

Supporting Information for

The reaction mechanism of the enantioselective Tsuji allylation: inner-sphere and outer-sphere pathways, internal rearrangements, and asymmetric C–C bond formation

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Cartesian coordinates for species mentioned in the text are below. Total calculated energies (in kcal/mol) are reported with each structure as the following:

A : B3LYP/BS3//B3LYP/BS2 electronic energies + Solvation

B : mPW1PW91/BS3//B3LYP/BS2 electronic energies + Solvation

C : B3LYP/BS3//B3LYP/BS2 electronic energies + Solvation + Dispersion

Where BS2 is the LACVP electronic core potential on Pd with the 6-31G** basis set on all other atoms, and BS3 is the LACV3P electronic core potential on Pd with the 6-311++G** basis set on all other atoms. See the main text for calculation details.

1:

	A	B	C
	-410669.0747	-410562.7627	-410685.4002
C	0.03078	-0.05642	-0.01536
C	0.01294	-0.03866	1.31673
C	1.24357	-0.01563	2.16656
O	1.14642	-1.10467	3.12130
C	2.11534	-1.11219	4.06045
O	3.00961	-0.30816	4.15004
O	1.99675	-2.14964	4.91415
C	0.89453	-3.03270	4.85713
C	1.07029	-4.27197	4.38326
H	-0.88509	-0.02621	-0.59724
H	0.96237	-0.09370	-0.57414
H	-0.93386	-0.00515	1.85313
H	2.15309	-0.13820	1.57123
H	1.33461	0.92173	2.72655
C	-1.56759	-3.39731	5.21404
C	-0.35875	-2.48943	5.48793
C	-0.06353	-5.27696	4.44820
C	-1.19054	-4.87044	5.40920
H	-1.90696	-3.24401	4.18127
H	-2.40090	-3.11636	5.86746
H	-0.19474	-2.37956	6.57004
H	-0.54594	-1.47990	5.10393
H	-0.46745	-5.42157	3.43438
H	0.34447	-6.25420	4.74041
H	-0.85733	-5.02313	6.44407
H	-2.06194	-5.51773	5.25976

C	2.35534	-4.74509	3.75878
H	2.74798	-5.61794	4.29622
H	2.18480	-5.06601	2.72245
H	3.12490	-3.97214	3.75881

CO2 (no solvation energies)

	A	B	C
	-118383.2468	-118348.7324	-118383.3659
C	-0.87534	0.68708	3.64034
O	0.03277	1.41941	3.55722
O	-1.78345	-0.04525	3.72345

(S)-2

	A	B	C
	-292320.6987	-292247.2272	-292337.914
C	-0.00571	-0.00795	-0.00212
C	0.00003	0.00139	1.33248
C	1.23678	-0.00360	2.18948
C	1.42537	-1.27088	3.07061
C	2.71542	-1.09894	3.90221
O	3.52749	-0.22434	3.66015
C	0.21865	-1.46615	4.03415
C	0.44540	-2.51288	5.13605
C	1.70054	-2.19342	5.95673
C	2.93797	-2.08385	5.04534
H	-0.00317	-0.50064	4.51094
H	-0.66731	-1.73123	3.44550
H	0.53942	-3.51412	4.69593
H	-0.43451	-2.54787	5.78909
H	1.55845	-1.24166	6.48633
H	1.87099	-2.95568	6.72537
H	3.82826	-1.76143	5.59171
H	3.15527	-3.07077	4.61346
C	1.60914	-2.51195	2.16303
H	2.49422	-2.39901	1.52804
H	1.72164	-3.43690	2.73455
H	0.74041	-2.62170	1.50698
H	1.21982	0.86849	2.85688
H	-0.95673	0.03407	1.85447
H	0.91776	-0.02841	-0.57631
H	-0.93137	0.01375	-0.57039
H	2.12528	0.11683	1.56259

Exo-3

	A	B	C
	-1056412.849	-1056242.798	-1056470.07
Pd	0.00437	-0.03175	-0.00796
C	0.01396	-0.08763	2.22608
C	1.32879	-0.07374	1.67686
C	-0.87208	-1.09850	1.86490
N	-1.49938	-0.28143	-1.53220
P	1.39385	0.88492	-1.63958
H	1.96946	0.78439	1.85376
H	-1.92319	-1.02449	2.12221
H	1.85570	-1.01447	1.52595
H	-0.50895	-2.08406	1.58175
H	-0.37386	0.81232	2.69933
C	-2.96681	-0.28477	-1.25953
C	-3.50651	-1.05537	-2.48358

