

Electronic Supplementary Information (ESI)

Design and Prediction of High Potent *ansa*-Zirconocene Catalyst for Olefin Polymerizations: Combined DFT Calculations and QSPR Approach

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Contents

1. **Table S1.** Geometry, α -agostic interaction (TS) and π coordination (reactant complex); Second Order Perturbation Theory Analysis ($E(2)$ / kcal mol⁻¹) of five monomers with the most favorable pathway (for the primary (1,2)-*si* insertion path of PP, BT, and HX monomers and the secondary (2,1)-*si* insertion path of ST monomer).
2. **Table S2.** Results of the intrinsic activation energy (E_a), the reaction energy (ΔE_r), the π -complexation energy (ΔE_π), and the apparent activation energy ($E_{a(\text{app})}$) in kcal/mol for ET, the primary (1,2)-*si* insertion of PP, BT, and HX monomers and the secondary (2,1)-*si* insertion of ST monomer in gas phase and in toluene and cyclohexane solvents.
3. **Fig. S1** Correlation between the activation energy and the experimental activity of *ansa*-zirconocene catalysts (Cat. 1-4).
4. Optimized cartesian coordinates (XYZ) of all structures.

Table S1. Geometry, α -agostic interaction (TS) and π coordination (reactant complex); Second Order Perturbation Theory Analysis ($E(2)$ / kcal mol⁻¹) of five monomers with the most favorable pathway (for the primary (1,2)-*si* insertion path of PP, BT, and HX monomers and the secondary (2,1)-*si* insertion path of ST monomer).

Monomer	TS structure				E(2) (kcal mol ⁻¹)	
	C _{α} -H _{α} (Å)	Zr-H _{α} (Å)	Zr-C _{α} (Å)	Zr-C _{α} -H _{α} (deg)	α -agostic Interaction (TS)	π coordination (Reactant complex)
					C-H _{α} → LP* Zr	C ₁ -C ₂ → LP* Zr
ET	1.151	2.090	2.272	66.1	LP*(4) 26.94 LP*(1) 4.97	LP*(5) 3.99 LP*(4) 4.88
PP	1.150	2.055	2.303	63.0	LP*(4) 26.40 LP*(1) 4.33	LP*(8) 4.52 LP*(4) 1.95
BT	1.153	2.061	2.295	63.7	LP*(4) 26.28 LP*(1) 4.34	LP*(8) 3.04 LP*(4) 3.20
HX	1.153	2.061	2.295	63.7	LP*(4) 26.84 LP*(1) 4.45	LP*(8) 4.59 LP*(4) 3.01
ST	1.153	2.087	2.294	65.0	LP*(4) 27.42 LP*(1) 5.04	LP*(8) 3.64 LP*(4) 13.96

Table S2. Results of the intrinsic activation energy (E_a), the reaction energy (ΔE_r), the π -complexation energy (ΔE_π), and the apparent activation energy ($E_{a(\text{app})}$) in kcal/mol for ET, the primary (1,2)-*si* insertion of PP, BT, and HX monomers and the secondary (2,1)-*si* insertion of ST monomer in gas phase and in toluene and cyclohexane solvents.

Cat. 3 with Olefin monomer	In gas phase				In toluene			
	E_a	ΔE_r	ΔE_π	$E_{a(\text{app})}$	E_a	ΔE_r	ΔE_π	$E_{a(\text{app})}$
ET	7.94	-9.79	-23.76	-15.82	8.29	-10.95	-20.57	-12.28
PP	8.77	-6.31	-27.04	-18.27	9.35	-7.27	-24.02	-14.67
BT	8.84	-6.91	-28.71	-19.87	9.16	-5.96	-25.18	-16.02
HX	9.63	-7.22	-30.45	-20.82	9.87	-4.55	-26.56	-16.69
ST	14.26	-3.13	-31.56	-17.30	13.66	-3.74	-26.59	-13.25
Cat. 3 with Olefin monomer	In cyclohexane							
	E_a	ΔE_r	ΔE_π	$E_{a(\text{app})}$				
ET	8.23	-10.71	-21.13	-12.90				
PP	9.24	-7.06	-24.56	-15.32				
BT	9.11	-5.96	-25.80	-16.69				
HX	9.81	-4.58	-27.20	-17.39				
ST	13.75	-3.65	-27.42	-13.66				

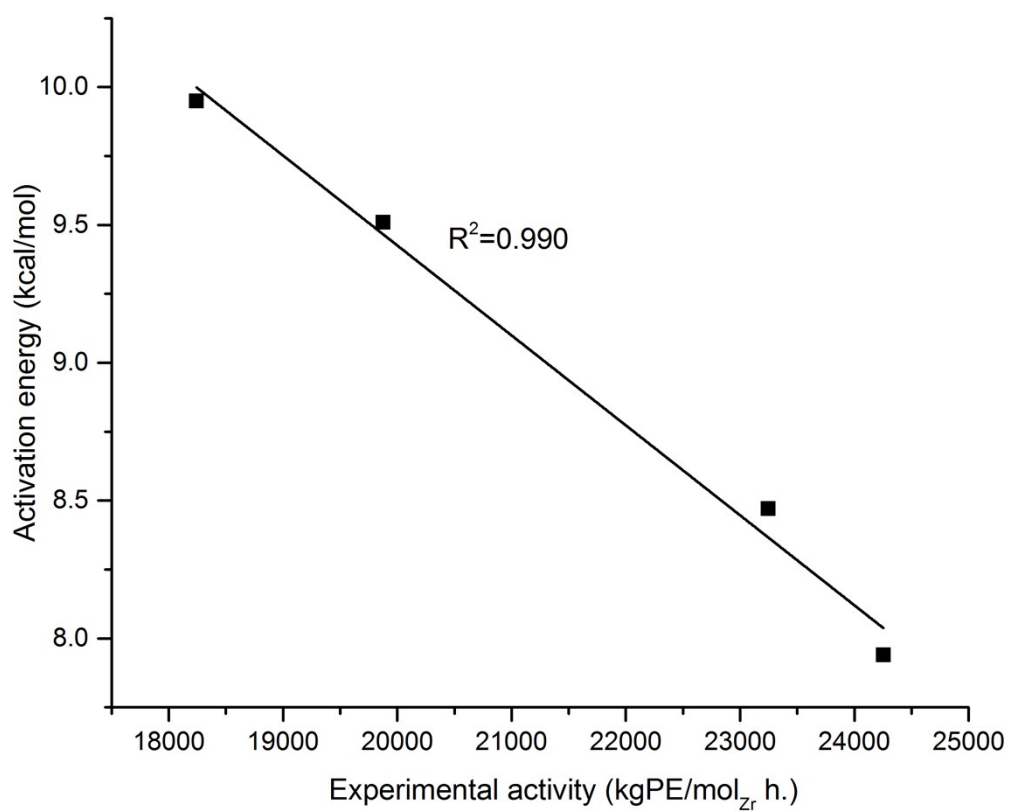


Fig. S1 Correlation between the activation energy and the experimental activity of *ansa*-zirconocene catalysts (Cat. 1-4).

Optimized cartesian coordinates (XYZ) of all structures.

12si-PP-TS(+)<i>i</i>Bu	H -3.6972 -0.1408 4.2479	H -4.4453 2.1525 -0.9482
C 0.8788 -0.1165 1.8683	H 3.3528 -3.8843 1.1885	H -3.7088 -1.2534 0.5438
C 0.1976 1.1330 1.8891	H 2.4326 -2.9369 2.3962	H -4.4615 0.3398 0.8669
C 0.9918 2.0391 1.1108	H 4.1805 -2.6576 2.1973	H -5.1964 -0.7690 -0.3257
C 2.1363 1.3188 0.5981	H 4.9365 -2.0701 -1.0420	
C 2.0719 -0.0464 1.0666	H 5.2170 -0.6280 -0.0315	12re-PP-TS(+)<i>i</i>Bu
H 0.5212 -1.0161 2.3768	H 4.2309 -0.5073 -1.5197	C 0.8879 0.2375 1.9109
Si 2.9381 -1.5733 0.3432	H -2.7834 -2.6498 -2.1937	C 0.1919 1.4642 1.7497
C 1.5010 -1.9888 -0.8334	H -3.4382 -3.8609 -0.1406	C 0.9540 2.2505 0.8270
C 1.2933 -1.4206 -2.1345	H -1.8339 -4.1829 1.7358	C 2.1102 1.4731 0.4145
C -0.0777 -1.5224 -2.5106	H 0.4999 -3.3758 1.5603	C 2.0803 0.2037 1.1073
C -0.7505 -2.2536 -1.4812	H 0.0199 3.9876 1.2940	H 0.5511 -0.5733 2.5551
C 0.2051 -2.4953 -0.4224	H 1.7465 5.1506 -0.0591	Si 2.9722 -1.4145 0.6890
H 2.0629 -0.9257 -2.7189	H 3.6958 3.9110 -0.9791	C 1.6281 -1.9958 -0.5209
H -0.5114 -1.1864 -3.4510	H 3.9847 1.4819 -0.5642	C 1.5478 -1.5680 -1.8872
C 3.2440 -2.8889 1.6526	Zr 0.1463 0.0527 -0.4796	C 0.2330 -1.7380 -2.3868
C 4.4680 -1.1486 -0.6569	C -2.0655 0.6919 -0.4254	C -0.5551 -2.3305 -1.3517
C -2.0799 -2.7652 -1.3715	H -1.7563 -0.1777 0.2610	C 0.2998 -2.4686 -0.1855
C -2.4335 -3.4494 -0.2267	H -2.2314 1.5386 0.2584	H 2.3721 -1.1292 -2.4496
C -1.5096 -3.6381 0.8429	H 0.7482 1.0773 -3.0134	H -0.0959 -1.5285 -3.3998
C -0.2143 -3.1776 0.7636	C 0.3733 1.6546 -2.1652	C 3.1281 -2.5039 2.2108
C 0.8544 3.4323 0.8652	C -1.0265 1.8675 -2.0743	C 4.5874 -1.1513 -0.2322
C 1.8243 4.0716 0.1250	H 1.0218 2.4581 -1.8073	C -1.9102 -2.7732 -1.3028
C 2.9451 3.3601 -0.4052	C -1.5317 3.2158 -1.6318	C -2.3888 -3.3075 -0.1281
C 3.1070 2.0101 -0.1882	H -0.8513 3.6658 -0.8993	C -1.5637 -3.4102 1.0361
C -1.0178 1.4873 2.6919	H -2.5494 3.2030 -1.2345	C -0.2484 -3.0008 1.0231
C -1.8397 0.2899 3.1806	H -1.6582 1.3126 -2.7721	C 0.7732 3.5771 0.3483
C -3.1233 0.7227 3.8904	H -1.5310 3.8657 -2.5295	C 1.7084 4.1002 -0.5220
H -0.6931 2.0776 3.5705	C -3.3905 0.2414 -1.0382	C 2.8336 3.3307 -0.9538
H -1.6599 2.1727 2.1085	C -4.2196 1.3656 -1.6837	C 3.0374 2.0406 -0.5094
H -1.2226 -0.3239 3.8577	C -4.2390 -0.4047 0.0769	C -1.0152 1.9244 2.5124
H -2.0945 -0.3605 2.3250	H -3.1842 -0.5225 -1.8045	C -1.8082 0.7981 3.1830
H -3.7676 1.2995 3.2045	H -3.7238 1.8259 -2.5455	C -3.0700 1.3210 3.8694
H -2.8955 1.3655 4.7584	H -5.1794 0.9495 -2.0278	H -0.6862 2.6461 3.2834

H -1.6828	2.5072	1.8495	H -4.1598	0.4063	1.3986	H 2.4343	-0.1927	3.8672
H -1.1620	0.2905	3.9198	H -5.2437	-0.6033	0.4010	H 1.8886	-1.5477	2.9002
H -2.0793	0.0412	2.4275	C -1.9518	0.7179	-3.3978	H 4.0318	0.5154	2.1122
H -3.7358	1.8165	3.1407	H -2.2477	1.5048	-4.1154	H 3.4402	-0.7328	1.0093
H -2.8171	2.0627	4.6456	H -1.2877	0.0237	-3.9280	H 4.1954	-2.5324	2.6063
H -3.6356	0.5053	4.3469	H -2.8677	0.1911	-3.1066	H 4.7830	-1.2870	3.7368
H 3.2965	-3.5578	1.9294	H -1.7597	2.2619	-1.8292	H 5.5596	-1.4797	2.1421
H 2.2237	-2.4527	2.8393				H 1.3821	5.0585	-1.4597
H 3.9810	-2.1707	2.8274	21si-PP-TS(+)<i>i</i>Bu			H 2.2694	4.2272	-0.1473
H 5.0764	-2.1216	-0.4268	C 1.4052	1.4926	1.3766	H 1.0482	5.4589	0.2514
H 5.2817	-0.5306	0.3601	C 1.2089	0.3690	2.2230	H -1.8835	4.6920	-1.3764
H 4.4250	-0.6548	-1.2035	C -0.1912	0.3255	2.5270	H -2.0467	4.6237	0.4005
H -2.5398	-2.7089	-2.1921	C -0.8410	1.4282	1.8400	H -2.5512	3.2310	-0.6001
H -3.4183	-3.6671	-0.0774	C 0.1615	2.1636	1.1003	H 1.8705	-1.8116	-3.5579
H -1.9858	-3.8418	1.9457	H 2.3718	1.7888	0.9738	H 4.2265	-1.1469	-3.1690
H 0.3833	-3.1164	1.9040	Si -0.0587	3.3304	-0.3810	H 4.7883	0.9772	-2.0068
H -0.0741	4.1748	0.6911	C 0.1534	1.9529	-1.6764	H 3.0082	2.5291	-1.2549
H 1.5990	5.1240	-0.8852	C -0.8953	1.1012	-2.1508	H -0.4489	-1.3455	3.9140
H 3.5515	3.7851	-1.6392	C -0.3629	-0.1172	-2.6533	H -2.8844	-0.9301	4.1927
H 3.9155	1.4746	-0.8217	C 1.0637	-0.0220	-2.5924	H -4.0053	0.9521	3.0199
Zr 0.1974	0.0270	-0.4805	C 1.3860	1.2378	-1.9522	H -2.7386	2.4693	1.5242
C -2.0538	0.4774	-0.3847	H -1.9556	1.3329	-2.0830	Zr 0.0882	0.0224	-0.1248
H -1.6967	-0.4167	0.2400	H -0.9272	-0.9332	-3.0989	C 1.0896	-2.0321	0.0525
H -2.0185	1.3625	0.2668	C 1.2894	4.6361	-0.4441	H 1.7810	-1.1654	-0.2478
H 0.6924	0.9904	-3.1204	C -1.7986	4.0308	-0.4967	H 1.2456	-2.2050	1.1265
C 0.1868	1.4813	-2.2832	C 2.1080	-0.8846	-3.0339	C -1.9513	-1.0870	0.1148
C -1.2350	1.4099	-2.2669	C 3.4148	-0.5071	-2.8173	C -1.1783	-2.2576	-0.0105
H 0.6504	2.4003	-1.9191	C 3.7384	0.7159	-2.1524	H -2.2233	-0.8450	1.1451
C -3.5194	0.1782	-0.6788	C 2.7536	1.5781	-1.7232	H -1.1434	-2.7843	-0.9676
C -4.2783	1.4283	-1.1465	C -0.9435	-0.5358	3.3732	C 1.5660	-3.2498	-0.7282
C -4.1885	-0.3564	0.6029	C -2.2931	-0.2948	3.5303	C 0.9598	-4.5578	-0.1977
H -3.5861	-0.6151	-1.4417	C -2.9385	0.7894	2.8550	C 3.1009	-3.3281	-0.6157
H -3.9185	1.8232	-2.1069	C -2.2409	1.6339	2.0169	H 1.2947	-3.1271	-1.7904
H -5.3490	1.1950	-1.2601	C 2.2660	-0.5113	2.8212	H -0.1240	-4.6314	-0.3658
H -4.1876	2.2271	-0.3892	C 3.6054	-0.5022	2.0762	H 1.4353	-5.4153	-0.6998
H -3.6800	-1.2603	0.9724	C 4.5942	-1.5046	2.6719	H 1.1511	-4.6554	0.8859

H 3.5793 -2.4173 -1.0069	C 1.8899 -2.8997 3.9718	H 3.3165 -2.8304 0.3202
H 3.3982 -3.4482 0.4406	H -0.2682 -1.1221 4.0663	H 2.2428 -3.9298 1.2367
H 3.4806 -4.1963 -1.1795	H -0.3625 -2.1620 2.6612	H 3.1586 -4.5472 -0.1679
C -3.0588 -0.7771 -0.8838	H 2.1593 -0.7599 3.7276	H -1.3914 -2.6748 -1.1444
H -2.7758 -1.0172 -1.9190	H 2.1260 -1.6659 2.2090	C -3.0353 -0.5636 -1.1091
H -3.3630 0.2796 -0.8361	H 1.4228 -3.7519 3.4454	H -3.3384 0.4490 -0.8199
H -0.9591 -2.8612 0.8709	H 1.4482 -2.8513 4.9822	H -3.1289 -1.2107 -0.2228
H -3.9488 -1.3806 -0.6320	H 2.9664 -3.1190 4.0800	H -1.4817 0.0038 -2.5786
	H 3.1392 4.5404 0.3391	H -3.7473 -0.9259 -1.8740
	H 2.9540 3.3451 1.6590	
21re-PP-TS(+)-iBu	H 2.0705 4.8885 1.7289	12si-PP-TS(-)-iBu
C 0.7689 0.9563 1.8390	H 0.3402 5.3566 -1.1813	C -0.5111 -0.8132 1.8290
C -0.1351 -0.0712 2.2251	H -0.7123 5.2005 0.2516	C 0.2117 -1.8802 1.2266
C -1.4455 0.3776 1.8585	H -1.0034 4.1842 -1.1902	C -0.6704 -2.4747 0.2617
C -1.3213 1.6622 1.1954	H 3.0297 -1.7029 -3.0982	C -1.8904 -1.6938 0.2260
C 0.0785 2.0307 1.1763	H 4.9478 -1.8891 -1.5358	C -1.8094 -0.6604 1.2388
H 1.8446 0.9205 2.0080	H 5.2737 -0.2485 0.3010	H -0.1157 -0.1759 2.6193
Si 0.9563 3.3469 0.1407	H 3.7354 1.6768 0.5818	Si -2.8560 0.9161 1.3661
C 1.4524 2.1207 -1.2233	H -2.8218 -1.0885 2.7170	C -1.9965 1.7684 -0.0890
C 0.6219 1.7144 -2.3188	H -4.8372 0.2536 2.1444	C -2.2004 1.3442 -1.4481
C 1.0636 0.4698 -2.8426	H -4.6333 2.4278 0.9633	C -1.1580 1.8160 -2.2787
C 2.2386 0.0892 -2.1252	H -2.4169 3.3494 0.3428	C -0.2754 2.5956 -1.4700
C 2.4572 1.0858 -1.0958	Zr 0.1878 0.1432 -0.4192	C -0.7738 2.5399 -0.1063
H -0.2550 2.2607 -2.6668	C 0.7323 -2.0819 -0.1444	H -3.0258 0.7189 -1.7866
H 0.6239 -0.0626 -3.6850	H 1.5630 -1.3434 0.1343	H -1.0753 1.6655 -3.3531
C 2.4212 4.0935 1.0499	H 0.2032 -2.3524 0.7810	C -2.5375 1.7595 3.0147
C -0.2173 4.6388 -0.5589	C -1.6270 -0.6053 -1.6787	C -4.6759 0.6328 0.9995
C 3.1591 -0.9896 -2.2836	C -0.9380 -1.8347 -1.6723	C 0.8877 3.3558 -1.7779
C 4.2227 -1.0835 -1.4164	H -0.2327 -2.0978 -2.4619	C 1.5552 3.9901 -0.7511
C 4.4138 -0.1338 -0.3612	C 1.4329 -3.3208 -0.6980	C 1.0926 3.9071 0.5999
C 3.5558 0.9290 -0.1960	C 0.4911 -4.5313 -0.7975	C -0.0456 3.2042 0.9290
C -2.7317 -0.1366 2.1808	C 2.6110 -3.6745 0.2274	C -0.5489 -3.6424 -0.5382
C -3.8443 0.6119 1.8703	H 1.8336 -3.0932 -1.6988	C -1.5665 -3.9574 -1.4161
C -3.7248 1.8652 1.1892	H -0.2709 -4.4140 -1.5834	C -2.7275 -3.1353 -1.5283
C -2.4972 2.3789 0.8342	H 1.0741 -5.4356 -1.0308	C -2.9021 -2.0267 -0.7245
C 0.1681 -1.2757 3.0645	H -0.0222 -4.6986 0.1629	C 1.5450 -2.4264 1.6531
C 1.6624 -1.5952 3.2087		

C	2.2296	-1.6133	2.7533	C	4.4409	0.3328	-1.1887	C	-1.6199	0.4594	2.7506
C	3.6400	-2.1228	3.0486	H	5.4809	0.2432	-0.8361	C	-1.8317	-0.9950	3.1843
H	1.3982	-3.4641	2.0071	H	4.2837	-0.4294	-1.9650	C	-3.1276	-1.1685	3.9775
H	2.2137	-2.5045	0.7815	H	4.3283	1.3273	-1.6550	H	-1.5710	1.0944	3.6555
H	1.6134	-1.6463	3.6682	H	3.5651	-0.7970	0.4514	H	-2.4992	0.8157	2.1926
H	2.2744	-0.5552	2.4467	C	2.3614	-2.1879	-1.7990	H	-0.9745	-1.3154	3.8009
H	4.2776	-2.0544	2.1494	H	1.6862	-2.9353	-1.3684	H	-1.8321	-1.6520	2.2939
H	3.6187	-3.1803	3.3622	H	3.2198	-2.0452	-1.1340	H	-4.0033	-0.8802	3.3719
H	4.1190	-1.5392	3.8505	H	2.2115	-0.1577	-2.6506	H	-3.1192	-0.5307	4.8776
H	-2.8721	2.8109	2.9899	H	2.7497	-2.5991	-2.7487	H	-3.2639	-2.2125	4.3012
H	-1.4677	1.7447	3.2824					H	4.3199	-2.7932	1.0751
H	-3.0924	1.2429	3.8170	12re-PP-TS(-)iBu				H	3.1311	-2.2900	2.3131
H	-5.2454	1.5624	1.1734	C	0.7429	-0.2068	1.8814	H	4.7300	-1.5087	2.2498
H	-5.0911	-0.1544	1.6524	C	-0.3572	0.6886	1.9684	H	5.3149	-0.1811	-0.8761
H	-4.8398	0.3342	-0.0491	C	0.0823	1.9278	1.3907	H	5.1285	1.0282	0.4245
H	1.2356	3.4352	-2.8101	C	1.4671	1.7708	0.9789	H	4.1479	1.1576	-1.0638
H	2.4450	4.5845	-0.9683	C	1.8756	0.4093	1.2477	H	-1.7224	-2.9701	-2.6920
H	1.6466	4.4329	1.3800	H	0.7159	-1.2340	2.2357	H	-2.1773	-4.4949	-0.7872
H	-0.4111	3.1790	1.9562	Si	3.2580	-0.6223	0.4508	H	-0.6281	-4.6225	1.1528
H	0.3258	-4.2873	-0.4401	C	2.1309	-1.3442	-0.9025	H	1.4275	-3.2402	1.2397
H	-1.4939	-4.8566	-2.0311	C	1.8596	-0.7284	-2.1669	H	-1.6029	3.3109	1.5688
H	-3.5061	-3.4126	-2.2414	C	0.6265	-1.1961	-2.6954	H	-0.3168	5.2313	0.6539
H	-3.8214	-1.4425	-0.7738	C	0.1180	-2.1889	-1.8015	H	2.0734	4.9859	0.0194
Zr	-0.2354	0.0638	-0.4952	C	1.0293	-2.2646	-0.6771	H	3.2310	2.7990	0.1996
C	2.0307	0.4649	-0.4064	H	2.4844	0.0350	-2.6283	Zr	0.1599	0.1011	-0.5137
H	1.4700	0.5917	0.5846	H	0.1826	-0.9085	-3.6449	C	-2.1051	-0.0023	-0.9176
H	2.0071	1.4358	-0.9259	C	3.9181	-1.9279	1.6304	H	-1.7025	-0.7126	-0.1039
H	-0.1134	-0.3657	-3.2985	C	4.5833	0.4482	-0.3402	H	-2.3172	-0.6577	-1.7727
C	0.2554	-1.0233	-2.5102	C	-1.0504	-3.0051	-1.8322	H	0.7697	1.7363	-2.8133
C	1.6189	-0.9272	-2.1508	C	-1.2942	-3.8526	-0.7738	C	0.1374	1.9523	-1.9473
H	-0.2093	-2.0130	-2.4555	C	-0.4040	-3.9262	0.3424	C	-1.2512	1.7370	-2.0992
C	3.4768	0.2040	0.0004	C	0.7360	-3.1545	0.4009	H	0.4484	2.7874	-1.3193
C	3.8833	1.2394	1.0692	C	-0.5666	3.1875	1.2467	C	-3.3947	0.5891	-0.3460
H	3.8488	2.2560	0.6429	C	0.1559	4.2517	0.7493	C	-4.1575	-0.5060	0.4210
H	3.2125	1.2170	1.9431	C	1.5316	4.1093	0.3799	H	-4.4642	-1.3056	-0.2750
H	4.9104	1.0400	1.4154	C	2.1809	2.8967	0.4755	H	-3.5411	-0.9587	1.2097

H -5.0666 -0.0886 0.8844	C -2.3464 -1.1847 2.0977	H 5.2228 -1.9141 -1.2156
C -4.3352 1.1739 -1.4106	C 2.7092 -1.0747 2.1514	C 3.0414 -2.8982 -2.5485
H -5.2686 1.5035 -0.9268	C 3.7329 0.0610 2.1114	H 3.9610 -3.5110 -2.5567
H -3.9138 2.0375 -1.9439	C 5.1619 -0.4577 2.2955	H 2.1861 -3.5920 -2.5659
H -4.5985 0.4028 -2.1551	H 2.7766 -1.5837 3.1362	H 3.0287 -2.3018 -3.4835
H -3.1270 1.3975 0.3579	H 2.9754 -1.8434 1.4095	H 2.9625 -2.6010 -0.4160
C -1.7988 1.3278 -3.4422	H 3.4983 0.7870 2.9081	H 0.6782 -3.0397 -0.6400
H -2.7415 0.7710 -3.3932	H 3.6440 0.6094 1.1614	C -2.1984 -1.7647 -2.0830
H -1.0568 0.7498 -4.0107	H 5.4242 -1.1777 1.5030	H -2.7032 -2.7372 -2.2249
H -1.8983 2.3514 -1.4691	H 5.2662 -0.9782 3.2615	H -1.7622 -1.4729 -3.0477
H -1.9946 2.2593 -4.0044	H 5.8951 0.3613 2.2650	H 0.3744 -2.5521 -2.4023
	H -1.2110 4.7788 1.7631	H -2.9785 -1.0338 -1.8235
21si-PP-TS(-)iBu	H 0.1821 3.8490 2.3943	
C 0.8227 0.7220 1.9700	H -1.3353 3.9177 3.3280	21re-PP-TS(-)iBu
C 1.2868 -0.6272 1.9642	H -3.9408 3.0294 1.2186	C 0.4059 -0.1292 1.7990
C 0.1179 -1.4585 1.9941	H -3.7331 1.9236 2.6034	C -0.2525 1.1206 1.6836
C -1.0520 -0.6037 2.0074	H -3.7810 1.2751 0.9365	C 0.6975 2.0314 1.0987
C -0.6136 0.7795 1.9690	H 1.7164 1.4232 -3.9243	C 1.9278 1.3058 0.8548
H 1.4780 1.5863 1.9605	H 3.6299 2.6691 -2.9479	C 1.7290 -0.0784 1.2365
Si -1.5645 2.3314 1.4345	H 3.4555 3.7345 -0.7067	H -0.0506 -1.0123 2.2409
C -1.0253 2.1861 -0.3799	H 1.3551 3.6173 0.6036	Si 2.6920 -1.6426 0.7636
C -1.6829 1.3841 -1.3655	H 0.8537 -3.5131 2.0920	C 1.4264 -2.1914 -0.5460
C -0.8033 1.0879 -2.4422	H -1.4315 -4.4814 2.2516	C 1.4349 -1.7831 -1.9195
C 0.4288 1.7707 -2.1852	H -3.4442 -3.0189 2.2859	C 0.1311 -1.8830 -2.4786
C 0.3095 2.4091 -0.8920	H -3.2329 -0.5481 2.1292	C -0.7294 -2.4373 -1.4800
H -2.7065 1.0201 -1.2797	Zr 0.0748 -0.0408 -0.2644	C 0.0585 -2.6008 -0.2753
H -1.0475 0.5280 -3.3336	C 1.8933 -0.9788 -1.3632	H 2.3058 -1.3874 -2.4451
C -0.9154 3.8606 2.3069	H 2.1403 -0.1382 -0.6162	H -0.1536 -1.6450 -3.5030
C -3.4304 2.1133 1.5584	H 1.8272 -0.5237 -2.3608	C 2.8625 -2.8457 2.1949
C 1.6375 1.8771 -2.9331	C -1.1422 -1.8975 -0.9993	C 4.3236 -1.2297 -0.0773
C 2.6994 2.5674 -2.3818	C 0.1321 -2.4084 -1.3439	C -2.1072 -2.7946 -1.4930
C 2.5957 3.1809 -1.0970	H -1.5246 -2.2643 -0.0469	C -2.6740 -3.2892 -0.3374
C 1.4314 3.1144 -0.3585	C 3.0448 -1.9729 -1.3226	C -1.9046 -3.4535 0.8570
C -0.0298 -2.8735 2.0749	C 4.3779 -1.2069 -1.2725	C -0.5673 -3.1225 0.8975
C -1.2992 -3.3990 2.1674	H 4.4977 -0.5984 -2.1925	C 0.6532 3.4425 0.9346
C -2.4538 -2.5583 2.1906	H 4.4298 -0.5292 -0.4069	C 1.8201 4.1063 0.6142

