.862641	-0.638075	2.992462
H	0.394391	4.719161	-0.681334	H	4.342762	1.085248	3.134579
H	1.855551	3.694409	-0.779385	C	5.059233	0.241658	0.616388
H	0.592995	3.597306	-2.050153	H	5.164762	0.404268	-0.474971
H	1.815691	-3.352009	0.841189	H	5.787036	0.912991	1.119632
H	2.052885	-3.568909	-0.922514	H	5.368491	-0.804797	0.832940
H	0.905784	-4.611771	-0.033074	C	2.565081	0.202441	-1.609493
C	-2.098348	2.571452	-1.599490	C	1.361253	0.599276	-2.293011
H	-3.017447	1.970774	-1.720723	H	3.206410	1.036875	-1.275060
H	-2.426879	3.625534	-1.448487	H	1.030718	-0.035707	-3.133799
H	-1.545199	2.538465	-2.561296	H	1.219907	1.677523	-2.468570
C	-0.826496	-2.648929	1.984286	C	3.339878	-0.969791	-2.189572
H	-1.150461	-3.714469	2.018909	H	4.134594	-1.364860	-1.527605
H	0.170908	-2.602402	2.470590	H	2.662989	-1.806741	-2.455829
H	-1.537013	-2.085363	2.614749	H	3.825122	-0.633942	-3.133118
C	2.569048	-0.415760	0.488942	<hr/>			
H	1.741251	-0.561387	1.235789	74			
H	2.967397	-1.427704	0.290870	6-re SCF Done: -1140.35962966 A.U.			
C	3.628429	0.504480	1.126692	Zr	-0.181439	-0.072694	-0.159546
				C	-1.572349	-1.703652	0.993054

C	0.429244	-2.418993	-0.022260	H	4.987532	0.810923	-1.793049
C	-1.396330	-0.609765	1.915527	H	3.465328	0.460895	-2.667127
C	-2.171605	0.500612	1.427588	H	3.430761	1.446690	-1.171781
C	-2.848472	0.113730	0.230272	C	-5.315094	0.259001	0.295058
C	-2.423850	-1.223034	-0.067022	H	-5.290933	0.494062	1.379254
C	0.289356	-2.137804	-1.434241	H	-6.234991	0.710091	-0.136113
C	1.416914	-1.360562	-1.838011	H	-5.389080	-0.843110	0.189964
C	2.269765	-1.141290	-0.715562	C	4.498383	-1.869034	-1.523773
C	1.627445	-1.750668	0.422602	H	4.125823	-2.022445	-2.557328
H	-2.782901	-1.822227	-0.912306	H	5.586219	-1.647365	-1.579069
H	-2.275937	1.465253	1.941224	H	4.368505	-2.823528	-0.972629
H	-0.835155	-0.628495	2.858413	C	4.372741	-0.520888	0.581753
H	1.621843	-1.043130	-2.869281	H	3.834820	0.235581	1.185684
H	-0.495338	-2.509063	-2.104929	H	4.375824	-1.471788	1.153476
H	2.049175	-1.805989	1.433341	H	5.428156	-0.189924	0.484626
C	-4.048941	0.807036	-0.424964	C	-4.157341	0.471304	-1.929874
C	3.740185	-0.710659	-0.813531	H	-3.258439	0.801119	-2.488626
C	-4.015217	2.338171	-0.245112	H	-4.282185	-0.617797	-2.100419
H	-3.939346	2.629544	0.822882	H	-5.042149	0.975529	-2.372520
H	-3.162677	2.791582	-0.787460	C	-1.435757	-4.138722	0.230180
H	-4.945974	2.792357	-0.645306	H	-0.751491	-5.003911	0.106301
C	3.911030	0.573109	-1.657055	H	-2.291794	-4.454956	0.862356

H	-1.835161	-3.886865	-0.772253	H	2.309972	4.233654	-0.098855
C	-0.154378	-3.400587	2.256810	H	1.775619	4.676614	1.556375
H	0.544574	-4.255098	2.143419	C	2.582154	2.270585	2.792639
H	0.391015	-2.588306	2.776753	H	2.481535	1.197698	3.062329
H	-0.990540	-3.717744	2.913849	H	3.633403	2.572047	2.994796
C	-0.690254	-2.958465	0.883434	H	1.928033	2.849249	3.481035
C	0.758543	2.027229	1.057136	<hr/>			
H	0.617696	1.117782	1.693953	74			
C	0.313825	2.425141	-1.114205	6-si SCF Done: -1140.36882966 A.U.			
C	-0.360890	1.462709	-1.943340	Zr	-0.015534	-0.185866	-0.232112
H	0.226547	0.987174	-2.747403	C	-1.112093	-2.088225	0.792296
H	-1.404484	1.689860	-2.223779	C	1.058942	-2.352211	-0.083907
C	-0.384804	3.748319	-0.860092	C	-1.111347	-1.057871	1.802862
H	0.112418	4.387379	-0.108458	C	-2.048984	-0.050374	1.401556
H	-0.419686	4.315672	-1.817149	C	-2.653830	-0.432030	0.164901
H	-1.432186	3.591043	-0.535728	C	-2.032071	-1.664188	-0.239249
H	-0.002925	2.755190	1.398143	C	1.076627	-1.967912	-1.479627
H	1.402352	2.514369	-1.278119	C	2.051036	-0.921539	-1.628352
C	2.190574	2.527507	1.318347	C	2.644652	-0.645097	-0.358359
H	2.887364	1.926423	0.692498	C	1.992659	-1.492376	0.599441
C	2.449175	4.006961	0.977082	H	-2.295897	-2.242924	-1.131679
H	3.492104	4.288000	1.236225	H	-2.309911	0.834971	1.996148
				H	-0.544590	-1.060131	2.742631

H	2.330964	-0.456944	-2.582726	H	3.171411	1.357870	1.579793
H	0.521804	-2.438095	-2.301276	H	3.971716	-0.164489	2.092664
H	2.238973	-1.545302	1.666882	H	4.958522	1.210036	1.520115
C	-3.932373	0.172651	-0.432008	C	-4.196845	-0.349073	-1.862159
C	3.936920	0.139720	-0.097784	H	-3.361342	-0.116329	-2.553507
C	-3.899999	1.718394	-0.442257	H	-4.347489	-1.448354	-1.872204
H	-3.708783	2.131041	0.569965	H	-5.117724	0.113715	-2.275110
H	-3.118092	2.110236	-1.123776	C	-0.532458	-4.333248	-0.277688
H	-4.876979	2.122180	-0.783030	H	0.278675	-5.075966	-0.427102
C	4.106226	1.322766	-1.073406	H	-1.395367	-4.846263	0.195777
H	5.084790	1.821017	-0.907739	H	-0.855260	-3.989010	-1.280068
H	4.081376	0.990822	-2.132130	C	0.430772	-3.746542	1.962389
H	3.312259	2.082518	-0.934342	H	1.279566	-4.446198	1.813934
C	-5.110037	-0.288715	0.473724	H	0.766782	-2.957362	2.664050
H	-4.995933	0.095284	1.508385	H	-0.396401	-4.298416	2.455430
H	-6.079333	0.080241	0.073599	C	-0.039597	-3.176096	0.611062
H	-5.158536	-1.396108	0.527943	C	0.582776	2.161867	0.609417
C	5.111111	-0.855586	-0.321440	H	0.834207	1.297225	1.283894
H	5.117071	-1.238194	-1.363009	H	1.556738	2.609870	0.340357
H	6.086504	-0.358038	-0.130196	C	-0.312327	3.138056	1.396123
H	5.029067	-1.728399	0.358646	H	-1.378481	2.889027	1.176030
C	4.006111	0.663428	1.354778	C	-0.097050	4.610059	0.994868

H	-0.756345	5.283111	1.583020	C	1.542529	-1.306507	-1.741210
H	0.953619	4.920981	1.187172	C	2.310781	-1.130537	-0.556133
H	-0.310963	4.794129	-0.077389	C	1.560228	-1.738792	0.503980
C	-0.117128	2.977726	2.919437	C	-1.318049	-0.462156	1.946582
H	-0.311703	1.934720	3.247420	C	-2.069242	0.663721	1.448069
H	0.924260	3.230683	3.215450	C	-2.778681	0.308319	0.264516
H	-0.799633	3.644815	3.490112	C	-2.411288	-1.043552	-0.028289
C	-0.194257	2.251312	-1.431202	H	1.892001	-1.815752	1.546409
C	-0.618238	1.069515	-2.133307	H	1.842198	-0.986720	-2.749071
H	-1.012933	2.860572	-1.007569	H	-2.124084	1.632629	1.963947
H	-0.016647	0.756409	-3.005468	H	-2.817109	-1.632928	-0.858403
H	-1.702304	0.916298	-2.257101	C	3.796466	-0.752566	-0.511808
C	0.911834	3.075684	-2.066991	C	-3.963624	1.055554	-0.357766
H	1.344191	3.850582	-1.403698	C	4.118826	0.444416	-1.434485
H	1.734715	2.428246	-2.430298	H	3.811159	0.244563	-2.481715
H	0.488590	3.593995	-2.956219	H	3.608198	1.370702	-1.103163
<hr/>							
80							
7-re SCF Done: -1218.91959158 A.U.							
Zr	-0.137965	0.003961	-0.201195	H	-4.713129	3.096192	-0.639162
C	0.380674	-2.371283	-0.041352	H	-3.699095	2.905019	0.821459
C	-1.559115	-1.558174	1.020044	H	-2.934226	2.950753	-0.799157
C	0.350760	-2.066308	-1.469101	C	4.582564	-1.991031	-1.033135

H	4.315532	-2.223345	-2.084617	H	-1.000444	-4.865003	-0.037612
H	5.677723	-1.805453	-0.988064	C	-0.774874	-2.875614	0.848124
H	4.359749	-2.889631	-0.421226	C	-0.513022	-2.617022	-2.581511
C	-5.226554	0.623745	0.442281	H	-0.283060	-2.090124	-3.530127
H	-5.134807	0.902701	1.512436	H	-0.313339	-3.699180	-2.750620
H	-6.135126	1.116742	0.033435	H	-1.601446	-2.508933	-2.410098
H	-5.376401	-0.474347	0.390557	C	-0.640386	-0.448650	3.299682
C	-4.172780	0.673794	-1.840418	H	-0.655258	0.578948	3.716885
H	-3.286103	0.920176	-2.458245	H	-1.171292	-1.101941	4.026778
H	-4.376543	-0.410348	-1.959917	H	0.418773	-0.775838	3.280319
H	-5.045288	1.219070	-2.257997	C	0.785832	2.228307	0.762538
C	4.271519	-0.465427	0.929767	H	0.597058	1.409419	1.502696
H	3.688373	0.345915	1.408525	H	0.183440	0.747735	-2.901388
H	4.182544	-1.367435	1.569861	C	-0.340058	1.345664	-2.136832
H	5.340146	-0.164393	0.930918	C	0.414220	2.362425	-1.456062
C	-0.260984	-3.464899	2.177944	H	-1.383154	1.595984	-2.398709
H	-1.115811	-3.720954	2.837875	H	0.021145	3.000342	0.977654
H	0.313784	-4.393777	1.980398	H	1.504731	2.345921	-1.630722
H	0.397787	-2.779720	2.739453	C	2.212071	2.732907	1.052778
C	-1.628863	-3.976719	0.182466	H	2.925554	1.983756	0.644836
H	-2.441855	-4.290715	0.870340	C	-0.179840	3.757580	-1.399902
H	-2.100983	-3.660502	-0.764252	H	-1.249180	3.726177	-1.111319

H	0.339090	4.451790	-0.715270	C	-1.993519	-1.592762	-0.160559
H	-0.132797	4.193826	-2.422982	H	2.200233	-1.382314	1.732809
C	2.593485	4.090918	0.434548	H	2.376213	-0.413404	-2.529946
H	1.931323	4.904395	0.804650	H	-2.347783	1.024936	1.904774
H	3.632593	4.363784	0.717301	H	-2.234276	-2.234089	-1.017173
H	2.547083	4.091935	-0.672679	C	3.917282	0.278315	-0.022924
C	2.453072	2.786947	2.579940	C	-3.912898	0.198358	-0.512707
H	3.492967	3.101460	2.818191	C	4.105746	1.430462	-1.031400
H	1.763558	3.513906	3.062673	H	4.119597	1.063071	-2.078574
H	2.281607	1.798691	3.057022	H	3.299197	2.184764	-0.944752

80

7-si SCF Done: -1218.92871554 A.U.

Zr	-0.013468	-0.089700	-0.235180	H	-4.875227	2.108730	-1.003591
C	1.064884	-2.253058	-0.017561	H	-3.741501	2.214594	0.375417
C	-1.083377	-1.943198	0.912223	H	-3.107834	2.104228	-1.298638
C	1.105766	-1.909493	-1.436279	C	5.107662	-0.711032	-0.176798
C	2.077948	-0.848892	-1.566475	H	5.148041	-1.129980	-1.203529
C	2.640909	-0.527747	-0.295919	H	6.072330	-0.196879	0.024952
C	1.976609	-1.359520	0.659344	H	5.013554	-1.559960	0.531337
C	-1.116850	-0.849811	1.872450	C	-5.103583	-0.223878	0.395369
C	-2.061912	0.110541	1.365975	H	-5.017094	0.224587	1.406515
C	-2.638580	-0.349092	0.144899	H	-6.068856	0.105892	-0.046651

H	-5.138695	-1.326517	0.516201	C	-0.514902	-0.744588	3.256484
C	-4.141174	-0.414802	-1.912136	H	-0.792526	0.227179	3.713026
H	-3.299973	-0.205620	-2.603953	H	-0.904077	-1.541554	3.927258
H	-4.266846	-1.515750	-1.855987	H	0.591936	-0.809092	3.280785
H	-5.065437	0.000236	-2.366175	C	0.531684	2.324383	0.477008
C	3.935780	0.849135	1.413484	H	0.731980	1.512955	1.229866
H	3.086848	1.540039	1.590443	H	1.527001	2.727816	0.213052
H	3.887040	0.044251	2.175826	C	-0.361504	3.382469	1.153677
H	4.876856	1.411284	1.591083	H	-1.428733	3.099647	0.986386
C	0.518104	-3.593051	2.091394	C	-0.134342	3.408459	2.681070
H	-0.308874	-4.050336	2.673681	H	0.911128	3.701750	2.919821
H	1.281470	-4.376389	1.901609	H	-0.809994	4.136344	3.181252
H	0.986860	-2.822441	2.728339	H	-0.312840	2.412750	3.138145
C	-0.559580	-4.263867	-0.030531	C	-0.169493	4.802948	0.586804
H	-1.329256	-4.786271	0.575463	H	-0.818492	5.530994	1.118127
H	-1.022873	-4.000552	-0.997763	H	0.882812	5.139255	0.717102
H	0.261549	-4.981106	-0.238769	H	-0.413793	4.872847	-0.492065
C	-0.016077	-3.047680	0.749435	H	0.024426	0.672287	-3.059179
C	0.517902	-2.614585	-2.638175	C	-0.596971	1.034826	-2.221054
H	0.721366	-2.024291	-3.554772	C	-0.198408	2.263585	-1.588976
H	0.976196	-3.618219	-2.786214	H	-1.676871	0.863717	-2.355454
H	-0.579007	-2.757897	-2.585297	H	-1.031954	2.890773	-1.226518

C	0.918450	3.053557	-2.248802	C	-3.588803	1.909551	-0.966633
H	1.333341	3.868657	-1.624486	C	3.839355	0.475161	-2.118150
H	1.751663	2.389946	-2.553267	H	3.190186	0.479875	-3.018532
H	0.513997	3.515639	-3.177020	H	3.581570	1.365877	-1.510802
<hr/>				H	4.888988	0.595463	-2.462106
82				C	-3.257853	3.415211	-0.934956
8-re SCF Done: -1546.45905650 A.U.				H	-4.076721	3.993225	-1.413029
Zr	-0.060876	0.159557	-0.229065	H	-3.149590	3.795500	0.102109
C	0.445155	-2.240886	0.131009	H	-2.326761	3.643591	-1.488107
C	-1.940069	-0.946565	0.904249	C	4.195078	-2.011222	-2.176916
C	0.162577	-2.210511	-1.291401	H	3.659265	-2.070856	-3.146147
C	1.219333	-1.493281	-1.922313	H	5.277866	-1.886870	-2.395188
C	2.212495	-1.138273	-0.948417	H	4.058619	-2.980154	-1.653140
C	1.700197	-1.557156	0.333152	C	-4.994602	1.713127	-0.326148
C	-1.594122	0.154314	1.778794	H	-5.006646	2.069228	0.724793
C	-2.000386	1.368576	1.113308	H	-5.763464	2.281605	-0.893045
C	-2.629504	1.046051	-0.132577	H	-5.287089	0.643047	-0.323409
C	-2.513080	-0.371334	-0.290733	C	-3.653069	1.439730	-2.438568
H	2.236378	-1.482259	1.287865	H	-2.661993	1.499974	-2.932495
H	1.314225	-1.348378	-3.008491	H	-4.009977	0.392949	-2.522937
H	-1.914445	2.376221	1.544523	H	-4.362025	2.074134	-3.011286
H	-2.915216	-0.929811	-1.142955	C	4.565965	-0.774900	-0.042322
C	3.679450	-0.829389	-1.305510				