O	-2.41984	-0.98504	-3.44273
C	-1.31512	-0.61857	-2.76976
H	-4.38401	-0.61432	-2.95410
C	0.43099	5.33277	-2.50101
C	0.47936	4.85098	-1.19108
C	0.74331	3.50335	-0.95277
C	0.97564	2.62556	-2.02533
C	0.92545	3.11617	-3.33900
C	0.65008	4.46466	-3.57139
H	0.22084	6.38193	-2.68647
H	0.30819	5.52312	-0.35548
H	0.77486	3.13260	0.06830
H	1.10385	2.45442	-4.18046
H	0.61118	4.83648	-4.59102
C	5.95802	0.73973	-0.84920
C	5.36474	1.94748	-1.21390
C	3.99233	2.01092	-1.46475
C	3.20255	0.85859	-1.34370
C	3.80539	-0.35434	-0.96736
C	5.17630	-0.41276	-0.72919
H	7.02592	0.69413	-0.65738
H	5.96859	2.84517	-1.30828
H	3.54396	2.95560	-1.75359
H	3.20482	-1.25536	-0.86913
H	5.63517	-1.35562	-0.44651
C	0.93743	-1.44543	-5.65669
C	2.14247	-0.84885	-5.30001
C	2.24555	-0.16393	-4.08765
C	1.15874	-0.05663	-3.21014
C	-0.07121	-0.66590	-3.57419
C	-0.15612	-1.35012	-4.79961
H	0.84283	-1.98334	-6.59446
H	3.00523	-0.91127	-5.95657
H	3.19209	0.29343	-3.82103
H	-1.09582	-1.81113	-5.07694
H	-3.69811	-2.11250	-2.27525
C	-3.57501	1.14177	-1.06279
C	-5.08617	0.97251	-0.79405
H	-5.62458	0.55507	-1.65101
H	-5.26968	0.32214	0.06898
H	-5.53736	1.94512	-0.57612
C	-3.35616	2.02705	-2.30485
H	-3.80214	1.59861	-3.20888
H	-3.82133	3.00566	-2.15032
H	-2.29200	2.19690	-2.49615
C	-2.94108	1.82204	0.16518
H	-3.41488	2.79333	0.34086
H	-3.07847	1.22073	1.07122
H	-1.86988	1.99628	0.02469
H	-3.13885	-0.85243	-0.34070

Endo-3

	A	B	C
	-1056412.737	-1056242.638	-1056470.224
Pd	-0.01208	0.03829	0.00640
C	0.00422	0.09290	2.22865
C	1.35257	0.06090	1.87470
C	-0.87250	-0.91176	1.73066
N	1.14937	1.00564	-1.53430
P	-1.71340	-0.19427	-1.58494
H	1.99358	0.91196	2.08013
H	-1.94167	-0.81476	1.88674

H	1.84799	-0.88448	1.66765
H	-0.50964	-1.93390	1.62911
H	-0.41430	1.00579	2.64776
C	2.63668	0.96659	-1.63508
C	2.92640	2.24581	-2.45258
O	1.64095	2.58519	-3.03711
C	0.70475	1.88104	-2.37887
H	3.63153	2.11558	-3.27225
C	-0.86357	-3.41789	-4.80185
C	-0.64154	-3.68270	-3.44862
C	-0.88287	-2.69468	-2.49530
C	-1.36017	-1.43253	-2.88776
C	-1.58317	-1.17393	-4.24889
C	-1.33115	-2.16464	-5.19932
H	-0.67076	-4.18640	-5.54453
H	-0.27725	-4.65677	-3.13575
H	-0.70399	-2.90575	-1.44418
H	-1.95414	-0.20611	-4.57080
H	-1.50443	-1.95622	-6.25097
C	-5.98925	-1.08647	-0.02051
C	-5.47101	-1.84133	-1.07210
C	-4.19120	-1.57868	-1.56638
C	-3.41560	-0.55588	-1.00224
C	-3.94103	0.19832	0.06187
C	-5.22234	-0.06214	0.54309
H	-6.98438	-1.29403	0.36082
H	-6.06168	-2.63808	-1.51442
H	-3.80290	-2.17182	-2.38752
H	-3.35101	0.99471	0.50900
H	-5.62129	0.53023	1.36123
C	-2.12548	3.89553	-3.80037
C	-3.23878	3.10548	-3.53434
C	-3.08432	1.88582	-2.87099
C	-1.82661	1.43098	-2.45745
C	-0.68971	2.23815	-2.73003
C	-0.86337	3.45852	-3.40425
H	-2.23140	4.84622	-4.31281
H	-4.22975	3.42870	-3.83877
H	-3.96168	1.28077	-2.67078
H	0.00700	4.06772	-3.61496
H	3.24207	3.09036	-1.83262
C	3.19865	-0.35166	-2.25927
C	4.73810	-0.23531	-2.29841
H	5.08611	0.55726	-2.96877
H	5.15191	-0.04103	-1.30221
H	5.17314	-1.17226	-2.65915
C	2.65249	-0.58355	-3.68127
H	2.89634	0.23965	-4.36156
H	3.09366	-1.49084	-4.10568
H	1.56648	-0.71579	-3.68064
C	2.83121	-1.55140	-1.36629
H	3.25389	-2.47228	-1.78135
H	3.23507	-1.43283	-0.35425
H	1.74743	-1.68767	-1.29496
H	3.04468	1.05631	-0.62374

enolate

	A	B	C
	-218789.8716	-218733.3019	-218798.7733
O	0.00299	-0.00084	0.00103
C	-0.00032	0.00033	1.27577
C	1.10715	0.00045	2.12067

C	-1.40956	-0.02570	1.92570
C	2.48012	0.07003	1.51537
C	-1.45050	0.34670	3.41225
C	-0.35042	-0.40281	4.16903
C	1.03058	-0.00709	3.62536
H	-1.28074	1.42828	3.52701
H	-2.44117	0.14128	3.85106
H	-0.50198	-1.48372	4.02904
H	-0.41395	-0.20940	5.25194
H	1.30222	0.97903	4.07385
H	1.78480	-0.70027	4.05141
H	-1.83788	-1.03205	1.78334
H	-2.04248	0.64868	1.33270
H	2.37348	0.05983	0.42545
H	3.04598	0.98382	1.79425
H	3.13691	-0.77494	1.80788