H -3.9453 -3.7593 1.2132	H -0.5052 0.1236 2.6715	H 1.0813 5.0336 -1.2611
H -5.2436 -1.8693 0.2598	Si -3.2611 0.2528 1.0403	H 0.0682 4.8957 1.0038
H -4.2671 0.4022 0.0917	C -2.4930 1.1653 -0.4294	H -1.6227 3.1690 1.5490
Zr -0.0983 0.0369 -0.4808	C -2.4017 0.5665 -1.7339	H 1.4235 -3.9737 0.2323
C 1.8066 -1.2531 -0.3023	C -1.4331 1.2315 -2.5204	H 0.0427 -5.1973 -1.4298
H 1.8752 -0.2171 0.1812	C -0.9058 2.3085 -1.7438	H -2.2454 -4.4196 -2.0113
H 1.5399 -1.9710 0.4856	C -1.5361 2.2492 -0.4360	H -3.2687 -2.4857 -0.8504
C -0.8048 -1.4912 -2.0975	H -2.9753 -0.2999 -2.0613	Zr -0.2962 0.0054 -0.4452
C 0.5400 -1.9151 -2.0787	H -1.1789 1.0041 -3.5535	C 1.7440 1.0462 -0.2029
H 1.2857 -1.4939 -2.7543	C -3.3941 1.3130 2.5859	H 1.0508 1.1055 0.7073
C 3.2019 -1.5747 -0.8259	C -4.8733 -0.5756 0.5491	H 1.5205 1.9123 -0.8456
C 3.3630 -3.0570 -1.1950	C 0.0336 3.3353 -2.0412	H 0.2878 -0.6499 -3.1448
C 4.2295 -1.2104 0.2622	C 0.3683 4.2339 -1.0500	C 0.7211 -1.0917 -2.2464
H 3.4059 -0.9577 -1.7157	C -0.2188 4.1577 0.2521	C 1.9502 -0.5732 -1.7796
H 2.7889 -3.3416 -2.0887	C -1.1529 3.1947 0.5652	H 0.5421 -2.1624 -2.1049
H 4.4236 -3.2734 -1.4004	C 0.4250 -3.6199 -0.0293	C 3.1437 1.2529 0.3651
H 3.0457 -3.7002 -0.3549	C -0.3496 -4.2998 -0.9475	C 3.1144 2.4631 1.3213
H 4.1555 -0.1485 0.5436	C -1.6678 -3.8606 -1.2726	H 2.8564 3.3790 0.7637
H 4.0614 -1.8191 1.1670	C -2.2382 -2.7738 -0.6408	H 2.3717 2.3371 2.1255
H 5.2520 -1.4077 -0.0998	C 1.8153 -1.6414 2.1655	H 4.1053 2.6023 1.7832
H 0.7527 -2.9177 -1.7036	C 2.1082 -0.5601 3.2073	C 4.1763 1.5327 -0.7373
C -1.8710 -2.5089 -1.7515	C 3.5558 -0.6115 3.6948	H 5.1486 1.7809 -0.2823
C -2.1714 -3.4156 -2.9546	H 1.9152 -2.6366 2.6378	H 4.3320 0.6837 -1.4178
H -2.7974 -2.0125 -1.4340	H 2.5832 -1.6115 1.3766	H 3.8548 2.4012 -1.3386
H -1.5327 -3.1175 -0.9010	H 1.4153 -0.6764 4.0583	H 3.4457 0.3697 0.9500
H -2.5173 -2.8220 -3.8186	H 1.8994 0.4302 2.7697	C 2.9659 -1.5239 -1.2064
H -1.2685 -3.9689 -3.2662	H 4.2574 -0.4537 2.8565	C 3.8431 -2.0474 -2.3591
H -1.0693 -0.8080 -2.9138	H 3.7860 -1.5937 4.1414	H 2.4534 -2.3672 -0.7273
H -2.9585 -4.1470 -2.7058	H 3.7527 0.1623 4.4535	H 3.6123 -1.0566 -0.4550
	H -3.9979 2.2164 2.3926	H 3.2304 -2.5592 -3.1186
12si-BT-TS(-)iBu	H -2.4032 1.6325 2.9500	H 4.3797 -1.2195 -2.8536
C -0.6092 -0.6762 1.9390	H -3.8819 0.7422 3.3950	H 2.3670 0.2797 -2.3198
C 0.4476 -1.5459 1.5507	H -5.6926 0.1643 0.5465	H 4.5921 -2.7582 -1.9748
C -0.1104 -2.4620 0.5957	H -5.1352 -1.3791 1.2591	
C -1.4833 -2.0713 0.3462	H -4.8169 -1.0123 -0.4617	
C -1.8155 -0.9620 1.2175	H 0.4725 3.4071 -3.0388	

12re-BT-TS(-)iBu

C -1.2378 0.6916 1.6547
C -0.0023 0.2321 2.1855
C -0.0189 -1.1993 2.0703
C -1.2901 -1.5929 1.4862
C -2.0463 -0.3979 1.1818
H -1.5200 1.7398 1.5999
Si -3.4385 -0.1327 -0.0839
C -2.2580 0.3911 -1.4821
C -1.6025 -0.5037 -2.3884
C -0.4293 0.0958 -2.9203
C -0.3542 1.4305 -2.4143
C -1.4665 1.6095 -1.5025
H -1.9284 -1.5222 -2.5939
H 0.2514 -0.3500 -3.6409
C -4.6056 1.2420 0.4454
C -4.2941 -1.7379 -0.5521
C 0.5766 2.4895 -2.6246
C 0.3999 3.6723 -1.9405
C -0.6901 3.8527 -1.0333
C -1.6097 2.8509 -0.8110
C 0.9176 -2.1924 2.4770
C 0.5751 -3.5213 2.3404
C -0.6926 -3.9114 1.8018
C -1.6089 -2.9767 1.3681
C 0.9890 1.0606 2.9537
C 0.7685 2.5721 2.8318
C 1.8019 3.3636 3.6345
H 0.9055 0.7761 4.0198
H 2.0208 0.8081 2.6653
H -0.2458 2.8181 3.1899
H 0.7978 2.8671 1.7658
H 2.8242 3.1554 3.2764
H 1.7586 3.0867 4.7014
H 1.6261 4.4482 3.5567
H -5.0748 1.7197 -0.4322

H -4.0777 2.0200 1.0220
H -5.4073 0.8374 1.0873
H -5.0269 -1.5606 -1.3584
H -4.8343 -2.1621 0.3119
H -3.5702 -2.4902 -0.9078
H 1.3982 2.3660 -3.3330
H 1.0955 4.4987 -2.0999
H -0.8008 4.8116 -0.5232
H -2.4574 3.0074 -0.1430
H 1.8674 -1.8984 2.9291
H 1.2696 -4.2972 2.6685
H -0.9340 -4.9743 1.7403
H -2.5753 -3.2824 0.9667
Zr -0.1279 -0.2120 -0.3758
C 2.0862 0.3981 -0.5479
H 1.3751 1.1905 -0.1061
H 2.3103 0.7642 -1.5586
H 0.1325 -2.6193 -1.9477
C 0.6091 -2.3444 -1.0023
C 1.9121 -1.8021 -1.0764
H 0.3780 -2.9758 -0.1441
C 3.3343 0.4270 0.3358
C 3.6536 1.8847 0.7134
H 3.9024 2.4604 -0.1946
H 2.8033 2.3759 1.2060
H 4.5214 1.9247 1.3924
C 4.5794 -0.1812 -0.3275
H 5.4460 -0.0485 0.3399
H 4.4846 -1.2552 -0.5404
H 4.8032 0.3404 -1.2741
H 3.1231 -0.1428 1.2584
C 2.6246 -1.7433 -2.4041
H 3.3314 -0.9063 -2.4697
H 1.8873 -1.6271 -3.2133
H 2.5421 -1.9592 -0.1979
C 3.3927 -3.0635 -2.5981

H 2.7078 -3.9265 -2.5701
H 4.1475 -3.1990 -1.8046
H 3.9140 -3.0602 -3.5685

21si-BT-TS(-)iBu

C -0.0831 0.7149 1.9588
C 0.5538 -0.5520 2.0596
C -0.4561 -1.5392 1.8014
C -1.7037 -0.8520 1.5285
C -1.4671 0.5757 1.5881
H 0.4257 1.6626 2.1122
Si -2.4621 1.9887 0.7905
C -1.3911 2.0406 -0.7810
C -1.5830 1.2331 -1.9508
C -0.3628 1.1008 -2.6671
C 0.6210 1.8983 -2.0052
C -0.0001 2.4584 -0.8234
H -2.5144 0.7437 -2.2220
H -0.2170 0.5597 -3.5992
C -2.3808 3.5609 1.8142
C -4.2093 1.4635 0.3422
C 1.9935 2.1591 -2.2870
C 2.7130 2.9430 -1.4110
C 2.1091 3.4923 -0.2387
C 0.7828 3.2623 0.0586
C -0.4149 -2.9608 1.8394
C -1.5867 -3.6606 1.6410
C -2.8237 -2.9850 1.3929
C -2.8914 -1.6102 1.3215
C 1.9529 -0.8155 2.5401
C 2.8361 0.4340 2.6071
C 4.2534 0.1059 3.0769
H 1.8927 -1.2669 3.5483
H 2.4344 -1.5791 1.9066
H 2.3758 1.1654 3.2936
H 2.8613 0.9223 1.6144

H	4.7399	-0.6101	2.3929	C	-3.2963	-1.8510	-2.4198	H	1.3470	-1.7315	3.6885
H	4.2340	-0.3509	4.0807	H	-1.6010	-2.8600	-3.2802	H	1.2427	-2.5435	2.1363
H	4.8800	1.0105	3.1263	H	-1.4762	-1.1070	-3.3492	H	3.3608	-0.4738	2.9632
H	-2.6298	4.4445	1.2012	H	-3.6359	-2.7456	-1.8715	H	3.2596	-1.1652	1.3443
H	-1.3809	3.7129	2.2531	H	-3.5426	-0.9794	-1.7894	H	3.5982	-3.4883	2.3234
H	-3.1038	3.5035	2.6467	H	0.8545	-2.5286	-2.4227	H	3.6879	-2.7768	3.9534
H	-4.7367	2.2920	-0.1615	H	-3.8757	-1.7792	-3.3539	H	4.9517	-2.4067	2.7504
H	-4.7849	1.1922	1.2440					H	1.8653	5.2250	0.4895
H	-4.2071	0.5966	-0.3396					H	2.4498	3.9111	1.5525
H	2.4531	1.7636	-3.1952					H	1.1381	4.9807	2.1058
H	3.7618	3.1651	-1.6188					H	-1.2637	5.0175	-0.5095
H	2.7096	4.1218	0.4207					H	-1.8405	4.5126	1.1017
H	0.3245	3.7141	0.9386					H	-2.1080	3.4543	-0.3124
H	0.5197	-3.4782	2.0663					H	2.9199	-0.8795	-3.4372
H	-1.5827	-4.7513	1.6924					H	5.0188	-0.7494	-2.1198
H	-3.7310	-3.5782	1.2631					H	5.2778	0.9051	-0.2812
H	-3.8391	-1.1047	1.1380					H	3.4408	2.4558	0.3081
Zr	-0.1293	-0.0480	-0.3771					H	-1.4003	-2.3518	2.8779
C	1.8902	-0.9326	-1.1042					H	-3.7545	-1.6070	3.1716
H	1.9193	-0.1152	-0.3002					H	-4.4388	0.7152	2.6163
H	2.0107	-0.4415	-2.0790					H	-2.8137	2.3457	1.6948
C	-0.9909	-2.0011	-1.3999					Zr	0.2037	0.1299	-0.3796
C	0.3969	-2.3805	-1.4404					C	0.7474	-2.0428	-0.9482
H	-1.5311	-2.5888	-0.6499					H	1.4523	-1.4221	-0.2814
C	3.1174	-1.7978	-0.8134					H	1.1479	-1.9201	-1.9659
C	4.3182	-0.8779	-0.5334					C	-1.8075	-0.4779	-1.3983
H	4.5532	-0.2774	-1.4289					C	-1.2443	-1.8171	-1.3527
H	4.1180	-0.1882	0.2998					C	1.0847	-3.4594	-0.4962
H	5.2065	-1.4791	-0.2810					C	2.6102	-3.6323	-0.4929
C	3.4594	-2.7403	-1.9762					H	3.0096	-3.4982	-1.5128
H	4.4287	-3.2270	-1.7839					H	3.1031	-2.9043	0.1677
H	2.7111	-3.5334	-2.1190					H	2.8731	-4.6458	-0.1496
H	3.5500	-2.1696	-2.9176					C	0.4388	-4.5064	-1.4154
H	2.9191	-2.4057	0.0866					H	0.7676	-5.5164	-1.1238
H	0.7656	-3.0429	-0.6523					H	-0.6603	-4.4803	-1.3674
C	-1.7929	-1.9372	-2.7008					H	0.7467	-4.3397	-2.4633

21re-BT-TS(-)iBu

H 0.7009 -3.6149 0.5267	C -0.2553 -3.6213 0.1495	H 2.1553 0.8179 -1.9954
H -1.6365 -2.4686 -0.5618	C 0.5130 0.3637 3.1670	C 1.4831 2.9370 -0.5237
H -1.0365 -2.3412 -2.2889	C -0.2303 1.6820 3.4074	C 2.9965 3.1117 -0.7107
C -3.1625 -0.2985 -0.7351	C 0.5698 2.6330 4.2978	C 0.9753 4.0518 0.4115
C -4.2904 -0.8921 -1.5940	H 0.6289 -0.1650 4.1319	H 0.9990 3.0587 -1.5055
H -3.3578 0.7715 -0.5605	H 1.5459 0.5724 2.8322	H 3.4341 2.3981 -1.4235
H -3.1555 -0.7847 0.2489	H -1.2094 1.4652 3.8688	H 3.1939 4.1271 -1.0902
H -4.3167 -0.4191 -2.5905	H -0.4421 2.1710 2.4407	H 3.5251 3.0091 0.2527
H -4.1409 -1.9762 -1.7360	H 1.5344 2.8900 3.8254	H -0.1157 3.9976 0.5471
H -1.7895 -0.0464 -2.4042	H 0.7891 2.1687 5.2743	H 1.4528 3.9605 1.4029
H -5.2698 -0.7379 -1.1123	H 0.0200 3.5696 4.4813	H 1.2284 5.0430 -0.0003
	H -5.6617 -0.8722 -0.0207	C 4.5434 -0.4722 -1.2135
12si-HX-TS(+)<i>i</i>Bu	H -4.7120 -0.4550 1.4380	C 5.8159 -0.6170 -0.3746
C -1.5230 -0.5541 1.7969	H -5.3165 -2.1136 1.2187	H 4.7011 0.2961 -1.9935
C -0.1565 -0.5628 2.1946	H -4.4073 -3.3679 -1.7386	H 4.3310 -1.4188 -1.7413
C 0.4299 -1.7349 1.6138	H -3.5461 -4.2211 -0.4273	C 7.0295 -0.9956 -1.2253
C -0.5840 -2.4089 0.8252	H -2.6352 -3.5442 -1.8099	H 6.0080 0.3338 0.1559
C -1.8227 -1.6713 0.9410	H -0.8045 3.5306 -2.6854	H 5.6470 -1.3819 0.4059
H -2.2379 0.2141 2.0886	H -2.0921 4.8817 -1.0565	H 6.8614 -1.9551 -1.7448
Si -3.3274 -1.7413 -0.2117	H -3.6387 3.8086 0.5674	H 7.2244 -0.2273 -1.9936
C -2.6592 -0.4040 -1.3832	H -4.0133 1.3600 0.5433	H 7.9363 -1.0968 -0.6075
C -1.7151 -0.6181 -2.4400	H 2.4688 -1.8325 2.3906	
C -1.0507 0.5949 -2.7690	H 2.9780 -3.9614 1.2162	12re-HX-TS(+)<i>i</i>Bu
C -1.6281 1.6335 -1.9731	H 1.2667 -5.0881 -0.1912	C -2.5269 0.7320 0.1876
C -2.5855 1.0109 -1.0792	H -1.0094 -4.1433 -0.4391	C -1.9893 1.1865 1.4203
H -1.4988 -1.5868 -2.8904	Zr -0.4126 -0.1200 -0.3672	C -1.7676 0.0230 2.2256
H -0.2995 0.7271 -3.5457	C 1.0560 1.5905 0.0633	C -2.1548 -1.1446 1.4522
C -4.8993 -1.2403 0.6874	H -0.0364 1.7597 0.3900	C -2.6520 -0.7003 0.1686
C -3.4863 -3.3724 -1.1302	H 1.6023 1.3921 0.9956	H -2.8008 1.3865 -0.6390
C -1.4659 3.0491 -1.9635	H 0.9701 -1.2397 -2.5343	Si -2.8625 -1.6756 -1.4414
C -2.1909 3.7945 -1.0612	C 1.3551 -1.1186 -1.5187	C -1.0543 -1.4517 -1.9739
C -3.0857 3.1785 -0.1318	C 2.1159 0.0402 -1.2293	C 0.0154 -2.2582 -1.4633
C -3.2891 1.8163 -0.1313	H 1.6306 -2.0368 -0.9930	C 1.2581 -1.5950 -1.6121
C 1.7227 -2.3100 1.7528	C 3.3321 -0.0846 -0.3478	C 1.0112 -0.3510 -2.2709
C 1.9964 -3.4964 1.1045	H 3.1574 -0.8662 0.4042	C -0.4247 -0.2464 -2.4719
C 1.0112 -4.1461 0.2980	H 3.5661 0.8465 0.1812	H -0.1164 -3.2273 -0.9817

H 2.2283 -1.9860 -1.3195	C 1.0775 1.5914 0.4698	C -0.8395 1.4268 1.8392
C -4.0862 -0.8203 -2.5809	H 0.3658 1.6919 -0.4279	C 0.1613 2.1636 1.0981
C -3.2254 -3.4973 -1.1627	H 0.5457 1.9989 1.3410	H 2.3716 1.7906 0.9707
C 1.8751 0.6847 -2.7371	H 1.4522 -2.2765 1.0871	Si -0.0643 3.3231 -0.3885
C 1.3193 1.7833 -3.3517	C 1.1775 -1.3274 1.5511	C 0.1613 1.9445 -1.6806
C -0.0964 1.9129 -3.5119	C 2.0662 -0.2336 1.4130	C -0.8840 1.0912 -2.1589
C -0.9609 0.9299 -3.0830	H 0.6042 -1.3974 2.4772	C -0.3488 -0.1285 -2.6542
C -1.3119 -0.1215 3.5645	C 2.2492 2.5174 0.1588	C 1.0779 -0.0328 -2.5856
C -1.2256 -1.3906 4.1011	C 2.9989 2.9293 1.4343	C 1.3960 1.2298 -1.9489
C -1.5685 -2.5467 3.3333	C 1.7199 3.7940 -0.5237	H -1.9442 1.3213 -2.0926
C -2.0173 -2.4409 2.0330	H 2.9389 2.0174 -0.5394	H -0.9122 -0.9456 -3.0989
C -1.8267 2.6101 1.8644	H 3.4310 2.0811 1.9845	C 1.2695 4.6429 -0.4512
C -1.8227 3.6334 0.7239	H 3.8202 3.6186 1.1807	C -1.8121 4.0043 -0.5111
C -1.5170 5.0447 1.2251	H 2.3117 3.4616 2.1155	C 2.1254 -0.8944 -3.0213
H -2.6452 2.8530 2.5678	H 1.1695 3.5573 -1.4469	C 3.4310 -0.5159 -2.7983
H -0.9022 2.7148 2.4634	H 1.0405 4.3372 0.1545	C 3.7499 0.7087 -2.1343
H -2.8044 3.6161 0.2196	H 2.5590 4.4633 -0.7758	C 2.7619 1.5716 -1.7136
H -1.0757 3.3381 -0.0328	C 3.3412 -0.3326 0.5921	C -0.9370 -0.5324 3.3793
H -0.5218 5.0821 1.7025	C 4.0764 -1.6715 0.7513	C -2.2876 -0.2963 3.5341
H -2.2585 5.3670 1.9755	H 4.0217 0.4787 0.8842	C -2.9365 0.7817 2.8523
H -1.5259 5.7749 0.4004	H 3.1290 -0.1711 -0.4731	C -2.2408 1.6264 2.0128
H -3.9581 -1.1587 -3.6237	C 5.3775 -1.6968 -0.0538	C 2.2739 -0.5067 2.8153
H -3.9692 0.2760 -2.5561	H 4.2891 -1.8585 1.8186	C 3.6138 -0.4791 2.0714
H -5.1191 -1.0522 -2.2679	H 3.4301 -2.5029 0.4178	C 4.6076 -1.4852 2.6519
H -3.3812 -4.0057 -2.1300	C 6.1138 -3.0314 0.0770	H 2.4389 -0.1981 3.8648
H -4.1379 -3.6278 -0.5556	H 5.1464 -1.4957 -1.1174	H 1.9052 -1.5470 2.8826
H -2.3930 -4.0045 -0.6469	H 6.0294 -0.8704 0.2831	H 4.0348 0.5401 2.1238
H 2.9571 0.5843 -2.6355	H 7.0472 -3.0340 -0.5081	H 3.4507 -0.6928 1.0004
H 1.9672 2.5755 -3.7313	H 6.3711 -3.2348 1.1308	H 4.2141 -2.5138 2.5705
H -0.4926 2.8031 -4.0042	H 5.4843 -3.8647 -0.2818	H 4.7950 -1.2826 3.7201
H -2.0357 1.0195 -3.2421	H 2.0909 0.4630 2.2540	H 5.5732 -1.4472 2.1231
H -1.0634 0.7601 4.1589		H 1.3437 5.0804 -1.4619
H -0.8962 -1.5217 5.1338	21si-HX-TS(+)<i>i</i>Bu	H 2.2580 4.2408 -0.1735
H -1.4865 -3.5314 3.7975	C 1.4059 1.4953 1.3753	H 1.0287 5.4532 0.2590
H -2.3080 -3.3274 1.4682	C 1.2121 0.3726 2.2236	H -1.9036 4.6563 -1.3970
Zr -0.2289 -0.2451 0.0350	C -0.1871 0.3279 2.5300	H -2.0676 4.6029 0.3802

H -2.5555 3.1951 -0.6075	H -5.2029 -1.3576 -2.4992	H 2.1756 -0.7413 3.7106
H 1.8913 -1.8215 -3.5465	H -7.5962 -1.7250 -1.8088	H 2.1374 -1.6471 2.1923
H 4.2453 -1.1558 -3.1442	H -6.5759 -3.0729 -1.2374	H 1.4568 -3.7363 3.4337
H 4.7986 0.9713 -1.9829	H -7.1004 -1.8077 -0.0964	H 1.4914 -2.8353 4.9695
H 3.0132 2.5239 -1.2462	H -0.9793 -2.8892 0.8231	H 3.0017 -3.0949 4.0551
H -0.4401 -1.3389 3.9224		H 3.1085 4.5757 0.3417
H -2.8774 -0.9317 4.1978	21re-HX-TS(+) iBu	H 2.9279 3.3733 1.6553
H -4.0046 0.9401 3.0138	C 0.7665 0.9619 1.8308	H 2.0268 4.9055 1.7274
H -2.7413 2.4573 1.5159	C -0.1305 -0.0651 2.2256	H 0.3023 5.3259 -1.2351
Zr 0.0921 0.0205 -0.1229	C -1.4472 0.3783 1.8655	H -0.7479 5.1859 0.2021
C 1.0757 -2.0418 0.0619	C -1.3288 1.6608 1.2032	H -1.0236 4.1308 -1.2131
H 1.7840 -1.1781 -0.2088	C 0.0689 2.0339 1.1692	H 3.0453 -1.7149 -3.0717
H 1.2079 -2.2273 1.1372	H 1.8417 0.9300 2.0007	H 4.9494 -1.9007 -1.4947
C -1.9517 -1.0794 0.1235	Si 0.9416 3.3502 0.1288	H 5.2719 -0.2456 0.3318
C -1.1921 -2.2545 -0.0375	C 1.4644 2.1223 -1.2230	H 3.7401 1.6851 0.5906
H -2.2165 -0.8648 1.1620	C 0.6428 1.7147 -2.3245	H -2.8148 -1.0926 2.7269
H -1.1614 -2.7511 -1.0112	C 1.0844 0.4686 -2.8415	H -4.8351 0.2432 2.1725
C 1.5571 -3.2514 -0.7287	C 2.2522 0.0850 -2.1137	H -4.6452 2.4215 0.9952
C 0.9340 -4.5636 -0.2299	C 2.4667 1.0853 -1.0851	H -2.4360 3.3499 0.3635
C 3.0897 -3.3397 -0.5956	H -0.2324 2.2602 -2.6785	Zr 0.1968 0.1427 -0.4254
H 1.3034 -3.1098 -1.7927	H 0.6505 -0.0670 -3.6838	C 0.7140 -2.0900 -0.1567
H -0.1457 -4.6301 -0.4256	C 2.3910 4.1179 1.0447	H 1.5487 -1.3606 0.1315
H 1.4179 -5.4168 -0.7314	C -0.2463 4.6123 -0.5963	H 0.1721 -2.3552 0.7616
H 1.0980 -4.6762 0.8568	C 3.1689 -0.9965 -2.2596	C -1.6221 -0.5824 -1.6957
H 3.5772 -2.4246 -0.9651	C 4.2278 -1.0889 -1.3855	C -0.9454 -1.8195 -1.6967
H 3.3716 -3.4788 0.4627	C 4.4160 -0.1341 -0.3368	H -0.2430 -2.0907 -2.4861
H 3.4739 -4.1999 -1.1684	C 3.5625 0.9348 -0.1798	C 1.4030 -3.3316 -0.7118
C -3.0720 -0.7346 -0.8481	C -2.7277 -0.1419 2.1969	C 0.4496 -4.5305 -0.8254
C -4.3410 -1.5377 -0.5257	C -3.8450 0.6071 1.8923	C 2.5713 -3.7019 0.2211
H -2.7715 -0.9372 -1.8882	C -3.7352 1.8599 1.2162	H 1.8141 -3.1027 -1.7081
H -3.3146 0.3391 -0.7788	C -2.5089 2.3779 0.8516	H -0.3073 -4.4038 -1.6130
C -5.5071 -1.1831 -1.4503	C 0.1855 -1.2720 3.0594	H 1.0253 -5.4392 -1.0632
H -4.1146 -2.6174 -0.6039	C 1.6798 -1.5815 3.1941	H -0.0690 -4.7031 0.1345
H -4.6293 -1.3548 0.5258	C 1.9252 -2.8835 3.9564	H 3.2869 -2.8706 0.3164
C -6.7675 -1.9907 -1.1330	H -0.2444 -1.1191 4.0672	H 2.1941 -3.9487 1.2282
H -5.7207 -0.1014 -1.3638	H -0.3450 -2.1583 2.6617	H 3.1060 -4.5827 -0.1710