H	4.237615	0.006235	0.670034	C	1.245823	1.948063	1.140777
H	4.559275	-1.746400	0.493651	H	0.990581	1.009909	1.690471
H	5.617519	-0.554175	-0.322481	C	0.919698	2.569538	-0.983582
C	-0.792250	-2.604941	3.059239	C	0.205218	1.760316	-1.938185
C	-1.867745	-4.034873	0.249037	H	0.805448	1.254357	-2.714014
Si	-1.069768	-2.589724	1.182671	H	-0.760483	2.150782	-2.303670
C	-1.155057	-0.005082	3.221528	H	2.018739	2.549698	-1.079576
C	-0.851816	-3.090229	-2.008632	H	0.597304	2.739218	1.561476
H	-2.836576	-4.345638	0.696783	C	2.739843	2.230780	1.386268
H	-0.088409	-3.410245	3.362940	H	3.329830	1.678859	0.619614
H	-0.270424	-3.976708	-2.358609	C	3.171553	1.680961	2.764736
H	-1.200937	-2.589215	-2.937881	C	3.149174	3.712543	1.281432
H	-1.187067	-4.914170	0.316269	C	0.362755	3.941482	-0.648301
H	-1.762204	-2.830915	3.559134	H	2.629330	2.200820	3.584576
H	-2.074788	-0.075737	3.852015	H	2.954557	0.596068	2.859083
H	-0.635805	0.916902	3.563547	H	4.260715	1.823585	2.938371
C	-2.088704	-3.616520	-1.230085	H	4.222609	3.838660	1.537849
C	-0.254156	-1.225574	3.529937	H	3.007342	4.127120	0.263983
H	-2.894407	-2.854732	-1.253665	H	2.564643	4.340002	1.990098
H	-0.076259	-1.253959	4.627970	H	-0.699000	3.883757	-0.346742
H	0.743476	-1.053364	3.068392	H	0.411100	4.576044	-1.561801
H	-2.495044	-4.479693	-1.802366	H	0.915211	4.466409	0.151941

82			H	4.760711	3.011389	-0.848952	
8-si SCF Done: -1546.46666394 A.U.			C	-3.999833	1.894042	-0.685846	
Zr	-0.001297	0.035192	-0.261375	H	-4.997790	2.259624	-1.008958
C	1.562761	-1.821683	0.022522	H	-3.808776	2.306210	0.326451
C	-1.205718	-1.946427	0.560613	H	-3.247610	2.321316	-1.378533
C	1.596152	-1.535050	-1.402369	C	5.192962	0.409581	-0.204158
C	2.300532	-0.291275	-1.563451	H	5.288733	0.022789	-1.239769
C	2.737292	0.184423	-0.286339	H	6.064962	1.067941	0.001028
C	2.218226	-0.724285	0.694224	H	5.244176	-0.457390	0.486325
C	-1.332066	-1.026948	1.673521	C	-5.150115	-0.163029	0.183672
C	-2.211124	0.023447	1.259329	H	-5.083354	0.225755	1.220693
C	-2.688458	-0.239497	-0.068185	H	-6.122574	0.164749	-0.243879
C	-2.012018	-1.424900	-0.519534	H	-5.152101	-1.271387	0.237589
H	2.415981	-0.659154	1.771000	C	-4.191855	-0.159828	-2.130962
H	2.544105	0.167755	-2.532164	H	-3.362518	0.124170	-2.811080
H	-2.553382	0.842662	1.908286	H	-4.293880	-1.264020	-2.162159
H	-2.185078	-1.916510	-1.483707	H	-5.127123	0.271017	-2.546287
C	3.862042	1.196548	-0.019834	C	3.820235	1.743362	1.425526
C	-3.967828	0.349947	-0.689474	H	2.875438	2.284194	1.635070
C	3.861283	2.379924	-1.008606	H	3.924070	0.932012	2.174904
H	3.881894	2.038174	-2.064299	H	4.661232	2.449591	1.590214
H	2.970478	3.021692	-0.872041	C	0.416874	-3.526510	2.428326

C	0.334049	-4.351897	-0.815402	H	-1.818179	2.900467	1.103733
Si	0.290788	-3.075918	0.588988	C	-0.593834	3.264269	2.836490
C	-0.897623	-1.336012	3.095983	C	-0.814770	4.785289	0.838401
C	1.305901	-2.554670	-2.488600	H	-1.557815	5.377150	1.414052
H	-0.482702	-5.100705	-0.723459	H	-1.073228	4.891885	-0.234390
H	1.352976	-4.080800	2.657527	H	0.179336	5.259702	0.994612
H	2.268236	-3.081750	-2.702429	H	-1.369499	3.851008	3.375695
H	1.037047	-2.035420	-3.434280	H	-0.633239	2.221297	3.216124
H	1.291453	-4.918071	-0.748536	H	0.397589	3.683796	3.114344
H	-0.426663	-4.206955	2.686604	C	-0.418973	2.413660	-1.513738
H	-1.764493	-1.843073	3.585485	C	-0.574420	1.182749	-2.241727
H	-0.751400	-0.392783	3.666580	H	-1.358618	2.854967	-1.140378
C	0.227897	-3.625471	-2.187031	H	0.143665	0.988389	-3.057843
C	0.351727	-2.231782	3.287305	H	-1.601894	0.851710	-2.462852
H	-0.773844	-3.153030	-2.263707	C	0.545364	3.438855	-2.082802
H	0.410663	-2.501900	4.365066	H	0.830359	4.243947	-1.378052
H	1.259225	-1.625548	3.086407	H	0.050647	3.920844	-2.955775
H	0.262947	-4.379756	-3.004240	H	1.469187	2.959333	-2.460791
C	0.234442	2.442797	0.579819	<hr/>			
H	0.552717	1.624938	1.283638	56			
H	1.160984	3.002198	0.355646	9-re SCF Done: -1054.60139310 A.U.			
C	-0.804475	3.317163	1.307436	Zr	-0.251236	-0.130550	-0.131624
				C	-1.590377	-1.734902	1.105086

C	-0.061038	-2.520801	-0.525751	C	3.458608	-2.186336	0.978464
C	-0.897833	-0.982430	2.123954	C	4.027854	-1.440130	-0.095242
C	-1.422264	0.346479	2.168327	H	-3.609279	-1.975673	-1.059412
C	-2.495894	0.437346	1.221581	H	-5.193262	-0.119003	-1.589186
C	-2.582735	-0.847065	0.525131	H	-5.144432	2.019992	-0.288938
C	-0.326588	-1.893326	-1.802622	H	-3.447445	2.402470	1.501991
C	0.842332	-1.162299	-2.206760	H	3.713022	-0.463605	-2.012341
C	1.876526	-1.389110	-1.235078	H	5.099665	-1.187018	-0.062674
C	1.307686	-2.205690	-0.165905	H	4.095223	-2.483772	1.826623
H	-1.114394	1.132296	2.870628	H	1.692365	-3.171169	1.773090
H	0.967702	-0.629934	-3.158366	C	1.300231	1.727084	0.567378
C	-1.106929	-3.024653	0.457534	H	1.504765	0.706300	1.008086
H	-0.100749	-1.372328	2.771079	C	-0.071711	2.396619	-1.008609
H	-1.932925	-3.561641	-0.051598	C	-1.017417	1.490557	-1.606418
H	-0.670735	-3.722418	1.200990	H	-0.791109	1.111471	-2.617670
H	-1.246836	-1.997776	-2.392279	H	-2.091065	1.672843	-1.415720
C	2.112860	-2.559816	0.958727	H	0.826972	2.600130	-1.615103
C	3.258364	-1.027923	-1.182581	H	0.871134	2.316701	1.401549
C	-3.543462	-1.018547	-0.518204	C	2.676492	2.271241	0.134969
C	-3.451354	1.462165	0.928096	H	2.976509	1.733149	-0.794406
C	-4.398724	1.240172	-0.065176	C	2.733447	3.784937	-0.153862
C	-4.436226	0.013802	-0.800600	H	2.447157	4.373957	0.745107

H	3.769457	4.081911	-0.421248	C	-1.233517	-2.262908	-0.153263
H	2.079758	4.102695	-0.989680	H	0.944680	1.681752	-2.561393
C	3.729769	1.937198	1.216497	H	-0.808590	-1.347945	3.093209
H	3.787162	0.846257	1.405069	C	1.186968	-2.853501	-1.005344
H	4.740787	2.285760	0.912196	H	0.059949	-0.844941	-2.936502
H	3.478621	2.438154	2.177375	H	2.046271	-3.447653	-0.633512
C	-0.631374	3.603299	-0.275777	H	0.754352	-3.404519	-1.864941
H	-1.479822	3.311452	0.375400	H	1.407248	-2.428010	1.971699
H	0.111308	4.148024	0.336483	C	-2.062831	-2.345502	-1.313116
H	-1.031555	4.315553	-1.031046	C	-3.159516	-1.342689	1.144094

56

9-si SCF Done: -1054.60536426 A.U.

Zr	0.215935	-0.180875	0.160841	C	3.554303	-0.943351	0.316864
C	1.600398	-1.440282	-1.389833	C	3.277003	1.767037	-0.596458
C	0.156045	-2.605098	0.086590	C	4.259521	1.411396	0.320085
C	0.847463	-0.544010	-2.232862	C	4.392014	0.065345	0.787547
C	1.300249	0.794788	-2.024227	C	-3.400936	-1.952475	-1.226569
C	2.384892	0.760728	-1.085975	C	-3.944959	-1.466434	-0.001292
C	2.557959	-0.627631	-0.658655	H	3.689598	-1.982774	0.655915
C	0.456062	-2.245811	1.454926	H	5.175574	-0.174829	1.523081
C	-0.715237	-1.668497	2.047721	H	4.957270	2.177765	0.694244
C	-1.779935	-1.711915	1.085619	H	3.187023	2.805345	-0.953529
				H	-3.593365	-0.974564	2.087547
				H	-5.011201	-1.191244	0.039274

H -4.051251 -2.032988 -2.111766
H -1.663034 -2.757587 -2.253373
C -1.604774 1.543374 -0.032437
H -1.497134 0.916387 -0.962953
H -2.423677 1.082169 0.553343
H -0.019476 2.986324 1.055338
C -0.246780 2.042644 1.581595
C 0.896610 1.219547 1.884207
H 0.879484 0.660975 2.837119
H 1.893925 1.598855 1.598859
C -1.325604 2.168091 2.644836
H -2.246865 2.672847 2.292496
H -1.605140 1.172729 3.046764
H -0.921139 2.766222 3.490690
C -1.989472 2.958942 -0.491642
H -1.991480 3.627136 0.402634
C -3.425896 2.978208 -1.057834
H -3.726965 4.006479 -1.353398
H -3.509058 2.330723 -1.957550
H -4.161632 2.609319 -0.313257
C -1.004801 3.561394 -1.507389
H 0.036666 3.568740 -1.123695

H -1.011441 2.982127 -2.456390
H -1.279361 4.607821 -1.756711

62

10-re SCF Done: -1133.15697719 A.U.

Zr 0.124539 0.153104 0.173709
C 1.911426 -1.020678 -0.967033
C 0.588802 -2.189099 0.611901
C 1.043570 -0.552169 -2.027985
C 1.132979 0.865029 -2.136080
C 2.106567 1.323480 -1.192383
C 2.577635 0.163416 -0.426324
C 0.698140 -1.484255 1.877746
C -0.604202 -1.075477 2.305228
C -1.562686 -1.574340 1.364414
C -0.833110 -2.247690 0.285616
H 0.608776 1.485986 -2.874325
H -0.840899 -0.570117 3.250325
C 1.793665 -2.424514 -0.328682
H 0.412763 -1.186127 -2.663879
H 1.619878 -1.324987 2.450383
C -1.591231 -2.826429 -0.783468
C -2.992618 -1.571419 1.376644

C	3.543900	0.386683	0.608570	C	-1.880006	1.463897	-0.643745
C	2.683812	2.614995	-0.974663	H	-1.775133	0.411417	-1.038986
C	3.641676	2.772493	0.017749	H	0.208039	1.609403	2.608415
C	4.056047	1.664695	0.819942	C	0.346013	1.991283	1.582607
C	-2.986333	-2.801725	-0.741814	C	-0.799871	2.563862	0.925637
C	-3.684057	-2.192869	0.341681	H	1.329043	2.462052	1.395319
H	3.921508	-0.449005	1.211647	H	-1.607588	2.118439	-1.495588
H	4.810583	1.820614	1.606768	H	-1.738945	2.529202	1.503960
H	4.100112	3.760347	0.185127	C	-3.366707	1.619855	-0.263449
H	2.386241	3.462401	-1.612542	H	-3.534983	1.074939	0.695044
H	-3.530229	-1.114175	2.222632	C	-4.251065	0.941217	-1.334843
H	-4.785319	-2.218635	0.357705	H	-3.995847	-0.130906	-1.454409
H	-3.558300	-3.278131	-1.553654	H	-5.328007	1.008345	-1.066485
H	-1.089443	-3.343192	-1.611526	H	-4.120969	1.436108	-2.322554
C	1.559118	-3.505286	-1.406373	C	-3.853723	3.070627	-0.074313
C	3.042898	-2.865737	0.464692	H	-3.715966	3.661752	-1.006464
H	3.950752	-2.805719	-0.170352	H	-4.939191	3.080140	0.159811
H	1.262640	-4.465737	-0.936747	H	-3.340364	3.607882	0.747241
H	3.220589	-2.264047	1.374230	C	-0.584471	3.846044	0.141456
H	0.781734	-3.231470	-2.141865	H	-1.433811	4.130964	-0.506748
H	2.917623	-3.917802	0.794825	H	-0.420542	4.675234	0.865054
H	2.498083	-3.670462	-1.974512	H	0.328622	3.775811	-0.482581

62

10-si SCF Done: -1133.16197229 A.U.

Zr 0.073216 -0.113927 -0.266953

C 1.986620 0.531426 1.072878

C 1.074131 2.076806 -0.476044

C 0.961681 0.211227 2.043056

C 0.704932 -1.190025 2.034993

C 1.605996 -1.802355 1.106313

C 2.393820 -0.739376 0.469957

C 1.131425 1.476083 -1.797226

C -0.187167 1.389672 -2.338450

C -1.099251 1.972761 -1.400036

C -0.330721 2.388034 -0.219968

H 0.007732 -1.718092 2.697452

H -0.444677 1.019049 -3.338684

C 2.231790 1.965998 0.545608

H 0.459501 0.930513 2.701694

H 2.042611 1.174641 -2.327940

C -1.048241 2.942229 0.889133

C -2.511952 2.192512 -1.458536

C 3.339856 -1.119355 -0.537864

C 1.852402 -3.176623 0.792831

C 2.808260 -3.492757 -0.163041

C 3.538772 -2.465962 -0.836930

C -2.433019 3.112923 0.810813

C -3.159149 2.751199 -0.360759

H 3.948065 -0.361995 -1.049264

H 4.282628 -2.744449 -1.599681

H 3.013106 -4.547776 -0.405943

H 1.289662 -3.966337 1.315909

H -3.070295 1.923333 -2.369083

H -4.246120 2.927978 -0.397726

H -2.970147 3.554418 1.664934

H -0.517440 3.275384 1.790138

C 2.170771 3.003776 1.687340

C 3.602110 2.156841 -0.140619

H 4.423893 1.863961 0.544912

H 2.132464 4.032416 1.273119

H 3.712383 1.574486 -1.072858

H 1.301337 2.875297 2.356749

H 3.736659 3.225148 -0.409484

H 3.079803 2.915954 2.318028

C -2.285976 -0.797380 0.241009

H -1.906396 0.110573 0.791683

H	-3.112313	-0.398216	-0.376973	Zr	0.132833	0.172665	0.201307
H	0.070205	-1.516891	-2.797810	C	1.695950	-1.187330	-1.058683
C	-0.106445	-1.874120	-1.767335	C	0.218090	-2.239416	0.458346
C	-1.480696	-2.013039	-1.347260	C	0.925064	-0.448959	-2.037068
H	0.614107	-2.637882	-1.424538	C	1.316538	0.926488	-1.973394
H	-1.679165	-2.881030	-0.693560	C	2.325331	1.067513	-0.981476
C	-2.775723	-1.812669	1.294138	C	2.546021	-0.221409	-0.369816
H	-1.941128	-2.521857	1.511699	C	0.542495	-1.666238	1.751795
C	-2.557747	-1.771246	-2.392841	C	-0.651308	-1.115962	2.312378
H	-2.507377	-2.588494	-3.145751	C	-1.716342	-1.314737	1.393953
H	-3.585678	-1.755631	-1.981034	C	-1.196489	-1.983217	0.221578
H	-2.386136	-0.817330	-2.932265	H	0.939603	1.729398	-2.621432
C	-3.977131	-2.645606	0.807042	H	-0.743915	-0.657879	3.306350
H	-4.298832	-3.370407	1.584485	C	1.309590	-2.604808	-0.575568
H	-4.845465	-1.987491	0.584249	H	0.204030	-0.868713	-2.749880
H	-3.751764	-3.226284	-0.110560	H	1.514201	-1.708014	2.259152
C	-3.131995	-1.109730	2.621445	C	-2.132447	-2.578355	-0.817917
H	-3.973078	-0.397636	2.479087	C	-3.192948	-1.090239	1.635292
H	-3.438422	-1.843865	3.397845	C	3.716163	-0.448353	0.571365
H	-2.272479	-0.531867	3.021417	C	3.177844	2.281920	-0.687589
<hr/>				C	4.545196	1.866882	-0.111933
70				C	4.361635	0.870285	1.042607
11-re SCF Done: -1137.97194865 A.U.							