Exo-Re-EXT-1

	A	B	C
	-1275181.254	-1274953.919	-1275255.735
Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.33735
C	0.33829	0.00000	5.13474
C	-1.30557	-0.08679	1.80668
C	-1.69509	-1.14602	0.97483
C	1.33898	-0.88457	4.66448
O	2.44051	-0.52359	4.15203
N	-0.00305	-0.61645	-2.16484
P	1.91886	1.24275	-0.62838
C	1.08832	-2.39874	4.75487
C	0.63481	1.47148	5.22768
C	-0.95042	-0.46344	5.77442
H	0.35446	0.90945	2.80830
H	0.65414	-0.86864	2.39336
H	-1.97194	0.77779	1.90956
H	-2.68740	-1.14175	0.51531
H	-1.20524	-2.12259	1.05400
H	1.70843	-2.78912	5.58240
H	1.48902	-2.86217	3.83962
H	-0.12815	2.10306	4.72680
H	0.65556	1.80855	6.28187
H	1.61881	1.68608	4.78716
H	-1.14276	0.12851	6.68906
H	-1.81955	-0.25792	5.11285
C	-1.21287	-1.13276	-2.85874
C	-0.63643	-2.29276	-3.71793
O	0.79664	-2.00172	-3.76979
C	1.04104	-1.10903	-2.75304
C	2.47575	-0.86841	-2.50301
C	2.99992	0.12020	-1.62491
H	-0.99958	-2.32982	-4.74696
H	-0.76885	-3.27410	-3.24325
H	-1.91204	-1.51304	-2.10568
C	3.27490	1.40924	1.79862
C	3.06611	2.04090	0.56060
C	3.72684	3.25290	0.28833
H	2.76714	0.48972	2.07995
C	2.18626	2.80172	-3.01826
C	1.50839	2.59996	-1.80613

C	0.47872	3.48853	-1.44953
H	2.98856	2.13031	-3.31297
C	-1.94674	-0.02698	-3.68387
C	-3.17931	-0.66606	-4.37442
H	-2.89378	-1.42480	-5.11804
H	-3.84600	-1.13721	-3.63486
H	-3.75263	0.11165	-4.90012
C	-1.01147	0.59271	-4.74630
H	-0.60417	-0.16827	-5.42760
H	-1.57179	1.31949	-5.35225
H	-0.17401	1.12243	-4.27281
C	-2.44417	1.07984	-2.72653
H	-3.00565	1.83735	-3.29370
H	-3.11401	0.66166	-1.95980
H	-1.60440	1.57495	-2.22362
C	4.13545	1.97410	2.74057
C	4.58304	3.81135	1.23646
H	-0.06057	3.34150	-0.51574
C	4.79060	3.17292	2.46164
H	4.25238	1.46061	3.69102
H	5.45526	3.61775	3.19929
H	5.08710	4.75121	1.01925
H	3.56728	3.76393	-0.65796
C	4.39235	0.20997	-1.47705
H	4.80380	0.95045	-0.79828
C	3.36965	-1.70394	-3.19692
H	2.96013	-2.45535	-3.86231
C	5.25941	-0.62998	-2.17273
H	6.33346	-0.53227	-2.03244
C	4.74456	-1.59026	-3.03943
H	5.40900	-2.25474	-3.58662
C	1.84296	3.86973	-3.85041
H	2.37741	4.01634	-4.78645
C	0.14732	4.55894	-2.27794
H	-0.64593	5.24293	-1.98483
C	0.82698	4.75035	-3.48178
H	0.56525	5.58367	-4.12956
C	-0.38415	-2.80314	4.98647
H	-0.45229	-3.87827	5.21085
H	-0.97795	-2.62205	4.07476
C	-0.96491	-1.96799	6.14260
H	-1.99117	-2.28624	6.37869
H	-0.35230	-2.13440	7.04375

Endo-Si-EXT-1

	A	B	C
	-1275182.563	-1274955.763	-1275257.94
Pd	0.00840	-0.01316	-0.03356
C	-0.01072	-0.02280	2.28332
C	1.90678	0.01082	4.83524
C	1.14484	-0.61128	1.74168
C	1.05676	-1.76615	0.94550
C	1.71589	1.33839	4.41392
O	2.27983	1.86371	3.39586
N	-0.09416	-0.48285	-2.20164
P	-0.70802	2.15341	-0.69656
C	0.73565	2.23435	5.19277
C	3.02402	-0.80710	4.25697
C	1.17763	-0.59326	6.01112
H	0.04849	0.95316	2.73654
H	-0.91479	-0.60820	2.43745
H	2.06680	-0.04159	1.82704