H -1.4088 -2.6538 -1.1672	C -2.7428 2.5436 0.0079	H 1.3489 -1.8488 -1.6246
C -3.0146 -0.5396 -1.1030	C 1.4277 -3.0723 0.5987	C 1.9285 2.4984 0.6773
C -4.0618 -1.0663 -2.0972	C 1.1582 -4.0730 -0.3132	C 1.2593 3.6598 1.4410
H -3.2855 0.4843 -0.8137	C -0.1438 -4.2302 -0.8755	H 0.7737 4.3492 0.7302
H -3.0394 -1.1431 -0.1846	C -1.1951 -3.4242 -0.4873	H 0.4899 3.3034 2.1446
C -5.4890 -1.0024 -1.5392	C 1.5184 -0.5451 2.6650	H 2.0168 4.2217 2.0112
H -3.9988 -0.4787 -3.0308	C 1.1746 0.6354 3.5752	C 2.9550 3.0907 -0.3002
H -3.8127 -2.1111 -2.3639	C 2.4140 1.2103 4.2603	H 3.6548 3.7438 0.2453
C -5.6992 -1.9013 -0.3163	H 1.9073 -1.3771 3.2815	H 3.5484 2.3299 -0.8268
H -5.7273 0.0455 -1.2775	H 2.3450 -0.2649 1.9934	H 2.4383 3.7080 -1.0559
H -6.1953 -1.2943 -2.3350	H 0.4379 0.3114 4.3302	H 2.4362 1.8587 1.4163
H -6.7500 -1.8824 0.0157	H 0.6828 1.4214 2.9784	C 3.1287 -0.2197 -0.4985
H -5.4382 -2.9487 -0.5521	H 3.1402 1.5767 3.5131	C 4.3476 -0.4277 -1.4153
H -5.0731 -1.5801 0.5333	H 2.9204 0.4411 4.8677	H 2.9042 -1.1606 0.0187
H -1.4883 0.0256 -2.5987	H 2.1542 2.0510 4.9228	H 3.3951 0.5230 0.2618
	H -5.2698 0.6344 1.5438	C 5.5839 -0.8641 -0.6253
12si-HX-TS(-)iBu	H -3.7043 0.7886 2.3925	H 4.1063 -1.1826 -2.1843
C -1.0051 -0.6635 1.9728	H -4.7779 -0.5887 2.7494	H 4.5665 0.5130 -1.9544
C 0.3574 -1.0569 1.8600	H -5.6708 -2.0575 -0.2123	C 6.8056 -1.0621 -1.5246
C 0.3818 -2.1879 0.9751	H -4.7002 -3.1864 0.7798	H 5.8034 -0.1059 0.1490
C -0.9648 -2.4058 0.4862	H -4.2401 -2.8494 -0.9148	H 5.3547 -1.8029 -0.0875
C -1.8532 -1.4652 1.1390	H -0.6975 3.1308 -3.3310	H 7.6851 -1.3798 -0.9418
H -1.3542 0.1613 2.5931	H -1.1010 4.9901 -1.7322	H 6.6082 -1.8310 -2.2916
Si -3.5974 -0.9563 0.5952	H -2.3770 4.6205 0.3679	H 7.0634 -0.1246 -2.0473
C -2.9876 0.0785 -0.8677	H -3.3372 2.4022 0.9112	H 2.0933 1.1000 -1.9258
C -2.4352 -0.5260 -2.0501	H 2.4194 -2.9714 1.0426	
C -1.6732 0.4144 -2.7807	H 1.9480 -4.7676 -0.6060	12re-HX-TS(-)iBu
C -1.7550 1.6665 -2.0976	H -0.3148 -5.0277 -1.6011	C -2.3382 0.2910 0.9971
C -2.5406 1.4533 -0.8941	H -2.1998 -3.5941 -0.8754	C -1.3571 0.7804 1.9011
H -2.5588 -1.5720 -2.3288	Zr -0.5503 -0.0905 -0.4172	C -0.6563 -0.3695 2.4002
H -1.1668 0.2343 -3.7267	C 0.8470 1.7018 -0.0439	C -1.2462 -1.5554 1.8022
C -4.4099 0.0696 1.9435	H 0.0313 1.5421 0.7445	C -2.2815 -1.1400 0.8812
C -4.6445 -2.4000 0.0072	H 0.4274 2.3535 -0.8263	H -3.0291 0.9283 0.4513
C -1.2486 2.9609 -2.4035	H 0.7240 -0.6495 -2.8914	Si -3.0048 -2.0499 -0.6219
C -1.4747 3.9881 -1.5115	C 1.1225 -0.8108 -1.8888	C -1.7621 -1.2974 -1.8517
C -2.2137 3.7766 -0.3052	C 1.9477 0.1936 -1.3341	C -0.4672 -1.8324 -2.1490

C 0.3912 -0.8148 -2.6452	H 1.5719 -1.8830 4.4881	21si-HX-TS(-)iBu
C -0.3730 0.3890 -2.7461	H 0.5134 -3.9143 3.5240	C 0.8160 0.7491 1.9264
C -1.6971 0.1039 -2.2304	H -1.2678 -3.7407 1.8058	C 1.3238 -0.5781 1.9277
H -0.1679 -2.8631 -1.9643	Zr -0.2346 -0.2603 -0.2037	C 0.1837 -1.4491 1.9696
H 1.4230 -0.9411 -2.9628	C 1.2994 1.4575 -0.1836	C -1.0140 -0.6282 1.9953
C -4.7790 -1.5308 -0.9603	H 0.1922 1.7677 -0.2651	C -0.6219 0.7629 1.9298
C -2.7463 -3.9079 -0.5249	H 1.7059 1.6264 -1.1895	H 1.4435 1.6360 1.9040
C -0.0482 1.7012 -3.1986	H 1.7179 -2.3618 -0.5286	Si -1.6095 2.2869 1.3673
C -1.0111 2.6839 -3.1265	C 1.5918 -1.6416 0.2850	C -0.9970 2.1863 -0.4314
C -2.3165 2.4118 -2.6112	C 2.3983 -0.4817 0.2436	C -1.5948 1.4118 -1.4782
C -2.6639 1.1535 -2.1700	H 1.3640 -2.0577 1.2666	C -0.6419 1.1236 -2.4917
C 0.3867 -0.4985 3.3615	C 1.9226 2.4195 0.8291	C 0.5720 1.7960 -2.1503
C 0.7905 -1.7632 3.7351	C 1.3450 3.8293 0.6101	C 0.3704 2.4246 -0.8618
C 0.1836 -2.9333 3.1766	H 1.6325 4.2004 -0.3886	H -2.6214 1.0559 -1.4796
C -0.8055 -2.8445 2.2200	H 0.2482 3.8370 0.6737	H -0.8247 0.5673 -3.4087
C -1.2644 2.1864 2.4241	H 1.7434 4.5293 1.3630	C -1.0514 3.8401 2.2645
C -2.0962 3.2033 1.6352	C 3.4538 2.5085 0.7405	C -3.4687 2.0247 1.4462
C -1.9666 4.6135 2.2124	H 3.8126 3.2770 1.4437	C 1.8276 1.9053 -2.8137
H -1.6198 2.1761 3.4720	H 3.9646 1.5672 0.9870	C 2.8442 2.6035 -2.1988
H -0.2165 2.5192 2.4758	H 3.7621 2.8137 -0.2744	C 2.6578 3.2142 -0.9207
H -3.1549 2.8925 1.6513	H 1.6563 2.0784 1.8456	C 1.4518 3.1345 -0.2579
H -1.7885 3.1904 0.5724	C 3.4600 -0.3450 -0.8185	C 0.0819 -2.8661 2.0545
H -0.9193 4.9583 2.1819	H 3.6540 0.6997 -1.0927	C -1.1694 -3.4318 2.1857
H -2.2941 4.6326 3.2657	H 3.1433 -0.8796 -1.7273	C -2.3502 -2.6240 2.2323
H -2.5811 5.3353 1.6515	H 2.6217 -0.0244 1.2101	C -2.2879 -1.2507 2.1290
H -5.0254 -1.6453 -2.0301	C 4.7708 -0.9626 -0.2989	C 2.7628 -0.9785 2.0991
H -4.9532 -0.4795 -0.6757	C 5.8824 -0.9106 -1.3502	C 3.7487 0.1919 2.0236
H -5.4782 -2.1546 -0.3768	H 4.5908 -2.0083 0.0077	C 5.1918 -0.2643 2.2422
H -3.0892 -4.3915 -1.4560	H 5.0952 -0.4192 0.6080	H 2.8631 -1.4651 3.0876
H -3.3176 -4.3411 0.3143	C 7.1969 -1.4947 -0.8291	H 3.0440 -1.7502 1.3643
H -1.6819 -4.1586 -0.3816	H 5.5536 -1.4629 -2.2497	H 3.4766 0.9413 2.7864
H 0.9396 1.9100 -3.6141	H 6.0330 0.1387 -1.6645	H 3.6482 0.6988 1.0452
H -0.7838 3.6912 -3.4815	H 7.5518 -0.9354 0.0541	H 5.4932 -1.0038 1.4810
H -3.0537 3.2166 -2.5859	H 7.0667 -2.5492 -0.5295	H 5.3023 -0.7394 3.2316
H -3.6717 0.9453 -1.8093	H 7.9855 -1.4539 -1.5975	H 5.8930 0.5837 2.1913
H 0.8214 0.3913 3.8222		H -1.3383 4.7444 1.7001

H	0.0397	3.8606	2.4206	H	-4.0023	-2.1288	-0.4787	C	3.0329	-1.3758	2.5162
H	-1.5296	3.8885	3.2586	H	-3.3869	-0.4951	-0.3267	C	3.8495	-2.5276	3.1031
H	-3.9913	2.9193	1.0650	C	-6.0421	-0.3663	-1.0902	H	1.2343	-1.8244	3.6243
H	-3.7928	1.8618	2.4888	H	-4.4720	0.1442	-2.5017	H	1.3048	-2.5998	2.0524
H	-3.7954	1.1605	0.8459	H	-5.0900	-1.5017	-2.6812	H	3.2465	-0.4471	3.0726
H	1.9674	1.4614	-3.8015	H	-6.8630	0.0172	-1.7168	H	3.3359	-1.1824	1.4699
H	3.8087	2.7099	-2.6995	H	-6.4178	-1.2438	-0.5359	H	3.6694	-3.4647	2.5495
H	3.4837	3.7718	-0.4750	H	-5.7874	0.4138	-0.3503	H	3.5709	-2.7031	4.1560
H	1.3093	3.6361	0.6992	H	0.1577	-2.4145	-2.5774	H	4.9292	-2.3124	3.0681
H	0.9833	-3.4825	2.0566					H	1.8715	5.1852	0.5378
H	-1.2685	-4.5155	2.2752	21re-HX-TS(-)iBu				H	2.4486	3.8367	1.5609
H	-3.3181	-3.1131	2.3574	C	1.1386	0.7625	1.6906	H	1.1477	4.9005	2.1495
H	-3.1913	-0.6429	2.1721	C	0.6796	-0.5323	2.0390	H	-1.2741	4.9909	-0.4929
Zr	0.0739	-0.0501	-0.2948	C	-0.7571	-0.4563	2.0898	H	-1.8317	4.4981	1.1292
C	1.8391	-1.0454	-1.4275	C	-1.1511	0.8958	1.7561	H	-2.1220	3.4326	-0.2746
H	2.1160	-0.2001	-0.7011	C	0.0407	1.6588	1.4372	H	2.8618	-0.7317	-3.6675
H	1.8259	-0.6086	-2.4340	H	2.1892	1.0275	1.6135	H	4.9867	-0.6557	-2.3878
C	-1.2172	-1.8774	-0.9852	Si	0.2548	3.2865	0.4879	H	5.2690	0.8908	-0.4612
C	-0.0001	-2.3733	-1.4971	C	0.8241	2.4392	-1.1191	H	3.4403	2.4030	0.2418
H	-1.4861	-2.3197	-0.0225	C	-0.0552	1.9722	-2.1476	H	-1.4174	-2.4009	2.8389
C	2.9280	-2.1062	-1.3267	C	0.5645	0.9366	-2.9021	H	-3.7574	-1.6324	3.1919
C	4.3029	-1.4228	-1.2304	C	1.8941	0.7762	-2.4098	H	-4.4280	0.7004	2.6662
H	4.5041	-0.8470	-2.1499	C	2.0505	1.6791	-1.2864	H	-2.8062	2.3205	1.7229
H	4.3544	-0.7331	-0.3762	H	-1.0795	2.3169	-2.2884	Zr	0.1923	0.1217	-0.4887
H	5.0976	-2.1785	-1.1180	H	0.1271	0.4036	-3.7444	C	0.9706	-1.9904	-1.0110
C	2.9174	-3.0476	-2.5406	C	1.5553	4.4043	1.2514	H	1.6764	-1.3476	-0.3724
H	3.7757	-3.7361	-2.4853	C	-1.3984	4.1281	0.1840	H	1.3541	-1.9362	-2.0388
H	2.0034	-3.6553	-2.6043	C	2.9698	-0.0735	-2.8029	C	-1.8141	-0.5317	-1.5037
H	3.0132	-2.4630	-3.4727	C	4.1479	-0.0222	-2.0922	C	-1.2393	-1.8187	-1.4986
H	2.7655	-2.7067	-0.4136	C	4.3105	0.8663	-0.9831	C	1.0570	-3.4216	-0.4922
H	0.5712	-3.0885	-0.9022	C	3.2936	1.7036	-0.5820	C	2.5295	-3.7677	-0.2095
C	-2.4298	-1.6531	-1.8850	C	-1.7195	-1.3861	2.5712	H	3.1119	-3.7331	-1.1462
C	-3.6669	-1.2600	-1.0720	C	-3.0134	-0.9494	2.7770	H	2.9836	-3.0640	0.5020
H	-2.6485	-2.5938	-2.4228	C	-3.3984	0.3920	2.4753	H	2.6098	-4.7856	0.2066
H	-2.2306	-0.9039	-2.6656	C	-2.5023	1.2970	1.9447	C	0.4902	-4.4375	-1.4964
C	-4.8184	-0.7384	-1.9300	C	1.5273	-1.6542	2.5710	H	0.6990	-5.4602	-1.1442

H -0.5968 -4.3478 -1.6333	C -3.7360 -3.4395 -0.3622	H 1.5227 1.5811 0.6512
H 0.9775 -4.3142 -2.4800	C -2.1121 2.9961 -1.7833	H 0.4491 -0.8067 -2.9363
H 0.4845 -3.5013 0.4485	C -2.6380 3.7477 -0.7576	C 0.9513 -0.8520 -1.9675
H -1.5201 -2.5142 -0.7018	C -3.2525 3.1334 0.3790	C 1.7897 0.2609 -1.6213
H -0.8837 -2.2753 -2.4213	C -3.3829 1.7655 0.4710	H 1.2961 -1.8428 -1.6617
C -3.0812 -0.2939 -0.7053	C 2.0878 -2.3198 0.8747	H 1.7523 1.1070 -2.3086
C -4.3177 -0.8429 -1.4310	C 2.1729 -3.4626 0.1057	C 1.0644 3.0894 -0.8474
H -3.2261 0.7813 -0.5182	C 1.0078 -4.0942 -0.4224	C 2.5024 3.4291 -1.2704
H -2.9985 -0.7832 0.2730	C -0.2550 -3.5946 -0.1751	C 0.6058 4.1496 0.1722
C -5.6016 -0.6061 -0.6332	C 1.3030 0.2173 2.7535	H 0.4151 3.1499 -1.7363
H -4.4057 -0.3747 -2.4291	C 0.6592 1.5115 3.2641	H 2.9639 2.6859 -1.9360
H -4.1807 -1.9267 -1.6054	C 1.6889 2.4431 3.9043	H 2.4958 4.3980 -1.7948
C -6.8384 -1.1699 -1.3357	H 1.6725 -0.3656 3.6180	H 3.1534 3.5412 -0.3881
H -5.4925 -1.0653 0.3669	H 2.2075 0.4447 2.1612	H -0.4294 3.9777 0.5017
H -5.7266 0.4797 -0.4637	H -0.1303 1.2601 3.9931	H 1.2614 4.1222 1.0604
H -7.7532 -0.9889 -0.7484	H 0.1579 2.0334 2.4303	H 0.6701 5.1583 -0.2683
H -6.9725 -0.7040 -2.3275	H 2.4557 2.7408 3.1666	C 3.1418 -0.0384 -1.0254
H -6.7411 -2.2591 -1.4876	H 2.2077 1.9440 4.7403	C 3.8086 0.7104 -0.0402
H -1.8081 -0.0343 -2.4782	H 1.2172 3.3592 4.2936	C 3.8222 -1.1511 -1.5637
	H -5.4963 -0.9299 1.3150	C 5.0700 0.3317 0.4281
12si-ST-TS(+)<i>i</i>Bu	H -4.1639 -0.5031 2.4314	H 3.3607 1.5994 0.3877
C -1.0300 -0.6613 1.9508	H -4.8066 -2.1622 2.4110	C 5.0922 -1.5176 -1.1153
C 0.3912 -0.6589 1.9475	H -4.7998 -3.4439 -0.6568	H 3.3500 -1.7371 -2.3514
C 0.8032 -1.7854 1.1558	H -3.5674 -4.2873 0.3239	C 5.7180 -0.7878 -0.1012
C -0.3860 -2.4393 0.6478	H -3.1356 -3.6044 -1.2721	H 5.5501 0.9261 1.2082
C -1.5482 -1.7364 1.1473	H -1.6602 3.4720 -2.6553	H 5.5900 -2.3818 -1.5602
H -1.6416 0.0733 2.4741	H -2.5904 4.8372 -0.8065	H 6.7056 -1.0783 0.2626
Si -3.3149 -1.8054 0.4639	H -3.6493 3.7689 1.1731	
C -2.9951 -0.4722 -0.8471	H -3.8966 1.3094 1.3169	12re-ST-TS(+)<i>i</i>Bu
C -2.3279 -0.6890 -2.0995	H 2.9855 -1.8376 1.2631	C 2.3041 -0.1324 1.3935
C -1.8195 0.5350 -2.6104	H 3.1529 -3.8906 -0.1111	C 1.4182 0.6761 2.1514
C -2.2137 1.5757 -1.7153	H 1.1222 -4.9979 -1.0244	C 1.3501 1.9448 1.4910
C -2.8983 0.9501 -0.5988	H -1.1410 -4.0981 -0.5605	C 2.2085 1.8930 0.3202
H -2.1918 -1.6619 -2.5725	Zr -0.5725 -0.1099 -0.4202	C 2.8205 0.5856 0.2593
H -1.2938 0.6694 -3.5538	C 0.8702 1.7086 -0.2144	H 2.5598 -1.1611 1.6438
C -4.5612 -1.2942 1.7744	H -0.1784 1.7771 0.2550	Si 3.6487 -0.2813 -1.2031

C	2.0086	-0.9364	-1.8962	H	2.5424	-3.2418	-0.1489	21si-ST-TS(+)<i>i</i>Bu			
C	1.1156	-0.1359	-2.6792	H	0.0495	3.1966	2.7259	C	-1.1658	-2.1094	0.5420
C	-0.1949	-0.6768	-2.6536	H	0.3510	5.1952	1.2794	C	-1.5212	-1.3589	1.6941
C	-0.1583	-1.8707	-1.8673	H	1.8024	5.1118	-0.7358	C	-0.3050	-1.1102	2.4110
C	1.2014	-2.0162	-1.3702	H	2.9971	3.0344	-1.3714	C	0.7871	-1.7299	1.6809
H	1.3940	0.7833	-3.1942	Zr	0.4455	0.1148	-0.2675	C	0.2564	-2.3323	0.4765
H	-1.0500	-0.2783	-3.1912	C	-1.3738	-0.4145	0.9901	H	-1.8830	-2.4496	-0.2009
C	4.8059	-1.6367	-0.6100	H	-0.6245	-1.2707	0.7963	Si	1.1552	-2.7569	-1.1477
C	4.4415	0.9063	-2.4233	H	-1.0531	0.0703	1.9205	C	0.6916	-1.1196	-2.0033
C	-1.1402	-2.8582	-1.5465	C	-0.9349	2.0063	-0.9674	C	1.4459	0.0954	-1.9296
C	-0.7762	-3.9225	-0.7546	C	-1.9317	1.4471	-0.1543	C	0.6026	1.2198	-2.1448
C	0.5499	-4.0486	-0.2314	H	-0.3497	2.8360	-0.5705	C	-0.7000	0.7267	-2.4786
C	1.5248	-3.1212	-0.5206	C	-2.6912	-1.1245	1.3042	C	-0.6594	-0.7163	-2.3600
C	0.6682	3.1475	1.8274	C	-3.5936	-0.2480	2.1838	H	2.5008	0.1590	-1.6716
C	0.8469	4.2563	1.0253	C	-2.4013	-2.4340	2.0646	H	0.9196	2.2583	-2.1649
C	1.6830	4.2086	-0.1345	H	-3.2139	-1.3756	0.3695	C	0.4305	-4.2774	-1.9774
C	2.3443	3.0539	-0.4982	H	-3.8536	0.7086	1.7139	C	3.0193	-2.8177	-0.9196
C	0.7885	0.3317	3.4682	H	-4.5333	-0.7793	2.4045	C	-1.9031	1.3763	-2.8755
C	0.7170	-1.1714	3.7597	H	-3.0873	-0.0435	3.1446	C	-3.0167	0.6074	-3.1356
C	-0.0770	-1.4701	5.0311	H	-1.7480	-3.1021	1.4833	C	-2.9881	-0.8146	-3.0039
H	1.3610	0.8323	4.2712	H	-1.9124	-2.2197	3.0295	C	-1.8397	-1.4739	-2.6231
H	-0.2239	0.7745	3.5297	H	-3.3475	-2.9601	2.2725	C	-0.0597	-0.4561	3.6513
H	1.7418	-1.5707	3.8512	H	-2.0108	1.8690	0.8522	C	1.2225	-0.4616	4.1604
H	0.2541	-1.6886	2.9016	C	-3.2393	1.0689	-0.7641	C	2.2932	-1.1069	3.4647
H	-1.1152	-1.1054	4.9369	C	-3.4118	0.0186	-1.6726	C	2.0954	-1.7191	2.2449
H	0.3738	-0.9717	5.9058	C	-4.3360	1.8974	-0.4703	C	-2.9071	-1.0200	2.1568
H	-0.1146	-2.5518	5.2358	C	-4.6484	-0.1989	-2.2865	C	-3.9764	-1.0673	1.0594
H	5.0014	-2.3689	-1.4125	H	-2.5839	-0.6554	-1.8638	C	-5.3342	-0.5836	1.5687
H	4.3926	-2.1764	0.2581	C	-5.5704	1.6888	-1.0905	H	-3.1867	-1.7246	2.9626
H	5.7712	-1.1990	-0.3012	H	-4.2169	2.7194	0.2402	H	-2.9098	-0.0255	2.6388
H	4.9426	0.3420	-3.2289	C	-5.7308	0.6398	-2.0022	H	-4.0612	-2.1012	0.6819
H	5.1998	1.5326	-1.9221	H	-4.7677	-1.0303	-2.9848	H	-3.6585	-0.4503	0.2005
H	3.6990	1.5735	-2.8919	H	-6.4099	2.3471	-0.8576	H	-5.2714	0.4648	1.9098
H	-2.1511	-2.7834	-1.9500	H	-6.6969	0.4725	-2.4826	H	-5.6749	-1.1934	2.4225
H	-1.5108	-4.6951	-0.5198	H	-1.0718	1.9652	-2.0495	H	-6.1022	-0.6398	0.7811
H	0.7912	-4.9101	0.3942					H	0.7263	-4.3237	-3.0400

H -0.6708 -4.2870 -1.9237	H 3.7288 -0.0254 1.1964	H -1.7548 -1.1264 3.5591
H 0.7964 -5.1908 -1.4765	C 4.0364 2.9599 -1.2578	H -1.1657 -2.0435 2.1883
H 3.5126 -3.0018 -1.8898	H 2.0718 3.5282 -0.5969	H 0.5716 -0.8909 4.4456
H 3.3097 -3.6300 -0.2312	C 5.0916 2.0465 -1.1464	H 1.2177 -1.7496 3.0431
H 3.4032 -1.8642 -0.5191	H 5.8033 0.2683 -0.1381	H -0.1009 -3.8105 3.6618
H -1.9287 2.4605 -2.9945	H 4.1234 3.8149 -1.9318	H -0.7772 -2.9562 5.0714
H -3.9410 1.0886 -3.4617	H 5.9993 2.1795 -1.7379	H 0.9687 -3.3150 5.0024
H -3.8901 -1.3856 -3.2321		H 4.1037 3.1662 0.7371
H -1.8153 -2.5622 -2.5613	21re-ST-TS(+)<i>i</i>Bu	H 3.4381 1.7011 1.5156
H -0.8839 -0.0017 4.2052	C 0.4908 0.8299 2.0731	H 3.3221 3.2805 2.3372
H 1.4279 0.0128 5.1219	C -0.6975 0.0576 2.1409	H 2.0372 5.4857 -0.0508
H 3.2868 -1.1131 3.9173	C -1.7421 0.8646 1.5596	H 0.9833 5.3706 1.3909
H 2.9158 -2.2174 1.7286	C -1.1419 2.0875 1.0710	H 0.3085 5.1027 -0.2429
Zr -0.1111 0.0616 0.0173	C 0.2734 2.0698 1.3838	H 1.4122 -1.0328 -4.2995
C -1.6374 1.6550 0.5880	H 1.4570 0.4993 2.4519	H 3.7414 -1.7614 -3.8312
H -2.0256 0.8311 -0.1172	Si 1.6123 3.1129 0.5405	H 5.0622 -0.7222 -2.0018
H -2.0364 1.4076 1.5814	C 1.4463 2.2150 -1.1258	H 4.1203 1.0988 -0.6118
C 1.5135 1.4535 1.1817	C 0.2269 2.2502 -1.8911	H -3.6094 -0.2178 1.8940
C 0.4116 2.3216 1.2463	C 0.1830 1.1768 -2.8112	H -5.0007 1.5628 0.8951
H 1.6804 0.8378 2.0669	C 1.4258 0.4710 -2.7116	H -3.9751 3.6269 -0.0426
H 0.3573 3.1761 0.5720	C 2.2041 1.1057 -1.6667	H -1.5297 4.0033 0.0879
C -2.2686 2.9553 0.1009	H -0.5741 2.9730 -1.7511	Zr 0.0755 0.3168 -0.3491
C -2.1846 4.0782 1.1471	H -0.6042 0.9845 -3.5377	C 1.1115 -1.6697 0.0661
C -3.7535 2.6894 -0.2151	C 3.2744 2.7800 1.3545	H 1.7315 -0.7325 0.3221
H -1.7605 3.2781 -0.8247	C 1.1907 4.9365 0.3973	H 0.6596 -2.0127 1.0082
H -1.1592 4.4239 1.3394	C 1.9854 -0.5842 -3.4851	C -1.6433 -1.1214 -1.4548
H -2.7700 4.9460 0.8036	C 3.2807 -0.9781 -3.2259	C -0.5442 -1.9911 -1.4174
H -2.6197 3.7382 2.1038	C 4.0411 -0.3775 -2.1761	H 0.1810 -1.9987 -2.2314
H -3.8691 1.9024 -0.9750	C 3.5210 0.6303 -1.3929	C 2.1214 -2.7035 -0.4218
H -4.2819 2.3675 0.6992	C -3.1490 0.6893 1.5037	C 1.5862 -4.1402 -0.3222
H -4.2363 3.6102 -0.5823	C -3.9176 1.6834 0.9378	C 3.3956 -2.5844 0.4358
H -0.1138 2.4306 2.1945	C -3.3291 2.8648 0.3985	H 2.3857 -2.4876 -1.4674
C 2.7329 1.7021 0.3723	C -1.9669 3.0737 0.4537	H 0.7862 -4.3548 -1.0463
C 3.8137 0.8082 0.4989	C -0.8853 -1.2357 2.8861	H 2.4027 -4.8534 -0.5187
C 2.8737 2.7939 -0.5023	C 0.3347 -1.6734 3.7039	H 1.2030 -4.3394 0.6949
C 4.9788 0.9754 -0.2531	C 0.0970 -3.0135 4.4005	H 3.8171 -1.5678 0.3893