C	-3.599221	-2.138008	-0.625776	C	-0.565889	2.666205	1.040374
C	-4.024512	-2.121828	0.850014	H	1.489858	2.327936	1.671614
H	4.482943	-1.056586	0.036333	H	-1.165136	2.596543	-1.456321
H	5.336617	0.647647	1.526242	H	-1.553388	2.677284	1.533594
H	5.100551	2.765750	0.231170	C	-3.110154	2.143229	-0.533626
H	3.302749	2.883258	-1.613731	H	-3.464306	1.502022	0.309063
H	-3.505354	-0.068216	1.322581	C	-3.920144	1.732531	-1.785998
H	-5.107075	-1.888538	0.939909	H	-3.745113	0.671861	-2.062324
H	-4.260481	-2.805680	-1.218231	H	-5.012867	1.866032	-1.627841
H	-2.076261	-3.688892	-0.736633	H	-3.628673	2.354055	-2.660754
C	0.803217	-3.473601	-1.746244	C	-3.471169	3.599259	-0.176766
C	2.467219	-3.388264	0.079872	H	-3.159496	4.296819	-0.985121
H	3.316959	-3.488346	-0.627240	H	-4.570656	3.705648	-0.060915
H	0.373450	-4.423314	-1.366259	H	-3.009339	3.946645	0.767982
H	2.849399	-2.919552	1.003702	C	-0.166424	3.985167	0.399979
H	0.032145	-2.978475	-2.362769	H	-0.949660	4.438056	-0.235467
H	2.119307	-4.407637	0.348625	H	0.073715	4.712200	1.207757
H	1.651398	-3.723145	-2.417571	H	0.748572	3.868367	-0.215558
C	-1.613366	1.862867	-0.759158	H	3.429927	-1.047905	1.459557
H	-1.543757	0.869248	-1.277622	H	3.723238	1.336964	1.826490
H	0.201571	1.518327	2.724519	H	5.163464	1.397944	-0.911315
C	0.458854	1.935307	1.736265	H	2.677988	2.955117	0.044891

H	-3.405648	-1.151958	2.724013	C	2.016075	-2.565775	1.056246
H	-3.879195	-3.133682	1.293223	C	3.229147	-1.284734	-1.443159
H	-3.738606	-1.115962	-1.042952	C	-3.672919	-0.251983	-0.595231
H	-1.818861	-2.342818	-1.855961	C	-2.909335	2.480608	0.552459
<hr/>							
70				C	-4.301345	2.157633	-0.023780
11-si SCF Done: -1137.98032616 A.U.							
Zr	-0.077073	0.110198	-0.272731	C	3.470921	-2.063201	0.951066
C	-1.703881	-1.081648	1.066012	C	4.025729	-2.182193	-0.476944
C	-0.265751	-2.299031	-0.369573	H	-4.492666	-0.765131	-0.038616
C	-0.873846	-0.360835	2.008327	H	-5.185035	0.938386	-1.613242
C	-1.162934	1.035095	1.891442	H	-4.776293	3.083541	-0.412706
C	-2.163686	1.210522	0.897381	H	-2.995639	3.118912	1.458211
C	-2.487501	-0.083350	0.339754	H	3.502029	-0.221166	-1.251299
C	-0.513874	-1.806526	-1.712656	H	5.101673	-1.906624	-0.501752
C	0.721794	-1.331228	-2.254047	H	4.105891	-2.628478	1.666111
C	1.741101	-1.504932	-1.277267	H	2.015260	-3.681479	1.047914
C	1.148539	-2.074891	-0.089835	C	-1.004274	-3.406044	1.857413
H	-0.729148	1.835286	2.506252	C	-2.607050	-3.257080	-0.018470
H	0.868577	-0.940857	-3.269970	H	-3.477337	-3.271484	0.670116
C	-1.410227	-2.542210	0.644189	H	-0.636334	-4.397534	1.520726
H	-0.179032	-0.803823	2.733055	H	-2.933121	-2.786739	-0.962574
H	-1.463582	-1.853402	-2.260112	H	-0.215669	-2.948926	2.480717

H -2.331132 -4.306989 -0.250606
H -1.887590 -3.568433 2.509718
C 1.895180 1.624046 0.342815
H 1.744214 0.700954 0.967292
H 2.861266 1.466624 -0.174701
H -0.354673 1.334723 -2.906375
C -0.360395 1.791287 -1.900489
C 0.868267 2.372615 -1.426856
H -1.293692 2.325831 -1.654486
H 0.744107 3.302344 -0.844965
C 1.934649 2.840331 1.287401
H 0.901101 3.258330 1.364071
C 2.048349 2.399225 -2.384614
H 1.820854 3.114472 -3.206075
H 2.999481 2.719833 -1.916159
H 2.210463 1.406575 -2.852895
C 2.851698 3.968492 0.775321
H 2.857494 4.828061 1.478687
H 3.899754 3.607851 0.680984
H 2.540420 4.357035 -0.215811
C 2.362447 2.432018 2.713946
H 3.397470 2.025976 2.715851

H 2.340880 3.299298 3.409504
H 1.696628 1.647329 3.130878
H -2.345041 3.090444 -0.191508
H -4.963164 1.778642 0.788306
H -3.515171 1.469041 -1.927520
H -3.437337 -0.912435 -1.454696
H 3.519935 -1.483262 -2.497259
H 3.962201 -3.242747 -0.812009
H 3.520253 -0.995889 1.266739
H 1.606232 -2.278419 2.046547

59

12-re SCF Done: -1093.89064635 A.U.

Zr 0.204368 -0.012994 0.152506
C 0.096811 -2.366762 0.915734
C 1.663296 -1.438643 -1.223574
C 0.161329 -1.518786 2.078321
C -1.073563 -0.791986 2.188396
C -1.972265 -1.279881 1.172035
C -1.233816 -2.233023 0.353160
C 0.909814 -0.647498 -2.163015
C 1.331799 0.714005 -2.080037
C 2.427187 0.787625 -1.154658

C	2.613877	-0.543813	-0.583086	C	1.177520	-3.300279	0.415615
H	-1.343786	-0.098223	2.994870	H	0.839504	-3.343428	-1.748233
H	0.946335	1.543297	-2.687211	H	2.054366	-3.218775	1.091205
H	1.007703	-1.462659	2.776204	H	2.553366	-3.420142	-1.299530
H	0.141547	-1.041311	-2.843067	H	0.844752	-4.362118	0.475535
C	3.631058	-0.748545	0.398835	C	-1.453252	1.753610	-0.593055
C	3.329959	1.839427	-0.802675	H	-1.600800	0.715164	-1.013703
C	-1.887722	-2.875650	-0.742289	C	-0.111510	2.527845	0.977428
C	-3.353878	-1.047794	0.907102	C	0.882005	1.690352	1.595027
C	-3.971128	-1.723270	-0.147351	H	0.676639	1.326417	2.615645
C	-3.240903	-2.621809	-0.975720	H	1.943073	1.929949	1.404390
C	4.469968	0.309737	0.747703	H	-1.061064	2.353455	-1.437377
C	4.328712	1.591640	0.133369	H	-1.026043	2.685801	1.573894
H	-1.347984	-3.608479	-1.361730	C	-2.852591	2.241313	-0.168138
H	-3.757555	-3.137376	-1.800818	H	-3.125061	1.722403	0.780075
H	-5.045216	-1.568448	-0.337368	C	0.372905	3.755335	0.226452
H	-3.935027	-0.374955	1.557236	H	1.244641	3.511610	-0.411905
H	3.251139	2.823549	-1.291024	H	-0.397942	4.239187	-0.401741
H	5.035665	2.393804	0.399925	H	0.716940	4.505850	0.972470
H	5.267826	0.151956	1.490223	C	-3.892314	1.829369	-1.236487
H	3.785320	-1.745398	0.840233	H	-4.918175	2.138844	-0.939239
C	1.584607	-2.939279	-1.032128	H	-3.665883	2.316770	-2.210219

H	-3.899376	0.732644	-1.397106	C	3.706379	-0.324924	0.193516
C	-2.981461	3.758691	0.077374	C	2.945977	2.368039	-0.441995
H	-2.723376	4.334836	-0.838323	C	-1.634064	-2.789754	-0.987310
H	-4.030769	4.013221	0.336833	C	-3.062691	-1.507177	1.146542
H	-2.344156	4.130737	0.903602	C	-3.721355	-1.948317	-0.000492
<hr/>							
59							
12-si SCF Done: -1093.89592204 A.U.							
Zr	0.196875	-0.044614	0.237992	C	4.411739	0.763974	0.705844
C	0.467947	-2.466447	0.579611	C	4.038754	2.102795	0.376982
C	1.735283	-0.985117	-1.441824	H	-1.106926	-3.314405	-1.799417
C	0.582256	-1.856097	1.880875	H	-3.565941	-2.915610	-1.955867
C	-0.693369	-1.334315	2.264479	H	-4.812698	-1.821217	-0.083916
C	-1.649511	-1.685747	1.249385	H	-3.621394	-1.036913	1.971213
C	-0.925314	-2.368833	0.179844	H	2.668575	3.403890	-0.695323
C	0.819678	-0.154178	-2.178255	H	4.633604	2.938701	0.778998
C	1.055365	1.216544	-1.847851	H	5.277542	0.591454	1.364262
C	2.192423	1.275617	-0.972600	H	4.030674	-1.352057	0.423113
C	2.600516	-0.095579	-0.682619	C	1.844476	-2.492664	-1.539271
H	-0.923194	-0.844290	3.218641	C	1.579480	-3.166777	-0.173637
H	0.534162	2.080493	-2.277860	H	1.103727	-2.844647	-2.287238
H	1.496255	-1.829722	2.489589	H	2.496035	-3.131594	0.451598
H	0.074391	-0.525974	-2.894846	H	2.841294	-2.791505	-1.937164
				H	1.346838	-4.247980	-0.308787

C	-1.886749	1.316812	-0.188037	67
H	-1.765400	0.396148	-0.826589	13-re SCF Done: -1098.70599794 A.U.
C	-0.730023	2.181635	1.445756	Zr -0.215418 0.050655 -0.152293
C	0.542605	1.629626	1.833922	C -1.637366 -1.194154 1.448395
H	0.611299	1.174685	2.837857	C -0.151427 -2.380704 -0.641140
H	1.451454	2.173543	1.526013	C -0.919239 -0.199767 2.203149
H	-0.672136	3.088456	0.817969	C -1.432133 1.088288 1.827972
H	-2.766744	1.089746	0.442013	C -2.484723 0.900524 0.880566
C	-1.831351	2.220522	2.492381	C -2.605021 -0.504992 0.623836
H	-1.549249	2.965018	3.269472	C -0.419801 -1.683309 -1.876821
H	-2.821876	2.511093	2.093117	C 0.783342 -1.007622 -2.267942
H	-1.937299	1.241060	3.000621	C 1.793418 -1.282799 -1.297699
C	-2.140279	2.512197	-1.130406	C 1.219311 -2.112472 -0.276462
H	-1.171544	3.037241	-1.309526	H -1.112067 2.052451 2.244059
C	-3.112432	3.552071	-0.539422	H 0.926236 -0.423082 -3.186398
H	-2.735492	4.003851	0.400438	H -0.155994 -0.400936 2.967434
H	-3.283864	4.382885	-1.256180	H -1.353508 -1.727566 -2.453467
H	-4.100458	3.090924	-0.320481	C 2.054926 -2.755296 0.812854
C	-2.658735	2.036500	-2.504579	C 3.281466 -1.047368 -1.417828
H	-2.807718	2.891705	-3.198846	C -3.731881 -1.088668 -0.206354
H	-1.950807	1.329643	-2.985665	C -3.479457 1.911285 0.363000
H	-3.632531	1.511672	-2.399693	C -4.387120 1.318173 -0.732654

C	-4.893273	-0.081564	-0.343196	H	-5.242167	2.001846	-0.920236
C	3.530441	-2.851945	0.369659	H	3.639364	-1.636781	-2.294377
C	4.048552	-1.503565	-0.160522	H	-4.111140	2.239903	1.221474
H	-4.097324	-2.028508	0.263606	C	1.514632	1.828637	0.722246
H	-5.439874	-0.013730	0.625264	H	1.498957	0.842816	1.257174
H	-3.822622	1.248813	-1.690143	H	-0.448612	1.365549	-2.685856
H	-2.976749	2.833219	-0.002205	C	-0.665514	1.780660	-1.687590
H	3.516836	0.011160	-1.663336	C	0.380126	2.542807	-1.051087
H	3.945478	-0.738849	0.640060	H	-1.692344	2.172685	-1.587367
H	3.623895	-3.621644	-0.430473	H	1.054386	2.555203	1.418886
H	1.658328	-3.767611	1.047088	H	1.342745	2.559889	-1.591374
C	-1.113835	-3.270601	0.118190	C	2.993657	2.164661	0.459739
C	-1.433608	-2.692472	1.515734	H	3.369546	1.487908	-0.341845
H	-2.046391	-3.368961	-0.475207	C	-0.021811	3.876957	-0.443782
H	-0.594719	-2.901442	2.212541	H	0.761814	4.358296	0.169796
H	-0.705362	-4.303509	0.210406	H	-0.278991	4.577107	-1.269943
H	-2.325936	-3.197972	1.953665	H	-0.930483	3.769568	0.183167
H	1.999573	-2.181521	1.766430	C	3.291924	3.609030	0.007824
H	-3.380510	-1.376985	-1.222385	H	2.965904	4.344735	0.775564
H	-5.625799	-0.452053	-1.091748	H	4.384990	3.749093	-0.132032
H	4.158985	-3.199571	1.217338	H	2.805082	3.879474	-0.949864
H	5.133846	-1.567525	-0.388930	C	3.826120	1.873337	1.731876

H	3.686553	0.831803	2.089714	C	3.704151	-0.998970	0.159831
H	4.912919	2.027879	1.553538	C	3.315604	2.010501	-0.280719
H	3.521652	2.550284	2.559929	C	4.273041	1.411030	0.769040
<hr/>							
67							
13-si SCF Done: -1098.71315926 A.U.							
Zr	0.163809	-0.010676	0.242191	C	-4.001463	-1.371704	-0.144740
C	1.577182	-1.123918	-1.456004	H	4.096772	-1.907032	-0.349281
C	0.114904	-2.463765	0.552082	H	5.347377	0.177607	-0.664845
C	0.797857	-0.127468	-2.145083	H	3.735181	1.278607	1.735119
C	1.272216	1.164127	-1.732140	H	2.776895	2.891833	0.133295
C	2.356697	0.978371	-0.822654	H	-3.517895	-0.033460	1.527105
C	2.538637	-0.430434	-0.625793	H	-3.757324	-0.554047	-0.860474
C	0.327473	-1.865074	1.848170	H	-3.759629	-3.530065	-0.012201
C	-0.889735	-1.210772	2.233355	H	-1.671067	-3.726767	-1.289230
C	-1.857734	-1.410126	1.200125	C	1.118416	-3.283945	-0.231817
C	-1.241829	-2.169240	0.150430	C	1.435817	-2.625594	-1.594324
H	0.908242	2.132725	-2.098276	H	2.046417	-3.375364	0.370642
H	-1.064294	-0.689140	3.183386	H	0.618020	-2.836373	-2.314845
H	0.029629	-0.327647	-2.904649	H	0.749919	-4.325676	-0.379326
H	1.234447	-1.958857	2.460667	H	2.355084	-3.072924	-2.039325
C	-2.020162	-2.700857	-1.037183	H	-1.838891	-2.089054	-1.950416
C	-3.333229	-1.084645	1.215192	H	3.381630	-1.333858	1.171058

H	5.590582	-0.318577	1.029213	H	-2.207881	3.425625	-3.283269
H	-4.101138	-2.947417	-1.661707	H	-1.597271	1.752635	-3.066498
H	-5.106014	-1.362950	-0.027170	C	-2.628385	4.040442	-0.622379
H	5.103834	2.121384	0.966307	H	-2.633823	4.912067	-1.310815
H	-3.814124	-1.713769	2.000591	H	-3.682671	3.709520	-0.494452
H	3.912908	2.405537	-1.135661	H	-2.267389	4.400955	0.362230
C	-1.736847	1.657369	-0.269881	<hr/>			
H	-1.674337	0.741079	-0.915486	62			
H	-2.673037	1.549725	0.308534	14-re SCF Done: -1384.54797225 A.U.			
H	0.609209	1.167914	2.875694	Zr	0.061045	0.219721	0.175422
C	0.638346	1.626050	1.870519	C	0.711437	-2.072600	0.806792
C	-0.550446	2.319192	1.436263	C	2.057006	-0.496196	-1.070312
H	1.602518	2.104174	1.633092	C	0.681398	-1.269335	2.018583
H	-0.361756	3.230069	0.839792	C	-0.676557	-0.972252	2.356129
C	-1.679581	2.473323	2.442974	C	-1.533328	-1.644546	1.419988
H	-1.350573	3.181221	3.236062	C	-0.679564	-2.296988	0.431920
H	-2.618729	2.869410	2.009811	C	1.079172	-0.159133	-2.088142
H	-1.909356	1.510622	2.942842	C	0.882514	1.250878	-2.123765
C	-1.762787	2.896543	-1.185701	C	1.776336	1.852971	-1.177107
H	-0.721290	3.290942	-1.277975	C	2.476466	0.772411	-0.484682
C	-2.234672	2.539642	-2.611759	H	-1.014071	-0.427516	3.247679
H	-3.279247	2.158850	-2.600598	H	0.224678	1.789433	-2.818998
				H	1.555873	-0.970858	2.613063