H	1.94602	-2.16265	0.46471
H	0.23125	-2.46254	1.07913
H	-0.15178	2.40961	4.56425
H	1.21800	3.21446	5.29406
H	3.67867	-1.20078	5.05133
H	2.67447	-1.69216	3.69484
H	3.63221	-0.19521	3.58536
H	0.88326	-1.62972	5.77618
H	1.86589	-0.69206	6.87346
C	-0.31916	-1.84586	-2.73831
C	0.49264	-1.81777	-4.05545
O	0.74456	-0.41210	-4.28449
C	0.44989	0.23677	-3.12778
C	0.81801	1.66517	-3.10802
C	0.40057	2.60041	-2.11741
H	-0.03608	-2.20390	-4.92786
H	1.45938	-2.32497	-3.96765
H	0.11328	-2.56349	-2.03415
C	0.47849	3.52633	1.40363
C	-0.55610	3.57351	0.45593
C	-1.41955	4.68201	0.42954
H	1.14077	2.67009	1.49487
C	-2.68475	2.94003	-2.62004
C	-2.40783	2.31588	-1.39435
C	-3.47717	1.80768	-0.63760
H	-1.87477	3.34363	-3.21968
C	-1.83296	-2.19406	-2.89684
C	-1.93865	-3.63245	-3.44510
H	-1.51518	-3.73114	-4.45092
H	-1.42495	-4.34761	-2.79176
H	-2.98894	-3.93570	-3.50689
C	-2.53891	-1.21381	-3.85328
H	-2.09541	-1.21714	-4.85561
H	-3.59242	-1.49169	-3.96472
H	-2.50638	-0.19015	-3.46944
C	-2.51772	-2.14295	-1.51731
H	-3.57210	-2.42684	-1.60947
H	-2.04601	-2.83709	-0.81206
H	-2.47453	-1.13922	-1.08560
C	0.66095	4.58243	2.29618
C	-1.23362	5.73189	1.32825
H	-3.27815	1.31350	0.31006
C	-0.19075	5.68632	2.25776
H	1.45891	4.49583	3.02639
H	-0.05425	6.50577	2.95861
H	-1.90625	6.58543	1.30348
H	-2.23360	4.72556	-0.28784
C	0.86776	3.91833	-2.21605
H	0.56862	4.64041	-1.46505
C	1.65641	2.10104	-4.15135
H	1.96557	1.38506	-4.90294
C	1.70564	4.32930	-3.25206
H	2.04525	5.36046	-3.29143
C	2.09819	3.41658	-4.22768
H	2.74964	3.72158	-5.04118
C	-4.00085	3.05591	-3.07452
H	-4.19877	3.54207	-4.02612
C	-4.79054	1.93508	-1.08852
H	-5.60605	1.54253	-0.48743
C	-5.05678	2.55832	-2.31015
H	-6.07946	2.65313	-2.66399
C	0.30469	1.69263	6.56159

H	-0.53810	2.27476	6.95795
H	1.12856	1.80769	7.28050
C	-0.05239	0.20737	6.45450
H	-0.43345	-0.17661	7.40976
H	-0.85825	0.08197	5.71654

Exo-Re EXT-2

	A	B	C
	-1275181.825	-1274955.525	-1275256.146
Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.43021
C	0.76069	0.00000	5.12049
C	-0.97433	-0.79732	1.80681
C	-1.94741	-0.23224	0.93756
C	1.40230	-1.17387	4.68085
O	2.38426	-1.18496	3.86119
N	2.22725	0.08624	-0.20567
P	-0.07147	0.64832	-2.24904
C	0.86243	-2.53806	5.12655
C	1.40088	1.33766	4.85784
C	-0.38277	-0.00772	6.11610
H	-2.66430	-0.87995	0.44069
H	-2.28751	0.78827	1.10510
H	-0.86165	-1.87938	1.84083
H	0.95168	-0.40615	2.73795
H	-0.15397	1.07253	2.51411
H	0.90266	-3.20725	4.25756
H	1.57595	-2.95525	5.85336
H	0.66461	2.11677	4.60881
H	1.94077	1.70530	5.74635
H	2.12993	1.26341	4.04688
H	-0.19041	0.74320	6.89987
H	-1.31610	0.32838	5.63058
C	3.15561	-0.66532	0.68847
C	4.44438	0.18203	0.60219
O	4.21877	1.06930	-0.52668
C	2.90367	0.98397	-0.83531
C	2.45402	1.98216	-1.84097
C	1.20379	1.96784	-2.51949
H	5.35279	-0.38413	0.39443
H	4.59947	0.80313	1.48958
H	2.76437	-0.64250	1.70989
C	3.32481	-2.16649	0.29810
C	4.28121	-2.79911	1.33365
H	5.29408	-2.38364	1.27528
H	3.89906	-2.64148	2.34836
H	4.36610	-3.87699	1.15453
C	3.87376	-2.32915	-1.13111
H	4.85000	-1.84752	-1.26085
H	4.00475	-3.39089	-1.36693
H	3.18711	-1.90828	-1.87332
C	1.96671	-2.88378	0.41562
H	2.08423	-3.95090	0.19271
H	1.57856	-2.79065	1.43473
H	1.22907	-2.47347	-0.28194
C	-4.00057	2.47953	-3.92615
C	-3.22256	1.67355	-4.75762
C	-2.03199	1.11792	-4.28582
C	-1.60991	1.36116	-2.96978
C	-2.40798	2.16108	-2.13605
C	-3.58964	2.72442	-2.61426
H	-4.92706	2.90966	-4.29633