C	0.1229	-1.9633	-1.6707	H	-2.9420	-2.1558	2.2862	C	-0.4426	0.9419	2.2327
H	-0.9747	-3.2191	1.2321	Zr	-0.3415	-0.3259	0.2261	C	0.0414	1.9548	1.3209
H	1.6638	-2.7658	1.2186	C	1.2981	1.1704	-0.5935	H	2.1029	2.2049	0.4736
C	-3.3617	-1.7994	-2.8377	H	0.5711	0.7008	-1.3480	Si	-0.9360	3.0894	0.1483
C	-3.8504	-3.4105	-0.1740	H	2.2489	0.7466	-0.9226	C	-0.7788	1.9165	-1.3399
C	2.5929	-1.6720	-1.4473	H	0.9843	-0.9384	2.6587	C	-1.6830	0.8456	-1.6360
C	2.6115	-1.1898	-2.7386	C	0.7477	0.0260	2.2007	C	-1.0390	-0.1443	-2.4261
C	1.4134	-1.0624	-3.5096	C	1.7999	0.6984	1.4727	C	0.2758	0.3270	-2.7286
C	0.1888	-1.4355	-2.9984	H	0.1118	0.6696	2.8175	C	0.4562	1.5839	-2.0311
C	-2.1039	1.6658	2.8318	C	1.2303	2.6782	-0.8934	H	-2.6979	0.7601	-1.2533
C	-2.2453	0.8006	3.9007	C	2.0358	2.9422	-2.1825	H	-1.4975	-1.0555	-2.7986
C	-2.5115	-0.5872	3.6949	H	3.1098	2.7508	-2.0104	C	-0.0816	4.7432	-0.0945
C	-2.6859	-1.1072	2.4274	H	1.7013	2.2819	-3.0019	C	-2.7445	3.2168	0.6426
C	-1.9882	3.2721	0.0275	H	1.9203	3.9890	-2.5071	C	1.3370	-0.2196	-3.5063
C	-2.2007	3.7317	-1.4225	C	1.6808	3.6377	0.2139	C	2.5330	0.4618	-3.5689
C	-1.9005	5.2234	-1.5885	H	1.6167	4.6726	-0.1592	C	2.7216	1.6968	-2.8751
H	-2.7467	3.7619	0.6681	H	1.0400	3.5758	1.1084	C	1.7127	2.2559	-2.1207
H	-1.0159	3.6404	0.4043	H	2.7251	3.4672	0.5222	C	0.4246	-1.0943	3.3807
H	-3.2395	3.5127	-1.7136	H	0.1841	2.9187	-1.1119	C	-0.7923	-1.2062	4.0198
H	-1.5606	3.1440	-2.1006	C	3.1586	0.1031	1.2968	C	-1.8387	-0.2541	3.7988
H	-0.8439	5.4360	-1.3503	C	3.5304	-1.1042	1.9179	C	-1.6847	0.7938	2.9160
H	-2.5255	5.8256	-0.9110	C	4.1381	0.7885	0.5526	C	3.1904	-0.1045	1.9204
H	-2.0951	5.5587	-2.6209	C	4.8098	-1.6384	1.7429	C	4.2201	0.5765	1.0130
H	-3.1255	-2.6776	-3.4685	H	2.8315	-1.6267	2.5632	C	5.6241	0.0065	1.2185
H	-2.8607	-0.9207	-3.2678	C	5.4167	0.2595	0.3742	H	3.4999	0.0296	2.9741
H	-4.4548	-1.6295	-2.8854	H	3.8872	1.7414	0.0858	H	3.2041	-1.1922	1.7484
H	-3.9002	-4.3275	-0.7927	C	5.7536	-0.9655	0.9592	H	4.2251	1.6597	1.2231
H	-4.8789	-3.0583	0.0005	H	5.0749	-2.5757	2.2360	H	3.9096	0.4699	-0.0436
H	-3.4103	-3.6839	0.7972	H	6.1538	0.8114	-0.2112	H	5.6499	-1.0735	0.9953
H	3.5089	-1.7589	-0.8640	H	6.7558	-1.3824	0.8233	H	5.9464	0.1387	2.2652
H	3.5611	-0.9015	-3.1938	H	1.8180	1.7810	1.5789	H	6.3599	0.5072	0.5695
H	1.4812	-0.6849	-4.5301					H	-0.4616	5.2541	-0.9963
H	-0.7178	-1.3717	-3.6041					H	1.0099	4.6256	-0.1974
H	-1.8990	2.7261	2.9855					H	-0.2661	5.3961	0.7765
H	-2.1542	1.1774	4.9189					H	-3.2949	3.8382	-0.0849
H	-2.6055	-1.2406	4.5641					H	-2.8526	3.6822	1.6375

21si-ST-TS(-)iBu

H -3.2214 2.2223 0.6688	H -5.9183 -0.0340 0.2574	H 4.4065 -2.9655 2.1889
H 1.1901 -1.1500 -4.0587	H -4.6045 -2.7501 -2.8281	H 4.2044 -2.3608 3.8512
H 3.3523 0.0645 -4.1716	H -6.3700 -1.2726 -1.8657	H 5.4203 -1.6201 2.7768
H 3.6793 2.2132 -2.9649		H 0.8479 5.2512 1.2195
H 1.8562 3.2165 -1.6247	21re-ST-TS(-)iBu	H 1.6313 3.9222 2.1244
H 1.2345 -1.7983 3.5831	C 1.0093 0.7153 1.8094	H 0.1176 4.6357 2.7329
H -0.9623 -2.0214 4.7257	C 0.8657 -0.6870 1.9514	H -2.1647 4.5755 -0.0343
H -2.7760 -0.3662 4.3471	C -0.5417 -0.9640 1.8631	H -2.6477 3.8074 1.5027
H -2.4834 1.5190 2.7599	C -1.2409 0.2928 1.6765	H -2.6967 2.8668 -0.0117
Zr 0.0858 -0.0547 -0.1174	C -0.2600 1.3565 1.5853	H 3.2296 0.1499 -3.4714
C 1.3522 -1.8808 -0.6873	H 1.9651 1.2279 1.8533	H 5.2254 0.5151 -2.0416
H 1.9166 -0.8751 -0.6943	Si -0.3562 3.1003 0.8408	H 5.0893 1.9002 0.0191
H 1.1286 -2.1071 -1.7389	C 0.4583 2.5907 -0.8080	H 2.9571 2.9400 0.7214
C -1.5975 -1.6754 0.6157	C -0.2429 2.0847 -1.9476	H -0.7410 -3.1089 2.2434
C -0.5587 -2.5683 0.3203	C 0.6138 1.2731 -2.7460	H -3.2208 -2.9888 2.4127
H -1.6501 -1.3628 1.6579	C 1.9149 1.3146 -2.1649	H -4.4131 -0.8285 2.1640
C 2.3112 -2.9259 -0.1252	C 1.8222 2.1049 -0.9527	H -3.1992 1.2623 1.6531
C 3.7304 -2.6584 -0.6553	H -1.2999 2.2506 -2.1462	Zr 0.2705 0.1370 -0.4705
H 3.7499 -2.7658 -1.7533	H 0.3445 0.7697 -3.6728	C 1.3603 -1.7362 -1.1885
H 4.0730 -1.6446 -0.4047	C 0.6593 4.3420 1.8167	H 1.9748 -1.0558 -0.4870
H 4.4417 -3.3838 -0.2271	C -2.1322 3.6347 0.5419	H 1.7469 -1.5356 -2.1985
C 1.8957 -4.3545 -0.5109	C 3.1573 0.7285 -2.5483	C -1.6450 -0.7517 -1.8027
H 2.6760 -5.0660 -0.1966	C 4.2619 0.9411 -1.7543	C -0.8178 -1.8853 -1.7754
H 0.9510 -4.6702 -0.0456	C 4.1833 1.7347 -0.5671	C 1.6655 -3.1763 -0.7865
H 1.7888 -4.4346 -1.6074	C 2.9982 2.3097 -0.1673	C 3.1774 -3.3154 -0.5310
H 2.3243 -2.8508 0.9774	C -1.2706 -2.1663 2.0888	H 3.7327 -3.1436 -1.4691
H 0.0739 -2.9022 1.1432	C -2.6414 -2.0889 2.1968	H 3.5361 -2.5922 0.2143
H -0.6400 -3.2450 -0.5302	C -3.3296 -0.8454 2.0529	H 3.4134 -4.3317 -0.1745
C -2.8894 -1.5958 -0.1030	C -2.6610 0.3217 1.7620	C 1.2573 -4.1942 -1.8642
C -3.9031 -0.7847 0.4432	C 1.9413 -1.6397 2.3897	H 1.6458 -5.1891 -1.5940
C -3.1664 -2.3064 -1.2832	C 3.3566 -1.0554 2.3285	H 0.1691 -4.2856 -1.9870
C -5.1451 -0.6666 -0.1843	C 4.4087 -2.0547 2.8113	H 1.6966 -3.9162 -2.8388
H -3.7037 -0.2465 1.3726	H 1.7212 -1.9332 3.4338	H 1.1183 -3.4112 0.1432
C -4.4076 -2.1878 -1.9127	H 1.8979 -2.5748 1.8111	H -1.0285 -2.6745 -1.0494
H -2.4101 -2.9645 -1.7167	H 3.3992 -0.1454 2.9511	H -0.3035 -2.1971 -2.6813
C -5.4006 -1.3622 -1.3718	H 3.5785 -0.7293 1.2947	H -1.5426 -0.1198 -2.6867

C -3.0114 -0.7040 -1.2264	C -2.2318 -2.4825 -0.2110	H -1.9573 2.8369 2.3184
C -3.7151 0.5143 -1.2265	C -1.7002 2.2465 -1.9194	H -0.7690 1.1118 3.6682
C -3.6932 -1.8646 -0.8267	C -0.5443 3.0283 -2.5474	H -3.0688 2.3207 3.5978
C -5.0503 0.5775 -0.8273	C -0.9647 4.4506 -2.9221	
H -3.2119 1.4218 -1.5670	H -2.5430 2.1953 -2.6358	Cat3-12si-BT-Reactant
C -5.0331 -1.8058 -0.4331	H -2.0858 2.7983 -1.0428	C 0.1544 -1.3777 1.8240
H -3.1864 -2.8300 -0.8523	H -0.1959 2.4890 -3.4463	C 1.5190 -1.2877 1.4508
C -5.7174 -0.5865 -0.4275	H 0.3031 3.0580 -1.8395	C 1.6425 -1.9681 0.1844
H -5.5768 1.5343 -0.8431	H -1.2856 5.0130 -2.0282	C 0.3146 -2.3779 -0.2292
H -5.5487 -2.7234 -0.1414	H -1.8090 4.4367 -3.6327	C -0.6317 -2.0188 0.8069
H -6.7673 -0.5454 -0.1308	H -0.1345 5.0019 -3.3912	H -0.2456 -0.9584 2.7459
	H 3.4006 -2.5474 -2.5397	Si -2.5159 -1.8794 0.6111
Cat3-12si-PP-Reactant	H 2.4430 -1.1529 -3.1199	C -2.4072 -0.2988 -0.4389
C -0.1913 0.1140 -1.8847	H 2.0004 -2.8022 -3.6225	C -1.8464 -0.2915 -1.7615
C -1.3471 0.8470 -1.5197	H 1.7083 -4.7963 -0.9017	C -1.4404 1.0182 -2.1208
C -2.2195 -0.0834 -0.8561	H 0.1192 -4.5854 -1.6892	C -1.8175 1.9005 -1.0523
C -1.5616 -1.3794 -0.8187	H 0.3036 -4.2805 0.0634	C -2.4032 1.0877 -0.0066
C -0.2742 -1.2631 -1.4584	H 2.9203 1.8712 3.1031	H -1.7053 -1.1749 -2.3820
H 0.6647 0.5528 -2.3959	H 4.0876 3.1981 1.3611	H -1.0273 1.3151 -3.0831
Si 1.2438 -2.3908 -1.2974	H 4.2366 2.3906 -0.9829	C -3.3052 -1.5853 2.2897
C 1.8871 -1.5366 0.2742	H 3.2677 0.2078 -1.6504	C -3.2901 -3.2936 -0.3511
C 1.3774 -1.7962 1.5851	H -4.0594 1.0208 -0.4480	C -1.7298 3.3084 -0.8983
C 1.6267 -0.6928 2.4497	H -5.2225 -0.9688 0.4950	C -2.2066 3.8767 0.2654
C 2.3876 0.2717 1.7126	H -4.0667 -3.1630 0.6611	C -2.7718 3.0785 1.3043
C 2.5054 -0.2250 0.3546	H -1.7467 -3.4579 -0.1625	C -2.8704 1.7081 1.1853
H 0.8198 -2.6925 1.8610	Zr -0.0101 0.0244 0.6041	C 2.7658 -2.3142 -0.6210
H 1.3754 -0.6354 3.5082	C 0.1897 2.2263 0.7687	C 2.5570 -2.9606 -1.8207
C 2.3807 -2.1997 -2.7792	H 1.0129 2.5482 0.0961	C 1.2431 -3.2958 -2.2673
C 0.7951 -4.1763 -0.9184	H -0.7260 2.7526 0.4513	C 0.1372 -3.0214 -1.4903
C 2.9799 1.5120 2.0739	H 0.4330 2.5513 1.7926	C 2.6061 -0.7195 2.3199
C 3.6235 2.2448 1.1015	H -1.0565 -1.1836 2.9625	C 3.6919 0.1095 1.6170
C 3.7108 1.7792 -0.2470	C -1.7372 -0.4108 2.5895	C 4.6289 0.7707 2.6298
C 3.1669 0.5723 -0.6279	C -1.6361 0.8536 3.0441	H 2.1304 -0.0947 3.0945
C -3.5493 0.0583 -0.3700	H -2.5797 -0.7160 1.9650	H 3.0986 -1.5509 2.8588
C -4.1904 -1.0502 0.1484	C -2.5399 1.9787 2.6865	H 3.2170 0.8842 0.9906
C -3.5279 -2.3130 0.2376	H -3.2925 1.6763 1.9431	H 4.2807 -0.5270 0.9365

H 5.1140 0.0110 3.2658	Cat3-12si-HX-Reactant	H 2.9022 -2.2962 2.3028
H 4.0688 1.4535 3.2916	C 2.2264 0.6052 1.3510	H 4.5696 -2.3526 1.6688
H 5.4205 1.3499 2.1279	C 1.6540 1.8833 1.1484	H 4.2983 -3.2986 -1.6608
H -4.3417 -1.2218 2.1816	C 1.7583 2.1612 -0.2635	H 5.0550 -1.6851 -1.5066
H -2.7391 -0.8452 2.8794	C 2.3248 0.9908 -0.9052	H 3.6383 -1.9192 -2.5720
H -3.3322 -2.5278 2.8635	C 2.6345 0.0042 0.1099	H -3.3702 -2.4557 -0.2128
H -4.3898 -3.1963 -0.3365	H 2.3021 0.1284 2.3270	H -3.3218 -3.4902 2.0486
H -3.0246 -4.2666 0.0975	Si 2.9643 -1.8457 -0.1576	H -1.1703 -3.9760 3.1864
H -2.9719 -3.3001 -1.4066	C 1.1505 -2.2327 -0.5675	H 0.9985 -3.4503 2.1075
H -1.3153 3.9265 -1.6959	C 0.5208 -1.7448 -1.7627	H 1.1332 4.2390 -0.5564
H -2.1637 4.9600 0.3953	C -0.8892 -1.7574 -1.6188	H 1.4781 4.1729 -3.0022
H -3.1447 3.5709 2.2044	C -1.1936 -2.3327 -0.3402	H 2.2986 2.1127 -4.1302
H -3.3229 1.1081 1.9745	C 0.0639 -2.6208 0.3157	H 2.9117 0.1042 -2.8168
H 3.7776 -2.0877 -0.2868	H 1.0494 -1.3799 -2.6412	Zr 0.1978 -0.0339 -0.0024
H 3.4127 -3.2398 -2.4388	H -1.6100 -1.5029 -2.3925	C -0.6609 -0.1431 2.0525
H 1.1209 -3.8116 -3.2216	C 3.5229 -2.6296 1.4546	H 0.0527 -0.4764 2.8222
H -0.8577 -3.3366 -1.8051	C 4.0923 -2.2150 -1.6119	H -0.9667 0.8884 2.3102
Zr -0.0012 0.1339 -0.1699	C -2.4235 -2.6468 0.2953	H -1.5384 -0.8081 2.0808
C 0.3624 1.6782 1.3982	C -2.3884 -3.2254 1.5478	H -0.6567 1.9582 -1.9090
H 0.0918 1.3654 2.4191	C -1.1512 -3.5062 2.2012	C -1.2727 1.8273 -1.0118
H 1.4594 1.8376 1.3886	C 0.0589 -3.2138 1.6080	C -2.3271 0.9704 -0.9885
H -0.1473 2.6275 1.1775	C 1.4803 3.3244 -1.0366	H -1.1067 2.5287 -0.1890
H 1.5740 -0.2690 -2.3602	C 1.6769 3.2834 -2.4009	C -3.2875 0.8282 0.1491
C 2.0173 0.5241 -1.7391	C 2.1551 2.1042 -3.0480	H -3.0464 1.5668 0.9299
C 1.7689 1.8361 -1.9769	C 2.4839 0.9772 -2.3231	H -3.1656 -0.1743 0.5978
H 2.8188 0.2320 -1.0580	C 1.2184 2.8142 2.2459	C -4.7514 0.9703 -0.3210
C 2.5008 2.9627 -1.3191	C -0.0996 3.5774 2.0423	H -4.8675 1.9056 -0.8976
H 3.2700 3.2836 -2.0504	C -0.4098 4.4752 3.2419	H -5.3874 1.0721 0.5744
H 3.0481 2.5897 -0.4370	H 1.1528 2.2374 3.1835	C -5.2445 -0.2190 -1.1513
C 1.6209 4.1686 -0.9678	H 2.0229 3.5584 2.4010	H -5.1573 -1.1384 -0.5426
H 1.0943 4.5412 -1.8628	H -0.9263 2.8608 1.8976	H -4.5934 -0.3641 -2.0337
H 2.2426 4.9878 -0.5751	H -0.0511 4.1899 1.1270	C -6.6923 -0.0367 -1.6117
H 1.0246 2.1119 -2.7320	H 0.3955 5.2134 3.3957	H -6.7912 0.8629 -2.2431
H 0.8702 3.9063 -0.2084	H -0.4963 3.8765 4.1648	H -7.3638 0.0862 -0.7447
	H -1.3541 5.0243 3.0993	H -7.0416 -0.9038 -2.1946
	H 3.4663 -3.7304 1.3973	H -2.5343 0.3729 -1.8793

Cat3-12si-PP-TS	H -2.5900 -1.0107 3.0547	C 2.3702 0.5667 -0.8465
C 0.2177 -0.1380 1.8876	H -2.4493 -2.7478 3.4155	C 1.7113 0.8533 -2.0908
C 1.4791 0.4163 1.5411	H -2.5204 -4.5275 0.5225	C 1.2822 -0.3423 -2.7184
C 2.1812 -0.5970 0.8031	H -0.9227 -4.6698 1.3095	C 1.7108 -1.4387 -1.9050
C 1.3035 -1.7429 0.6595	H -1.0402 -4.1838 -0.4070	C 2.3592 -0.8782 -0.7318
C 0.0612 -1.4638 1.3523	H -2.4816 2.5772 -2.8738	H 1.5159 1.8569 -2.4702
H -0.5471 0.3946 2.4511	H -3.3173 3.9652 -0.9907	H 0.7640 -0.4182 -3.6725
Si -1.6355 -2.2867 1.1191	H -3.5999 3.0030 1.2831	C 3.8206 1.3311 1.8545
C -2.1208 -1.1996 -0.3649	H -3.1186 0.6158 1.7339	C 2.7625 3.5489 -0.1120
C -1.6822 -1.4351 -1.7134	H 4.1812 0.2031 0.4465	C 1.5967 -2.8515 -2.0555
C -1.7409 -0.2421 -2.4753	H 4.9319 -1.8211 -0.7894	C 2.0715 -3.6645 -1.0505
C -2.2797 0.7842 -1.6363	H 3.3978 -3.7418 -1.1457	C 2.6724 -3.1188 0.1273
C -2.4886 0.2021 -0.3220	H 1.1020 -3.7388 -0.2137	C 2.8202 -1.7586 0.2959
H -1.3011 -2.3875 -2.0838	Zr 0.0043 0.0360 -0.5783	C -2.9091 1.6039 1.0206
H -1.4763 -0.1364 -3.5258	C 0.4653 2.2722 -0.9167	C -3.1652 2.7685 0.3227
C -2.7179 -2.0200 2.6300	H -0.3586 2.1117 -0.1499	C -2.1028 3.5814 -0.1740
C -1.5121 -4.0825 0.5844	H 1.3079 2.7124 -0.3728	C -0.7794 3.2539 0.0484
C -2.5970 2.1531 -1.8741	H 0.0225 2.9929 -1.6125	C -1.7602 -0.9738 2.6435
C -3.0595 2.9171 -0.8257	H 0.8681 -0.7368 -3.1323	C -0.9130 -2.1656 3.1005
C -3.2255 2.3627 0.4821	C 1.4310 -0.2136 -2.3540	C -1.7650 -3.2511 3.7593
C -2.9510 1.0370 0.7425	C 1.4782 1.2180 -2.4529	H -2.2555 -0.5253 3.5253
C 3.5018 -0.6357 0.2832	H 2.3494 -0.7082 -2.0234	H -2.5875 -1.3263 1.9998
C 3.9142 -1.7646 -0.3981	C 2.8003 1.9235 -2.2632	H -0.1451 -1.8090 3.8089
C 3.0350 -2.8704 -0.5972	H 3.3432 1.5116 -1.3990	H -0.3698 -2.5862 2.2356
C 1.7502 -2.8709 -0.0899	H 2.6945 3.0122 -2.1506	H -2.5186 -3.6422 3.0533
C 2.0575 1.7220 2.0019	H 0.8188 1.6640 -3.2023	H -2.3032 -2.8494 4.6346
C 1.0338 2.6947 2.5958	H 3.4056 1.7301 -3.1661	H -1.1457 -4.0962 4.0990
C 1.6743 4.0279 2.9834		H 4.8003 1.1526 1.3785
H 2.8345 1.5100 2.7604	Cat3-12si-BT-TS	H 3.5299 0.4193 2.4020
H 2.5972 2.2074 1.1679	C 0.4168 0.3041 1.9444	H 3.9390 2.1408 2.5954
H 0.5687 2.2285 3.4819	C -0.9892 0.1017 1.9352	H 3.8096 3.6908 -0.4310
H 0.2195 2.8639 1.8685	C -1.5594 1.2302 1.2532	H 2.5313 4.3106 0.6526
H 2.1154 4.5232 2.1006	C -0.4752 2.0836 0.8040	H 2.1174 3.7316 -0.9876
H 2.4821 3.8746 3.7192	C 0.7798 1.5077 1.2445	H 1.1485 -3.2725 -2.9579
H 0.9359 4.7146 3.4264	H 1.1292 -0.3880 2.3915	H 2.0015 -4.7493 -1.1522
H -3.7843 -2.1596 2.3815	Si 2.5323 1.8172 0.5775	H 3.0404 -3.8006 0.8962

H 3.3145 -1.3542 1.1793	H 1.6540 1.7435 -2.6521	Zr 0.3417 -0.0449 -0.4363
H -3.7236 0.9911 1.4118	H 0.5943 -0.4807 -3.7049	C -0.8251 -2.0209 -0.2026
H -4.1966 3.0823 0.1501	C 4.5367 1.0563 1.2986	H 0.2389 -2.0943 0.1936
H -2.3472 4.4922 -0.7240	C 3.3865 3.3488 -0.5231	H -1.4779 -2.1539 0.6659
H 0.0229 3.9029 -0.3036	C 1.5037 -2.9592 -2.2007	H -0.8986 -2.8712 -0.8888
Zr 0.0070 -0.0424 -0.4811	C 2.0704 -3.7994 -1.2681	H -1.1919 0.7972 -2.6406
C -1.0791 -2.0704 -0.4613	C 2.8715 -3.2906 -0.1981	C -1.5164 0.5687 -1.6217
H -0.0784 -2.1251 0.0753	C 3.1271 -1.9422 -0.0686	C -2.0363 -0.7505 -1.3919
H -1.8515 -2.2038 0.3027	C -2.1986 1.8581 1.4137	H -2.0265 1.3840 -1.0998
H -1.0449 -2.9219 -1.1492	C -2.4611 3.0231 0.7189	C -3.2893 -0.9091 -0.5583
H -1.1815 0.8328 -2.8664	C -1.4218 3.7334 0.0477	H -3.1604 -0.3744 0.3962
C -1.6726 0.5193 -1.9411	C -0.1093 3.3055 0.0950	C -4.5086 -0.3351 -1.2958
C -2.1167 -0.8396 -1.8712	C -1.0401 -0.7832 2.9178	H -3.4723 -1.9698 -0.3256
H -2.3211 1.2666 -1.4745	C -0.2231 -2.0168 3.3135	H -4.6257 -0.8398 -2.2725
C -3.4947 -1.1376 -1.3187	C -1.0588 -3.0195 4.1099	H -4.3322 0.7331 -1.5116
H -3.6244 -0.5957 -0.3680	H -1.3936 -0.2761 3.8354	C -5.7921 -0.4936 -0.4765
C -4.5596 -0.6848 -2.3300	H -1.9606 -1.0950 2.3900	H -5.6557 0.0019 0.5033
H -3.6096 -2.2132 -1.1158	H 0.6476 -1.6942 3.9107	C -7.0112 0.0912 -1.1920
H -4.4254 -1.1912 -3.3008	H 0.1817 -2.4987 2.4055	H -5.9574 -1.5654 -0.2632
H -4.5007 0.4021 -2.4997	H -1.9186 -3.3742 3.5149	H -7.1772 -0.4128 -2.1598
H -1.7950 -1.4920 -2.6877	H -1.4565 -2.5551 5.0283	H -6.8699 1.1674 -1.3941
H -5.5659 -0.9293 -1.9542	H -0.4616 -3.8971 4.4035	H -7.9248 -0.0250 -0.5871
	H 5.4184 0.7897 0.6904	H -1.9443 -1.4483 -2.2287
	H 4.2537 0.1789 1.9033	
	H 4.8301 1.8600 1.9963	Cat3-12si-ST-TS
	H 4.3922 3.4127 -0.9735	C 2.4308 0.3611 0.6506
	H 3.3092 4.1285 0.2542	C 2.4811 -0.9902 0.2086
	H 2.6511 3.5742 -1.3132	C 1.6000 -1.7332 1.0752
	H 0.9015 -3.3532 -3.0223	C 0.9900 -0.7889 2.0008
	H 1.9190 -4.8778 -1.3466	C 1.5209 0.5321 1.7463
	H 3.3059 -3.9928 0.5161	H 3.0015 1.1657 0.1867
	H 3.7707 -1.5694 0.7283	Si 0.8124 2.2287 2.2313
	H -2.9944 1.3233 1.9352	C -0.2952 2.3454 0.6961
	H -3.4791 3.4160 0.6832	C -1.5862 1.7252 0.5819
	H -1.6715 4.6463 -0.4965	C -1.9397 1.5495 -0.7776
	H 0.6822 3.8791 -0.3880	C -0.8849 2.0955 -1.5742
Cat3-12si-HX-TS		
C 1.1130 0.3075 1.8961		
C -0.2926 0.2154 2.0834		
C -0.8635 1.3781 1.4623		
C 0.2080 2.1324 0.8413		
C 1.4647 1.4683 1.1236		
H 1.8268 -0.4329 2.2553		
Si 3.1213 1.6408 0.2116		
C 2.6601 0.4046 -1.1583		
C 1.8410 0.7308 -2.2937		
C 1.2496 -0.4363 -2.8371		
C 1.7250 -1.5561 -2.0838		
C 2.5751 -1.0359 -1.0268		