H	0.575203	-0.877973	-2.749960	H	3.848559	-1.857829	1.616193
C	3.398610	1.100128	0.557201	H	3.084162	-3.610534	-2.185990
C	2.115481	3.214381	-0.897885	H	3.863947	-3.543866	1.023085
C	-1.285762	-3.036908	-0.628957	Si	2.227232	-2.217039	-0.307166
C	-2.949200	-1.827619	1.369261	C	-2.120845	1.178186	-0.683235
C	-3.496821	-2.602261	0.348288	H	-1.861288	0.143204	-1.050774
C	-2.673845	-3.187273	-0.657752	C	-1.265806	2.427505	0.932386
C	3.673220	2.438005	0.837647	C	-0.034549	2.068495	1.584943
C	3.049513	3.487869	0.095323	H	-0.095544	1.673412	2.612374
H	-0.660534	-3.537483	-1.382594	H	0.843605	2.712234	1.396357
H	-3.139888	-3.786805	-1.455652	H	-1.912562	1.853069	-1.536326
H	-4.585305	-2.770088	0.317094	H	-2.183748	2.199106	1.500739
H	-3.589744	-1.395109	2.154504	C	-1.291167	3.743490	0.175243
H	1.663252	4.029747	-1.484370	H	-0.355885	3.884746	-0.401057
H	3.325782	4.532824	0.310076	H	-2.149398	3.862949	-0.510529
H	4.399536	2.692286	1.625358	H	-1.339255	4.569496	0.919489
H	3.925156	0.301350	1.099602	C	-3.629101	1.131701	-0.361635
C	3.808207	-2.482115	0.701018	H	-3.760867	0.553633	0.581080
C	2.120520	-3.561956	-1.635612	C	-4.363585	0.352185	-1.477326
H	1.937102	-4.558048	-1.180609	H	-3.950920	-0.669330	-1.599517
H	4.711029	-2.262660	0.092923	H	-5.448343	0.257921	-1.252241
H	1.322142	-3.371086	-2.380496	H	-4.268594	0.878382	-2.452805

C -4.328895 2.493538 -0.177146
H -4.237739 3.120442 -1.091429
H -5.413811 2.338360 0.002495
H -3.940697 3.080915 0.677698

C -0.808543 3.639661 0.768620
C 0.430672 -3.153950 0.735252
C 2.231519 -2.591161 -1.427880
C 2.644978 -3.324340 -0.316602

62

C 1.757685 -3.592546 0.765687

14-si SCF Done: -1384.55449919 A.U.

C -2.679321 3.410113 -0.810105

Zr 0.002565 0.145353 -0.279500

C -1.666868 4.194166 -0.174365

C -1.345549 -1.854678 -0.732017

H -0.257288 -3.412555 1.553828

C -2.015175 0.139113 1.126318

H 2.118195 -4.175262 1.627936

C -1.174014 -1.173035 -2.004936

H 3.674475 -3.715278 -0.275339

C 0.184883 -1.291034 -2.429238

H 2.921126 -2.399253 -2.265117

C 0.892303 -2.094447 -1.471698

H -0.032229 4.251030 1.255729

C -0.042553 -2.417702 -0.394386

H -1.571155 5.259870 -0.437986

C -0.910817 0.150379 2.065301

H -3.332320 3.880845 -1.561535

C -0.249874 1.410171 2.026689

H -3.673148 1.488178 -0.948046

C -0.952679 2.257270 1.106249

C -4.394632 -1.231311 -0.479928

C -2.031655 1.465627 0.514886

C -3.023059 -2.731306 1.834179

H 0.595673 -0.912277 -3.373949

H -3.198270 -3.742676 1.410446

H 0.592954 1.713736 2.660250

H -5.146834 -0.721022 0.157880

H -1.969423 -0.678141 -2.578691

H -2.165479 -2.797883 2.533722

H -0.624509 -0.686795 2.717110

H -4.279577 -0.643340 -1.412618

C -2.862865 2.067271 -0.480517

H -3.917212 -2.451218 2.430885

H -4.803924 -2.224585 -0.762172
Si -2.763977 -1.462382 0.453189
C 2.449951 0.286693 0.292479
H 1.864551 -0.514142 0.827571
H 3.153985 -0.283203 -0.341654
H 2.248520 2.501202 -0.543347
C 1.947306 1.708906 -1.252467
C 0.597433 1.831924 -1.750577
H 0.417890 1.517438 -2.793601
H 0.019546 2.720990 -1.444210
C 3.177902 1.123270 1.365747
H 2.540622 2.002939 1.621415
C 3.025661 1.328880 -2.254669
H 3.162502 2.178403 -2.959688
H 4.009723 1.110163 -1.797935
H 2.722322 0.449446 -2.858259
C 4.537987 1.673830 0.894023
H 5.032386 2.247104 1.706548
H 5.222905 0.846319 0.606008
H 4.445038 2.353886 0.023592
C 3.370907 0.306015 2.661422
H 2.403588 -0.065768 3.060088

H 4.014471 -0.580688 2.476004
H 3.854466 0.915080 3.455692

70

15-re SCF Done: -1389.36163704 A.U.

Zr 0.111302 0.250010 0.202132
C 1.877607 -0.781093 -1.181735
C 0.271046 -2.171482 0.635116
C 1.012284 -0.046959 -2.084911
C 1.224949 1.354219 -1.873380
C 2.225757 1.517767 -0.870533
C 2.597355 0.212623 -0.400182
C 0.634652 -1.493810 1.869055
C -0.545051 -0.939130 2.447106
C -1.646883 -1.226840 1.593025
C -1.156399 -1.966187 0.456161
H 0.749098 2.168268 -2.437049
H -0.606033 -0.412744 3.409288
H 0.352440 -0.482716 -2.847976
H 1.632607 -1.473302 2.327726
C -2.094552 -2.674603 -0.502324
C -3.119376 -1.043108 1.886778
C 3.764459 0.006869 0.543818

C	2.930320	2.783362	-0.435070	H	-1.804086	-2.524255	-1.563888
C	4.301979	2.468338	0.197167	H	3.460339	1.597037	2.006927
C	4.197673	1.322691	1.218477	H	-3.751786	-1.279979	-0.791911
C	-3.567351	-2.259817	-0.299671	H	5.023279	2.178522	-0.600864
C	-3.944592	-2.142641	1.186874	H	-3.762868	-3.118492	1.693018
H	4.621757	-0.400881	-0.043338	H	-3.285024	-1.067967	2.985241
H	5.169932	1.174714	1.735119	H	3.048156	3.464419	-1.305718
H	4.713893	3.382547	0.675286	Si	1.563558	-2.577664	-0.683440
H	2.317499	3.348783	0.303545	C	-1.846564	1.599125	-0.891872
H	-3.482665	-0.045359	1.552692	H	-1.658360	0.579866	-1.319246
H	-5.029828	-1.929687	1.294045	C	-0.964323	2.642109	0.889649
H	-4.229777	-2.990124	-0.811609	C	0.118816	2.095128	1.663728
H	-2.000307	-3.771706	-0.323212	H	-0.121539	1.715291	2.670005
C	0.910228	-3.584470	-2.149025	H	1.088450	2.620190	1.611072
C	3.063076	-3.476772	0.045422	H	-1.449521	2.319991	-1.631021
H	3.903280	-3.492505	-0.680770	H	-1.963675	2.552795	1.348519
H	0.491431	-4.555225	-1.809865	C	-3.374129	1.740085	-0.753509
H	3.429734	-3.010530	0.981242	H	-3.715303	1.074530	0.073453
H	0.121774	-3.053757	-2.719145	C	-0.718429	3.960712	0.176316
H	2.791151	-4.528680	0.277257	H	0.237737	3.942166	-0.384174
H	1.743778	-3.800724	-2.850878	H	-1.521139	4.252402	-0.525015
H	3.544432	-0.761374	1.314726	H	-0.633479	4.764483	0.941704

C	-4.055759	1.239128	-2.049791	H	-0.869947	0.737749	-3.350509
H	-3.756909	0.200632	-2.303246	H	0.363610	0.557606	2.783396
H	-5.164200	1.261265	-1.962158	H	1.578506	1.467307	-2.452564
H	-3.774177	1.882916	-2.911596	C	-1.690463	2.886079	0.821094
C	-3.909267	3.153416	-0.445135	C	-3.137650	1.550939	-1.527086
H	-3.632250	3.870752	-1.248625	C	3.641428	-0.567582	-0.592944
H	-5.018708	3.138052	-0.393313	C	2.326291	-3.143941	0.430917
H	-3.546207	3.565323	0.517309	C	3.735004	-3.084228	-0.197201
<hr/>							
70							
15-si SCF Done: -1389.36977460 A.U.							
Zr	0.030800	-0.168591	-0.276509	C	3.844200	-1.954157	-1.236273
C	1.921746	0.563541	1.121267	C	-3.198563	2.562269	0.804318
C	0.475974	2.224457	-0.603895	C	-3.779270	2.620536	-0.619312
C	0.939057	0.002436	2.029200	H	4.556358	-0.296838	-0.013317
C	0.910589	-1.415912	1.844795	H	4.833451	-1.989260	-1.740524
C	1.858076	-1.765399	0.838885	H	3.983887	-4.063551	-0.658783
C	2.455048	-0.550538	0.349606	H	1.621834	-3.611723	-0.295905
C	0.637034	1.578258	-1.897116	H	-3.544873	0.552469	-1.248372
C	-0.655574	1.199277	-2.377161	H	-4.881471	2.483298	-0.595373
C	-1.629760	1.580502	-1.408271	H	-3.737360	3.267580	1.472405
C	-0.944491	2.182988	-0.295505	H	-1.553941	3.986512	0.693841
H	0.309001	-2.128444	2.425053	C	1.558730	3.509393	2.103531
				C	3.491299	2.986594	-0.231761
				H	4.371353	2.846819	0.431109

H	1.313420	4.539585	1.769220	H	-3.654270	-1.311627	2.888832
H	3.695453	2.457750	-1.183808	C	-3.575190	-3.368130	0.988828
H	0.719604	3.146321	2.729489	H	-3.747871	-4.182815	1.723620
H	3.404275	4.070268	-0.460317	H	-4.526404	-2.799552	0.892239
H	2.460929	3.566351	2.749213	H	-3.368690	-3.846719	0.010361
H	3.550355	0.206767	-1.383368	C	-1.342869	-2.282603	-1.282949
H	-1.262814	2.650263	1.818620	C	-0.069454	-1.920689	-1.849355
H	3.081181	-2.110440	-2.031656	H	-1.327053	-3.182975	-0.643790
H	-3.369702	1.544180	1.222679	H	-0.071379	-1.516528	-2.876733
H	4.490045	-2.913584	0.604057	H	0.776467	-2.595850	-1.642073
H	-3.596465	3.631971	-1.049176	C	-2.559916	-2.191940	-2.188318
H	-3.432617	1.707815	-2.587143	H	-3.528498	-2.280375	-1.659269
H	2.323714	-3.815173	1.317132	H	-2.564454	-1.245635	-2.766189
Si	1.909105	2.386121	0.618838	H	-2.505319	-3.022276	-2.927242
C	-2.160316	-1.278626	0.480576	<hr/>			
H	-1.815429	-0.392330	1.077791	71			
H	-3.085335	-0.945292	-0.027214	16-re SCF Done: -1753.77208883 A.U.			
C	-2.431406	-2.444204	1.452061	Zr	-0.419710	-0.058209	0.150193
H	-1.509317	-3.071546	1.517415	C	1.414552	1.352321	-0.824149
C	-2.729407	-1.928502	2.876791	C	1.487327	-1.697804	0.686682
H	-2.877398	-2.768496	3.590172	C	1.018190	0.320711	-1.764219
H	-1.903187	-1.296523	3.264969	C	-0.291497	0.579698	-2.281631
				C	-0.695063	1.869420	-1.773910

C	0.358324	2.352864	-0.888327	H	-2.122345	-4.707837	-1.923530
C	0.708198	-1.473200	1.871631	H	0.089674	-4.346491	-3.044563
C	-0.615344	-1.995587	1.706973	H	1.859576	-2.970756	-1.974999
C	-0.655333	-2.676722	0.429578	C	3.038468	2.285452	1.709570
C	0.640915	-2.474894	-0.210197	C	4.482782	1.962995	-0.996939
H	-0.817578	-0.007223	-3.046144	C	4.176628	-1.402593	2.170485
H	-1.406301	-2.004700	2.468184	C	4.234854	-1.961089	-0.856477
H	1.634584	-0.539088	-2.055145	Si	3.068969	1.280098	0.089894
H	1.076522	-0.974850	2.777665	Si	3.277204	-1.058823	0.524835
C	0.880838	-3.081101	-1.485121	H	2.174000	2.010490	2.347386
C	-1.646900	-3.480476	-0.205744	H	5.463064	1.882839	-0.479784
C	0.244363	3.661440	-0.329728	H	5.219887	-1.022723	2.131854
C	-1.821594	2.696342	-2.064536	H	3.846967	-1.734816	-1.871071
C	-1.881594	3.976908	-1.522274	H	3.674111	-0.911376	3.029279
C	-0.849873	4.457389	-0.659438	H	4.211287	-3.062412	-0.713390
C	-0.109398	-3.861504	-2.075394	H	2.983371	3.376698	1.507202
C	-1.368550	-4.067138	-1.439422	H	4.557397	1.412239	-1.957545
H	1.040181	4.053770	0.321570	H	5.297815	-1.638986	-0.834162
H	-0.919899	5.480231	-0.256046	H	4.216291	-2.493477	2.377457
H	-2.728878	4.636616	-1.768443	H	3.967683	2.107317	2.291333
H	-2.605747	2.338978	-2.751214	H	4.309845	3.034788	-1.234630
H	-2.606340	-3.670937	0.299053	C	-2.959210	-0.010078	0.021212

H -2.435724 -0.563712 -0.808539
 C -2.191255 1.113675 1.794074
 C -0.782447 1.307957 2.021167
 H -0.395494 2.329336 1.859495
 H -0.342294 0.790183 2.889657
 H -3.390370 0.890160 -0.457208
 H -2.659786 0.334724 2.419360
 C -3.045989 2.346338 1.572026
 H -4.084743 2.127531 1.263624
 H -3.091891 2.907619 2.532106
 H -2.591216 3.020734 0.820015
 C -4.046510 -0.959126 0.558561
 H -3.549428 -1.741178 1.178972
 C -5.134614 -0.308396 1.436721
 H -4.737046 0.151472 2.363056
 H -5.684943 0.478275 0.875628
 H -5.880924 -1.070506 1.746040
 C -4.735564 -1.681161 -0.624394
 H -4.002420 -2.215473 -1.262620
 H -5.483013 -2.422997 -0.266865
 H -5.272103 -0.949812 -1.267656

16-si SCF Done: -1753.77267987 A.U.
 Zr 0.537512 0.204299 -0.346166
 C -1.309259 0.984615 1.149101
 C -1.305776 -1.320702 -1.092789
 C -0.171630 0.763714 2.013347
 C 0.825390 1.749949 1.761833
 C 0.313376 2.671346 0.788560
 C -0.988435 2.172707 0.360581
 C -0.662203 -0.806785 -2.282292
 C 0.651214 -1.357248 -2.389365
 C 0.838412 -2.299770 -1.319416
 C -0.353196 -2.242651 -0.480670
 H 1.776678 1.852633 2.297489
 H 1.355484 -1.175866 -3.210745
 H -0.105985 -0.019745 2.781111
 H -1.126336 -0.133969 -3.015910
 C -0.405951 -3.043598 0.701346
 C 1.893475 -3.205863 -1.002180
 C -1.694828 2.874535 -0.663471
 C 0.808012 3.910938 0.278724
 C 0.062215 4.591080 -0.679968
 C -1.172826 4.067085 -1.168080

71

C	0.657112	-3.898515	1.003803	H	-4.151326	2.097093	2.457267
C	1.792353	-3.988400	0.148003	H	-2.172308	-1.664607	2.907592
H	-2.666288	2.498096	-1.019964	H	-5.076787	-2.680454	-0.293028
H	-1.725948	4.620606	-1.942909	H	-3.952556	-0.761362	-3.014854
H	0.429382	5.552431	-1.074191	H	-5.354186	0.993252	1.707215
H	1.763325	4.319593	0.645224	H	-2.840352	-0.262470	3.804441
H	2.768213	-3.291498	-1.666348	C	2.872463	-0.426591	0.420537
H	2.598495	-4.696883	0.397651	H	2.025310	-0.925337	0.968937
H	0.609884	-4.527665	1.906698	H	3.345435	-1.245324	-0.151170
H	-1.296419	-3.016074	1.348112	H	3.441687	1.693739	-0.496714
C	-4.364962	1.477204	1.560093	C	2.955988	1.011945	-1.217539
C	-2.983839	-0.908549	2.911694	C	1.757621	1.526117	-1.831846
C	-3.988888	-0.164066	-2.078539	H	1.477705	2.569169	-1.610989
C	-3.994330	-2.808936	-0.507824	H	1.561512	1.224399	-2.875270
Si	-3.009361	0.156037	1.329784	C	3.829181	0.164015	1.479099
Si	-3.141566	-1.110889	-0.656641	H	3.593394	1.246143	1.614056
H	-4.448210	2.161324	0.691072	C	3.625363	-0.521102	2.848036
H	-3.947079	-1.446949	3.035227	H	4.277622	-0.070552	3.627202
H	-5.056179	0.025447	-1.837785	H	2.574558	-0.437172	3.195926
H	-3.560664	-3.434218	0.299186	H	3.868446	-1.603724	2.787532
H	-3.509647	0.815187	-2.283133	C	5.315666	0.082637	1.078730
H	-3.899566	-3.373836	-1.460004	H	5.547452	0.673267	0.169920

H 5.962005 0.471591 1.893874
H 5.618834 -0.970011 0.886799
C 3.926597 0.257732 -2.111740
H 4.724319 -0.283647 -1.569433
H 3.395216 -0.468188 -2.758355
H 4.417485 0.994478 -2.785696

H -1.561027 -0.566374 -2.076489
C 0.905064 -3.084430 1.153773
C 2.504173 -2.891034 -1.224876
C -2.312868 1.949449 -0.521898
C -0.421418 3.880843 0.443707
C -1.326838 4.200275 -0.562538

65

C -2.250895 3.232982 -1.062607

17-re SCF Done: -1588.08626736 A.U.