H	-3.54124	1.47481	-5.77724
H	-1.43464	0.49311	-4.94236
H	-2.10098	2.33415	-1.10801
H	-4.19531	3.34484	-1.95961
C	0.98350	-2.74760	-5.24018
C	1.53571	-1.48096	-5.43293
C	1.24508	-0.44462	-4.54369
C	0.40113	-0.66931	-3.44537
C	-0.13906	-1.95126	-3.25236
C	0.14481	-2.98077	-4.14842
H	1.21110	-3.55191	-5.93417
H	2.19361	-1.29558	-6.27785
H	1.67650	0.53816	-4.70763
H	-0.77830	-2.13958	-2.39364
H	-0.28167	-3.96707	-3.98843
C	3.05904	4.03946	-3.01235
C	3.36057	3.02193	-2.11247
C	0.92233	3.00698	-3.41818
C	1.83176	4.03477	-3.66623
H	3.78015	4.83095	-3.19330
H	4.31234	3.02538	-1.59644
H	-0.02924	3.01319	-3.93787
H	1.57591	4.82225	-4.36978
C	-0.62689	-1.37353	6.77635
H	-1.59891	-1.37933	7.28649
H	0.13576	-1.54694	7.54878
C	-0.54201	-2.49856	5.74039
H	-1.28721	-2.31979	4.95171
H	-0.79177	-3.46733	6.19297

Exo-Si EXT-2

	A	B	C
	-1275182.332	-1274955.372	-1275255.98
Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.43460
C	0.65221	0.00000	5.16313
C	-1.19912	-0.41694	1.83564
C	-1.91273	0.41090	0.92630
C	1.88827	0.24035	4.53438
O	2.51187	-0.62058	3.82611
N	2.17571	-0.41363	-0.23302
P	0.01375	0.50363	-2.27961
C	2.49174	1.65125	4.56780
C	0.16639	-1.41162	5.36360
C	-0.06656	1.05304	5.97491
H	-2.81799	0.02598	0.44582
H	-1.89105	1.50025	1.05605
H	-1.48295	-1.47301	1.91966
H	0.72721	-0.70774	2.82495
H	0.27456	1.05762	2.45711
H	3.58145	1.53585	4.68171
H	2.34034	2.11831	3.57439
H	0.23171	-1.70699	6.43118
H	-0.89319	-1.54354	5.07328
H	0.78339	-2.11510	4.78759
H	-1.15867	0.96673	5.82002
H	0.08706	0.87177	7.06151
C	2.93621	-1.23878	0.75264
C	4.34872	-0.60410	0.69412
O	4.33270	0.17947	-0.55249
C	3.01806	0.29165	-0.91052
C	2.79171	1.22858	-2.03901

C	1.56638	1.40782	-2.73306
H	5.17821	-1.31050	0.61920
H	4.51022	0.08254	1.53421
H	2.53000	-1.07863	1.75942
C	2.88901	-2.76174	0.41753
C	3.72326	-3.50519	1.49357
H	4.79656	-3.27923	1.41022
H	3.38673	-3.22184	2.50202
H	3.60399	-4.59223	1.37186
C	3.44588	-3.05425	-0.99327
H	4.47334	-2.67810	-1.11191
H	3.46443	-4.14039	-1.17061
H	2.81577	-2.59532	-1.76886
C	1.42952	-3.26580	0.50991
H	1.39460	-4.34701	0.30493
H	1.02687	-3.09461	1.51895
H	0.78429	-2.75402	-0.21783
C	-3.30986	3.18905	-4.11270
C	-2.85252	2.08918	-4.83777
C	-1.85341	1.26643	-4.31410
C	-1.30436	1.53555	-3.05025
C	-1.78398	2.63714	-2.32089
C	-2.77325	3.46164	-2.85300
H	-4.08764	3.82864	-4.52418
H	-3.27338	1.86946	-5.81676
H	-1.50483	0.41249	-4.88921
H	-1.38330	2.84357	-1.33020
H	-3.13281	4.31399	-2.28062
C	-0.01063	-3.32187	-4.91909
C	0.90483	-2.30943	-5.20384
C	0.93919	-1.15132	-4.42436
C	0.05709	-0.99839	-3.34343
C	-0.85229	-2.03205	-3.05562
C	-0.88995	-3.18036	-3.84401
H	-0.03627	-4.22164	-5.52974
H	1.59510	-2.41800	-6.03781
H	1.65309	-0.36696	-4.66205
H	-1.52891	-1.93449	-2.20874
H	-1.60165	-3.97028	-3.61429
C	3.84535	2.89390	-3.48096
C	3.90928	1.98423	-2.43261
C	1.52511	2.33335	-3.78886
C	2.64693	3.06930	-4.16479
H	4.72869	3.46489	-3.75655
H	4.83704	1.84283	-1.89091
H	0.59297	2.48737	-4.32360
H	2.57825	3.77788	-4.98727
C	0.38077	2.50001	5.65884
H	-0.04766	3.19679	6.39502
H	0.00474	2.79828	4.66553
C	1.92074	2.57650	5.66492
H	2.29165	2.25591	6.65262
H	2.26329	3.61177	5.51099

Endo-Re EXT-2

	A	B	C
	-1275181.683	-1274955.675	-1275256.676
Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.43136
C	0.44076	0.00000	5.09180
C	-0.73507	1.03179	1.82295
C	-1.80692	0.75715	0.93470