C	0.1464	2.5667	-0.6663	H	-0.4229	-0.5371	3.6476	H	-1.7247	-1.6966	-2.1273
H	-2.1948	1.3825	1.4187	Zr	0.1381	0.0847	-0.2241	H	-1.5204	0.7081	-3.2711
H	-2.8668	1.1189	-1.1434	C	0.6435	-0.6504	-2.3528	C	-2.7615	-1.6277	2.7122
C	2.1748	3.5203	2.2822	H	1.2710	0.2517	-2.0498	C	-2.5111	-3.6715	0.3389
C	-0.2384	2.1761	3.7870	H	1.3775	-1.3850	-2.7000	C	-2.1995	2.9271	-1.3047
C	-0.7132	2.2250	-2.9829	H	-0.0022	-0.3078	-3.1688	C	-2.4868	3.6208	-0.1484
C	0.4619	2.7614	-3.4610	C	-1.3598	-1.7506	-0.3240	C	-2.7035	2.9397	1.0882
C	1.4967	3.1946	-2.5735	C	-0.5730	-2.1037	-1.4548	C	-2.6782	1.5598	1.1693
C	1.3552	3.1066	-1.2050	H	-1.0698	-2.2415	0.6092	C	3.1526	-1.4876	-0.6090
C	1.2719	-3.1160	1.1792	H	-1.0491	-2.1941	-2.4324	C	3.0322	-2.3707	-1.6609
C	0.3631	-3.5224	2.1358	H	0.2484	-2.7980	-1.2776	C	1.8151	-3.0669	-1.9131
C	-0.2620	-2.5907	3.0178	C	-2.7979	-1.3975	-0.4070	C	0.7220	-2.9135	-1.0852
C	0.0317	-1.2446	2.9541	C	-3.4983	-1.1567	0.7895	C	2.7566	0.5649	2.0395
C	3.4450	-1.4604	-0.8511	C	-3.4962	-1.2883	-1.6228	C	3.9113	1.1084	1.1824
C	3.2986	-2.8958	-1.3664	C	-4.8463	-0.7934	0.7729	C	4.5362	2.3533	1.8147
C	4.2320	-3.1530	-2.5511	H	-2.9690	-1.2557	1.7414	H	2.1664	1.4129	2.4343
H	3.3878	-0.7642	-1.7081	C	-4.8455	-0.9249	-1.6405	H	3.1828	0.0723	2.9326
H	4.4694	-1.3416	-0.4528	H	-2.9891	-1.4789	-2.5710	H	3.5548	1.3374	0.1621
H	2.2545	-3.0911	-1.6667	C	-5.5264	-0.6685	-0.4445	H	4.6819	0.3290	1.0707
H	3.5303	-3.6030	-0.5532	H	-5.3708	-0.6107	1.7134	H	4.8880	2.1370	2.8377
H	5.2820	-2.9701	-2.2661	H	-5.3705	-0.8476	-2.5951	H	3.7975	3.1719	1.8836
H	3.9928	-2.4793	-3.3927	H	-6.5802	-0.3843	-0.4608	H	5.3954	2.7147	1.2281
H	4.1514	-4.1914	-2.9090					H	-3.8434	-1.4266	2.6278
H	1.7580	4.5374	2.1814	Cat3-ET-Product				H	-2.2834	-0.7581	3.1930
H	2.9125	3.3668	1.4775	C	0.5115	-0.7107	1.8727	H	-2.6273	-2.4950	3.3818
H	2.7141	3.4622	3.2438	C	1.8072	-0.3962	1.3690	H	-3.6015	-3.8081	0.4452
H	-0.5721	3.1957	4.0466	C	2.0366	-1.2745	0.2493	H	-2.0072	-4.4879	0.8848
H	0.3367	1.7778	4.6407	C	0.8215	-2.0424	0.0406	H	-2.2670	-3.7695	-0.7318
H	-1.1386	1.5532	3.6539	C	-0.1334	-1.7157	1.0826	H	-2.0379	3.4494	-2.2497
H	-1.5078	1.9093	-3.6623	H	0.0582	-0.2091	2.7299	H	-2.5537	4.7102	-0.1712
H	0.6083	2.8754	-4.5370	Si	-2.0116	-1.9998	1.0306	H	-2.9195	3.5261	1.9835
H	2.4074	3.6246	-2.9951	C	-2.3161	-0.6213	-0.2445	H	-2.8897	1.0516	2.1104
H	2.1340	3.4765	-0.5377	C	-1.9329	-0.7510	-1.6285	H	4.0903	-0.9630	-0.4407
H	1.7404	-3.8484	0.5254	C	-1.7975	0.5170	-2.2372	H	3.8862	-2.5432	-2.3186
H	0.1180	-4.5823	2.2268	C	-2.1319	1.5034	-1.2542	H	1.7587	-3.7505	-2.7624
H	-0.9728	-2.9572	3.7608	C	-2.4343	0.8002	-0.0164	H	-0.1916	-3.4844	-1.2520

Zr -0.0331	0.2675	-0.3452	C -2.8032	1.9030	0.4125	H -2.9040	-3.6541	-2.6395
C 0.9398	2.7196	-0.2006	C -0.2466	-1.8898	2.6036	H -1.0774	-1.9986	-3.0589
H 1.7603	2.3660	0.4406	C 1.1273	-2.3727	2.1133	H -3.5947	-2.0632	-3.0911
H 0.8930	3.8146	-0.1085	C 1.4351	-3.8106	2.5263			
H -0.0459	2.4497	0.2721	H -0.2532	-1.8717	3.7078	Cat3-12si-BT-Product		
H 2.3138	0.4779	-1.9106	H -1.0234	-2.6145	2.3037	C 1.0083	0.5734	1.8225
C 1.2770	0.8176	-2.0415	H 1.9119	-1.6925	2.4840	C -0.1038	-0.1941	2.2580
C 1.1388	2.3357	-1.7051	H 1.1772	-2.2972	1.0045	C -1.2821	0.5657	1.9372
H 0.9657	0.6166	-3.0736	H 0.6811	-4.5076	2.1216	C -0.8664	1.7651	1.2353
H 2.0653	2.8530	-2.0061	H 1.4232	-3.9053	3.6252	C 0.5822	1.7607	1.1302
H 0.3124	2.7828	-2.2761	H 2.4270	-4.1282	2.1673	H 2.0446	0.2583	1.9242
			H 2.8666	4.1230	0.7950	Si 1.7078	2.6563	-0.1190
Cat3-12si-PP-Product			H 2.4908	2.8938	2.0410	C 1.6945	1.2087	-1.3639
C 0.3084	0.5560	1.9021	H 1.6294	4.4505	2.0449	C 0.6932	0.9953	-2.3726
C -0.5878	-0.5350	2.0486	H 0.2816	4.9722	-1.1110	C 0.6150	-0.3749	-2.7200
C -1.8569	-0.1004	1.5294	H -0.9427	4.8240	0.1803	C 1.6246	-1.0711	-1.9760
C -1.6911	1.2400	1.0007	H -1.0529	3.7992	-1.2800	C 2.2999	-0.0941	-1.1421
C -0.3133	1.6499	1.2035	H 2.6890	-2.3918	-2.4316	H 0.0265	1.7675	-2.7527
H 1.3541	0.5299	2.2009	H 4.2837	-2.7240	-0.5579	H -0.0712	-0.8158	-3.4396
Si 0.7133	2.9639	0.2842	H 4.6471	-0.9524	1.1482	C 3.4027	3.0066	0.6071
C 1.3682	1.7253	-1.0129	H 3.3972	1.1844	1.0567	C 0.8746	4.1504	-0.8915
C 0.6873	1.3601	-2.2250	H -3.2523	-1.7444	1.8823	C 1.9785	-2.4506	-1.8878
C 1.0858	0.0714	-2.6558	H -5.1675	-0.5280	0.8682	C 2.9844	-2.8230	-1.0197
C 2.0963	-0.3963	-1.7518	H -4.8916	1.7646	-0.0429	C 3.6720	-1.8610	-0.2182
C 2.2802	0.6269	-0.7393	H -2.6942	2.9151	0.0226	C 3.3426	-0.5239	-0.2666
H -0.0919	1.9553	-2.6987	Zr -0.0574	-0.1764	-0.3957	C -2.6582	0.3204	2.1842
H 0.7119	-0.4568	-3.5302	C -0.8567	-2.7422	-1.0556	C -3.5821	1.2529	1.7557
C 2.0552	3.6700	1.3905	H 0.2372	-2.5071	-1.0259	C -3.1786	2.4337	1.0629
C -0.3533	4.2565	-0.5604	H -1.2964	-2.6394	-0.0440	C -1.8501	2.6911	0.7907
C 2.8202	-1.6230	-1.6671	H -0.8610	-3.8183	-1.2895	C -0.0458	-1.5540	2.8960
C 3.7089	-1.7981	-0.6262	H -1.8919	0.1979	-2.6182	C 1.0007	-2.4550	2.2219
C 3.9148	-0.7821	0.3568	C -1.8306	-0.4402	-1.7260	C 0.9723	-3.8908	2.7418
C 3.2184	0.4062	0.3142	C -1.6498	-1.9355	-2.1186	H 0.1864	-1.4690	3.9724
C -3.1204	-0.7439	1.4653	H -2.7605	-0.3214	-1.1530	H -1.0397	-2.0303	2.8331
C -4.1816	-0.0603	0.9056	C -3.0169	-2.6022	-2.3241	H 2.0048	-2.0195	2.3562
C -4.0232	1.2581	0.3824	H -3.5938	-2.5788	-1.3833	H 0.8329	-2.4663	1.1223

H -0.0157 -4.3524 2.5719	Cat3-12si-HX-Product	H 4.5269 1.8647 0.3613
H 1.1690 -3.9106 3.8270	C 1.8601 0.5406 1.5975	H 4.2939 3.6287 0.3684
H 1.7342 -4.5128 2.2455	C 0.8142 -0.1133 2.3006	H 1.9575 4.4370 -2.0619
H 4.1435 3.1884 -0.1908	C -0.3399 0.7405 2.2143	H 1.4374 4.8458 -0.4031
H 3.7621 2.1718 1.2313	C 0.0061 1.8807 1.3868	H 0.3827 3.8564 -1.4535
H 3.3576 3.9049 1.2474	C 1.3887 1.7446 0.9658	H 1.0404 -3.3513 -2.5787
H 1.5439 4.6188 -1.6337	H 2.8628 0.1347 1.4802	H 3.0875 -4.1568 -1.4277
H 0.6325 4.9068 -0.1251	Si 2.2780 2.5029 -0.5375	H 4.7014 -2.5624 -0.4116
H -0.0598 3.8688 -1.4052	C 1.8663 1.0333 -1.6847	H 4.2960 -0.1180 -0.4788
H 1.4769 -3.1875 -2.5188	C 0.6491 0.8858 -2.4353	H -1.8977 -0.2211 3.4075
H 3.2786 -3.8725 -0.9541	C 0.3844 -0.4799 -2.6987	H -3.5578 1.5696 2.9484
H 4.4793 -2.1967 0.4352	C 1.4762 -1.2446 -2.1696	H -2.9767 3.5216 1.5278
H 3.8848 0.2076 0.3331	C 2.3992 -0.3119 -1.5491	H -0.7227 3.7472 0.5174
H -2.9705 -0.5714 2.7312	H -0.0206 1.7051 -2.6913	Zr 0.3263 -0.1380 -0.1743
H -4.6436 1.0949 1.9562	H -0.4803 -0.8755 -3.2269	C -1.4683 -2.2378 0.0814
H -3.9420 3.1485 0.7500	C 4.1157 2.7091 -0.2161	H -0.4563 -2.4468 -0.3472
H -1.5507 3.6019 0.2720	C 1.4304 4.0533 -1.1713	H -1.3758 -1.9111 1.1356
Zr -0.0302 -0.1474 -0.2653	C 1.7290 -2.6475 -2.1062	H -1.9269 -3.2387 0.1055
C -1.6500 -2.3858 -0.4638	C 2.8714 -3.0873 -1.4695	H -2.0539 0.7839 -1.5536
H -0.5526 -2.4998 -0.6489	C 3.7971 -2.1716 -0.8818	C -1.8247 0.2153 -0.6431
H -1.8298 -2.0862 0.5872	C 3.5745 -0.8119 -0.9110	C -2.3244 -1.2533 -0.7574
H -2.0145 -3.4204 -0.5605	C -1.6420 0.6260 2.7679	H -2.3278 0.7066 0.2011
H -2.1162 0.6476 -2.1194	C -2.5582 1.6270 2.5130	C -3.7918 -1.3720 -0.3085
C -2.0467 0.0543 -1.1986	C -2.2238 2.7494 1.6970	H -3.8567 -1.0814 0.7572
C -2.3675 -1.4436 -1.4654	C -0.9728 2.8798 1.1287	C -4.7570 -0.5199 -1.1307
H -2.7680 0.4583 -0.4746	C 0.9007 -1.4635 2.9558	H -4.0958 -2.4341 -0.3686
C -3.8839 -1.7072 -1.3920	C 1.6852 -2.4615 2.0892	H -4.6635 -0.7906 -2.1999
H -4.2264 -1.4730 -0.3669	C 1.6433 -3.8871 2.6351	H -4.4708 0.5438 -1.0508
C -4.6830 -0.8960 -2.4112	H 1.3801 -1.3876 3.9478	C -6.2126 -0.6866 -0.6886
H -4.0582 -2.7874 -1.5502	H -0.1179 -1.8485 3.1357	H -6.2954 -0.4252 0.3830
H -4.3375 -1.1084 -3.4382	H 2.7285 -2.1206 1.9861	C -7.1734 0.1749 -1.5103
H -4.5719 0.1858 -2.2322	H 1.2774 -2.4611 1.0537	H -6.4978 -1.7515 -0.7709
H -2.0176 -1.7167 -2.4755	H 0.6047 -4.2554 2.6962	H -7.1217 -0.0918 -2.5805
H -5.7550 -1.1437 -2.3560	H 2.0715 -3.9216 3.6510	H -6.9167 1.2453 -1.4197
	H 2.2183 -4.5782 1.9986	H -8.2162 0.0459 -1.1782
	H 4.6759 2.7887 -1.1639	H -2.2562 -1.5791 -1.8092

Cat3-21si-ST-Product	H 2.5247 3.9598 -0.6189	C 1.1700 -0.3430 -2.3220
C 1.9470 1.2583 1.1727	H 1.4105 5.1830 0.0390	C 2.2430 -0.3480 -1.3740
C 1.8820 0.1444 2.0432	H -1.8058 4.2916 -1.1290	C 2.0400 0.7800 -0.4770
C 0.5636 0.1377 2.6171	H -1.6718 4.3482 0.6501	C 0.8440 1.4820 -0.8770
C -0.1731 1.2546 2.0552	H -2.2769 2.8698 -0.1593	H -0.5640 1.0230 -2.5650
C 0.6786 1.9384 1.1009	H 1.6169 -2.4232 -3.1976	Si -0.2380 2.6370 0.1720
H 2.8278 1.5193 0.5892	H 4.0284 -1.8420 -3.0898	C -1.1860 1.2000 0.9790
Si 0.2063 3.0518 -0.3685	H 4.7735 0.4168 -2.3659	C -0.6850 0.4220 2.0700
C 0.2331 1.6100 -1.6170	H 3.1300 2.1456 -1.6843	C -1.3450 -0.8360 2.1330
C -0.8902 0.7613 -1.9004	H 0.5114 -1.5467 4.0089	C -2.3560 -0.8460 1.1140
C -0.4583 -0.4993 -2.3739	H -1.8174 -1.0619 4.7320	C -2.2300 0.3920 0.3730
C 0.9717 -0.4611 -2.4742	H -3.0667 0.8749 3.8113	H 0.1330 0.7300 2.7240
C 1.4044 0.8461 -2.0153	H -2.0504 2.3658 2.1065	H -1.1940 -1.6070 2.8870
H -1.9288 1.0065 -1.6885	Zr 0.3931 -0.2292 -0.0006	C -1.3090 3.7280 -0.9160
H -1.1120 -1.3288 -2.6282	C -0.0985 -3.2516 -0.4922	C 0.7300 3.5850 1.4720
C 1.5029 4.3668 -0.6988	H 0.8423 -2.7000 -0.7021	C -3.3540 -1.7920 0.7620
C -1.5519 3.6980 -0.2336	H 0.2303 -4.2751 -0.2511	C -4.1750 -1.5180 -0.3120
C 1.9386 -1.4410 -2.8464	H -0.6560 -3.2756 -1.4378	C -4.0350 -0.3140 -1.0650
C 3.2772 -1.1088 -2.7886	C -1.5524 -1.2639 0.5472	C -3.0820 0.6300 -0.7450
C 3.7062 0.1871 -2.3682	C -0.9460 -2.6907 0.6749	C 3.3870 -1.1860 -1.2190
C 2.7977 1.1511 -1.9843	H -1.7739 -0.9223 1.5657	C 4.2850 -0.9060 -0.2100
C -0.0448 -0.7112 3.5789	H -1.7814 -3.3943 0.8409	C 4.0780 0.1900 0.6860
C -1.3359 -0.4328 3.9810	H -0.3418 -2.7262 1.5999	C 2.9740 1.0110 0.5790
C -2.0550 0.6811 3.4503	C -2.8010 -1.1215 -0.2589	H -2.1810 4.1080 -0.3560
C -1.4987 1.5115 2.4985	C -3.6021 0.0249 -0.0673	H -1.6760 3.1910 -1.8070
C 2.9573 -0.8905 2.2164	C -3.2365 -2.0657 -1.2052	H -0.7230 4.5950 -1.2680
C 2.8250 -1.9691 1.1264	C -4.7644 0.2350 -0.8094	H 0.0590 4.2810 2.0050
C 3.9476 -3.0082 1.1343	H -3.2978 0.7552 0.6861	H 1.5370 4.1780 1.0090
H 3.9494 -0.4165 2.1441	C -4.4038 -1.8584 -1.9518	H 1.1800 2.9140 2.2220
H 2.8911 -1.3622 3.2100	H -2.6779 -2.9903 -1.3541	H -3.4680 -2.7140 1.3360
H 2.8246 -1.4736 0.1262	C -5.1691 -0.7049 -1.7671	H -4.9540 -2.2290 -0.5930
H 1.8531 -2.4808 1.2523	H -5.3646 1.1312 -0.6348	H -4.7110 -0.1350 -1.9040
H 3.9756 -3.5311 2.1047	H -4.7181 -2.6125 -2.6770	H -3.0040 1.5620 -1.3050
H 4.9248 -2.5210 0.9820	H -6.0782 -0.5449 -2.3499	H 3.5630 -2.0090 -1.9150
H 3.8068 -3.7597 0.3414	CAT-1-REACTANT	H 5.1810 -1.5200 -0.0950
H 1.3790 4.7971 -1.7078	C 0.3490 0.7690 -2.0270	H 4.8200 0.3830 1.4630

H 2.8410 1.8600 1.2490	C 4.2810 -1.0400 -0.0470	H -0.0750 0.4080 2.8270
Zr 0.0270 -0.6990 -0.0330	C 4.0820 0.0900 0.8030	Si 0.8860 2.5710 0.6010
C -0.9900 -2.2400 -1.2900	C 3.0080 0.9410 0.6290	C 1.6120 1.2820 -0.5920
H -0.2830 -2.7020 -2.0010	H -2.0090 4.1710 -0.6260	C 1.0140 0.9890 -1.8620
H -1.4120 -3.0190 -0.6320	H -1.4950 3.1490 -2.0000	C 1.4380 -0.2800 -2.3290
H -1.8290 -1.8070 -1.8630	H -0.5080 4.5500 -1.5200	C 2.3890 -0.7980 -1.3870
H 2.5220 -1.5460 1.5980	H 0.1770 4.3980 1.8040	C 2.5000 0.1640 -0.3110
C 1.6490 -2.1980 1.7040	H 1.6670 4.1990 0.8390	H 0.2950 1.6280 -2.3720
C 1.3150 -3.0640 0.7260	H 1.2530 3.0110 2.1110	H 1.1920 -0.7250 -3.2900
H 1.0940 -2.1620 2.6440	H -3.5540 -2.5160 1.4060	C 1.9060 2.7730 2.1640
H 1.9160 -3.1390 -0.1850	H -4.9020 -2.1500 -0.6460	C 0.5130 4.1890 -0.2770
H 0.4600 -3.7390 0.8250	H -4.5500 -0.1460 -2.0710	C 3.1690 -1.9830 -1.3740
H 1.0280 -1.0470 -3.1380	H -2.8770 1.5790 -1.4670	C 4.0370 -2.1890 -0.3190
	H 3.5640 -2.1960 -1.7210	C 4.1500 -1.2450 0.7430
CAT-1-TS	H 5.1560 -1.6730 0.1140	C 3.3960 -0.0890 0.7630
C 0.4240 0.6540 -2.0110	H 4.8060 0.2900 1.5950	C -3.6550 -0.3250 -0.1580
C 1.2020 -0.5170 -2.2130	H 2.8820 1.8190 1.2630	C -4.0550 0.3690 -1.2810
C 2.2810 -0.4850 -1.2700	Zr -0.0110 -0.6590 0.0390	C -3.3100 1.4810 -1.7770
C 2.0940 0.6880 -0.4360	C -0.7830 -2.6250 -0.8860	C -2.1730 1.9180 -1.1290
C 0.9250 1.4130 -0.9000	H -0.3660 -3.2020 -1.7200	C -2.2370 -1.4910 2.6620
H -0.4700 0.9120 -2.5800	H -1.5900 -3.1710 -0.3850	C -2.7110 -2.8130 2.0440
Si -0.1400 2.6690 0.0550	H -1.2760 -1.7180 -1.3670	H -1.3930 -1.6930 3.3420
C -1.1750 1.3310 0.9250	H 2.2960 -1.7400 1.2300	H -3.0500 -1.0900 3.2960
C -0.7370 0.6010 2.0830	C 1.2720 -2.1040 1.3490	H -1.9220 -3.2910 1.4420
C -1.4420 -0.6240 2.2000	C 0.8320 -3.1140 0.4630	H -3.5990 -2.6840 1.4060
C -2.3930 -0.6820 1.1320	H 0.8670 -2.1000 2.3640	H 2.9200 3.1390 1.9290
C -2.2100 0.5130 0.3250	H 1.4930 -3.3970 -0.3600	H 2.0010 1.8210 2.7120
H 0.0630 0.9200 2.7530	H 0.1600 -3.8970 0.8190	H 1.4270 3.5060 2.8360
H -1.3250 -1.3600 2.9920	H 1.0570 -1.2580 -2.9970	H 1.4370 4.7840 -0.3720
C -1.1350 3.7280 -1.1330		H -0.2220 4.7830 0.2930
C 0.8350 3.6560 1.3190	CAT-2-REACTANT	H 0.1150 4.0280 -1.2920
C -3.3860 -1.6400 0.7760	C -0.7550 0.5110 1.9830	H 3.1010 -2.6990 -2.1950
C -4.1310 -1.4310 -0.3630	C -1.8140 -0.3950 1.7190	H 4.6610 -3.0850 -0.2990
C -3.9300 -0.2760 -1.1820	C -2.4750 0.0870 0.5300	H 4.8570 -1.4420 1.5510
C -2.9950 0.6830 -0.8580	C -1.7460 1.2490 0.0560	H 3.5010 0.6340 1.5720
C 3.3980 -1.3390 -1.0650	C -0.6550 1.5230 0.9700	H -4.2560 -1.1530 0.2180

H -4.9710 0.0730 -1.7980	C 3.0430 -0.2340 1.1180	H -2.6400 -3.7630 2.7110
H -3.6650 2.0070 -2.6650	C -3.5760 -0.4410 0.1230	
H -1.6340 2.7980 -1.4800	C -4.1810 0.3640 -0.8210	CAT-3-REACTANT
Zr 0.0240 -0.5360 -0.1580	C -3.5900 1.5910 -1.2480	C 0.6970 0.3410 -1.9190
C 0.8670 -2.0200 1.2680	C -2.3920 2.0240 -0.7200	C 1.9150 -0.1220 -1.3580
H 0.0550 -2.7700 1.3660	C -1.6340 -1.8500 2.5330	C 2.2570 0.8060 -0.3070
H 1.7690 -2.5080 0.8680	C -2.7030 -2.8550 2.0920	C 1.1880 1.7840 -0.2130
H 1.0830 -1.6490 2.2820	H -0.6560 -2.3570 2.6060	C 0.1970 1.4950 -1.2280
H -2.0970 -0.8190 -2.4400	H -1.8670 -1.5190 3.5610	H 0.1870 -0.1600 -2.7400
C -1.3840 -1.6490 -2.3770	H -2.5820 -3.1540 1.0380	Si -1.6070 2.0920 -1.2550
C -1.4060 -2.5020 -1.3310	H -3.7150 -2.4410 2.2140	C -2.1230 0.9520 0.1750
H -0.6910 -1.7920 -3.2070	H 2.9440 3.3200 1.8920	C -1.6730 1.1560 1.5220
H -2.1660 -2.4170 -0.5510	H 1.9910 2.1360 2.8360	C -1.8020 -0.0390 2.2730
H -0.7140 -3.3500 -1.2760	H 1.4430 3.8250 2.7210	C -2.4120 -1.0250 1.4280
H -2.9870 -3.5170 2.8440	H 1.2820 4.8010 -0.4970	C -2.6090 -0.4180 0.1280
	H -0.3660 4.7130 0.1880	H -1.2480 2.0840 1.9010
CAT-2-TS	H 0.0160 3.8820 -1.3500	H -1.5960 -0.1560 3.3340
C -0.4080 0.3190 1.8880	H 3.2320 -2.6960 -1.9770	C -2.4040 1.6210 -2.8880
C -1.4630 -0.6140 1.6850	H 4.2560 -3.3000 0.2020	C -1.8170 3.9010 -0.7990
C -2.3390 -0.0280 0.6980	H 4.1340 -1.7590 2.1480	C -2.8250 -2.3610 1.6660
C -1.7540 1.2390 0.2860	H 3.0310 0.4520 1.9640	C -3.4220 -3.0610 0.6350
C -0.5390 1.4680 1.0390	H -4.0540 -1.3670 0.4340	C -3.6130 -2.4700 -0.6480
H 0.4160 0.1560 2.5840	H -5.1370 0.0610 -1.2510	C -3.2120 -1.1750 -0.9130
Si 0.9190 2.6170 0.6190	H -4.1050 2.1970 -1.9960	C 3.3980 0.9350 0.5400
C 1.7580 1.3580 -0.5340	H -1.9560 2.9750 -1.0240	C 3.4450 1.9710 1.4510
C 1.3700 1.1300 -1.8980	Zr 0.0290 -0.4030 -0.4310	C 2.3720 2.9040 1.5770
C 1.7800 -0.1580 -2.3270	C 0.1610 -2.6820 -0.0980	C 1.2580 2.8170 0.7690
C 2.4940 -0.7690 -1.2480	H -0.5020 -3.3310 0.4840	C 2.7260 -1.2450 -1.9460
C 2.4560 0.1550 -0.1270	H 0.8920 -3.2620 -0.6700	C 3.5060 -2.1550 -0.9870
H 0.7970 1.8310 -2.5060	H 0.7630 -2.1080 0.6800	C 4.2000 -3.2860 -1.7500
H 1.6340 -0.5830 -3.3190	H -2.2400 -0.4510 -2.0830	H 2.0460 -1.8700 -2.5490
C 1.9200 3.0040 2.1590	C -1.3220 -1.0300 -2.2220	H 3.4470 -0.8050 -2.6610
C 0.4090 4.1410 -0.3520	C -1.2780 -2.3250 -1.6510	H 2.8220 -2.5870 -0.2370
C 3.1640 -2.0210 -1.1210	H -0.7710 -0.8590 -3.1490	H 4.2610 -1.5750 -0.4330
C 3.7300 -2.3500 0.0900	H -2.1120 -2.6270 -1.0140	H 4.8990 -2.8780 -2.4990
C 3.6620 -1.4620 1.2100	H -0.7680 -3.1340 -2.1760	H 3.4610 -3.9070 -2.2840