C 2.148985 -3.712802 1.067391

Zr 0.656659 0.290209 -0.088870

C 2.931352 -3.630171 -0.122462

C -1.293677 0.409703 1.384286

H -3.063770 1.229878 -0.878574

C -0.832664 -1.658119 -0.218111

H -2.940791 3.513966 -1.873551

C -0.176760 0.645844 2.272945

H -1.339573 5.220265 -0.979360

C 0.378533 1.926694 1.996989

H 0.272926 4.640348 0.836557

C -0.421432 2.557765 0.985105

H 3.112728 -2.839181 -2.140873

C -1.430876 1.595660 0.546411

H 3.889736 -4.172168 -0.170737

C -0.748719 -1.078819 -1.545702

H 2.522657 -4.303160 1.918788

C 0.537751 -1.382387 -2.092656

H 0.277647 -3.183413 2.053787

C 1.254407 -2.206024 -1.157122

C -3.631533 -1.067125 0.405269

C 0.422041 -2.350646 0.030538

C -4.577684 -0.212373 1.019890

H 1.213169 2.394143 2.536507

C -4.040094 -1.853199 -0.696930

H 0.875811 -1.129010 -3.106076

C -5.889698 -0.127559 0.526908

H 0.165824 -0.053279 3.048405

H -4.280448 0.401421 1.886498

C	-5.356630	-1.769109	-1.184060	H	5.136591	0.770183	2.299296
H	-3.320782	-2.534228	-1.179899	H	5.083254	-0.964814	1.848511
C	-6.284771	-0.904454	-0.578111	C	5.046775	-0.550447	-0.945352
H	-6.610130	0.551647	1.010596	H	4.493328	-0.366214	-1.890133
H	-5.656906	-2.384200	-2.047801	H	6.128990	-0.432809	-1.163977
H	-7.314268	-0.836588	-0.964052	H	4.869315	-1.607133	-0.659952
P	-1.972771	-1.294560	1.181387	H	4.940099	1.425251	-0.100259
C	3.092090	0.423462	0.438656	<hr/>			
H	2.772187	-0.647430	0.555706	65			
H	1.142433	1.260494	-2.736490	17-si SCF Done: -1588.08926082 A.U.			
C	1.245403	1.781201	-1.770057	Zr	-0.643764	0.164833	0.191993
C	2.558112	1.820237	-1.176670	C	1.197449	0.487651	-1.372161
H	0.609059	2.678554	-1.663959	C	0.971170	-1.653791	0.203396
H	2.887384	0.947189	1.395008	C	0.017805	0.608087	-2.200955
H	3.356766	1.327295	-1.754604	C	-0.675041	1.806145	-1.865304
C	4.613792	0.398803	0.184795	C	0.096275	2.511530	-0.880742
C	2.981737	3.110069	-0.496353	C	1.240111	1.673407	-0.518622
H	2.139082	3.563203	0.059531	C	0.924933	-1.129349	1.557292
H	3.842134	3.001550	0.192336	C	-0.321898	-1.501826	2.147779
H	3.281725	3.837873	-1.282543	C	-1.068212	-2.286154	1.202691
C	5.365449	0.047727	1.487645	C	-0.275032	-2.373845	-0.020625
H	6.465410	0.054685	1.328958	H	-1.582962	2.180923	-2.354841
				H	-0.623146	-1.289273	3.181649

H	-0.276706	-0.113581	-2.975392	H	4.129740	0.786491	-1.922159
H	1.736040	-0.593508	2.066530	C	5.535483	-1.434494	0.974747
C	-0.803419	-3.050502	-1.160257	H	3.578757	-2.383133	1.009051
C	-2.330327	-2.956009	1.274079	C	6.354042	-0.457796	0.381027
C	2.125531	2.116531	0.512528	H	6.475304	1.104158	-1.134122
C	-0.052503	3.807486	-0.295779	H	5.928369	-2.062762	1.790459
C	0.862947	4.222336	0.665545	H	7.389613	-0.315506	0.728529
C	1.933328	3.374593	1.084693	P	2.025029	-1.159809	-1.229361
C	-2.054068	-3.666825	-1.065331	C	-3.118106	0.019235	-0.179590
C	-2.802603	-3.628092	0.148422	H	-2.483307	-0.608106	-0.869641
H	2.978177	1.491050	0.812879	H	-3.684402	-0.726663	0.408728
H	2.626901	3.726741	1.864127	H	-0.976547	1.157855	2.890753
H	0.763784	5.223165	1.115944	C	-1.325060	1.557583	1.922507
H	-0.879885	4.463186	-0.610928	C	-2.685627	1.265609	1.544037
H	-2.912004	-2.944328	2.209251	H	-0.930895	2.560246	1.683129
H	-3.771664	-4.150671	0.195903	H	-3.202052	2.076000	0.999018
H	-2.461567	-4.208820	-1.933090	C	-3.560154	0.552724	2.562032
H	-0.206858	-3.111788	-2.084197	H	-4.538487	0.223058	2.162107
C	3.685406	-0.813679	-0.503734	H	-3.044205	-0.331674	2.987048
C	4.521369	0.157314	-1.105600	H	-3.757836	1.253301	3.403206
C	4.211529	-1.614463	0.536492	C	-4.034798	0.897443	-1.056230
C	5.841455	0.336541	-0.661572	H	-3.552868	1.896693	-1.180377

C	-5.421253	1.135578	-0.427107	H	-1.562636	0.822482	-3.126187
H	-6.054538	1.760960	-1.091231	H	0.567835	1.077611	2.650778
H	-5.953343	0.171948	-0.268654	H	0.461928	-0.765966	-2.317830
H	-5.362678	1.652597	0.552044	C	0.600696	3.270483	0.220277
C	-4.198466	0.291341	-2.466385	C	-1.471760	3.527126	-1.733196
H	-3.217560	0.148617	-2.966396	C	0.186018	-2.908899	0.036580
H	-4.692078	-0.702907	-2.414831	C	-1.934520	-2.892348	1.966155
H	-4.819581	0.943701	-3.117447	C	-1.745463	-3.980268	1.117610
<hr/>							
78							
18-re SCF Done: -1732.59520062 A.U.							
Zr	-1.118164	0.327295	0.186424	C	-0.142310	4.446481	0.111631
C	0.910853	-0.617980	1.166703	C	-1.160267	4.580631	-0.881647
C	1.009050	0.880956	-0.866137	H	0.994011	-2.940187	-0.706561
C	0.228069	0.133064	2.208422	H	-0.605961	-4.835773	-0.542710
C	-0.966921	-0.547129	2.609675	H	-2.413383	-4.853533	1.192915
C	-1.042284	-1.778036	1.880136	H	-2.739008	-2.894913	2.719244
C	0.087457	-1.808167	0.949279	H	-2.242775	3.642337	-2.511757
C	0.240201	0.230582	-1.912168	H	-1.701266	5.536362	-0.972331
C	-0.840520	1.058162	-2.332875	H	0.064797	5.287582	0.791881
C	-0.755318	2.292936	-1.614371	H	1.396081	3.208558	0.974780
C	0.361119	2.174809	-0.668741	B	1.982742	-0.012430	0.097318
H	-1.649407	-0.236395	3.411644	C	2.934043	-1.059827	-0.720120
				C	3.386434	-2.274542	-0.141312

C	3.409116	-0.765640	-2.024214	C	-3.261004	-0.662913	-0.759358
C	4.254637	-3.147147	-0.820677	H	-2.324347	-1.269025	-0.924698
H	3.033255	-2.548042	0.867623	C	-3.671398	1.119551	0.477703
C	4.283282	-1.627748	-2.713104	C	-2.613713	1.838572	1.139127
H	3.068611	0.159709	-2.519640	H	-2.378981	2.852806	0.766196
C	4.710678	-2.824984	-2.112637	H	-2.523050	1.721749	2.232267
H	4.573883	-4.087936	-0.342556	H	-3.492302	-0.210965	-1.744074
H	4.626322	-1.366657	-3.727967	H	-4.264276	0.453355	1.127576
H	5.388974	-3.507219	-2.650296	C	-4.475690	1.878215	-0.563219
P	3.460049	1.079192	1.018180	H	-3.805405	2.467739	-1.219902
C	3.172822	1.958314	2.622694	H	-5.121102	1.242631	-1.197061
H	4.102800	2.469912	2.944762	H	-5.133236	2.604101	-0.034800
H	2.359103	2.703717	2.548000	C	-4.342218	-1.679646	-0.338351
H	2.888440	1.207603	3.386633	H	-4.126080	-1.991903	0.709574
C	4.160512	2.338262	-0.126256	C	-5.799427	-1.177802	-0.390568
H	5.019571	2.868247	0.332580	H	-6.077822	-0.860496	-1.419837
H	4.497717	1.815463	-1.043425	H	-6.492722	-1.997322	-0.105125
H	3.375381	3.066166	-0.410005	H	-6.002482	-0.329455	0.292188
C	4.916877	0.042962	1.468754	C	-4.229450	-2.943099	-1.222442
H	5.337566	-0.432285	0.562868	H	-3.219631	-3.395422	-1.158419
H	5.687867	0.670847	1.960037	H	-4.970182	-3.714416	-0.917162
H	4.598656	-0.758971	2.163848	H	-4.425394	-2.693805	-2.288874

78				C	0.751169	-3.865437	-0.467920
18-si SCF Done: -1732.60155784 A.U.				C	0.366627	4.392837	0.203391
Zr	1.121737	0.289922	-0.271435	C	1.442572	4.380968	1.143163
C	-0.966379	-0.484883	-1.252501	H	-0.973819	-2.930280	0.455548
C	-0.936725	0.815637	0.923261	H	0.703561	-4.750394	0.186356
C	-0.315644	0.342861	-2.256046	H	2.458508	-4.636005	-1.595869
C	0.845907	-0.315411	-2.768529	H	2.646954	-2.627122	-3.080111
C	0.944352	-1.599081	-2.140228	H	2.566614	3.233432	2.605398
C	-0.149415	-1.697972	-1.169293	H	2.050433	5.290498	1.276025
C	-0.158018	0.038364	1.868748	H	0.177322	5.300612	-0.390885
C	0.981208	0.771999	2.310707	H	-1.283032	3.318941	-0.680095
C	0.929364	2.070161	1.709063	B	-1.972232	0.046161	-0.083029
C	-0.234643	2.093804	0.815160	C	-2.920612	-1.056737	0.659204
H	1.500718	0.062673	-3.564364	C	-3.409121	-2.202084	-0.022552
H	1.718029	0.436871	3.052119	C	-3.355425	-0.884549	1.998595
H	-0.655439	1.329023	-2.596256	C	-4.278250	-3.121244	0.590971
H	-0.414150	-0.978719	2.194990	H	-3.083692	-2.383919	-1.061136
C	-0.448444	3.272163	0.032493	C	-4.229637	-1.794577	2.622819
C	1.732495	3.241790	1.885470	H	-2.980929	-0.020578	2.574119
C	-0.187654	-2.841531	-0.306411	C	-4.697052	-2.918502	1.919171
C	1.864331	-2.681909	-2.306514	H	-4.627512	-4.005110	0.032019
C	1.756338	-3.794950	-1.475624	H	-4.541262	-1.629395	3.667509

H	-5.376308	-3.637606	2.405088	C	4.027851	-0.971073	1.626141
P	-3.447822	1.263363	-0.829751	H	3.856929	0.007220	2.136267
C	-3.195608	2.295746	-2.347377	C	3.568913	-2.077649	2.600391
H	-4.111131	2.885775	-2.557487	H	2.486876	-1.992662	2.833834
H	-2.338667	2.987250	-2.240195	H	3.733622	-3.084769	2.160523
H	-2.994546	1.621375	-3.203249	H	4.129404	-2.031075	3.559503
C	-4.064636	2.426237	0.457682	C	5.543914	-1.094885	1.378072
H	-4.942828	2.996205	0.092812	H	5.945075	-0.267950	0.757778
H	-4.354757	1.830811	1.346276	H	6.102419	-1.085788	2.338106
H	-3.258275	3.125182	0.755167	H	5.782762	-2.050917	0.862479
C	-4.955471	0.320128	-1.317030	C	4.595103	0.247486	-1.774028
H	-5.358835	-0.224182	-0.442632	H	5.244021	1.054153	-2.181486
H	-5.721640	1.015718	-1.715820	H	5.254118	-0.571998	-1.427366
H	-4.693093	-0.422287	-2.096516	H	3.981678	-0.136800	-2.614458
C	3.195417	-0.998786	0.327533	<hr/>			
H	2.218414	-1.507823	0.563417	71			
H	3.645322	-1.645756	-0.448266	19-re SCF Done: -1251.02567904 A.U.			
H	4.263706	1.115980	0.237341	Zr	-0.172583	-0.042607	-0.176272
C	3.717820	0.839545	-0.682470	C	-1.602257	-1.610739	1.084802
C	2.704565	1.783888	-1.088130	C	0.414708	-2.380884	-0.733157
H	2.595676	2.704191	-0.488139	C	-0.966874	-0.796442	2.089544
H	2.565471	1.932985	-2.173841	C	-1.481612	0.526136	2.029089
				C	-2.509777	0.558950	1.029831

C	-2.574897	-0.763347	0.399079	C	-1.370397	-3.107099	0.959705
C	0.190068	-1.671997	-1.969831	H	-1.142880	-3.777694	-1.109209
C	1.254442	-0.738214	-2.170030	H	-0.880630	-3.438472	1.898712
C	2.211477	-0.915874	-1.113825	H	0.095492	-4.416991	-0.027812
C	1.684190	-1.915430	-0.184900	H	-2.338312	-3.651996	0.931466
H	-1.192222	1.356462	2.684828	C	2.047492	-3.379493	1.927401
H	1.382747	-0.088967	-3.044709	C	4.122276	0.492709	-2.049084
H	-0.217185	-1.158399	2.806880	C	-3.722604	-2.345741	-1.306042
H	-0.630640	-1.871478	-2.672086	C	-3.549962	2.834309	1.567480
C	2.471791	-2.297463	0.961906	H	2.810362	-3.520770	2.718781
C	3.527777	-0.365538	-0.959741	H	-3.929425	2.592015	2.585914
C	-3.547874	-1.001287	-0.640173	H	-4.498090	-2.295020	-2.095905
C	-3.467223	1.586902	0.721631	H	4.289178	-0.102681	-2.974999
C	-4.377224	1.310882	-0.293485	H	1.085251	-3.151057	2.431854
C	-4.398829	0.055420	-0.972095	H	3.454625	1.333308	-2.338096
C	3.724629	-1.689597	1.108042	H	-2.562525	3.320517	1.713161
C	4.249575	-0.762665	0.165612	H	-2.785821	-2.707861	-1.778014
H	-5.151786	-0.103487	-1.761542	H	-4.038950	-3.125687	-0.580326
H	-5.135144	2.067587	-0.557223	H	1.914416	-4.357659	1.417200
H	5.271438	-0.375321	0.313807	H	5.097431	0.921700	-1.743655
H	4.350727	-1.977331	1.968916	H	-4.237128	3.582304	1.123703
C	-0.491927	-3.501079	-0.253816	C	1.099364	2.010255	0.674299

H	1.294106	1.042599	1.218764
H	-0.658454	1.077035	-2.733024
C	-0.943279	1.496926	-1.754260
C	-0.064699	2.471160	-1.162253
H	-2.030055	1.657795	-1.629361
H	0.482273	2.617442	1.364874
H	0.900095	2.616099	-1.679594
C	-0.705098	3.749353	-0.653011
H	-1.675641	3.532412	-0.168433
H	-0.083631	4.340395	0.044353
H	-0.924102	4.394734	-1.533079
C	2.487597	2.642491	0.456128
H	2.995125	2.080106	-0.356328
C	2.501471	4.132660	0.063547
H	3.548925	4.490429	-0.028442
H	2.003211	4.337645	-0.904568
H	2.010768	4.760674	0.839674
C	3.343421	2.453995	1.730674
H	3.440329	1.381882	1.998429
H	4.368332	2.863042	1.591517
H	2.886627	2.983428	2.596033

19-si SCF Done: -1251.03282016 A.U.