C	1.07765	-1.18785	4.67548
O	2.15145	-1.21986	3.98708
C	0.42616	-2.53938	5.00459
C	1.17042	1.31606	5.00325
C	-0.84091	0.00897	5.90239
H	-2.32937	1.57834	0.45306
H	-2.39690	-0.14892	1.06578
H	-0.35255	2.04896	1.88901
H	0.99947	0.13932	2.80482
H	-0.40247	-1.00608	2.47769
H	0.55214	-3.19338	4.13279
H	1.02173	-3.00135	5.80667
H	0.56738	2.10818	4.53176
H	1.43413	1.69203	6.00509
H	2.10023	1.19993	4.43990
H	-0.74650	0.73545	6.72544
H	-1.67833	0.38925	5.28996
N	2.11902	-0.67123	-0.25637
P	-0.12256	-0.17985	-2.34075
C	2.90641	-1.40974	0.77107
C	4.32958	-0.87123	0.52030
O	4.25810	-0.28620	-0.81198
C	2.94177	-0.14267	-1.09334
C	2.65721	0.61918	-2.33591
C	1.39528	0.67694	-2.99020
H	5.11247	-1.62940	0.50184
H	4.60930	-0.07569	1.21855
H	2.55620	-1.12847	1.76909
C	2.76003	-2.96119	0.65924
C	3.55543	-3.57388	1.83302
H	4.63434	-3.40262	1.73578
H	3.22066	-3.14307	2.78338
H	3.40477	-4.65918	1.86222
C	3.27646	-3.49946	-0.68804
H	4.33334	-3.26220	-0.85621
H	3.18339	-4.59085	-0.71543
H	2.70011	-3.10026	-1.52936
C	1.27888	-3.34823	0.82885
H	1.17041	-4.43898	0.80596
H	0.89859	-2.99043	1.78962
H	0.65735	-2.93188	0.03025
C	-3.65476	1.89761	-4.53907
C	-3.17158	0.68455	-5.02935
C	-2.10176	0.04638	-4.39840
C	-1.50829	0.61528	-3.26181
C	-2.00915	1.83122	-2.76932
C	-3.06781	2.47225	-3.40928
H	-4.48821	2.39129	-5.03130
H	-3.62636	0.23090	-5.90599
H	-1.73270	-0.89546	-4.79162
H	-1.56792	2.26959	-1.87834
H	-3.44293	3.41460	-3.01974
C	-0.02304	-4.45937	-4.15024
C	0.85052	-3.49391	-4.65099
C	0.84627	-2.20058	-4.12459
C	-0.02953	-1.86361	-3.08196
C	-0.89647	-2.84625	-2.57545
C	-0.89822	-4.13253	-3.11209
H	-0.01792	-5.46458	-4.56246
H	1.53656	-3.74428	-5.45573
H	1.52416	-1.45562	-4.52948
H	-1.56688	-2.60159	-1.75548

H	-1.57549	-4.88218	-2.71268
C	3.61390	2.06475	-4.05570
C	3.74476	1.31496	-2.89019
C	1.29134	1.43508	-4.16408
C	2.38115	2.12546	-4.69594
H	4.47224	2.59741	-4.45446
H	4.70259	1.26168	-2.38738
H	0.33639	1.49120	-4.67439
H	2.25844	2.70529	-5.60664
C	-1.22592	-1.36062	6.48219
H	-2.25808	-1.33845	6.85534
H	-0.58314	-1.58531	7.34521
C	-1.04395	-2.46213	5.43426
H	-1.67676	-2.23833	4.56251
H	-1.38193	-3.43239	5.82208

Endo-Si EXT-2

	A	B	C
	-1275181.545	-1274955.431	-1275256.919
Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	2.40919
C	1.28893	0.00000	4.88502
C	-0.72791	-1.05584	1.84302
C	-0.13913	-1.95797	0.92083
C	1.33375	1.33900	4.46861
O	2.03232	1.76706	3.48623
C	0.40563	2.36756	5.13016
C	2.33429	-0.97767	4.41685
C	0.41401	-0.46964	6.02493
H	-0.75142	-2.72651	0.45872
H	0.91966	-2.19857	1.00477
H	-1.81104	-1.06180	1.95613
H	-0.52639	0.82823	2.86144
H	1.07862	0.06392	2.40626
H	0.98268	3.29411	5.23757
H	-0.40132	2.60715	4.41642
H	2.99394	-1.28590	5.24502
H	1.89739	-1.90677	4.01743
H	2.96381	-0.52506	3.64599
H	0.00346	-1.46519	5.79066
H	1.02685	-0.62835	6.93348
N	0.28713	2.18725	-0.27563
P	-0.02100	-0.07694	-2.34890
C	1.04000	3.08272	0.64802
C	0.24638	4.39760	0.50610
O	-0.48741	4.23835	-0.74411
C	-0.46351	2.91481	-1.02512
C	-1.32344	2.49999	-2.16094
C	-1.23195	1.25027	-2.83553
H	0.85726	5.29504	0.41280
H	-0.49023	4.54010	1.30440
H	0.98768	2.68005	1.66534
C	2.56014	3.19138	0.29853
C	3.20511	4.09980	1.36904
H	2.83270	5.13090	1.32319
H	3.01405	3.69493	2.36827
H	4.28889	4.14459	1.21303
C	2.79303	3.76871	-1.11022
H	2.36129	4.76929	-1.23230
H	3.86802	3.85673	-1.30251
H	2.37506	3.12092	-1.88780
C	3.20692	1.79690	0.40754