H	4.7700	-3.9380	-1.0700	C	2.1000	0.8320	-1.6110	H	-4.1330	0.5270	-0.1450
H	-3.5040	1.6820	-2.8220	C	2.0120	-0.4270	-2.2580	H	-4.3090	2.5180	-1.5810
H	-2.1320	0.5960	-3.1910	C	2.2660	-1.4380	-1.2780	H	-2.4120	4.1070	-1.8300
H	-2.0710	2.3090	-3.6840	C	2.4500	-0.7670	-0.0030	H	-0.2870	3.7510	-0.5950
H	-2.8700	4.2020	-0.9400	H	1.9430	1.7920	-2.1040	Zr	0.0680	-0.1980	-0.5580
H	-1.1870	4.5430	-1.4380	H	1.8440	-0.5940	-3.3200	C	-0.7770	-2.3380	-0.6800
H	-1.5550	4.0950	0.2540	C	2.7950	1.6680	2.7610	H	-1.7240	-2.7250	-0.2880
H	-2.6960	-2.8130	2.6520	C	2.2270	3.6930	0.4250	H	-0.2640	-3.0820	-1.2990
H	-3.7640	-4.0840	0.8020	C	2.3530	-2.8580	-1.3580	H	-0.1190	-2.1920	0.2380
H	-4.0970	-3.0550	-1.4320	C	2.5690	-3.5760	-0.2030	H	-1.7830	0.9670	-2.3240
H	-3.3790	-0.7270	-1.8930	C	2.7130	-2.9240	1.0620	C	-1.1500	0.0980	-2.5220
H	4.2390	0.2500	0.4460	C	2.6570	-1.5520	1.1750	C	-1.6910	-1.1800	-2.2420
H	4.3270	2.0900	2.0830	C	-3.2860	1.2010	-0.2410	H	-0.4420	0.1850	-3.3500
H	2.4520	3.7120	2.3070	C	-3.3790	2.3210	-1.0440	H	-2.6680	-1.2240	-1.7550
H	0.4610	3.5580	0.8350	C	-2.2920	3.2340	-1.1860	H	-1.4490	-2.0260	-2.8880
Zr	-0.0490	-0.3410	0.3720	C	-1.1060	3.0370	-0.5100				
C	-0.1960	-2.3300	-0.6180	C	-2.4200	-1.2560	1.9380	CAT-4-REACTANT			
H	0.7850	-2.7970	-0.3880	C	-3.7200	-1.6550	1.2300	C	1.1740	0.4410	-1.8340
H	-1.0010	-2.9510	-0.1990	C	-4.2490	-2.9900	1.7580	C	2.2500	-0.1530	-1.1230
H	-0.2900	-2.3140	-1.7150	H	-1.7430	-2.1300	1.9660	C	2.4820	0.6820	0.0290
H	1.7210	0.6330	2.7630	H	-2.6550	-1.0390	2.9960	C	1.5220	1.7780	-0.0160
C	1.2620	-0.3490	2.9110	H	-3.5560	-1.7200	0.1400	C	0.7000	1.6370	-1.1900
C	1.6480	-1.4110	2.1710	H	-4.4780	-0.8700	1.3860	H	0.7530	0.0190	-2.7470
H	0.5180	-0.4520	3.7010	H	-4.4180	-2.9390	2.8470	Si	-1.0100	2.3940	-1.5120
H	2.4630	-1.3260	1.4480	H	-3.5230	-3.8010	1.5710	C	-1.9230	1.0710	-0.5040
H	1.2100	-2.4030	2.3300	H	-5.2010	-3.2640	1.2770	C	-2.0220	1.0590	0.9260
				H	3.8870	1.5760	2.6300	C	-2.3280	-0.2430	1.4120
CAT-3-TS				H	2.4270	0.7540	3.2560	C	-2.4890	-1.0860	0.2550
C	-0.3530	0.2760	1.8260	H	2.6010	2.5150	3.4410	C	-2.2140	-0.2880	-0.9210
C	-1.6560	-0.0830	1.3790	H	3.3020	3.9400	0.4630	H	-1.8480	1.9250	1.5680
C	-2.0780	0.9610	0.4770	H	1.6810	4.4490	1.0150	C	-1.4160	2.3530	-3.3450
C	-0.9820	1.9120	0.3580	H	1.9020	3.7730	-0.6260	C	-1.2390	4.0880	-0.7320
C	0.1070	1.4890	1.2130	H	2.2580	-3.3600	-2.3240	C	-2.8670	-2.4470	0.1250
H	0.2320	-0.3250	2.5230	H	2.6480	-4.6640	-0.2470	C	-2.9300	-2.9980	-1.1390
Si	1.9450	1.9690	1.1140	H	2.8930	-3.5310	1.9510	C	-2.6290	-2.2260	-2.3000
C	2.3560	0.6650	-0.2070	H	2.8070	-1.0620	2.1380	C	-2.2690	-0.8970	-2.2080

C	3.4430	0.6460	1.0880	H	-0.2760	-0.3620	3.4000	C	3.9040	-2.0390	-0.6650
C	3.4250	1.6330	2.0500	H	2.2750	-1.5040	2.0550	C	4.3720	-3.3670	-1.2630
C	2.4580	2.6860	2.0240	H	0.7890	-2.4730	2.6400	H	2.2120	-2.0220	-2.0110
C	1.5120	2.7580	1.0250	C	-2.7040	-0.6230	2.8150	H	3.5370	-0.9780	-2.5020
C	3.0290	-1.3330	-1.6380	C	-4.2320	-0.7330	2.9730	H	3.4050	-2.2180	0.3040
C	3.9170	-2.0820	-0.6370	H	-2.3200	0.1340	3.5190	H	4.7780	-1.4020	-0.4530
C	4.4140	-3.4050	-1.2220	H	-2.2390	-1.5880	3.0850	H	4.8710	-3.2030	-2.2330
H	2.3130	-2.0430	-2.0880	H	-4.4950	-1.0150	4.0050	H	3.5160	-4.0420	-1.4390
H	3.6640	-0.9830	-2.4730	H	-4.7130	0.2300	2.7380	H	5.0830	-3.8810	-0.5970
H	3.3560	-2.2730	0.2950	H	-4.6420	-1.4930	2.2880	H	-2.4640	2.6030	-3.4390
H	4.7810	-1.4520	-0.3670					H	-0.9920	1.6430	-3.7760
H	4.9710	-3.2310	-2.1580	CAT-4-TS				H	-0.8950	3.4190	-3.7010
H	3.5660	-4.0710	-1.4550	C	1.1590	0.5340	-1.7820	H	-2.2430	4.5450	-0.8100
H	5.0820	-3.9290	-0.5210	C	2.2170	-0.1070	-1.0770	H	-0.4810	4.8380	-0.8180
H	-2.5060	2.4060	-3.5090	C	2.4830	0.7050	0.0840	H	-1.2470	3.9990	0.5630
H	-1.0360	1.4390	-3.8290	C	1.5280	1.8050	0.0820	H	-3.0240	-3.1090	0.8400
H	-0.9500	3.2170	-3.8510	C	0.6980	1.7090	-1.0990	H	-2.9760	-4.0540	-1.4590
H	-2.2130	4.5110	-1.0350	H	0.7340	0.1510	-2.7100	H	-2.4190	-2.6270	-3.4160
H	-0.4470	4.7840	-1.0610	Si	-1.0160	2.4730	-1.4110	H	-1.9410	-0.2120	-3.1500
H	-1.2240	4.0410	0.3690	C	-1.9570	1.0960	-0.5010	H	4.2010	-0.1610	1.1320
H	-3.1010	-3.0410	1.0100	C	-2.1050	1.0250	0.9290	H	4.1960	1.5370	2.9140
H	-3.2240	-4.0420	-1.2600	C	-2.3890	-0.2980	1.3540	H	2.5120	3.3680	2.9530
H	-2.7010	-2.6990	-3.2810	C	-2.4620	-1.1050	0.1700	H	0.8140	3.5700	1.1540
H	-2.0710	-0.3080	-3.1030	C	-2.1800	-0.2540	-0.9720	Zr	-0.0080	-0.1910	0.2680
H	4.1970	-0.1380	1.1230	H	-1.9770	1.8680	1.6110	C	0.4630	-2.4440	0.1640
H	4.1700	1.6180	2.8480	C	-1.3780	2.5340	-3.2530	H	1.4290	-2.9170	-0.0350
H	2.4840	3.4500	2.8030	C	-1.2640	4.1150	-0.5330	H	-0.2950	-3.1800	0.4530
H	0.7970	3.5800	0.9880	C	-2.7660	-2.4840	-0.0180	H	0.1230	-2.0350	-0.8420
Zr	0.0220	-0.2240	0.2720	C	-2.7380	-3.0010	-1.2940	H	1.4250	0.2880	2.6430
C	0.2890	-2.3890	-0.2300	C	-2.4200	-2.1790	-2.4200	C	0.6190	-0.4370	2.4970
H	1.3400	-2.7090	-0.2280	C	-2.1440	-0.8350	-2.2790	C	0.9820	-1.7560	2.1340
H	-0.2860	-3.0200	0.4680	C	3.4520	0.6280	1.1260	H	-0.2740	-0.3080	3.1110
H	-0.1280	-2.5620	-1.2390	C	3.4450	1.5830	2.1230	H	2.0380	-1.9670	1.9480
H	1.2160	0.6000	2.7910	C	2.4810	2.6350	2.1450	H	0.3920	-2.5970	2.5030
C	0.6900	-0.3560	2.8940	C	1.5290	2.7470	1.1530	C	-2.7350	-0.7560	2.7400
C	1.2790	-1.5050	2.5050	C	2.9560	-1.3040	-1.6190	C	-4.2520	-0.9510	2.9070

H -2.3750 -0.0140 3.4720
H -2.2160 -1.7060 2.9610
H -4.4890 -1.2970 3.9260
H -4.7860 -0.0040 2.7260
H -4.6320 -1.6960 2.1890

CAT-5-REACTANT

C -0.4430 -0.6280 -1.9070
C -1.7190 -0.5860 -1.2920
C -1.6970 -1.5690 -0.2360
C -0.3650 -2.1420 -0.1900
C 0.4370 -1.5480 -1.2410
H -0.1600 0.0040 -2.7470
Si 2.3360 -1.5350 -1.3320
C 2.5110 -0.3280 0.1270
C 2.1580 -0.6900 1.4700
C 1.9240 0.4690 2.2500
C 2.2000 1.6140 1.4280
C 2.5700 1.1260 0.1160
H 2.0330 -1.7100 1.8280
H 1.7040 0.4930 3.3140
C 2.8840 -0.7830 -2.9630
C 3.1290 -3.1950 -0.9570
C 2.1850 3.0070 1.6970
C 2.5440 3.8770 0.6860
C 2.9140 3.4010 -0.6060
C 2.9250 2.0520 -0.9010
C -2.7030 -2.0600 0.6470
C -2.3770 -3.0500 1.5520
C -1.0540 -3.5810 1.6310
C -0.0600 -3.1400 0.7820
C -2.8950 0.1870 -1.8270
C -3.8040 0.9000 -0.8180
C -4.9700 1.6140 -1.5070
H -2.5170 0.9300 -2.5490
H -3.5190 -0.5150 -2.4130

H -3.2250 1.6430 -0.2420
H -4.2130 0.1840 -0.0840
H -5.5540 0.8740 -2.0830
H -4.5660 2.3340 -2.2420
H 3.9510 -0.5030 -2.9300
H 2.2980 0.1180 -3.2110
H 2.7480 -1.5120 -3.7800
H 4.2180 -3.1350 -1.1280
H 2.7200 -3.9830 -1.6120
H 2.9740 -3.5000 0.0910
H 1.9250 3.3760 2.6910
H 2.5580 4.9520 0.8770
H 3.2030 4.1230 -1.3720
H 3.2210 1.6960 -1.8870
H -3.7250 -1.6890 0.5830
H -3.1480 -3.4490 2.2140
H -0.8390 -4.3690 2.3550
H 0.9350 -3.5850 0.8100
Zr 0.1460 0.2690 0.3610
C -0.2620 2.1850 -0.6980
H -1.3550 2.3330 -0.5890
H 0.2750 3.0270 -0.2310
H -0.0440 2.1840 -1.7770
H -1.2120 -1.1410 2.7980
C -1.0860 -0.0600 2.9200
C -1.7800 0.8090 2.1530
H -0.4180 0.2910 3.7070
H -2.5240 0.4580 1.4350
H -1.6760 1.8920 2.2870
C -5.8780 2.3370 -0.5100
H -6.3090 1.6260 0.2180
H -5.3130 3.0990 0.0570
H -6.7110 2.8450 -1.0200

CAT-5-TS

C 0.1290 -0.3870 1.8000
C 1.4550 -0.4690 1.2880
C 1.4780 -1.6100 0.4050
C 0.1330 -2.1650 0.3630
C -0.7210 -1.4030 1.2490
H -0.2000 0.3820 2.5000
Si -2.6190 -1.2730 1.2470
C -2.6630 0.0610 -0.1070
C -2.5420 -0.2140 -1.5120
C -2.1000 0.9370 -2.2120
C -1.9720 2.0000 -1.2630
C -2.2940 1.4530 0.0450
H -2.7170 -1.1880 -1.9710
H -1.9420 1.0160 -3.2860
C -3.2410 -0.6690 2.9130
C -3.4720 -2.8350 0.6460
C -1.6150 3.3730 -1.3970
C -1.5360 4.1510 -0.2630
C -1.8110 3.6090 1.0320
C -2.1820 2.2930 1.1970
C 2.5110 -2.2350 -0.3530
C 2.2050 -3.3400 -1.1230
C 0.8790 -3.8620 -1.1900
C -0.1480 -3.2860 -0.4730
C 2.5780 0.4080 1.7780
C 3.8950 0.3710 0.9980
C 4.8500 1.4830 1.4390
H 2.2130 1.4500 1.8180
H 2.7880 0.1350 2.8290
H 3.7050 0.4640 -0.0860
H 4.3880 -0.6050 1.1440
H 5.0200 1.3990 2.5270
H 4.3600 2.4620 1.2780
H -4.2470 -0.2250 2.8180
H -2.5700 0.0860 3.3540

H -3.3020 -1.5140 3.6200	C 2.7710 0.1260 0.0120	H -3.0370 -2.4810 0.6820
H -4.5660 -2.7230 0.7420	C 2.5840 -0.3540 1.3520	H -2.0340 -4.1590 2.1880
H -3.1630 -3.7080 1.2470	C 2.1680 0.6990 2.2020	H 0.4150 -4.6030 2.1750
H -3.2480 -3.0460 -0.4130	C 2.1540 1.9090 1.4280	H 1.9110 -3.4140 0.5950
H -1.4180 3.7960 -2.3840	C 2.5270 1.5590 0.0730	Zr 0.3520 0.2120 0.4030
H -1.2720 5.2070 -0.3470	H 2.6960 -1.3920 1.6620	C -0.5200 2.0530 -0.4930
H -1.7450 4.2650 1.9030	H 2.0150 0.6340 3.2770	H -1.6080 1.9610 -0.3010
H -2.4280 1.9000 2.1840	C 3.0610 -0.1260 -3.1110	H -0.1340 2.9620 -0.0040
H 3.5320 -1.8620 -0.3130	C 3.8820 -2.5120 -1.2320	H -0.3920 2.1560 -1.5810
H 2.9970 -3.8320 -1.6910	C 1.8760 3.2570 1.7700	H -0.5250 -1.5540 2.8200
H 0.6840 -4.7390 -1.8100	C 1.9800 4.2220 0.7870	C -0.6270 -0.4770 2.9940
H -1.1550 -3.7050 -0.5010	C 2.3460 3.8820 -0.5480	C -1.5450 0.2490 2.3200
Zr -0.2400 0.1500 -0.5780	C 2.6110 2.5770 -0.9140	H 0.0030 -0.0210 3.7590
C 1.2240 1.9150 -0.7960	C -1.9600 -2.6430 0.6780	H -2.2420 -0.2280 1.6270
H 2.2610 2.0000 -0.4570	C -1.3950 -3.5860 1.5130	H -1.6690 1.3210 2.5070
H 0.9320 2.7660 -1.4220	C 0.0090 -3.8440 1.5030	C -6.0020 1.1100 -0.1080
H 0.5990 1.9970 0.1530	C 0.8470 -3.1780 0.6340	H -6.2410 0.2630 0.5630
H 1.0600 -1.5690 -2.3840	C -2.7250 -0.3600 -1.6550	H -5.5200 1.8820 0.5220
C 0.7360 -0.5440 -2.5800	C -3.7130 0.0860 -0.5680	C -7.2890 1.6670 -0.7190
C 1.6710 0.4920 -2.3450	C -5.0050 0.6400 -1.1700	H -7.7920 0.9020 -1.3350
H 0.0050 -0.4050 -3.3790	H -2.5340 0.4930 -2.3280	H -7.9950 1.9970 0.0600
H 2.6230 0.2200 -1.8830	H -3.2220 -1.1310 -2.2740	H -7.0710 2.5320 -1.3700
H 1.6970 1.3620 -3.0030	H -3.2560 0.8640 0.0660	
C 6.1840 1.4360 0.6930	H -3.9670 -0.7550 0.1000	CAT-6-TS
H 6.8560 2.2450 1.0200	H -5.4760 -0.1350 -1.8020	C -0.0840 -0.4030 1.7800
H 6.6980 0.4750 0.8690	H -4.7590 1.4830 -1.8430	C 1.1810 -0.7210 1.2110
H 6.0320 1.5400 -0.3960	H 4.0490 0.3660 -3.1080	C 0.9680 -1.8710 0.3670
	H 2.2930 0.6430 -3.2970	C -0.4520 -2.1910 0.4040
CAT-6-REACTANT	H 3.0380 -0.8380 -3.9540	C -1.1200 -1.2730 1.3020
C -0.1700 -0.6690 -1.8860	H 4.9270 -2.2320 -1.4500	H -0.2410 0.4280 2.4690
C -1.3950 -0.9120 -1.2160	H 3.6020 -3.3440 -1.9010	Si -2.9670 -0.8250 1.3850
C -1.1220 -1.9210 -0.2220	H 3.8470 -2.8770 -0.1920	C -2.8590 0.4610 -0.0110
C 0.2970 -2.2200 -0.2690	H 1.6140 3.5250 2.7960	C -2.8550 0.1300 -1.4100
C 0.9080 -1.4290 -1.3180	H 1.7890 5.2680 1.0330	C -2.2600 1.1700 -2.1690
H -0.0610 0.0500 -2.6970	H 2.4260 4.6770 -1.2920	C -1.9110 2.2230 -1.2650
Si 2.7580 -1.0320 -1.4950	H 2.9050 2.3300 -1.9340	C -2.2550 1.7750 0.0730

H -3.2130 -0.8120 -1.8250	C 1.2490 1.6130 -0.9400	C 1.7850 4.3610 0.7730
H -2.1450 1.1910 -3.2510	H 2.3000 1.5250 -0.6460	C 2.2000 4.0530 -0.5550
C -3.3870 -0.0840 3.0580	H 1.0780 2.4840 -1.5820	C 2.6020 2.7800 -0.9090
C -4.0970 -2.2360 0.8760	H 0.6930 1.8290 0.0300	C -1.4360 -2.8650 0.6610
C -1.3340 3.5110 -1.4640	H 0.4280 -1.8330 -2.3940	C -0.7920 -3.7460 1.5050
C -1.0720 4.2970 -0.3630	C 0.2670 -0.7740 -2.6140	C 0.6310 -3.8660 1.5140
C -1.3750 3.8480 0.9610	C 1.3710 0.0990 -2.4620	C 1.4110 -3.1200 0.6560
C -1.9530 2.6180 1.1890	H -0.4690 -0.5410 -3.3870	C -2.3840 -0.6640 -1.6990
C 1.8420 -2.6830 -0.4130	H 2.2890 -0.3130 -2.0370	C -3.4400 -0.3460 -0.6320
C 1.3180 -3.7400 -1.1290	H 1.5030 0.9350 -3.1510	C -4.7530 0.1240 -1.2610
C -0.0790 -4.0300 -1.1210	C 6.1350 0.3480 0.3480	H -2.2600 0.2210 -2.3440
C -0.9590 -3.2690 -0.3810	H 6.4480 -0.6970 0.5300	H -2.7860 -1.4610 -2.3520
C 2.4590 -0.0360 1.6210	H 5.9120 0.4230 -0.7330	H -3.0710 0.4430 0.0450
C 3.7110 -0.3130 0.7820	C 7.2740 1.3030 0.7120	H -3.6430 -1.2310 -0.0060
C 4.8590 0.6310 1.1430	H 7.5260 1.2210 1.7830	H -5.1260 -0.6560 -1.9500
H 2.2760 1.0540 1.6460	H 8.1840 1.0840 0.1310	H -4.5560 1.0180 -1.8830
H 2.6750 -0.3160 2.6680	H 6.9870 2.3510 0.5140	H 4.2950 0.7040 -3.0740
H 3.4850 -0.2130 -0.2950		H 2.5220 0.8150 -3.2740
H 4.0380 -1.3540 0.9360	CAT-7-REACTANT	H 3.4060 -0.5940 -3.9200
H 5.0700 0.5490 2.2250	C 0.1870 -0.7360 -1.8910	H 5.4090 -1.7690 -1.3660
H 4.5390 1.6770 0.9700	C -1.0180 -1.0930 -1.2360	H 4.2150 -3.0150 -1.8360
H -4.3100 0.5180 3.0030	C -0.6610 -2.0660 -0.2320	H 4.3750 -2.5170 -0.1260
H -2.5750 0.5580 3.4380	C 0.7820 -2.2240 -0.2580	H 1.4700 3.6420 2.7830
H -3.5460 -0.8910 3.7950	C 1.3260 -1.3810 -1.3030	H 1.4850 5.3830 1.0100
H -5.1510 -1.9410 1.0160	H 0.2340 -0.0160 -2.7070	H 2.2080 4.8480 -1.3030
H -3.9090 -3.1330 1.4910	Si 3.1280 -0.8010 -1.4610	H 2.9320 2.5590 -1.9240
H -3.9630 -2.5080 -0.1840	C 3.0010 0.3630 0.0360	H -2.5240 -2.8080 0.6520
H -1.1150 3.8650 -2.4730	C 2.8490 -0.1260 1.3770	H -1.3810 -4.3790 2.1720
H -0.6390 5.2900 -0.4970	C 2.3190 0.8850 2.2160	H 1.1010 -4.5800 2.1930
H -1.1610 4.5080 1.8040	C 2.1880 2.0820 1.4320	H 2.4940 -3.2490 0.6300
H -2.2170 2.3020 2.1990	C 2.6110 1.7640 0.0840	Zr 0.5810 0.2070 0.4000
H 2.9120 -2.4880 -0.4290	H 3.0610 -1.1450 1.6950	C -0.4750 1.9420 -0.5110
H 1.9870 -4.3760 -1.7130	H 2.1600 0.8120 3.2890	H -1.5460 1.7480 -0.2920
H -0.4490 -4.8770 -1.7020	C 3.3570 0.1220 -3.0800	H -0.1720 2.8950 -0.0490
H -2.0210 -3.5100 -0.3520	C 4.3940 -2.1560 -1.1670	H -0.3840 2.0340 -1.6050
Zr -0.4790 0.1280 -0.5970	C 1.7690 3.3960 1.7620	H -0.1400 -1.6510 2.8120

C -0.3390 -0.5880 2.9850	C -2.1070 2.6770 1.1880	H -0.7350 -0.5310 -3.3850
C -1.3130 0.0530 2.3030	C 1.4630 -2.7770 -0.4050	H 2.0260 -0.4020 -2.0300
H 0.2410 -0.0790 3.7560	C 0.8980 -3.8080 -1.1290	H 1.2840 0.8770 -3.1370
H -1.9580 -0.4860 1.6050	C -0.5110 -4.0350 -1.1330	C 5.8750 0.0660 0.3930
H -1.5350 1.1090 2.4890	C -1.3620 -3.2390 -0.3960	H 6.1440 -0.9930 0.5670
C -5.8280 0.4510 -0.2250	C 2.1790 -0.1650 1.6420	H 5.6700 0.1590 -0.6910
H -6.0290 -0.4470 0.3910	C 3.4220 -0.4900 0.8070	C 7.0640 0.9570 0.7620
H -5.4460 1.2250 0.4690	C 4.6080 0.4010 1.1800	H 7.2620 0.8620 1.8450
C -7.1360 0.9370 -0.8530	H 2.0420 0.9310 1.6710	H 6.7900 2.0150 0.5880
H -7.5090 0.1640 -1.5500	H 2.3780 -0.4590 2.6880	C 8.3250 0.6080 -0.0310
H -6.9290 1.8340 -1.4660	H 3.2060 -0.3740 -0.2700	H 9.1700 1.2590 0.2480
C -8.2060 1.2570 0.1930	H 3.7040 -1.5450 0.9560	H 8.6260 -0.4380 0.1530
H -9.1390 1.6070 -0.2790	H 4.8080 0.3040 2.2630	H 8.1510 0.7210 -1.1150
H -8.4450 0.3630 0.7960	H 4.3360 1.4600 1.0110	
H -7.8580 2.0450 0.8840	H -4.5690 0.6770 2.9820	CAT-8-REACTANT
	H -2.8360 0.6470 3.4270	C 1.7820 0.8530 -1.4040
CAT-7-TS	H -3.8650 -0.7630 3.7750	C 2.6050 -0.0860 -0.7280
C -0.3780 -0.4220 1.7830	H -5.5020 -1.7350 0.9860	C 2.6210 0.3150 0.6560
C 0.8760 -0.7940 1.2210	H -4.3160 -2.9820 1.4650	C 1.7880 1.5050 0.7840
C 0.6190 -1.9300 0.3710	H -4.3340 -2.3510 -0.2090	C 1.2620 1.8530 -0.5110
C -0.8140 -2.1880 0.3990	H -1.1960 3.8980 -2.4660	H 1.5610 0.7970 -2.4710
C -1.4470 -1.2460 1.2960	H -0.6690 5.2950 -0.4820	Si -0.2600 2.9190 -0.8980
H -0.5030 0.4120 2.4740	H -1.2360 4.5290 1.8130	C -1.4850 1.5040 -0.5850
Si -3.2730 -0.7170 1.3680	H -2.3890 2.3700 2.1960	C -1.9180 1.0760 0.7130
C -3.0990 0.5660 -0.0240	H 2.5400 -2.6290 -0.4140	C -2.4330 -0.2490 0.6750
C -3.1010 0.2390 -1.4230	H 1.5420 -4.4700 -1.7100	C -2.3850 -0.6680 -0.7010
C -2.4570 1.2540 -2.1760	H -0.9140 -4.8620 -1.7200	C -1.7770 0.3950 -1.4720
C -2.0680 2.2880 -1.2670	H -2.4340 -3.4330 -0.3760	H -1.8280 1.6700 1.6250
C -2.4390 1.8520 0.0680	Zr -0.7330 0.1310 -0.5950	C -0.2230 3.4980 -2.6840
H -3.4980 -0.6860 -1.8430	C 1.0550 1.5490 -0.9190	C -0.5400 4.3080 0.3360
H -2.3340 1.2720 -3.2570	H 2.0970 1.4110 -0.6120	C -2.8310 -1.8530 -1.3410
C -3.6710 0.0380 3.0410	H 0.9350 2.4300 -1.5590	C -2.6380 -1.9840 -2.7010
C -4.4610 -2.0760 0.8510	H 0.4950 1.7900 0.0430	C -2.0080 -0.9550 -3.4610
C -1.4350 3.5510 -1.4580	H 0.1150 -1.8560 -2.3940	C -1.5750 0.2160 -2.8720
C -1.1450 4.3210 -0.3540	C -0.0100 -0.7920 -2.6110	C 3.2980 -0.1840 1.8140
C -1.4740 3.8810 0.9670	C 1.1230 0.0420 -2.4530	C 3.1300 0.4570 3.0230