Zr	0.140520	-0.064297	0.212239
C	1.581573	-1.468996	-1.227392
C	-0.401798	-2.453110	0.528776
C	0.936497	-0.534023	-2.112640
C	1.440840	0.774633	-1.872714
C	2.476027	0.678941	-0.883585
C	2.557473	-0.715584	-0.443676
C	-0.156275	-1.883952	1.832352
C	-1.226429	-0.994911	2.161316
C	-2.208976	-1.068614	1.114643
C	-1.690299	-1.946627	0.066203
H	1.150492	1.680460	-2.413790
H	-1.334754	-0.446170	3.104464
H	0.188679	-0.801931	-2.872187
H	0.689697	-2.139574	2.484577
C	-2.482654	-2.184030	-1.115229
C	-3.517366	-0.486203	1.025355
C	3.547228	-1.091695	0.537843
C	3.401437	1.672485	-0.409552
C	4.340024	1.258431	0.529111
C	4.400046	-0.087024	0.999981

71

C	-3.725173	-1.542972	-1.190920	H	2.394783	3.585079	-0.695954
C	-4.236752	-0.727339	-0.144879	H	2.828943	-2.917688	1.505962
H	5.173301	-0.351761	1.739789	H	3.980071	-3.199951	0.173527
H	5.075984	1.985977	0.910556	H	-1.985188	-4.188991	-1.816500
H	-5.249220	-0.302621	-0.249929	H	-5.125609	0.631569	1.967197
H	-4.352953	-1.715523	-2.080774	H	4.173860	3.700067	-0.520624
C	0.495200	-3.505132	-0.101064	C	-1.441561	1.872446	-0.259200
C	1.346871	-2.969126	-1.280768	H	-1.428268	1.118655	-1.094622
H	1.165560	-3.882512	0.698828	H	-2.302065	1.604411	0.380575
H	0.832924	-3.183281	-2.240964	C	-1.673391	3.254051	-0.895856
H	-0.098938	-4.387207	-0.423378	H	-1.545236	4.032652	-0.106731
H	2.312631	-3.515135	-1.341553	C	-0.697499	3.606803	-2.029737
C	-2.074630	-3.150612	-2.202333	H	0.357874	3.604824	-1.688850
C	-4.094008	0.288804	2.183344	H	-0.786133	2.887711	-2.873483
C	3.737318	-2.513270	1.012198	H	-0.912306	4.618564	-2.433630
C	3.356393	3.081833	-0.941656	C	-3.130893	3.373773	-1.395212
H	-2.826763	-3.164991	-3.016039	H	-3.857150	3.195738	-0.575041
H	3.447093	3.103220	-2.050010	H	-3.330993	4.383506	-1.814874
H	4.567857	-2.574164	1.743032	H	-3.341271	2.628158	-2.192279
H	-4.128455	-0.333073	3.105512	H	0.702142	1.030183	2.855456
H	-1.095818	-2.894914	-2.658474	C	0.907932	1.419479	1.842586
H	-3.486671	1.185540	2.435292	C	-0.022569	2.387938	1.319858

H 1.980481 1.562839 1.629852
H 0.410808 3.152211 0.650631
C -1.064444 2.928966 2.284957
H -0.558721 3.635020 2.980049
H -1.898786 3.479192 1.807300
H -1.489565 2.113618 2.904873

H -2.062311 -3.310285 0.093630
H -0.756179 -3.526073 1.284484
C 2.107959 -2.587930 0.860806
C 3.209747 -1.064469 -1.301258
C -3.606161 -0.715042 -0.311433
C -3.253144 1.813112 0.995011

62

C -4.277553 1.616534 0.076374

20-re SCF Done: -1133.16651897 A.U.

C -4.450040 0.359602 -0.583288

Zr -0.209253 -0.000178 -0.137416
C -1.577799 -1.486700 1.202943
C -0.149435 -2.396162 -0.494022
C -0.819001 -0.756873 2.202651
C -1.253420 0.608408 2.185799
C -2.352559 0.738263 1.276779
C -2.548866 -0.561076 0.635762
C -0.434218 -1.799395 -1.791799
C 0.755662 -1.108579 -2.222457
C 1.813371 -1.365026 -1.287910
C 1.252586 -2.153227 -0.194881
H -0.887265 1.392366 2.863082
H 0.875295 -0.608245 -3.193007
C -1.183529 -2.811273 0.551411

C 3.469595 -2.282566 0.815621
C 4.016750 -1.530480 -0.264570
H -3.791566 -1.691764 -0.781659
H -5.279146 0.234409 -1.297241
H -4.985357 2.434281 -0.134538
H -3.153242 2.771115 1.529753
H 3.645889 -0.513606 -2.149889
H 5.099706 -1.328851 -0.285612
H 4.136175 -2.646949 1.613234
H 1.713033 -3.218059 1.671154
C 0.111104 -1.329281 3.243515
C -1.615884 -2.072364 -2.687297
H 0.306102 -2.404983 3.078188
H -2.436976 -2.582135 -2.149001

H	-0.350148	-1.231967	4.251270	C	3.919988	1.890120	1.003731
H	1.091697	-0.811671	3.278647	H	3.928082	0.800445	1.208492
H	-1.311380	-2.742403	-3.522989	H	4.934779	2.178635	0.652419
H	-2.031663	-1.148203	-3.139410	H	3.736220	2.418843	1.964980
C	1.455789	1.807182	0.459476	<hr/>			
H	1.618989	0.792757	0.929666	62			
C	0.062365	2.492083	-1.090818	20-si SCF Done: -1133.17261168 A.U.			
C	-0.945018	1.616437	-1.633383	Zr	-0.183124	-0.062767	-0.199738
H	-0.771721	1.209926	-2.644261	C	-1.596133	-1.007945	1.530584
H	-2.001451	1.856515	-1.412287	C	-0.445737	-2.454417	-0.001838
H	0.949053	2.634975	-1.731033	C	-0.665937	-0.200638	2.297133
H	1.089343	2.449129	1.285201	C	-0.906882	1.177877	1.987654
C	-0.414687	3.746796	-0.380243	C	-2.049365	1.271064	1.127938
H	-1.247605	3.514462	0.312935	C	-2.481084	-0.092094	0.820173
H	0.374603	4.278099	0.183893	C	-0.797946	-2.150523	-1.381941
H	-0.813895	4.450671	-1.143885	C	0.400059	-1.728459	-2.056166
C	2.841754	2.262696	-0.039806	C	1.515006	-1.850219	-1.163209
H	3.075302	1.693353	-0.969825	C	0.995321	-2.296430	0.128125
C	2.968024	3.765050	-0.363809	H	-0.391532	2.027440	2.455927
H	2.752760	4.387220	0.532710	H	0.461996	-1.476868	-3.123444
H	4.006013	3.999594	-0.681182	C	-1.416826	-2.484739	1.178811
H	2.296706	4.100492	-1.178719	H	-2.383152	-2.958045	0.909675
				H	-1.004921	-3.066330	2.028795

C	1.903713	-2.494696	1.210614	H	-1.949893	-3.329948	-2.772920
C	2.919405	-1.643090	-1.332299	H	-2.454189	-1.612779	-2.704798
C	-3.630269	-0.283226	-0.006440	C	1.846323	1.427375	-0.193338
C	-2.801707	2.385801	0.641629	H	1.852178	0.585259	0.556523
C	-3.922950	2.153521	-0.146018	H	2.688486	1.182841	-0.868143
C	-4.334616	0.823970	-0.475130	C	0.507031	1.976057	-1.796474
C	3.268982	-2.270315	1.016527	C	-0.774010	1.331966	-1.958683
C	3.771602	-1.847684	-0.249074	H	0.464041	2.973750	-1.325370
H	-3.990935	-1.298359	-0.227604	H	-0.924279	0.735916	-2.876579
H	-5.233352	0.675250	-1.094009	H	-1.669414	1.888146	-1.629393
H	-4.517553	3.005294	-0.513596	C	2.079522	2.744358	0.576322
H	-2.501029	3.411682	0.908496	H	1.086351	3.191125	0.823745
H	3.318049	-1.342001	-2.314164	C	2.805405	2.485662	1.913719
H	4.856447	-1.700459	-0.374155	H	2.235355	1.783150	2.556825
H	3.971863	-2.443338	1.846735	H	3.808393	2.039843	1.740063
H	1.540236	-2.872111	2.177249	H	2.947846	3.428012	2.485945
C	0.243424	-0.668472	3.406834	C	2.863183	3.787132	-0.244720
C	-2.091575	-2.462190	-2.089812	H	2.345944	4.069475	-1.184045
H	0.224078	-1.769037	3.517767	H	3.014892	4.719123	0.339788
H	-2.898088	-2.737569	-1.384259	H	3.868201	3.396762	-0.517523
H	-0.097926	-0.238414	4.374252	C	1.490576	1.877722	-2.952014
H	1.300418	-0.364257	3.264112	H	2.494804	2.283236	-2.721205

H	1.610950	0.826890	-3.285787	C	-4.569765	1.678800	-0.204583
H	1.083617	2.452789	-3.812841	C	3.281431	-3.151932	0.076119
<hr/>							
76							
21-re SCF Done: -1467.92361545 A.U.							
Zr	-0.029981	0.323494	-0.206488	H	-3.501916	0.257720	-1.443480
C	-1.813679	-0.671023	1.184588	H	-5.039968	1.697072	0.805364
C	-0.321029	-2.061766	-0.774639	H	-3.207857	2.890871	-1.379645
C	-0.866550	-0.062029	2.116313	H	-1.852013	3.774313	0.466184
C	-0.980916	1.359227	1.973459	H	3.674039	-0.248160	-1.848553
C	-1.983568	1.664312	1.009311	H	4.094784	-1.168411	0.391749
C	-2.492743	0.425508	0.498745	H	3.195827	-3.897512	-0.747452
C	-0.490235	-1.297743	-2.014291	H	1.975938	-2.252165	1.560297
C	0.804814	-0.807811	-2.390268	C	-0.069349	-0.728082	3.212188
C	1.776539	-1.259321	-1.453301	C	-1.678646	-1.250547	-2.941628
C	1.096797	-2.006291	-0.437109	H	0.489398	-1.624637	2.876948
H	-0.425093	2.096695	2.570387	H	-2.648461	-1.262136	-2.411323
H	1.025633	-0.250836	-3.312534	H	-0.734421	-1.058127	4.041881
C	1.870770	-2.805383	0.598134	H	0.667379	-0.020885	3.645794
C	3.277519	-1.265020	-1.633116	H	-1.677441	-2.127444	-3.629330
C	-3.742847	0.385739	-0.365395	H	-1.654854	-0.337810	-3.572786
C	-2.615041	3.007484	0.722921	Si	-1.699962	-2.431708	0.479453
C	-3.691282	2.927618	-0.377067	C	-3.299706	-3.085515	-0.308304
				C	-1.264887	-3.739021	1.786845

H	-3.712517	-2.463744	-1.124226	C	0.992305	4.051488	-0.458514
H	-0.370403	-3.513199	2.396347	H	1.890950	4.331870	0.119904
H	-4.084908	-3.193079	0.470462	H	0.874871	4.792875	-1.280344
H	-1.109802	-4.725412	1.299561	H	0.110291	4.161292	0.204835
H	-3.100807	-4.096402	-0.725558	C	3.500300	1.703741	0.498397
H	-2.126927	-3.840626	2.481078	H	3.739260	0.957215	-0.290857
H	3.493243	-1.860698	-2.550828	C	4.128419	3.039971	0.054851
H	5.055847	-2.153441	-0.733492	H	3.958283	3.837592	0.811069
H	3.870938	-3.639103	0.882404	H	5.228129	2.926556	-0.053550
H	1.322029	-3.737703	0.841236	H	3.742634	3.404880	-0.917713
H	-3.086968	3.368316	1.666669	C	4.207305	1.239012	1.794728
H	-4.309690	3.850283	-0.362816	H	3.836276	0.250611	2.138755
H	-5.402203	1.684446	-0.940522	H	5.307325	1.156850	1.653050
H	-4.362368	-0.490607	-0.083367	H	4.028582	1.963982	2.619041
C	1.976080	1.701988	0.715599	<hr/>			
H	1.736853	0.742417	1.246813	76			
C	1.046993	2.662534	-1.072068	21-si SCF Done: -1467.93023358 A.U.			
C	-0.159829	2.160035	-1.674839	Zr	-0.062800	-0.230017	-0.280566
H	-0.080011	1.733122	-2.688452	C	1.845872	0.248221	1.205546
H	-1.077460	2.750095	-1.509639	C	0.749826	2.062089	-0.675787
H	1.975801	2.445422	-1.628821	C	0.761651	-0.156620	2.096652
H	1.669191	2.511144	1.405253	C	0.522539	-1.551768	1.875187
				C	1.438460	-2.046321	0.902790

C	2.251169	-0.947183	0.465784	H	-1.384507	2.536871	1.712477
C	0.773670	1.374919	-1.970057	C	0.159572	0.620097	3.242563
C	-0.588945	1.181397	-2.374923	C	1.944444	1.144668	-2.892797
C	-1.462323	1.734729	-1.394522	H	-0.216903	1.624534	2.963158
C	-0.655998	2.269878	-0.337582	H	2.855925	0.794151	-2.372378
H	-0.203230	-2.161703	2.431769	H	0.909940	0.773853	4.049851
H	-0.901817	0.738718	-3.331128	H	-0.690011	0.063988	3.688509
C	-1.264618	3.115149	0.767744	H	2.218710	2.083457	-3.426293
C	-2.955821	1.944183	-1.494761	H	1.693336	0.388851	-3.665097
C	3.487359	-1.178073	-0.386504	Si	2.155925	2.025320	0.604371
C	1.711559	-3.489696	0.545207	C	3.879301	2.316900	-0.137417
C	2.832829	-3.634106	-0.505823	C	2.006702	3.326492	1.978869
C	3.975099	-2.636526	-0.255679	H	4.137245	1.655561	-0.985024
C	-2.646745	3.661411	0.352851	H	1.058145	3.296790	2.545458
C	-3.546559	2.547400	-0.205262	H	4.652352	2.183560	0.649449
H	3.297053	-0.964291	-1.462381	H	2.116571	4.343482	1.545005
H	4.390048	-2.797615	0.765750	H	3.944170	3.366228	-0.497821
H	2.423601	-3.458803	-1.526615	H	2.836825	3.179173	2.702941
H	0.787933	-4.009792	0.205531	H	-3.146157	2.639366	-2.345760
H	-3.482345	1.002098	-1.763175	H	-4.569150	2.932188	-0.405909
H	-3.657236	1.750795	0.565298	H	-3.131705	4.152544	1.223663
H	-2.515641	4.451375	-0.421968	H	-0.584975	3.957476	1.012892

H	2.018315	-4.017171	1.478343	C	-3.327901	-1.595587	2.618846
H	3.214190	-4.677391	-0.501576	H	-4.174592	-0.880463	2.530517
H	4.808476	-2.818949	-0.967655	H	-3.643174	-2.405599	3.312272
H	4.293405	-0.482989	-0.072634	H	-2.484286	-1.053754	3.094662
C	-2.440502	-1.040123	0.294902	<hr/>			
H	-2.029658	-0.204750	0.924237	74			
H	-3.270199	-0.593372	-0.283925	22-re SCF Done: -1691.62788091 A.U.			
C	-1.617053	-2.156536	-1.399208	Zr	0.173173	0.228123	-0.092359
C	-0.265252	-1.972295	-1.860367	C	1.460341	2.033183	0.964008
H	-1.778100	-3.051848	-0.772968	C	-0.802296	2.429411	-0.616269
H	-0.136896	-1.566894	-2.879498	C	1.059879	1.172037	2.059926
H	0.462737	-2.756538	-1.599956	C	1.780022	-0.054829	1.991129
C	-2.935735	-2.156775	1.235167	C	2.683743	0.013598	0.884346
H	-2.096641	-2.876156	1.398353	C	2.458564	1.283252	0.209930
C	-2.735036	-1.900079	-2.396420	C	-0.446067	1.807373	-1.880862
H	-3.747746	-1.884075	-1.949019	C	-1.357528	0.742086	-2.155444
H	-2.578607	-0.944706	-2.936639	C	-2.323024	0.691515	-1.102107
H	-2.718045	-2.711072	-3.158221	C	-1.968152	1.708745	-0.126336
C	-4.119939	-2.959928	0.660428	H	1.696929	-0.879780	2.710699
H	-4.448715	-3.744403	1.374610	H	-1.361960	0.127907	-3.064539
H	-4.991854	-2.294856	0.473538	C	-2.792164	1.889732	1.038308
H	-3.873505	-3.467193	-0.293764	C	-3.557099	-0.063817	-0.967279
				C	3.216361	1.595543	-0.971903