H	4.28074	1.86835	0.19683
H	3.07641	1.40209	1.41936
H	2.77308	1.09741	-0.31419
C	-1.60933	-3.93386	-4.40523
C	-0.61952	-3.18467	-5.04128
C	-0.13616	-2.01393	-4.45422
C	-0.63660	-1.58248	-3.21624
C	-1.62648	-2.34902	-2.57977
C	-2.11509	-3.51101	-3.17403
H	-1.98117	-4.84628	-4.86313
H	-0.21923	-3.51062	-5.99752
H	0.63386	-1.44036	-4.95999
H	-2.00673	-2.03286	-1.61222
H	-2.88217	-4.09294	-2.67057
C	3.88724	0.85978	-4.68140
C	2.71097	1.51798	-5.04102
C	1.52403	1.26433	-4.35073
C	1.50584	0.35122	-3.28596
C	2.69748	-0.29818	-2.92389
C	3.87807	-0.05008	-3.62219
H	4.80941	1.05962	-5.21998
H	2.71369	2.23022	-5.86172
H	0.61349	1.77683	-4.64540
H	2.69996	-0.99444	-2.08928
H	4.79267	-0.55931	-3.33189
C	-3.14890	3.16630	-3.63656
C	-2.27946	3.43722	-2.58338
C	-2.11656	1.00384	-3.89370
C	-3.06792	1.94366	-4.29355
H	-3.88380	3.90785	-3.93534
H	-2.33482	4.38770	-2.06654
H	-2.06403	0.05625	-4.41803
H	-3.73812	1.71321	-5.11709
C	-0.72942	0.49440	6.36473
H	-1.22055	0.18943	7.29784
H	-1.49427	0.44981	5.57553
C	-0.19818	1.92709	6.46872
H	0.57418	1.96412	7.25014
H	-0.99038	2.62031	6.78170

R-4

	A	B	C
	-1275216.128	-1274993.689	-1275289.721
Pd	0.23152	0.12915	-0.08725
C	-0.07453	0.33076	2.99761
C	0.49370	0.44947	4.43887
C	0.86604	0.76708	1.88665
C	0.62581	1.89820	1.09115
C	1.54572	-0.64739	4.69609
O	1.91331	-1.43080	3.83397
N	0.60841	-2.21976	-0.38485
P	-0.48134	-0.15281	-2.30954
C	2.04914	-0.77826	6.12955
C	1.11274	1.84880	4.66236
C	-0.66273	0.20286	5.45965
H	1.44818	2.41695	0.60279
H	-0.27495	2.49300	1.23639
H	1.88807	0.40194	1.97612
H	-0.37994	-0.71199	2.86025
H	-0.99109	0.93346	2.94408
H	2.57585	0.14023	6.41918
H	2.76532	-1.60379	6.16280

H	1.46690	1.99880	5.68551
H	0.35756	2.61544	4.45542
H	1.94965	2.02481	3.98167
H	-1.39292	1.01547	5.35538
H	-1.18392	-0.72091	5.17046
C	0.81364	-3.06265	0.81676
C	2.14563	-3.78412	0.50042
O	2.32931	-3.57830	-0.92045
C	1.44708	-2.60218	-1.28449
C	1.58766	-2.13275	-2.68172
C	0.79988	-1.10212	-3.27159
H	2.14305	-4.86039	0.68185
H	2.99543	-3.33286	1.02327
H	0.93981	-2.40733	1.68266
C	-0.40261	-4.00149	1.09845
C	-0.10629	-4.79364	2.38892
H	0.74540	-5.47381	2.27525
H	0.11455	-4.11888	3.22391
H	-0.97292	-5.40348	2.66765
C	-0.65180	-4.97196	-0.07194
H	0.21925	-5.60205	-0.28489
H	-1.48716	-5.64053	0.16431
H	-0.91075	-4.42801	-0.98528
C	-1.66794	-3.15066	1.31982
H	-2.52625	-3.79910	1.53273
H	-1.54550	-2.47128	2.17044
H	-1.90331	-2.54902	0.43922
C	-4.38932	-2.66900	-2.65176
C	-3.28889	-3.02777	-3.42972
C	-2.10068	-2.29653	-3.34912
C	-1.99560	-1.20160	-2.48007
C	-3.10604	-0.85790	-1.69101
C	-4.29511	-1.57980	-1.78250
H	-5.31327	-3.23739	-2.71728
H	-3.35328	-3.87644	-4.10598
H	-1.25545	-2.58004	-3.96913
H	-3.02934	-0.02388	-0.99792
H	-5.14564	-1.29761	-1.16746
C	-1.51210	3.55085	-4.94125
C	-0.58000	3.62892	-3.90525
C	-0.28398	2.49804	-3.14381
C	-0.90149	1.26849	-3.41903
C	-1.84004	1.20200	-4.46162
C	-2.14302	2.33613	-5.21575
H	-1.75347	4.43435	-5.52638
H	-0.09381	4.57432	-3.67935
H	0.41549	2.56196	-2.31388
H	-2.34312	0.26439	-4.67908
H	-2.87659	2.27154	-6.01540
C	1.06293	-0.75834	-4.60664
H	0.48190	0.03054	-5.07072
C	2.57729	-2.76605	-3.45624
H	3.16991	-3.54796	-2.99733
C	2.04792	-1.39806	-5.35976
H	2.21344	-1.10152	-6.39199
C	2.80848	-2.41097	-4.78158
H	3.57996	-2.92016	-5.35166
C	0.86037	-1.01057	7.08958
H	0.41818	-1.99242	6.87222
H	1.22051	-1.05119	8.12413
C	-0.20822	0.07908	6.92319
H	-1.07497	-0.14682	7.55622