C	2.2820	1.6010	3.1520	H	0.1110	-3.1880	1.6900	C	-3.2480	-1.3200	1.3860
C	1.6090	2.1140	2.0640	C	-3.1560	-0.9750	1.7700	C	-3.8830	-2.3880	0.4890
C	3.3830	-1.1610	-1.4380	C	-4.6850	-0.9130	1.5870	C	-4.3410	-3.5980	1.3070
C	3.9530	-2.2990	-0.5830	H	-2.9000	-0.5330	2.7480	H	-2.5340	-1.8090	2.0740
C	4.4580	-3.4480	-1.4580	H	-2.8460	-2.0360	1.7990	H	-4.0370	-0.9010	2.0380
H	2.7330	-1.5890	-2.2200	H	-4.9950	0.1460	1.5600	H	-3.1660	-2.7090	-0.2870
H	4.2190	-0.6780	-1.9770	H	-4.9450	-1.3410	0.6030	H	-4.7470	-1.9550	-0.0420
H	3.1800	-2.6730	0.1110	C	-5.4190	-1.6580	2.7020	H	-5.0610	-3.2920	2.0840
H	4.7820	-1.9180	0.0360	H	-5.1800	-1.2250	3.6890	H	-3.4840	-4.0740	1.8150
H	5.2280	-3.0910	-2.1640	H	-6.5100	-1.6060	2.5640	H	-4.8270	-4.3540	0.6710
H	3.6320	-3.8770	-2.0520	H	-5.1280	-2.7230	2.7230	H	1.1500	3.7420	3.1430
H	4.9000	-4.2530	-0.8500					H	-0.2420	2.6560	3.4340
H	-1.2350	3.7690	-3.0310	CAT-8-TS				H	-0.5210	4.3270	2.8860
H	0.1800	2.7240	-3.3580	C	-1.7560	0.7780	1.4150	H	1.3080	4.9680	0.1230
H	0.4220	4.3890	-2.7760	C	-2.5440	-0.1730	0.7080	H	-0.4280	4.9600	-0.2960
H	-1.3700	4.9490	-0.0080	C	-2.6280	0.3010	-0.6520	H	0.7280	3.9670	-1.2320
H	0.3610	4.9390	0.4350	C	-1.8310	1.5160	-0.7460	H	3.2880	-2.6280	0.6970
H	-0.8070	3.9240	1.3340	C	-1.2870	1.8280	0.5580	H	2.8110	-3.0130	3.1060
H	-3.3180	-2.6410	-0.7640	H	-1.5150	0.6910	2.4760	H	1.6660	-1.2830	4.4750
H	-2.9790	-2.8860	-3.2130	Si	0.2160	2.9140	0.9830	H	1.0050	0.8940	3.4990
H	-1.8830	-1.0940	-4.5370	C	1.4860	1.5400	0.6580	H	-3.9470	-1.0540	-1.7590
H	-1.1260	1.0090	-3.4680	C	1.9670	1.1660	-0.6470	H	-3.7280	0.1780	-3.8790
H	3.9580	-1.0450	1.7390	C	2.4840	-0.1550	-0.6480	H	-2.3030	2.2090	-4.0550
H	3.6600	0.0890	3.9040	C	2.3710	-0.6430	0.6970	H	-1.0980	3.0900	-2.0720
H	2.1830	2.0810	4.1280	C	1.7430	0.3900	1.4990	Zr	-0.0790	-0.1900	-0.1180
H	0.9910	3.0070	2.1580	H	1.9070	1.7950	-1.5370	C	-0.3000	-2.4130	0.4490
Zr	0.1120	-0.2410	0.0880	C	0.1470	3.4540	2.7800	H	-1.2270	-2.9810	0.5770
C	0.3270	-2.1670	-1.0350	C	0.4750	4.3310	-0.2220	H	0.5820	-3.0600	0.4980
H	1.3060	-2.6450	-0.8830	C	2.7720	-1.8730	1.2940	H	-0.2350	-1.7420	1.3670
H	-0.4720	-2.8710	-0.7510	C	2.5050	-2.0800	2.6290	H	-0.9650	-0.4760	-2.7710
H	0.2080	-1.9580	-2.1150	C	1.8480	-1.0830	3.4170	C	-0.1460	-1.0180	-2.2900
H	0.7400	-0.4060	2.9220	C	1.4690	0.1280	2.8780	C	-0.4550	-2.2610	-1.6840
C	0.1270	-1.2570	2.6020	C	-3.3160	-0.1700	-1.8090	H	0.8460	-0.9000	-2.7310
C	0.6940	-2.3090	1.9770	C	-3.1890	0.5250	-2.9950	H	-1.5030	-2.5690	-1.6560
H	-0.9260	-1.2690	2.8850	C	-2.3740	1.6910	-3.0960	H	0.2730	-3.0730	-1.7190
H	1.7630	-2.3200	1.7510	C	-1.6950	2.1810	-2.0010	C	3.1840	-0.8620	-1.7670

C 4.7140 -0.8620 -1.5860	C -5.0590 -2.3680 1.3090	H 5.1540 -0.5740 -0.4900
H 2.9360 -0.3800 -2.7270	H -3.2950 -0.5040 1.9900	H 4.7100 -1.7270 0.7790
H 2.8340 -1.9090 -1.8320	H -4.5650 0.4440 1.2260	C 5.5110 -2.6530 -1.0150
H 5.0640 0.1830 -1.5270	H -3.4410 -2.0910 -0.0950	H 6.5140 -2.6860 -0.5570
H 4.9600 -1.3290 -0.6160	H -4.9250 -1.2150 -0.5090	H 5.0460 -3.6370 -0.8210
C 5.4190 -1.5990 -2.7240	H -5.8680 -1.7620 1.7570	C -5.6450 -3.6090 0.6350
H 5.1960 -1.1270 -3.6970	H -4.3950 -2.6650 2.1410	H -6.2050 -4.2300 1.3520
H 6.5120 -1.5940 -2.5860	H 1.2420 4.4170 2.3900	H -6.3350 -3.3270 -0.1800
H 5.0870 -2.6510 -2.7780	H -0.3590 3.6560 2.6330	H -4.8460 -4.2340 0.1980
	H -0.2210 5.1440 1.6650	C 5.6490 -2.4330 -2.5250
CAT-9-REACTANT	H 2.0660 4.8140 -0.7390	H 4.6720 -2.4840 -3.0370
C -1.8510 1.5330 0.8620	H 0.4500 4.8880 -1.4970	H 6.0910 -1.4430 -2.7370
C -2.6780 0.5510 0.2570	H 1.5810 3.5660 -1.9120	H 6.2980 -3.1980 -2.9790
C -2.4010 0.6060 -1.1570	H 2.7100 -2.5200 2.0360	
C -1.3920 1.6360 -1.3720	H 1.9410 -2.1180 4.3640	CAT-9-TS
C -1.0450 2.2280 -0.1050	H 0.9210 0.0500 5.0170	C -1.8690 1.2630 1.1570
H -1.8250 1.7130 1.9380	H 0.6680 1.8930 3.3790	C -2.6630 0.3210 0.4440
Si 0.5290 3.1910 0.3350	H -3.7220 -0.8280 -2.1590	C -2.5470 0.6660 -0.9510
C 1.5680 1.6250 0.5880	H -2.9050 -0.2820 -4.4170	C -1.6260 1.7890 -1.0540
C 2.1440 0.8500 -0.4730	H -1.1330 1.4310 -4.7720	C -1.2040 2.1780 0.2740
C 2.4450 -0.4720 -0.0430	H -0.1610 2.6700 -2.8550	H -1.7600 1.2590 2.2420
C 2.1060 -0.5360 1.3550	Zr -0.1340 -0.0560 0.0130	Si 0.3430 3.1600 0.7860
C 1.5420 0.7410 1.7370	C -0.8110 -1.6140 1.4710	C 1.4980 1.6530 0.7410
H 2.2970 1.2110 -1.4920	H -1.8200 -1.9980 1.2600	C 2.0830 1.1140 -0.4600
C 0.2770 4.1880 1.9060	H -0.0980 -2.4550 1.4880	C 2.4610 -0.2420 -0.2860
C 1.2150 4.2050 -1.0910	H -0.8120 -1.1710 2.4840	C 2.1470 -0.5870 1.0710
C 2.2580 -1.5670 2.3170	H -0.3020 -0.8310 -2.8020	C 1.5410 0.5700 1.7020
C 1.8270 -1.3390 3.6080	C 0.1340 -1.6270 -2.1870	H 2.1870 1.6590 -1.3990
C 1.2410 -0.0930 3.9830	C -0.6590 -2.4350 -1.4540	C 0.1180 3.8810 2.5050
C 1.0880 0.9340 3.0740	H 1.2090 -1.8010 -2.2520	C 0.8800 4.4210 -0.4980
C -2.9390 -0.0840 -2.2880	H -1.7420 -2.2940 -1.4370	C 2.3530 -1.7860 1.8130
C -2.4800 0.2280 -3.5500	H -0.2490 -3.2610 -0.8660	C 1.9170 -1.8390 3.1190
C -1.4640 1.2120 -3.7550	C 3.2270 -1.5150 -0.7840	C 1.2780 -0.7170 3.7340
C -0.9130 1.8970 -2.6930	C 4.6940 -1.5630 -0.3120	C 1.0870 0.4670 3.0540
C -3.7190 -0.2330 1.0080	H 3.2040 -1.3000 -1.8650	C -3.1460 0.1470 -2.1350
C -4.2680 -1.4950 0.3320	H 2.7760 -2.5130 -0.6370	C -2.8200 0.7070 -3.3550

C -1.8850	1.7790	-3.4590	C	3.2070	-1.1110	-1.2510	C	0.8880	1.3590	3.9460
C -1.2850	2.3110	-2.3370	C	4.6980	-1.2290	-0.8870	C	0.8000	2.0610	2.7610
C -3.5520	-0.6860	1.1260	H	3.1160	-0.7010	-2.2700	C	-2.7400	-0.6730	-2.3290
C -4.1570	-1.7950	0.2590	H	2.7650	-2.1240	-1.2720	C	-2.1790	-0.7420	-3.5870
C -4.7770	-2.9080	1.1060	H	5.1470	-0.2200	-0.8810	C	-1.1610	0.1710	-4.0030
H -2.9810	-1.1480	1.9520	H	4.7920	-1.6170	0.1430	C	-0.7100	1.1660	-3.1610
H -4.3770	-0.1380	1.6170	C	5.4630	-2.1340	-1.8540	C	-3.7890	0.1540	0.7900
H -3.3880	-2.2300	-0.4050	H	5.3510	-1.7420	-2.8820	C	-4.2740	-1.2680	0.4850
H -4.9320	-1.3710	-0.4020	H	4.9980	-3.1380	-1.8520	C	-5.1480	-1.8210	1.6130
H -5.5240	-2.4650	1.7900	C	6.9460	-2.2450	-1.4950	H	-3.4420	0.2020	1.8360
H -3.9920	-3.3480	1.7500	H	7.0740	-2.6560	-0.4790	H	-4.6560	0.8380	0.7320
H 1.0930	4.1180	2.9660	H	7.4820	-2.9020	-2.1990	H	-3.4120	-1.9430	0.3350
H -0.4220	3.1890	3.1730	H	7.4300	-1.2530	-1.5190	H	-4.8470	-1.2690	-0.4550
H -0.4710	4.8130	2.4460	C	-5.4280	-3.9980	0.2540	H	-6.0080	-1.1420	1.7660
H 1.7310	5.0090	-0.1120	H	-5.8580	-4.7960	0.8800	H	-4.5640	-1.8050	2.5510
H 0.0600	5.1210	-0.7340	H	-6.2390	-3.5790	-0.3670	H	0.9750	5.1840	1.0610
H 1.2040	3.9380	-1.4350	H	-4.6900	-4.4610	-0.4260	H	-0.6260	4.4670	1.4060
H 2.8550	-2.6370	1.3490					H	-0.4370	5.5990	0.0460
H 2.0720	-2.7460	3.7070	CAT-10-REACTANT				H	2.0570	4.6480	-1.9660
H 0.9570	-0.7990	4.7740	C	-1.9390	1.8600	0.2530	H	0.5080	4.4330	-2.8300
H 0.6330	1.3270	3.5460	C	-2.7000	0.7100	-0.0850	H	1.6850	3.0890	-2.7400
H -3.8650	-0.6680	-2.0820	C	-2.3060	0.3450	-1.4230	H	2.5510	-1.4820	2.9430
H -3.2890	0.3240	-4.2630	C	-1.2960	1.2990	-1.8650	H	1.5780	-0.4310	4.9740
H -1.6550	2.1900	-4.4440	C	-1.0640	2.2590	-0.8170	H	0.4770	1.7920	4.8600
H -0.5940	3.1510	-2.4150	H	-2.0040	2.3590	1.2210	H	0.3420	3.0490	2.7290
Zr -0.1360	0.0040	-0.0660	Si	0.4550	3.3680	-0.5710	H	-3.5220	-1.3720	-2.0410
C -0.6430	-2.1270	0.6600	C	1.4870	1.9920	0.2270	H	-2.5230	-1.5060	-4.2870
H -1.6300	-2.5960	0.7180	C	2.1620	0.9570	-0.5010	H	-0.7480	0.0840	-5.0100
H 0.1580	-2.8420	0.8760	C	2.4410	-0.1620	0.3310	H	0.0420	1.8810	-3.4920
H -0.6210	-1.3790	1.5180	C	1.9830	0.1850	1.6520	Zr	-0.1370	0.1520	0.0580
H -0.7450	-0.4640	-2.7710	C	1.3720	1.4950	1.5840	C	-0.9130	-0.9290	1.8590
C -0.0400	-1.0230	-2.1500	H	2.3980	1.0000	-1.5660	H	-1.9000	-1.3870	1.6980
C -0.5280	-2.1730	-1.4820	C	0.0570	4.7820	0.6000	H	-0.1970	-1.7070	2.1710
H 1.0020	-1.0280	-2.4740	C	1.2460	3.9310	-2.1800	H	-0.9940	-0.2100	2.6950
H -1.5950	-2.3960	-1.5590	C	2.0650	-0.5060	2.8880	H	-0.0500	-1.4310	-2.3780
H 0.1240	-3.0390	-1.3540	C	1.5200	0.0820	4.0120	C	0.3270	-2.0000	-1.5200

C -0.5310 -2.5880 -0.6610	C 1.4210 1.8720 0.8500	H -2.8030 0.4290 -4.6020
H 1.4030 -2.1530 -1.4340	C 2.1060 1.2460 -0.2510	H -1.0490 2.1900 -4.6830
H -1.6120 -2.4830 -0.7840	C 2.4120 -0.1100 0.0320	H -0.1940 3.2290 -2.5980
H -0.1770 -3.1970 0.1750	C 1.9450 -0.3670 1.3650	Zr -0.1810 0.2360 -0.0440
C 3.2980 -1.3480 0.0020	C 1.3210 0.8450 1.8650	C -0.8600 -1.8100 0.7770
C 4.7240 -1.1870 0.5660	H 2.3270 1.7320 -1.2030	H -1.8750 -2.2190 0.7460
H 3.3560 -1.4750 -1.0910	C -0.0610 4.2320 2.3340	H -0.1380 -2.5450 1.1450
H 2.8560 -2.2720 0.4180	C 1.0570 4.5980 -0.5820	H -0.8900 -0.9960 1.5720
H 5.1770 -0.2810 0.1250	C 2.0230 -1.5270 2.1870	H -0.5570 -0.4560 -2.7560
H 4.6560 -1.0090 1.6530	C 1.4520 -1.4910 3.4400	C 0.0900 -0.9480 -2.0250
C 5.6130 -2.4030 0.2900	C 0.7970 -0.3150 3.9240	C -0.4460 -2.0490 -1.3110
H 6.5780 -2.2610 0.8070	C 0.7240 0.8340 3.1640	H 1.1570 -0.9670 -2.2540
H 5.1510 -3.3050 0.7350	C -2.9260 0.3780 -2.4660	H -1.4880 -2.3220 -1.4860
C -5.6610 -3.2410 1.3470	C -2.4240 0.8430 -3.6650	H 0.2140 -2.8730 -1.0310
H -6.1760 -3.6070 2.2510	C -1.4210 1.8560 -3.7130	C 3.2200 -1.0550 -0.8020
H -4.7970 -3.9140 1.1870	C -0.9340 2.4290 -2.5570	C 4.6680 -1.1870 -0.2950
C 5.8820 -2.6540 -1.1980	C -3.7460 -0.2520 0.7600	H 3.2380 -0.7070 -1.8480
H 4.9310 -2.8610 -1.7230	C -4.2650 -1.3980 -0.1150	H 2.7520 -2.0560 -0.8040
H 6.2940 -1.7310 -1.6480	C -5.0000 -2.4590 0.7030	H 5.1380 -0.1880 -0.2920
C -6.6150 -3.3300 0.1510	H -3.3020 -0.6740 1.6800	H 4.6570 -1.5300 0.7550
H -6.1140 -3.0550 -0.7930	H -4.6100 0.3460 1.1030	C 5.4930 -2.1500 -1.1480
H -7.0090 -4.3520 0.0310	H -3.4290 -1.8730 -0.6600	H 5.4880 -1.8030 -2.1990
H -7.4730 -2.6480 0.2860	H -4.9470 -0.9990 -0.8840	H 5.0090 -3.1450 -1.1490
C 6.8480 -3.8190 -1.4220	H -5.8230 -1.9810 1.2660	C 6.9380 -2.2860 -0.6650
H 7.0340 -3.9900 -2.4950	H -4.3110 -2.8760 1.4630	H 6.9370 -2.6310 0.3860
H 7.8180 -3.6210 -0.9350	H 0.8640 4.4690 2.8880	H 7.4130 -1.2880 -0.6640
H 6.4430 -4.7520 -0.9930	H -0.6900 3.5870 2.9700	C -5.5590 -3.5950 -0.1560
	H -0.6130 5.1740 2.1670	H -6.2490 -3.1710 -0.9090
CAT-10-TS	H 1.8720 5.1860 -0.1250	H -4.7300 -4.0610 -0.7220
C -1.9910 1.6320 0.8910	H 0.2910 5.3020 -0.9490	C 7.7530 -3.2510 -1.5300
C -2.7400 0.6830 0.1400	H 1.4780 4.0610 -1.4490	H 7.7850 -2.9060 -2.5780
C -2.4430 0.9380 -1.2480	H 2.5350 -2.4210 1.8250	H 8.7910 -3.3370 -1.1690
C -1.4600 2.0100 -1.3000	H 1.5080 -2.3680 4.0880	H 7.3050 -4.2600 -1.5220
C -1.1830 2.4640 0.0460	H 0.3650 -0.3260 4.9260	C -6.2830 -4.6560 0.6750
H -2.0080 1.6870 1.9800	H 0.2560 1.7360 3.5580	H -7.1310 -4.2110 1.2240
Si 0.3310 3.4190 0.6870	H -3.6920 -0.3940 -2.4560	H -6.6770 -5.4660 0.0400

H -5.6020 -5.1060 1.4180	H -0.6450 -4.8880 -0.6040	C 5.8240 2.7000 0.2840
	H -0.3600 -5.7690 0.9170	H 4.8860 3.0020 0.7880
CAT-11-REACTANT	H 2.2650 -4.5020 2.5480	H 6.2740 1.9070 0.9120
C -1.9350 -2.1510 0.2100	H 0.7880 -4.1220 3.4790	C -6.5960 3.0480 -0.2990
C -2.6850 -0.9610 0.3960	H 1.9510 -2.8270 3.0640	H -5.9860 2.9250 0.6150
C -2.1790 -0.3490 1.5990	H 2.3590 0.6970 -3.3590	H -7.4450 2.3450 -0.2020
C -1.1110 -1.1980 2.1140	H 1.2960 -0.7060 -5.1140	C 6.7650 3.9060 0.2350
C -0.9580 -2.3390 1.2480	H 0.2420 -2.8810 -4.5470	H 7.7090 3.6060 -0.2540
H -2.0800 -2.8220 -0.6370	H 0.2500 -3.7430 -2.2210	H 6.3170 4.6870 -0.4070
Si 0.5560 -3.4690 1.0790	H -3.3740 1.4450 1.9960	C 7.0560 4.4790 1.6240
C 1.5030 -2.2450 -0.0150	H -2.1740 2.0070 4.0730	H 7.7350 5.3450 1.5700
C 2.1940 -1.0900 0.4790	H -0.2990 0.5960 4.9050	H 6.1240 4.8080 2.1170
C 2.4100 -0.1360 -0.5530	H 0.3870 -1.4530 3.6850	H 7.5270 3.7180 2.2710
C 1.8890 -0.7170 -1.7640	Zr -0.1520 -0.4300 -0.0810	C -7.1160 4.4860 -0.3730
C 1.3100 -2.0000 -1.4320	C -1.1130 0.2200 -1.9950	H -7.7560 4.6240 -1.2610
H 2.4850 -0.9390 1.5200	H -2.0500 0.7710 -1.8170	H -7.7090 4.7490 0.5190
C 0.0910 -5.0620 0.1980	H -0.4290 0.8470 -2.5870	H -6.2790 5.2020 -0.4510
C 1.4710 -3.7500 2.6960	H -1.3540 -0.6720 -2.6020	
C 1.8920 -0.2570 -3.1050	H 0.0910 1.6550 1.9980	CAT-11-TS
C 1.2990 -1.0390 -4.0750	C 0.3850 2.0220 1.0080	C 2.0150 -1.9750 0.8080
C 0.6940 -2.2890 -3.7480	C -0.5520 2.3710 0.1030	C 2.7820 -1.0230 0.0790
C 0.6870 -2.7720 -2.4550	H 1.4450 2.1770 0.8080	C 2.4530 -1.2150 -1.3110
C -2.5510 0.8190 2.3350	H -1.6170 2.2750 0.3290	C 1.4320 -2.2500 -1.3850
C -1.8780 1.1270 3.4980	H -0.2800 2.7740 -0.8760	C 1.1650 -2.7470 -0.0530
C -0.8030 0.3160 3.9780	C 3.2590 1.0970 -0.4850	H 2.0500 -2.0730 1.8940
C -0.4100 -0.8170 3.2990	C 4.6600 0.8610 -1.0860	Si -0.3680 -3.6780 0.5780
C -3.8560 -0.5800 -0.4680	H 3.3670 1.4150 0.5640	C -1.4060 -2.1050 0.8170
C -4.3290 0.8760 -0.4030	H 2.7780 1.9290 -1.0330	C -2.0870 -1.4130 -0.2460
C -5.2980 1.2090 -1.5400	H 5.1660 0.0730 -0.5000	C -2.3430 -0.0610 0.0970
H -3.6010 -0.8310 -1.5120	H 4.5460 0.4710 -2.1110	C -1.8470 0.1260 1.4320
H -4.7060 -1.2350 -0.2020	C 5.5160 2.1320 -1.1040	C -1.2570 -1.1250 1.8710
H -3.4640 1.5630 -0.4600	H 6.4670 1.9080 -1.6180	H -2.3400 -1.8530 -1.2120
H -4.8210 1.0650 0.5640	H 5.0090 2.9060 -1.7120	C 0.0250 -4.5620 2.1880
H -6.1730 0.5350 -1.4740	C -5.7720 2.6660 -1.5320	C -1.1500 -4.7870 -0.7200
H -4.8020 0.9850 -2.5020	H -6.3800 2.8500 -2.4360	C -1.8750 1.2530 2.3010
H 0.9800 -5.5430 -0.2440	H -4.8950 3.3380 -1.6080	C -1.2850 1.1480 3.5420

C -0.6620 -0.0680 3.9660	C 0.5300 1.8450 -1.2120	C -1.1590 -0.7200 2.3530
C -0.6390 -1.1860 3.1600	H -1.0980 0.8250 -2.1800	C -2.1510 -0.9090 1.3440
C 2.9360 -0.6270 -2.5160	H 1.5730 2.1160 -1.3890	C -2.1860 0.3130 0.5320
C 2.3960 -1.0260 -3.7220	H -0.1170 2.6610 -0.8840	C -1.1790 1.2210 1.0210
C 1.3540 -1.9990 -3.7890	C -3.1310 0.9450 -0.6820	H 0.2680 0.9350 2.7090
C 0.8670 -2.6000 -2.6470	C -4.5660 1.1030 -0.1450	Si -0.2350 2.5570 0.0300
C 3.8290 -0.1460 0.7130	H -3.1770 0.6450 -1.7430	C 0.8380 1.2960 -0.9140
C 4.3560 1.0270 -0.1230	H -2.6290 1.9300 -0.6470	C 0.4240 0.6150 -2.1040
C 5.1130 2.0430 0.7320	H -5.0720 0.1220 -0.1840	C 1.1580 -0.5920 -2.2760
H 3.4220 0.2440 1.6630	H -4.5270 1.3920 0.9200	C 2.1500 -0.6460 -1.2380
H 4.6850 -0.7820 1.0040	C -5.3680 2.1370 -0.9350	C 1.9140 0.4850 -0.3610
H 3.5220 1.5330 -0.6420	H -5.3870 1.8470 -2.0030	H -0.3890 0.9430 -2.7520
H 5.0250 0.6490 -0.9140	H -4.8510 3.1140 -0.8900	H 1.0660 -1.2850 -3.1110
H 5.9260 1.5280 1.2740	C -6.8010 2.2950 -0.4260	C 0.7370 3.6530 1.2010
H 4.4320 2.4430 1.5080	H -6.7810 2.5810 0.6430	C -1.3240 3.5140 -1.1650
H -0.8950 -4.7700 2.7610	H -7.3160 1.3160 -0.4740	C 3.2030 -1.5570 -0.9680
H 0.7050 -3.9730 2.8240	C 5.6920 3.2000 -0.0820	C 3.9650 -1.3670 0.1660
H 0.5210 -5.5250 1.9740	H 6.3770 2.7990 -0.8520	C 3.7060 -0.2890 1.0640
H -1.9730 -5.3690 -0.2690	H 4.8750 3.7090 -0.6300	C 2.7020 0.6260 0.8210
H -0.4100 -5.4980 -1.1260	C -7.6050 3.3310 -1.2150	C -2.6860 -2.1350 0.8360
H -1.5710 -4.2080 -1.5590	H -7.6160 3.0420 -2.2830	C -3.0970 -2.1870 -0.4840
H -2.3630 2.1770 1.9840	H -7.0880 4.3070 -1.1620	C -3.0890 -1.0080 -1.3040
H -1.3020 1.9990 4.2260	C 6.4380 4.2220 0.7780	C -2.7000 0.2290 -0.8020
H -0.2140 -0.1120 4.9610	H 7.2500 3.7080 1.3240	H 1.5370 4.1860 0.6590
H -0.1940 -2.1180 3.5090	H 5.7490 4.6180 1.5480	H 1.2010 3.0810 2.0220
H 3.7300 0.1160 -2.4900	C -9.0400 3.4730 -0.7010	H 0.0670 4.4050 1.6530
H 2.7740 -0.5910 -4.6490	H -9.0480 3.7840 0.3580	H -0.7610 4.3670 -1.5820
H 0.9520 -2.2800 -4.7640	H -9.6030 4.2230 -1.2800	H -2.2160 3.9130 -0.6510
H 0.0970 -3.3690 -2.7040	H -9.5790 2.5120 -0.7720	H -1.6610 2.8960 -2.0140
Zr 0.2360 -0.4850 -0.0360	C 7.0140 5.3750 -0.0470	H 3.4000 -2.3880 -1.6470
C 0.9920 1.5030 0.8560	H 7.5460 6.1010 0.5900	H 4.7860 -2.0520 0.3880
H 2.0230 1.8680 0.8210	H 7.7260 5.0000 -0.8020	H 4.3320 -0.1790 1.9520
H 0.3100 2.2560 1.2660	H 6.2120 5.9150 -0.5810	H 2.5390 1.4700 1.4910
H 0.9970 0.6610 1.6230		H -2.6630 -3.0370 1.4510
H 0.6030 0.3110 -2.7220	CAT-1	H -3.4330 -3.1300 -0.9170
C -0.0290 0.7830 -1.9660	C -0.5730 0.5450 2.1370	H -3.4150 -1.0870 -2.3430