C	3.770726	-0.859172	0.474009	C	4.156540	-2.013509	1.203175
C	4.517989	-0.492108	-0.703117	C	5.590136	-1.332953	-1.117660
C	4.196377	0.726005	-1.412757	C	5.936417	-2.475487	-0.394503
C	-3.952277	1.150787	1.182923	C	5.222734	-2.813438	0.779144
C	-4.374744	0.187230	0.193626	C	-6.020811	-1.433271	-0.644555
H	3.045723	2.544925	-1.500265	C	-5.221476	-1.665444	-1.790449
H	4.783145	0.971300	-2.312551	H	3.613597	-2.275120	2.125281
H	-4.599066	1.309112	2.061022	H	5.507921	-3.703681	1.361695
H	-2.525230	2.651777	1.785030	H	6.773419	-3.107676	-0.731308
Si	0.415280	3.487159	0.362690	H	6.157106	-1.058268	-2.022428
C	1.325547	4.715313	-0.753130	H	-6.227340	-0.335866	1.214278
C	-0.335908	4.426679	1.824398	H	-6.976377	-1.967915	-0.523216
H	1.627156	4.274672	-1.724225	H	-5.556107	-2.377310	-2.561521
H	-0.743933	3.755735	2.606919	H	-3.395004	-1.166498	-2.841470
H	2.237167	5.104321	-0.252655	C	-0.821427	-1.829086	0.998658
H	-1.153111	5.097940	1.486015	H	-1.124864	-0.838423	1.446575
H	0.660690	5.577706	-0.972488	H	2.094761	-1.353285	-1.588052
H	0.446465	5.055157	2.300545	C	0.989946	-1.340892	-1.612710
H	0.333061	1.427987	2.843580	C	0.303340	-2.351007	-0.851869
H	0.359436	2.130600	-2.553785	H	0.565896	-1.064370	-2.591629
C	-4.010032	-0.987076	-1.945517	H	-0.101352	-2.268523	1.716791
C	-5.602337	-0.522806	0.325482	H	-0.660979	-2.686984	-1.272033

C	-2.118220	-2.660322	0.923262	C	2.377640	1.332639	0.262244
H	-2.740073	-2.259763	0.092578	C	-0.599570	1.968277	-1.894259
C	1.148807	-3.448621	-0.234363	C	-1.482762	0.883893	-2.183908
H	2.076673	-3.037747	0.209066	C	-2.390029	0.733494	-1.086912
H	0.628994	-4.056400	0.528015	C	-2.026291	1.714557	-0.076534
H	1.463757	-4.135306	-1.051656	H	1.447541	-0.928645	2.616642
C	-1.944795	-4.172372	0.681012	H	-1.496155	0.310883	-3.119502
H	-1.339538	-4.645744	1.485489	C	-2.742821	1.743873	1.169527
H	-2.937960	-4.668907	0.686222	C	-3.542421	-0.131162	-0.896170
H	-1.469090	-4.413604	-0.289841	C	3.216787	1.694788	-0.847426
C	-2.921654	-2.461382	2.230643	C	3.576260	-0.889912	0.433863
H	-3.886785	-3.010771	2.194730	C	4.417515	-0.463378	-0.657244
H	-2.349265	-2.840837	3.106146	C	4.198016	0.822820	-1.281888
H	-3.149467	-1.390912	2.410773	C	-3.798919	0.873432	1.379411
<hr/>							
74							
22-si SCF Done: -1691.63486345 A.U.							
Zr	0.105756	0.309715	-0.196137	H	3.104834	2.681055	-1.321317
C	1.350435	2.064525	0.996416	H	4.853688	1.108356	-2.120139
C	-0.915564	2.509972	-0.583254	H	-4.352547	0.901620	2.331715
C	0.881716	1.162292	2.028112	H	-2.469003	2.478395	1.940979
C	1.576558	-0.077519	1.936838	Si	0.319276	3.538852	0.409462
C	2.526487	0.017262	0.869632	C	1.242986	4.759877	-0.703088
				C	-0.420000	4.479620	1.876605

H	1.555969	4.313612	-1.668080	H	-5.502552	-2.497912	-2.462102
H	-0.829670	3.810340	2.659918	H	-3.518490	-1.048052	-2.873714
H	2.149098	5.150648	-0.194100	C	-1.011620	-1.800593	0.582268
H	-1.235357	5.155021	1.541752	H	-1.311607	-0.860368	1.128382
H	0.582428	5.622539	-0.933973	H	-1.933075	-2.108854	0.054415
H	0.367302	5.102880	2.351451	H	2.106418	-1.125321	-1.614014
H	0.113797	1.396060	2.778198	C	1.013620	-1.144084	-1.762359
H	0.164642	2.354554	-2.582162	C	0.274695	-2.203860	-1.120544
C	-4.025323	-1.013762	-1.896411	H	0.700483	-0.868420	-2.785019
C	-5.365212	-0.902629	0.572865	H	0.874888	-2.843760	-0.448996
C	3.818950	-2.147315	1.041932	C	-0.732379	-2.957349	-1.972928
C	5.461792	-1.330040	-1.088173	H	-0.168850	-3.563940	-2.716049
C	5.678882	-2.564844	-0.474533	H	-1.388786	-3.644226	-1.406387
C	4.853597	-2.977347	0.597603	H	-1.378602	-2.259015	-2.541715
C	-5.811089	-1.771077	-0.422437	C	-0.576774	-2.830831	1.646465
C	-5.141489	-1.823644	-1.669539	H	0.531315	-2.773623	1.762198
H	3.184235	-2.470529	1.882372	C	-1.199115	-2.497097	3.019608
H	5.026575	-3.949652	1.085447	H	-0.860988	-3.211319	3.801410
H	6.494648	-3.217584	-0.824035	H	-0.928266	-1.473822	3.355375
H	6.106367	-1.006467	-1.922028	H	-2.308020	-2.547139	2.971891
H	-5.893890	-0.850096	1.538959	C	-0.913208	-4.285234	1.264436
H	-6.690361	-2.410188	-0.242989	H	-0.397808	-4.613679	0.339795

H	-0.609764	-4.982822	2.073497	C	4.281918	0.744135	-1.240876
H	-2.006702	-4.411440	1.107434	C	-3.972343	1.183833	1.171502
<hr/>							
80				C	-4.417196	0.194680	0.219721
23-re SCF Done: -1770.19144190 A.U.							
Zr	0.162105	0.106932	-0.127381	H	3.140233	2.566070	-1.247047
C	1.394339	1.866241	1.061920	H	4.924641	1.065004	-2.076461
C	-0.777964	2.322342	-0.665098	H	-4.618471	1.397578	2.038340
C	0.976714	0.948186	2.118670	H	-2.528659	2.685976	1.708198
C	1.718623	-0.263511	1.981735	Si	0.412756	3.348608	0.398564
C	2.651483	-0.133722	0.907931	C	1.438660	4.609985	-0.579492
C	2.437929	1.170876	0.306910	C	-0.419405	4.375445	1.760700
C	-0.460035	1.679549	-1.941721	H	1.860800	4.234790	-1.529973
C	-1.400020	0.616116	-2.149851	H	-0.929613	3.788426	2.547006
C	-2.354851	0.610397	-1.088683	H	2.275268	4.984571	0.047924
C	-1.964641	1.642287	-0.148244	H	-1.161466	5.068636	1.310352
H	1.628920	-1.122789	2.660257	H	0.788537	5.476752	-0.826244
H	-1.437339	-0.011060	-3.050406	H	0.356847	4.993544	2.260877
C	-2.795480	1.889720	0.999128	C	-4.088601	-1.039664	-1.890779
C	-3.606027	-0.108342	-0.932830	C	-5.664031	-0.477251	0.370442
C	3.271612	1.573884	-0.793348	C	4.119352	-2.173032	1.164923
C	3.761284	-0.973895	0.495122	C	5.666017	-1.331301	-1.026914
C	4.568066	-0.525077	-0.611881	C	5.982360	-2.519475	-0.366543
				C	5.211582	-2.937859	0.743671

C	-6.109760	-1.397289	-0.577506	H	0.606390	-1.110758	-2.660288
C	-5.318965	-1.677411	-1.719386	H	2.118655	-1.418272	-1.635709
H	3.533348	-2.497835	2.039194	H	-0.141879	-2.449712	1.596805
H	5.473274	-3.864002	1.279507	H	-0.636244	-2.771269	-1.412715
H	6.840155	-3.124420	-0.700999	C	1.155621	-3.558257	-0.363483
H	6.278050	-0.991850	-1.878859	H	0.623758	-4.191556	0.369353
H	-6.282997	-0.250406	1.254213	H	1.490721	-4.217802	-1.194979
H	-7.080256	-1.901148	-0.443716	H	2.071977	-3.157427	0.111651
H	-5.676075	-2.395546	-2.474488	C	-2.140203	-2.822622	0.748453
H	-3.480748	-1.257325	-2.783152	H	-2.740682	-2.406032	-0.090040
C	0.483197	2.140903	-3.025881	C	-1.955002	-4.328889	0.479492
C	0.049882	1.216501	3.281444	H	-2.945687	-4.829676	0.450392
H	1.455192	2.503896	-2.646582	H	-1.453948	-4.547885	-0.483919
H	-0.941130	1.605313	2.977635	H	-1.367235	-4.816046	1.288745
H	0.024638	2.968336	-3.613936	C	-2.981187	-2.651087	2.035828
H	0.699170	1.313934	-3.732513	H	-2.432194	-3.044758	2.920014
H	0.498818	1.957956	3.978581	H	-3.218829	-1.584913	2.228900
H	-0.126204	0.285929	3.857791	H	-3.943028	-3.202452	1.962576
C	-0.848439	-1.991280	0.877643	<hr/>			
H	-1.165824	-1.016539	1.348576	80			
C	0.317466	-2.444586	-0.962022	23-si SCF Done: -1770.19771528 A.U.			
C	1.014101	-1.409366	-1.680618	Zr	0.101172	0.185572	-0.183022
				C	1.281301	1.915500	1.108881

C	-0.887858	2.393157	-0.633433	H	-2.621141	2.589424	1.771629
C	0.834603	0.971793	2.128680	Si	0.292159	3.404026	0.461308
C	1.552827	-0.250013	1.963563	C	1.318497	4.680484	-0.495457
C	2.503445	-0.103655	0.905859	C	-0.561468	4.402669	1.830150
C	2.338982	1.233571	0.358660	H	1.759206	4.310507	-1.439491
C	-0.562525	1.814285	-1.938151	H	-1.084228	3.797710	2.594092
C	-1.464085	0.726132	-2.180316	H	2.141053	5.061864	0.146240
C	-2.396596	0.628063	-1.101942	H	-1.298311	5.101502	1.379858
C	-2.041293	1.645549	-0.131274	H	0.664038	5.541488	-0.750704
H	1.445129	-1.122840	2.620914	H	0.203069	5.013070	2.356985
H	-1.477411	0.129533	-3.101904	C	-4.004523	-1.164023	-1.868093
C	-2.842875	1.787366	1.053533	C	-5.466304	-0.869016	0.515973
C	-3.563366	-0.214148	-0.909517	C	3.825647	-2.254232	1.013185
C	3.216390	1.666197	-0.694706	C	5.518565	-1.307369	-1.022534
C	3.578228	-0.972859	0.458108	C	5.738862	-2.567044	-0.462661
C	4.446141	-0.480845	-0.582994	C	4.888296	-3.044062	0.562021
C	4.226156	0.834519	-1.142300	C	-5.868437	-1.805554	-0.434905
C	-3.931287	0.959314	1.262793	C	-5.136443	-1.950243	-1.639283
C	-4.320113	-0.048323	0.307352	H	3.171880	-2.628323	1.817075
H	3.120314	2.680148	-1.108704	H	5.063876	-4.035920	1.007906
H	4.908870	1.179851	-1.935325	H	6.576590	-3.188613	-0.816965
H	-4.548100	1.082161	2.167790	H	6.182688	-0.932144	-1.818620

H	-6.042285	-0.743457	1.447728	C	-0.618877	-3.032396	-2.097783
H	-6.760005	-2.427190	-0.254959	H	-0.024910	-3.615129	-2.836314
H	-5.461698	-2.679506	-2.398066	H	-1.287685	-3.738744	-1.571522
H	-3.448453	-1.274608	-2.812223	H	-1.250479	-2.324521	-2.671030
C	0.378696	2.339360	-2.995549	C	-1.344025	-2.830420	2.847172
C	-0.080984	1.233324	3.301491	H	-1.036611	-3.578604	3.609656
H	1.387393	2.582221	-2.612340	H	-1.143088	-1.820672	3.262316
H	-1.088835	1.585661	3.011135	H	-2.442974	-2.919302	2.708694
H	-0.032715	3.261451	-3.464735	C	-0.847776	-4.494498	1.023501
H	0.510308	1.590036	-3.802010	H	-0.252183	-4.752316	0.125226
H	0.361111	2.000272	3.974195	H	-0.576283	-5.223637	1.815968
H	-0.216324	0.309821	3.899514	H	-1.920609	-4.654087	0.778383
C	-1.001679	-1.971912	0.483193				
H	-1.305268	-1.056980	1.070261				
H	-1.912104	-2.246987	-0.082216				
C	0.350975	-2.289899	-1.194007				
C	1.081980	-1.193336	-1.778473				
H	0.945586	-2.941491	-0.528929				
H	0.786723	-0.887827	-2.797645				
H	2.169694	-1.154977	-1.601305				
C	-0.604186	-3.052638	1.510269				
H	0.487710	-2.956849	1.716006				

86

24-re SCF Done: -1698.81018491 A.U.

Zr	0.127842	0.087345	-0.157393
C	1.535369	1.827548	0.850164
C	-0.948378	2.287620	-0.394666
C	1.358208	0.861563	1.930753
C	2.088480	-0.320931	1.610199
C	2.809095	-0.123390	0.387384
C	2.434800	1.194056	-0.117855
C	-0.885632	1.691158	-1.729668

C	-1.824557	0.605503	-1.776272	H	0.741719	2.746622	-2.760421
C	-2.575219	0.566283	-0.553488	H	1.250450	1.779188	3.892154
C	-2.005319	1.576203	0.328579	H	0.612830	0.109103	3.818506
H	2.156062	-1.200473	2.264609	H	-0.874683	2.945544	-3.492016
H	-2.032104	0.007070	-2.673402	H	0.014650	1.404200	-3.684413
C	-2.576437	1.757200	1.624628	Si	0.408387	3.302258	0.455728
C	-3.760361	-0.162844	-0.187036	C	1.203696	4.635710	-0.637240
C	2.993914	1.637477	-1.355303	C	-0.158649	4.258923	1.995594
C	3.832486	-0.906634	-0.256688	H	1.499433	4.309023	-1.651749
C	4.341438	-0.414478	-1.458999	H	-0.462504	3.630370	2.852841
C	3.914611	0.829149	-2.015455	H	2.106383	5.039277	-0.130785
C	-3.692558	1.004796	1.988806	H	-1.007391	4.926613	1.735376
C	-4.284048	0.074789	1.087428	H	0.481640	5.471899	-0.757290
H	2.743543	2.628799	-1.756713	H	0.680690	4.901917	2.337645
H	4.355228	1.168873	-2.966065	C	-4.461515	-1.031379	-1.231235
H	5.125818	-0.978007	-1.987746	C	4.408657	-2.131506	0.452533
H	-5.198038	-0.449742	1.405929	H	-3.666322	-1.602473	-1.767079
H	-4.152488	1.158188	2.978143	H	3.557206	-2.664443	0.935749
H	-2.191398	2.530623	2.303441	C	5.363290	-1.692234	1.589836
C	0.673908	1.066179	3.262055	C	5.109686	-3.132614	-0.481014
C	-0.207969	2.222258	-2.968384	C	-5.450188	-2.054570	-0.647904
H	-0.356481	1.460702	3.173814	C	-5.172959	-0.145048	-2.283365

H	-4.978317	-2.696024	0.124190	C	1.126884	-3.536391	-0.838960
H	-6.005966	0.418566	-1.812332	H	0.751584	-4.237736	-0.071540
H	6.252494	-1.174249	1.172375	H	1.308074	-4.121458	-1.768036
H	4.451932	-3.456013	-1.314086	H	2.107535	-3.146054	-0.507146
H	-5.598012	-0.764502	-3.101763	C	-1.777082	-4.428616	0.501365
H	-4.482791	0.595091	-2.735951	H	-1.065113	-4.962231	1.169143
H	-5.839953	-2.715235	-1.449903	H	-2.758682	-4.938731	0.600532
H	-6.327499	-1.556013	-0.183649	H	-1.439880	-4.576840	-0.543376
H	5.718427	-2.569884	2.171053	C	-2.534930	-2.866144	2.312853
H	4.867300	-0.992356	2.292599	H	-2.740748	-1.816940	2.607105
H	5.417297	-4.037738	0.082831	H	-3.494410	-3.426373	2.361810
H	6.030654	-2.700080	-0.926514	H	-1.851377	-3.308702	3.070796
<hr/>							
C	-0.613956	-2.116566	0.864042	86			
H	-0.830195	-1.189819	1.469653	24-si SCF Done: -1698.81735837 A.U.			
H	1.823924	-1.277192	-2.071469	Zr	0.037681	0.170493	-0.203330
C	0.727479	-1.296956	-1.928858	C	1.347527	1.954489	0.881749
C	0.182713	-2.397394	-1.176698	C	-1.192442	2.292994	-0.308062
H	0.150910	-0.938486	-2.797345	C	1.230824	0.937021	1.920573
H	-0.832760	-2.713730	-1.473474	C	1.998300	-0.202117	1.535476
H	0.209295	-2.627727	1.399961	C	2.692207	0.080362	0.311729
C	-1.912178	-2.946138	0.899610	C	2.276101	1.413675	-0.115554
H	-2.635746	-2.473322	0.199096	C	-1.134426	1.769297	-1.673512