H -2.7090 1.1120 -1.4400	H -2.4190 -1.3540 3.3030	C -1.8810 1.3690 0.0560
Zr -0.2270 -0.7690 -0.1350	H -3.6930 -2.5300 0.7520	H -2.6590 -1.3330 -1.7660
C 0.7570 -2.5880 0.7190	H -4.4910 -1.2980 1.7770	H -1.9590 0.7790 -3.2700
H 0.1000 -3.1510 1.4020	H 3.4100 2.0760 2.3840	C -2.6190 -0.6220 3.1070
H 1.0350 -3.2450 -0.1290	H 2.0840 1.1200 3.1040	C -3.0530 -2.8840 0.9750
H 1.6890 -2.3300 1.2510	H 2.0560 2.8970 3.2150	C -1.3830 3.2120 -1.5410
H -0.8610 -1.4510 3.1010	H 2.4700 4.2830 0.2240	C -1.1570 4.0380 -0.4600
	H 0.7870 4.5870 0.7370	C -1.2580 3.5540 0.8790
CAT-2	H 1.1290 3.9010 -0.8790	C -1.6100 2.2480 1.1480
C -0.6340 0.2880 1.9160	H 2.2280 -3.2250 -2.3110	C 2.5720 -1.5400 -1.0900
C -1.8400 -0.3530 1.5400	H 2.7900 -4.4010 -0.1980	C 1.9870 -2.1460 -2.1880
C -2.3680 0.4050 0.4390	H 2.8810 -3.1810 1.9630	C 0.6840 -2.7400 -2.0990
C -1.4840 1.5630 0.2310	H 2.4930 -0.7360 2.0710	C -0.0180 -2.7630 -0.9010
C -0.3820 1.4770 1.1520	H -3.9350 -0.8370 -0.4650	C 2.9940 0.5470 1.5170
H 0.0330 -0.1070 2.6820	H -3.7530 0.2280 -2.6880	C 4.3400 0.3720 0.8070
Si 1.3850 2.1740 0.9390	H -2.1660 2.1140 -3.0820	C 5.4180 1.2440 1.4550
C 1.8970 0.8600 -0.3410	H -0.7900 3.0350 -1.2310	H 2.6450 1.5870 1.3830
C 1.6300 0.9470 -1.7450	Zr -0.2810 -0.2250 -0.6490	H 3.1570 0.4240 2.6030
C 1.6330 -0.3450 -2.3410	C -0.7350 -2.4120 -0.5150	H 4.2440 0.6500 -0.2570
C 2.0200 -1.2870 -1.3280	H -1.7770 -2.6110 -0.2190	H 4.6410 -0.6900 0.8410
C 2.1240 -0.5560 -0.0800	H -0.5470 -2.8770 -1.5010	H 5.5600 0.9670 2.5140
H 1.3950 1.8710 -2.2730	H -0.0590 -2.8990 0.2110	H 5.1310 2.3090 1.4200
H 1.4890 -0.5650 -3.3990	H -4.0780 -2.8970 2.4430	H 6.3850 1.1330 0.9390
C 2.3200 2.0480 2.5600		H -3.6380 -0.1990 3.0890
C 1.4390 3.8920 0.1800	CAT-3	H -1.9260 0.1650 3.4470
C 2.2750 -2.6820 -1.3660	C 0.6150 -0.3950 1.7730	H -2.5960 -1.4340 3.8540
C 2.5820 -3.3300 -0.1880	C 1.8780 -0.3870 1.1330	H -4.1200 -2.7930 1.2440
C 2.6360 -2.6280 1.0540	C 1.8160 -1.4050 0.1200	H -2.6350 -3.7400 1.5320
C 2.4100 -1.2690 1.1240	C 0.5090 -2.0720 0.2360	H -3.0050 -3.1130 -0.1020
C -3.2540 -0.0020 -0.6120	C -0.2520 -1.4210 1.2680	H -1.2990 3.5850 -2.5630
C -3.1410 0.5880 -1.8590	H 0.3380 0.3240 2.5440	H -0.8980 5.0850 -0.6250
C -2.2330 1.6770 -2.0840	Si -2.1530 -1.2950 1.4180	H -1.0710 4.2430 1.7050
C -1.4670 2.2010 -1.0510	C -2.3160 -0.0210 0.0130	H -1.7260 1.8990 2.1740
C -2.3690 -1.5860 2.2250	C -2.3870 -0.3520 -1.3780	H 3.5530 -1.0800 -1.1790
C -3.7360 -2.1000 1.7660	C -1.9710 0.7480 -2.1810	H 2.5220 -2.1820 -3.1380
H -1.6170 -2.3890 2.1240	C -1.7290 1.8570 -1.3010	H 0.2510 -3.2050 -2.9870

H -1.0010 -3.2290 -0.8440	H 4.0620 -1.6600 0.8040	C 0.0960 -2.1260 0.2200
Zr 0.0100 -0.0320 -0.7680	H 4.9910 -0.1900 0.4370	C -0.5710 -1.4090 1.2750
C 1.3460 1.7390 -1.0700	H 6.1150 -1.3880 -1.4810	H 0.2100 0.2810 2.5210
H 2.4130 1.4820 -0.9760	H 5.1540 -2.8490 -1.1350	Si -2.4460 -1.1150 1.4910
H 1.1660 2.1660 -2.0740	H 6.3620 -2.2760 0.0470	C -2.5460 0.1610 0.0820
H 1.1040 2.5230 -0.3300	H -2.1300 2.2780 -3.6990	C -2.6960 -0.1700 -1.3030
	H -0.4860 1.5800 -3.7540	C -2.2170 0.8850 -2.1290
	H -0.6970 3.3460 -3.6510	C -1.8500 1.9740 -1.2690
CAT-4	H -2.7880 4.1070 -1.1510	C -1.9930 1.5090 0.0980
C 1.4680 0.9070 -1.4460	H -1.1630 4.7020 -0.7140	H -3.0650 -1.1270 -1.6720
C 2.4460 0.3570 -0.5820	H -2.0910 3.6870 0.4290	H -2.2420 0.9090 -3.2180
C 2.2260 0.9610 0.7030	H -2.3140 -3.6360 0.4310	C -2.7880 -0.3960 3.1900
C 1.1400 1.9430 0.5550	H -1.5570 -4.4870 -1.7790	C -3.5010 -2.6180 1.0950
C 0.6540 1.8960 -0.7990	H -0.8470 -2.9240 -3.5740	C -1.3990 3.2930 -1.5330
H 1.3430 0.5870 -2.4800	H -0.9430 -0.4700 -3.2510	C -1.0640 4.1030 -0.4690
Si -1.1000 2.3130 -1.4330	H 3.4010 -0.2070 2.1400	C -1.1540 3.6370 0.8770
C -1.8920 0.7350 -0.7220	H 1.9920 0.4150 4.0750	C -1.6050 2.3670 1.1700
C -2.3480 0.5940 0.6310	H 0.0600 1.9710 3.8060	C 2.1470 -1.7730 -1.1810
C -2.3850 -0.7740 1.0270	H -0.4430 3.0200 1.6140	C 1.4710 -2.3230 -2.2560
C -2.0480 -1.5470 -0.1390	Zr 0.0340 -0.1060 0.5200	C 0.1260 -2.8050 -2.1180
C -1.6880 -0.6260 -1.1980	C 0.9150 -2.1610 0.4380	C -0.5300 -2.7700 -0.8950
H -2.5730 1.4270 1.2980	H 1.9890 -2.1700 0.6860	C 2.8390 0.2730 1.4010
C -1.1020 2.3790 -3.3080	H 0.3770 -2.8140 1.1520	C 4.1370 -0.0120 0.6410
C -1.8490 3.8410 -0.6350	H 0.7790 -2.5970 -0.5680	C 5.3180 0.7600 1.2330
C -2.0110 -2.9480 -0.3600	C -2.8890 -1.3320 2.3280	H 2.5720 1.3380 1.2780
C -1.5860 -3.4130 -1.5860	C -4.3670 -1.7490 2.2220	H 3.0320 0.1360 2.4800
C -1.1790 -2.5140 -2.6180	H -2.7710 -0.5790 3.1260	H 4.0280 0.2740 -0.4210
C -1.2190 -1.1470 -2.4420	H -2.2830 -2.2080 2.6150	H 4.3550 -1.0950 0.6640
C 2.5780 0.4920 2.0110	H -4.7210 -2.1690 3.1770	H 5.4400 0.4720 2.2930
C 1.7800 0.8320 3.0890	H -4.9970 -0.8830 1.9650	H 5.0800 1.8400 1.2280
C 0.6730 1.7310 2.9350	H -4.5000 -2.5110 1.4360	H -3.7660 0.1160 3.2060
C 0.3920 2.3270 1.7130		H -2.0170 0.3280 3.4990
C 3.4640 -0.6580 -1.0280		H -2.8110 -1.2030 3.9420
C 4.5300 -1.0860 -0.0150	CAT-5	H -4.5480 -2.4240 1.3860
C 5.6030 -1.9490 -0.6810	C 0.3990 -0.4610 1.7450	H -3.1510 -3.5030 1.6540
H 2.9290 -1.5540 -1.3920	C 1.6350 -0.5640 1.0620	H -3.5010 -2.8650 0.0200
H 3.9750 -0.2350 -1.9120	C 1.4510 -1.5750 0.0570	

H -1.3210 3.6520 -2.5610	C -1.0570 4.1300 -0.5550	H 6.5320 -1.0850 0.1330
H -0.7230 5.1240 -0.6530	C -1.1150 3.7050 0.8060	H 6.2170 0.2920 -0.9370
H -0.8790 4.3130 1.6890	C -1.6410 2.4780 1.1550	C 7.6470 0.7060 0.6440
H -1.7100 2.0360 2.2030	C 1.6850 -1.9760 -1.2600	H 7.8460 0.4180 1.6910
H 3.1610 -1.3990 -1.3060	C 0.9180 -2.4920 -2.2900	H 8.5330 0.4430 0.0450
H 1.9660 -2.4020 -3.2250	C -0.4510 -2.8690 -2.0790	H 7.5290 1.8040 0.6150
H -0.3760 -3.2300 -2.9890	C -1.0420 -2.7660 -0.8260	
H -1.5460 -3.1510 -0.8000	C 2.6490 0.0590 1.2430	CAT-7
Zr -0.2590 -0.0540 -0.7790	C 3.8810 -0.3320 0.4240	C -0.1350 -0.5000 1.7220
C 1.2120 1.5920 -1.1450	C 5.1440 0.3610 0.9380	C 1.0620 -0.7210 0.9990
H 2.2560 1.2490 -1.0720	H 2.4550 1.1390 1.1170	C 0.7550 -1.7260 0.0180
H 1.0400 2.0100 -2.1550	H 2.8860 -0.0800 2.3130	C -0.6360 -2.1550 0.2390
H 1.0550 2.4110 -0.4200	H 3.7380 -0.0570 -0.6360	C -1.1990 -1.3670 1.3040
C 6.6180 0.5080 0.4680	H 4.0230 -1.4270 0.4580	H -0.2320 0.2690 2.4880
H 6.8800 -0.5650 0.4830	H 5.3070 0.0830 1.9960	Si -3.0320 -0.9060 1.5830
H 6.5220 0.8170 -0.5870	H 4.9890 1.4560 0.9250	C -3.0770 0.3470 0.1510
H 7.4580 1.0670 0.9100	H -3.8480 0.4490 3.3460	C -3.3040 -0.0000 -1.2200
	H -2.0740 0.5270 3.5500	C -2.7700 0.9940 -2.0870
CAT-6	H -2.9640 -0.9230 4.0760	C -2.2830 2.0670 -1.2660
C 0.1800 -0.4820 1.7120	H -4.9110 -2.0700 1.6340	C -2.4140 1.6440 0.1150
C 1.3720 -0.6910 0.9770	H -3.5900 -3.2450 1.8820	H -3.7630 -0.9300 -1.5530
C 1.0660 -1.7050 0.0050	H -3.9620 -2.6370 0.2420	H -2.8340 0.9980 -3.1750
C -0.3170 -2.1510 0.2440	H -1.4440 3.6470 -2.6200	C -3.2410 -0.1230 3.2760
C -0.8780 -1.3650 1.3110	H -0.6520 5.1190 -0.7820	C -4.2300 -2.3180 1.2650
H 0.0810 0.2900 2.4750	H -0.7530 4.3770 1.5860	C -1.7350 3.3370 -1.5790
Si -2.7140 -0.9270 1.6080	H -1.7180 2.1800 2.2010	C -1.2940 4.1390 -0.5470
C -2.7890 0.3200 0.1720	H 2.7150 -1.6810 -1.4420	C -1.3720 3.7100 0.8120
C -3.0260 -0.0330 -1.1950	H 1.3570 -2.6240 -3.2800	C -1.9150 2.4880 1.1520
C -2.5140 0.9650 -2.0710	H -1.0260 -3.2690 -2.9160	C 1.3840 -1.9970 -1.2420
C -2.0300 2.0450 -1.2590	H -2.0780 -3.0650 -0.6760	C 0.6220 -2.4980 -2.2830
C -2.1410 1.6250 0.1250	Zr -0.5660 -0.0800 -0.7880	C -0.7530 -2.8600 -2.0880
H -3.4780 -0.9690 -1.5210	C 1.0000 1.4500 -1.2510	C -1.3570 -2.7560 -0.8420
H -2.5880 0.9640 -3.1590	H 2.0200 1.0350 -1.2150	C 2.3460 0.0120 1.2820
C -2.9150 -0.1400 3.3000	H 0.8160 1.8630 -2.2600	C 3.5820 -0.3870 0.4710
C -3.8960 -2.3550 1.3060	H 0.9330 2.2890 -0.5350	C 4.8470 0.2900 1.0010
C -1.4990 3.3210 -1.5800	C 6.3890 0.0110 0.1200	H 2.1660 1.0950 1.1620

H 2.5710 -0.1370 2.3540	CAT-8	H -0.7880 4.5530 2.2150
H 3.4500 -0.1030 -0.5880	C -2.0390 1.0800 0.8590	H 1.6110 4.8470 -0.0960
H 3.7110 -1.4840 0.5000	C -2.7250 0.0620 0.1510	H 0.0440 4.8490 -0.9510
H 4.9980 0.0020 2.0580	C -2.3540 0.2190 -1.2290	H 1.3520 3.7390 -1.4600
H 4.7030 1.3870 0.9940	C -1.4910 1.4070 -1.3270	H 2.7100 -2.8720 1.3360
H -4.1660 0.4790 3.3140	C -1.2830 1.9400 -0.0060	H 1.6770 -3.0500 3.5910
H -2.3940 0.5320 3.5380	H -2.0710 1.1720 1.9440	H 0.3870 -1.1600 4.5570
H -3.3090 -0.9080 4.0480	Si 0.2210 2.9290 0.6360	H 0.1530 0.9860 3.3450
H -5.2450 -2.0190 1.5780	C 1.3780 1.4200 0.6870	H -3.0230 -1.5990 -2.2580
H -3.9440 -3.2120 1.8450	C 2.1110 0.9230 -0.4430	H -1.3760 -1.3880 -4.0900
H -4.2850 -2.5990 0.2000	C 2.4410 -0.4530 -0.2840	H 0.1990 0.5460 -4.1810
H -1.6650 3.6660 -2.6170	C 2.0060 -0.8290 1.0350	H 0.0820 2.3710 -2.5020
H -0.8760 5.1230 -0.7670	C 1.3030 0.2990 1.6130	Zr -0.1020 -0.2030 -0.3780
H -1.0100 4.3760 1.5980	H 2.3290 1.5020 -1.3410	C -0.6370 -2.2540 0.3480
H -2.0060 2.1880 2.1960	C -0.1630 3.6490 2.3250	H -1.6240 -2.5870 -0.0100
H 2.4200 -1.7130 -1.4120	C 0.8620 4.2030 -0.5880	H 0.1320 -2.9680 -0.0060
H 1.0700 -2.6290 -3.2700	C 2.1510 -2.0380 1.7630	H -0.6280 -2.2880 1.4520
H -1.3240 -3.2480 -2.9340	C 1.5710 -2.1310 3.0100	C 3.2680 -1.3040 -1.2020
H -2.3980 -3.0440 -0.7040	C 0.8310 -1.0450 3.5660	C 4.7480 -1.3430 -0.7710
Zr -0.8480 -0.0770 -0.7860	C 0.6870 0.1510 2.8920	H 3.2020 -0.9220 -2.2350
C 0.7400 1.4380 -1.2190	C -2.3620 -0.7370 -2.2980	H 2.8750 -2.3370 -1.2120
H 1.7550 1.0120 -1.1710	C -1.4310 -0.6220 -3.3140	H 5.1420 -0.3110 -0.7650
H 0.5740 1.8600 -2.2280	C -0.5310 0.4940 -3.3710	H 4.8060 -1.7070 0.2690
H 0.6710 2.2720 -0.4970	C -0.5950 1.5210 -2.4380	C 5.5850 -2.2300 -1.6930
C 6.0940 -0.0660 0.1900	C -3.6340 -0.9360 0.8140	H 5.5470 -1.8630 -2.7340
H 6.2310 -1.1640 0.1930	C -4.3890 -1.9170 -0.0880	H 6.6400 -2.2470 -1.3770
H 5.9390 0.2250 -0.8670	C -5.4160 -2.7190 0.7140	H 5.2100 -3.2680 -1.6880
C 7.3630 0.6050 0.7180	H -3.0470 -1.5050 1.5580	
H 7.5120 0.3140 1.7740	H -4.3760 -0.3600 1.3970	CAT-9
H 7.2200 1.7020 0.7150	H -3.6770 -2.6140 -0.5630	C -1.9740 1.6150 0.3070
C 8.6030 0.2390 -0.1010	H -4.8910 -1.3620 -0.8990	C -2.6890 0.4890 -0.1690
H 9.5070 0.7300 0.2930	H -6.1620 -2.0480 1.1740	C -2.1590 0.2040 -1.4740
H 8.7740 -0.8510 -0.0880	H -4.9240 -3.2820 1.5250	C -1.1660 1.2430 -1.7890
H 8.4810 0.5460 -1.1550	H -5.9510 -3.4380 0.0740	C -1.0420 2.1250 -0.6590
	H 0.7670 3.9350 2.8460	H -2.1100 2.0230 1.3090
	H -0.7110 2.9390 2.9660	Si 0.4810 3.1510 -0.1360

C 1.4650 1.6450 0.4820	H -1.0720 -2.2380 -3.6140	C 2.4320 -0.1160 0.3900
C 2.2460 0.7830 -0.3590	H 0.7040 -0.5380 -4.0410	C 1.8110 0.2030 1.6470
C 2.4140 -0.5030 0.2280	H 0.6160 1.7010 -2.9720	C 1.1150 1.4640 1.4950
C 1.8170 -0.4380 1.5360	Zr -0.0650 -0.1140 -0.2480	H 2.5790 1.0600 -1.4920
C 1.1850 0.8580 1.6740	C -0.8970 -1.7920 0.9780	C -0.2120 4.7150 0.2980
H 2.6080 1.0500 -1.3520	H -1.8730 -2.1420 0.6060	C 1.1990 3.8090 -2.3510
C 0.0040 4.3500 1.2270	H -0.1850 -2.6390 0.9710	C 1.7830 -0.4900 2.8840
C 1.3710 3.9750 -1.5730	H -1.0100 -1.4690 2.0290	C 1.0450 0.0380 3.9220
C 1.7620 -1.3830 2.5930	C 3.2350 -1.6400 -0.3050	C 0.3120 1.2530 3.7640
C 1.0570 -1.0580 3.7330	C 4.6690 -1.6170 0.2620	C 0.3320 1.9610 2.5800
C 0.3860 0.1960 3.8570	H 3.2730 -1.5890 -1.4050	C -2.0830 -1.3740 -1.8990
C 0.4350 1.1430 2.8550	H 2.7650 -2.6030 -0.0390	C -1.0270 -1.7630 -2.7030
C -2.1610 -1.0200 -2.2210	H 5.1470 -0.6620 -0.0210	C -0.0610 -0.8100 -3.1680
C -1.1230 -1.2780 -3.0990	H 4.6110 -1.6280 1.3640	C -0.1770 0.5410 -2.8670
C -0.1060 -0.2970 -3.3500	C 5.5240 -2.7920 -0.2280	C -3.7560 -0.0380 0.6990
C -0.1540 0.9600 -2.7610	H 6.4930 -2.7620 0.2990	C -4.4450 -1.3370 0.2760
C -3.7670 -0.2000 0.6240	H 5.0380 -3.7410 0.0640	C -5.6350 -1.6630 1.1830
C -4.5080 -1.3610 -0.0450	C -6.4210 -3.0220 0.1680	H -3.3110 -0.1700 1.7010
C -5.6900 -1.8370 0.8030	H -7.2680 -3.3500 0.7910	H -4.5290 0.7430 0.8140
H -3.3320 -0.5510 1.5760	H -6.8140 -2.7530 -0.8280	H -3.7320 -2.1800 0.3200
H -4.5090 0.5710 0.8990	H -5.7400 -3.8820 0.0420	H -4.7830 -1.2520 -0.7710
H -3.8230 -2.2130 -0.2010	C 5.7680 -2.7780 -1.7410	H -6.3760 -0.8450 1.1090
H -4.8710 -1.0500 -1.0420	H 4.8280 -2.8980 -2.3070	H -5.2880 -1.6800 2.2320
H -6.3900 -0.9950 0.9490	H 6.2330 -1.8270 -2.0530	H 0.6600 5.2060 0.7630
H -5.3210 -2.1150 1.8070	H 6.4400 -3.5980 -2.0410	H -0.8990 4.4030 1.1020
H 0.8970 4.6790 1.7870		H -0.7390 5.4630 -0.3200
H -0.7050 3.9010 1.9420	CAT-10	H 1.9300 4.6040 -2.1220
H -0.4780 5.2430 0.7920	C -2.0510 1.7550 -0.0070	H 0.4750 4.2100 -3.0800
H 2.1420 4.6630 -1.1850	C -2.7050 0.5170 -0.2240	H 1.7510 2.9830 -2.8280
H 0.6660 4.5640 -2.1850	C -2.1500 -0.0180 -1.4370	H 2.3370 -1.4230 3.0030
H 1.8790 3.2500 -2.2300	C -1.2070 0.9760 -1.9730	H 1.0160 -0.4750 4.8840
H 2.2690 -2.3440 2.4970	C -1.1360 2.0870 -1.0610	H -0.2620 1.6360 4.6100
H 1.0090 -1.7670 4.5610	H -2.2180 2.3670 0.8800	H -0.2000 2.9070 2.4860
H -0.1620 0.4130 4.7760	Si 0.3340 3.2730 -0.7710	H -2.7970 -2.1120 -1.5400
H -0.0490 2.1120 2.9770	C 1.3780 1.9850 0.1600	H -0.9230 -2.8090 -2.9940
H -2.9120 -1.7810 -2.0260	C 2.2130 1.0000 -0.4660	H 0.7630 -1.1540 -3.7960

H	0.5540	1.2570	-3.2430	H	2.2070	-2.7680	0.3980	H	0.2350	-3.5920	1.9810
Zr	-0.0580	0.0420	-0.1730	Si	-0.4330	-3.3610	-1.2640	H	2.7280	2.0610	-1.2270
C	-0.8140	-1.3840	1.3780	C	-1.4200	-2.2560	-0.0710	H	0.7950	3.0130	-2.4400
H	-1.7660	-1.8590	1.0920	C	-2.2620	-1.1670	-0.4780	H	-0.9530	1.5310	-3.4300
H	-0.0530	-2.1740	1.5350	C	-2.4240	-0.2160	0.5690	H	-0.7490	-0.9390	-3.3180
H	-0.9500	-0.8690	2.3460	C	-1.7580	-0.7600	1.7230	Zr	0.0300	-0.2920	-0.1240
C	3.3180	-1.2990	0.1310	C	-1.0930	-1.9820	1.3210	C	0.8780	0.8250	1.6200
C	4.7180	-1.0980	0.7450	H	-2.6690	-1.0430	-1.4820	H	1.8240	1.3340	1.3760
H	3.4100	-1.4680	-0.9540	C	0.1470	-4.9720	-0.4960	H	0.1400	1.5790	1.9550
H	2.8690	-2.2100	0.5660	C	-1.3770	-3.6030	-2.8710	H	1.0500	0.1400	2.4690
H	5.1760	-0.2000	0.2930	C	-1.6660	-0.2970	3.0610	C	-3.2750	1.0190	0.5510
H	4.6010	-0.8850	1.8210	C	-0.8950	-1.0090	3.9550	C	-4.6760	0.7600	1.1440
C	5.6380	-2.3070	0.5480	C	-0.1910	-2.1840	3.5540	H	-3.3740	1.3870	-0.4830
H	6.5720	-2.1350	1.1120	C	-0.2750	-2.6720	2.2660	H	-2.7880	1.8190	1.1370
H	5.1670	-3.2040	0.9920	C	1.9880	1.4010	-1.6740	H	-5.1820	-0.0080	0.5320
C	-6.3110	-2.9970	0.8430	C	0.8990	1.9310	-2.3420	H	-4.5570	0.3330	2.1540
H	-7.0920	-3.1990	1.5950	C	-0.1020	1.0790	-2.9160	C	-5.5360	2.0260	1.2090
H	-5.5690	-3.8120	0.9380	C	0.0100	-0.3040	-2.8620	H	-6.4810	1.7850	1.7270
C	5.9900	-2.5900	-0.9160	C	3.7710	-0.3790	0.5590	H	-5.0250	2.7840	1.8330
H	5.0710	-2.8260	-1.4840	C	4.4370	0.9840	0.3580	C	6.2930	2.5430	1.1800
H	6.4110	-1.6720	-1.3670	C	5.6620	1.1490	1.2610	H	7.1110	2.6110	1.9180
C	-6.9340	-3.0240	-0.5560	H	3.3840	-0.4470	1.5910	H	5.5440	3.3020	1.4770
H	-6.1710	-2.9130	-1.3460	H	4.5490	-1.1600	0.4790	C	-5.8600	2.6310	-0.1590
H	-7.4630	-3.9740	-0.7370	H	3.7220	1.7950	0.5870	H	-4.9280	2.9440	-0.6670
H	-7.6620	-2.2020	-0.6750	H	4.7310	1.1000	-0.6990	H	-6.3200	1.8560	-0.8010
C	6.9840	-3.7440	-1.0580	H	6.4140	0.3860	0.9880	C	6.8470	2.8960	-0.2050
H	7.2300	-3.9390	-2.1150	H	5.3640	0.9390	2.3040	H	6.0290	2.8870	-0.9500
H	7.9240	-3.5170	-0.5250	H	-0.7040	-5.5330	-0.0740	H	7.5600	2.1110	-0.5170
H	6.5720	-4.6730	-0.6270	H	0.8830	-4.8060	0.3080	C	-6.7990	3.8370	-0.0660
				H	0.6280	-5.6030	-1.2650	H	-7.7360	3.5240	0.4300
				H	-2.1030	-4.4260	-2.7530	H	-6.3410	4.6000	0.5900
				H	-0.6920	-3.8710	-3.6940	C	-7.1110	4.4450	-1.4350
				H	-1.9440	-2.7060	-3.1700	H	-7.7890	5.3090	-1.3480
				H	-2.1970	0.6060	3.3670	H	-6.1860	4.7870	-1.9330
				H	-0.8160	-0.6740	4.9910	H	-7.5910	3.7000	-2.0950
				H	0.4110	-2.7180	4.2930	C	7.5350	4.2630	-0.2210
CAT-11											
C	2.0070	-2.0110	-0.3610								
C	2.6670	-0.7580	-0.3910								
C	2.0600	-0.0150	-1.4610								
C	1.0780	-0.8950	-2.1150								
C	1.0370	-2.1490	-1.4100								

H 8.3760 4.2850 0.4930

H 7.9310 4.5060 -1.2210

H 6.8290 5.0610 0.0700