C	-1.977657	0.610642	-1.743477	H	0.510623	2.782173	-2.719200
C	-2.652819	0.427389	-0.488849	H	1.170312	1.777553	3.912789
C	-2.147397	1.450608	0.417668	H	0.574290	0.094407	3.803379
H	2.119616	-1.100226	2.154777	H	-1.130668	3.249505	-3.258295
H	-2.163223	0.041344	-2.663472	H	-0.445033	1.661830	-3.721105
C	-2.643968	1.488483	1.755700	Si	0.121747	3.366930	0.543110
C	-3.678053	-0.494125	-0.077591	C	0.806252	4.761977	-0.546781
C	2.828278	1.952050	-1.317742	C	-0.471921	4.252590	2.115194
C	3.698442	-0.657727	-0.407021	H	1.069495	4.466773	-1.579567
C	4.207645	-0.068997	-1.564808	H	-0.743710	3.587411	2.956063
C	3.774365	1.212868	-2.022547	H	1.709295	5.200566	-0.071179
C	-3.601425	0.556990	2.156458	H	-1.351987	4.888327	1.879973
C	-4.111231	-0.414591	1.249447	H	0.039343	5.563136	-0.616430
H	2.554636	2.961807	-1.654445	H	0.340421	4.921797	2.471884
H	4.216416	1.629236	-2.941507	C	-4.310603	-1.428871	-1.105615
H	4.981063	-0.593358	-2.147342	C	4.201028	-1.988345	0.146823
H	-4.894476	-1.100978	1.606669	H	-3.485918	-1.794420	-1.759447
H	-3.994731	0.588556	3.185063	H	3.315483	-2.507192	0.584262
H	-2.319906	2.277299	2.448854	C	5.207421	-1.755917	1.299324
C	0.588347	1.071464	3.279997	C	4.798203	-2.927512	-0.914770
C	-0.511015	2.398195	-2.894898	C	-4.994276	-2.666848	-0.501694
H	-0.453269	1.439963	3.241100	C	-5.297180	-0.650353	-2.009416

H -4.310936 -3.232887 0.164816
H -6.159793 -0.282454 -1.414330
H 6.127121 -1.264564 0.916848
H 4.095443 -3.097817 -1.756473
H -5.691709 -1.299244 -2.820406
H -4.815464 0.231439 -2.479019
H -5.333415 -3.352601 -1.305818
H -5.893353 -2.392848 0.090168
H 5.503055 -2.717833 1.770166
H 4.784130 -1.102273 2.089035
H 5.042762 -3.913024 -0.466480
H 5.741772 -2.522224 -1.338030
C -0.693011 -2.114468 0.585867
H -0.953103 -1.246823 1.257510
H -1.673525 -2.481643 0.227874
H 1.841093 -0.910691 -2.091756
C 0.750881 -1.071740 -2.033649
C 0.278905 -2.249832 -1.347222
H 0.206544 -0.780450 -2.948970
H 1.068631 -2.845433 -0.854582
C -0.772073 -3.085824 -2.059301
H -0.279958 -3.611990 -2.907193

H -1.258445 -3.851724 -1.426116
H -1.564118 -2.442668 -2.493943
C 0.032502 -3.162923 1.454689
H 1.126745 -2.946308 1.420967
C -0.408555 -3.052184 2.929938
H 0.141655 -3.773317 3.572643
H -0.231158 -2.033457 3.333081
H -1.494217 -3.265230 3.034838
C -0.156602 -4.614378 0.971078
H 0.257172 -4.789934 -0.042032
H 0.351895 -5.322992 1.658593
H -1.234047 -4.889326 0.950218

83

25-re SCF Done: -1910.91654369 A.U.

Zr -0.009864 -0.435809 0.048109
C 1.301618 -1.895571 1.575178
C -1.475749 -1.888774 1.414729
C 1.968144 -1.885260 0.304480
C 2.571851 -0.591111 0.059752
C 2.330242 0.190425 1.266625
C 1.525274 -0.601864 2.188137
C -2.026967 -0.573931 1.577185

C	-2.655643	-0.121052	0.365776	H	3.442157	2.069227	1.021526
C	-2.525731	-1.214905	-0.576614	H	-2.003546	-0.015266	2.524327
C	-1.769034	-2.297824	0.052459	H	-3.715647	-0.657512	-2.342252
C	-1.490426	-3.491153	-0.680717	H	-0.911253	-4.305246	-0.217284
C	-3.075478	-1.425428	-1.881598	H	2.052033	-2.758791	-0.357156
C	1.156773	-0.060982	3.457938	Si	4.010647	-0.360562	-1.153148
C	2.791387	1.475180	1.681792	Si	-3.916504	1.296833	0.385423
C	2.448982	1.958803	2.947048	C	5.615758	-0.432888	-0.132855
C	1.626253	1.201812	3.826175	C	4.006853	1.276424	-2.119958
C	-2.012502	-3.642070	-1.965433	C	4.044697	-1.800151	-2.395995
C	-2.818514	-2.618199	-2.550670	C	-5.592988	0.521796	0.843176
H	1.369535	1.612235	4.815689	C	-4.140609	2.214906	-1.263721
H	2.827407	2.940427	3.274058	C	-3.433786	2.550237	1.728713
H	-3.250411	-2.783461	-3.550980	H	5.654406	0.374360	0.628100
H	-1.818356	-4.567142	-2.530370	H	3.126792	1.364510	-2.789662
C	-0.870135	-2.742371	2.508298	H	4.122401	-2.780421	-1.880040
C	0.604024	-3.080405	2.203164	H	-3.394571	2.081127	2.734283
H	-0.943336	-2.183195	3.464285	H	-3.217756	2.726412	-1.602707
H	0.664677	-3.936423	1.498982	H	-5.903879	-0.235016	0.092413
H	-1.469011	-3.670259	2.653814	H	6.508255	-0.327565	-0.786514
H	1.134910	-3.407094	3.126841	H	5.696927	-1.401115	0.404585
H	0.556770	-0.655707	4.164117	H	4.917190	1.332783	-2.754971

H 4.015234 2.161873 -1.450876
H 4.934255 -1.700997 -3.054306
H 3.148816 -1.830336 -3.051039
H -4.185425 3.367045 1.774157
H -2.443850 3.010227 1.529408
H -4.926377 2.990607 -1.136041
H -4.474584 1.541813 -2.080737
H -6.390264 1.293921 0.899615
H -5.538014 0.012928 1.828340
C -0.155071 2.029128 -0.505035
H -0.151247 1.756679 0.591886
C 0.130233 0.817539 -2.324407
C 0.246967 -0.613510 -2.254762
H -0.576583 -1.215832 -2.677674
H 1.249556 -1.049231 -2.392210
H -1.192560 2.349182 -0.715772
H 1.082918 1.358162 -2.444038
C -1.023306 1.381892 -3.131159
H -1.204206 2.461766 -2.976994
H -0.792586 1.233361 -4.209688
H -1.960823 0.831538 -2.921568
C 0.835462 3.200816 -0.653631

H 1.867501 2.786610 -0.597178
C 0.728364 3.999272 -1.968753
H 1.461497 4.833340 -1.968349
H 0.929445 3.391942 -2.872833
H -0.281066 4.452915 -2.080330
C 0.666431 4.183150 0.529092
H 1.404181 5.013041 0.469087
H -0.348013 4.638742 0.518549
H 0.802825 3.674821 1.504826

83

25-si SCF Done: -1910.91533101 A.U.

Zr 0.060522 -0.095048 0.199061
C 1.616397 -0.683914 2.064407
C -1.151678 -1.194818 2.061653
C 2.151052 -1.302294 0.883619
C 2.699720 -0.321176 -0.014894
C 2.528884 0.956649 0.650653
C 1.859507 0.737605 1.934303
C -2.053323 -0.210579 1.532590
C -2.506131 -0.593942 0.212989
C -1.914748 -1.901960 -0.039958
C -1.089125 -2.278032 1.095652

C	-0.438572	-3.551159	1.104111	H	0.167859	-3.860347	1.969222
C	-2.061239	-2.815870	-1.128378	H	2.177429	-2.388091	0.716217
C	1.598675	1.833421	2.807620	Si	3.945923	-0.841966	-1.346051
C	2.966581	2.279591	0.321333	Si	-4.151062	-0.036635	-0.560337
C	2.700530	3.327142	1.199899	C	5.656790	-0.835091	-0.512083
C	2.009380	3.114005	2.430951	C	4.057339	0.272108	-2.882380
C	-0.625899	-4.426699	0.035519	C	3.543505	-2.610866	-1.912266
C	-1.432661	-4.057907	-1.078990	C	-5.339031	-1.522936	-0.481219
H	1.823478	3.968466	3.100495	C	-4.039280	0.516263	-2.377206
H	3.041365	4.344640	0.948489	C	-4.941556	1.331881	0.497367
H	-1.561066	-4.767735	-1.911684	H	5.926778	0.182510	-0.158683
H	-0.145457	-5.417779	0.051881	H	3.145483	0.228872	-3.510793
C	-0.476459	-1.155157	3.414679	H	3.634705	-3.338583	-1.078703
C	1.048420	-1.382271	3.282314	H	-5.125619	0.967992	1.530408
H	-0.670625	-0.162357	3.873206	H	-3.527241	1.492974	-2.496851
H	1.269815	-2.466643	3.203470	H	-4.990144	-2.383933	-1.087211
H	-0.926352	-1.904965	4.106474	H	6.448716	-1.173587	-1.214495
H	1.572118	-1.037292	4.202139	H	5.668940	-1.509396	0.369805
H	1.101899	1.665842	3.776677	H	4.908612	-0.076374	-3.506664
H	3.518334	2.464713	-0.613335	H	4.251608	1.335114	-2.629128
H	-2.394156	0.678117	2.083027	H	4.252581	-2.927973	-2.706501
H	-2.686545	-2.548991	-1.995195	H	2.514868	-2.694074	-2.321041

H -5.924855 1.614279 0.063772
H -4.330096 2.253527 0.566688
H -5.062317 0.625757 -2.797367
H -3.500590 -0.227315 -3.001392
H -6.344445 -1.231006 -0.854451
H -5.452850 -1.876832 0.565120
C -0.306708 2.312053 -0.340531
H -0.084124 2.114729 0.743452
H 0.541285 2.935903 -0.677544
C -0.199601 1.093323 -2.198363
C 0.080860 -0.314490 -2.135839
H -1.259597 1.350968 -2.358892
H -0.744559 -1.010215 -2.355851
H 1.064609 -0.649964 -2.506496
C 0.782746 1.998502 -2.916705
H 0.782798 1.729629 -3.996571
H 0.534106 3.073707 -2.839864
H 1.814269 1.853549 -2.541778
C -1.642910 3.073923 -0.399788
H -2.464434 2.328696 -0.483546
C -1.760651 4.028632 -1.602998
H -2.734494 4.562432 -1.587635

H -0.959340 4.799474 -1.576225
H -1.690587 3.504506 -2.577517
C -1.876231 3.862202 0.907853
H -1.083797 4.627306 1.054546
H -2.855810 4.388383 0.896828
H -1.858979 3.194866 1.794976

65

26-re SCF Done: -1172.46272988 A.U.

Zr 0.207609 -0.121679 0.163382
C 1.709996 -1.546386 -1.150090
C -0.113231 -2.493749 0.753707
C 1.086119 -0.695147 -2.131364
C 1.564999 0.645453 -2.000344
C 2.551575 0.639946 -0.950121
C 2.629691 -0.711551 -0.398570
C -0.159307 -1.740336 1.980036
C -1.362185 -0.950874 2.016669
C -2.134385 -1.304236 0.843968
C -1.350549 -2.236563 0.043900
C -1.893738 -2.743929 -1.176299
C -3.459977 -0.970232 0.438158
C 3.533566 -0.982039 0.673338

C	3.466442	1.640293	-0.491124	C	-1.886352	-0.164170	3.188423
C	4.359029	1.327417	0.529577	H	0.295981	1.654448	-3.447135
C	4.381899	0.029439	1.126237	H	-1.072848	0.143793	3.875825
C	-3.191507	-2.386961	-1.549845	H	2.050821	1.852250	-3.729983
C	-3.973954	-1.516657	-0.740130	H	1.255886	2.766486	-2.420843
H	5.095208	-0.178897	1.938927	H	-2.604664	-0.771114	3.785194
H	5.073285	2.090084	0.879818	H	-2.427227	0.753530	2.874387
H	-5.006567	-1.281455	-1.043813	C	-1.242675	1.831982	-0.551123
H	-3.624985	-2.800651	-2.474269	H	-1.415424	0.852284	-1.087255
C	0.975484	-3.456290	0.333191	H	0.599273	0.965433	2.757723
C	1.562334	-3.049870	-1.037302	C	0.891624	1.403636	1.789783
H	1.771345	-3.446646	1.107210	C	-0.006340	2.357159	1.196015
H	0.895677	-3.395818	-1.854083	H	1.975505	1.591455	1.687010
H	0.592528	-4.502598	0.303097	H	-0.729430	2.476491	-1.290512
H	2.540569	-3.553236	-1.212950	H	-0.954796	2.506770	1.740025
H	3.595624	-1.993320	1.104890	C	0.600863	3.626938	0.626937
H	3.483040	2.635757	-0.962458	H	1.533980	3.403849	0.072948
H	0.588136	-1.795435	2.784162	H	-0.074399	4.204311	-0.031445
H	-4.085377	-0.320550	1.070310	H	0.883328	4.286487	1.477607
H	-1.319559	-3.456939	-1.787768	C	-2.643737	2.377463	-0.209885
H	0.373042	-1.037132	-2.895454	H	-3.038987	1.792302	0.652413
C	1.272032	1.784672	-2.937365	C	-2.702934	3.869870	0.174601

H	-3.754538	4.171092	0.365966	C	3.670404	-0.926467	-0.046974
H	-2.123273	4.117239	1.085391	C	3.413941	1.849368	0.601199
H	-2.326110	4.510067	-0.653188	C	4.391332	1.060469	1.202405
C	-3.599963	2.141949	-1.402397	C	4.515860	-0.323810	0.884567
H	-3.657550	1.068332	-1.672493	C	-3.328693	-1.951326	-1.500209
H	-4.629039	2.492713	-1.168447	C	-3.865373	-1.740668	-0.194590
H	-3.251743	2.702410	-2.297550	H	5.299659	-0.922737	1.374741
<hr/>							
65							
26-si SCF Done: -1172.46219466 A.U.							
Zr	0.213951	-0.053023	0.137682	H	-4.951880	-1.594763	-0.081059
C	1.718082	-0.431852	-1.763133	H	-4.006949	-1.954534	-2.367966
C	0.318683	-2.459891	-0.404716	C	1.261134	-2.899139	-1.506039
C	1.037975	0.802843	-2.062927	C	1.550941	-1.745931	-2.495107
C	1.487906	1.834925	-1.171023	H	2.204461	-3.255857	-1.043078
C	2.531490	1.261426	-0.355017	H	0.706098	-1.642421	-3.208727
C	2.673602	-0.142674	-0.707177	H	0.842804	-3.778137	-2.046946
C	0.614956	-2.363362	1.002615	H	2.448306	-1.975221	-3.116057
C	-0.564393	-2.016646	1.733529	H	3.807818	-1.986853	-0.308162
C	-1.642144	-1.929237	0.778647	H	3.337753	2.922691	0.838741
C	-1.098701	-2.198163	-0.552981	H	1.592730	-2.576643	1.456930
C	-1.963996	-2.189893	-1.686390	H	-3.485216	-1.598376	1.938614
C	-3.050602	-1.736358	0.935983	H	-1.566547	-2.402435	-2.691393
				H	0.324484	0.943671	-2.887614

C 1.215217 3.312612 -1.272462
C -0.696405 -2.019553 3.231293
H 0.432704 3.534602 -2.023696
H 0.279891 -1.840855 3.725687
H 2.135751 3.851712 -1.590778
H 0.900006 3.767833 -0.308742
H -1.072971 -3.004250 3.589659
H -1.407722 -1.253635 3.602733
C -1.929994 1.226769 -0.049616
H -1.778336 0.440577 -0.840394
H -2.794940 0.859559 0.532977
H 0.396497 0.475872 3.027359
C 0.413582 1.144316 2.148614
C -0.816605 1.798685 1.798718
H 1.349800 1.716665 2.043228
H -0.709889 2.800218 1.344649
C -1.992845 1.667131 2.748983
H -2.943710 2.064360 2.347522
H -2.158440 0.611341 3.042938
H -1.755672 2.231730 3.678162
C -2.243379 2.550002 -0.774466
H -1.290388 3.092215 -0.954727

C -2.872386 2.275596 -2.158927
H -3.839746 1.738912 -2.054639
H -3.065869 3.221748 -2.710083
H -2.210882 1.644911 -2.789339
C -3.157698 3.496353 0.027399
H -2.705303 3.821496 0.985846
H -3.379053 4.414861 -0.556639
H -4.130060 3.008809 0.259739

References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; et al. Gaussian 03; Gaussian, Inc.: Pittsburgh, PA, 2004.
2. Perdew J P (1986) Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Phys Rev B* 33: 8822-8824
3. P Perdew J P (1986) Erratum: density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Phys Rev B* 34: 7406-7410
4. Becke A D (1988) Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys Rev A* 38: 3098-3100
5. Schäfer A, Horn H, Ahlrichs R (1992) SV SVP TVP Ahlrichs basis set. *J Chem Phys* 97: 2571-2580
6. Kuechle W, Dolg M, Stoll H, Preuss H (1994) ECP SDD. *J Chem Phys* 100: 7535-7540