H 0.18746 1.03900 7.27920

S-4

	A	B	C
	-1275215.032	-1274992.752	-1275288.457
Pd	0.08836	-0.04733	-0.02569
C	-0.01518	-0.09513	3.08648
C	0.67668	-0.04640	4.47706
C	0.80398	0.48598	1.94689
C	0.43862	1.65291	1.25308
C	1.91928	-0.96296	4.47874
O	2.05725	-1.87043	3.67287
N	0.50886	-2.33595	-0.48341
P	-0.62828	-0.14449	-2.26371
C	2.95114	-0.75040	5.58382
C	-0.29822	-0.64223	5.52708
C	1.05290	1.41167	4.85679
H	1.19408	2.26565	0.76523
H	-0.48757	2.17111	1.49802
H	1.85452	0.19497	1.93970
H	-0.26122	-1.14373	2.89235
H	-0.96948	0.44327	3.15901
H	3.83764	-1.33730	5.32631
H	2.53396	-1.18565	6.50435
H	0.12009	-0.64940	6.53832
H	-1.21776	-0.04718	5.55164
H	-0.56781	-1.67117	5.26644
H	1.53046	1.88170	3.98891
H	0.12430	1.97067	5.03251
C	0.67636	-3.30938	0.62154
C	1.97472	-4.05055	0.22331
O	2.16568	-3.70384	-1.16913
C	1.32802	-2.65699	-1.42331
C	1.49380	-2.04608	-2.76252
C	0.70517	-0.97246	-3.26904
H	1.92442	-5.13877	0.28922
H	2.84391	-3.69465	0.78630
H	0.83294	-2.75575	1.55148
C	-0.58183	-4.21703	0.80472
C	-0.32523	-5.15662	2.00118
H	0.50116	-5.85235	1.81659
H	-0.08683	-4.58699	2.90686
H	-1.21648	-5.75970	2.20796
C	-0.87231	-5.04417	-0.46260
H	-0.03256	-5.69143	-0.74059
H	-1.74135	-5.69125	-0.29887
H	-1.09882	-4.39509	-1.31372
C	-1.80689	-3.33745	1.12080
H	-2.69202	-3.96565	1.27702
H	-1.64967	-2.74986	2.03211
H	-2.01990	-2.64295	0.30514
C	-4.47452	-2.66394	-3.02634
C	-3.34365	-2.91285	-3.80383
C	-2.17101	-2.18156	-3.59584
C	-2.11244	-1.19708	-2.59890
C	-3.25333	-0.96511	-1.81260
C	-4.42651	-1.68630	-2.02994
H	-5.38650	-3.23146	-3.19179
H	-3.37224	-3.67428	-4.57932
H	-1.30218	-2.37667	-4.21737
H	-3.21395	-0.21744	-1.02419
H	-5.30132	-1.49048	-1.41545

C	-1.62710	3.78654	-4.55887
C	-0.71893	3.77043	-3.49892
C	-0.43351	2.57446	-2.84016
C	-1.03683	1.37349	-3.24351
C	-1.95133	1.40172	-4.30900
C	-2.24436	2.60063	-4.96005
H	-1.86045	4.72000	-5.06414
H	-0.24348	4.69227	-3.17445
H	0.24686	2.56299	-1.99220
H	-2.44299	0.48705	-4.62650
H	-2.95918	2.60841	-5.77909
C	1.00021	-0.49286	-4.55373
H	0.41884	0.32950	-4.95493
C	2.51400	-2.58577	-3.56728
H	3.10542	-3.40241	-3.17215
C	2.01782	-1.03908	-5.33596
H	2.20847	-0.63623	-6.32725
C	2.77820	-2.09478	-4.84200
H	3.57429	-2.53211	-5.43728
C	3.27698	0.73278	5.83558
H	3.95644	0.82168	6.69135
H	3.81295	1.13941	4.96703
C	1.99335	1.54038	6.06328
H	1.49885	1.19339	6.98091
H	2.23533	2.59764	6.22615

Exo-5

	A	B	C
	-1275186.07	-1274962.105	-1275269.019
Pd	0.14141	-0.10303	0.00512
C	0.29480	-0.16403	2.28836
O	2.73196	-0.13582	-0.06000
C	-0.33037	1.01560	1.87451
C	0.34300	1.82797	0.92068
C	3.59139	-1.04266	-0.43658
C	4.53913	-0.61917	-1.56505
C	3.69439	-2.30578	0.11123
C	2.87062	-2.67140	1.31641
C	4.73252	-3.31703	-0.32946
H	-0.17423	2.67487	0.47924
H	-0.25129	-0.89683	2.87489
H	1.42919	1.88760	0.94153
H	1.37806	-0.24731	2.26332
H	-1.38825	1.17272	2.07579
N	-0.11562	-2.17528	-0.62798
P	0.18149	0.46127	-2.23952
H	3.97457	-0.59418	-2.50852
H	4.83586	0.41900	-1.36718
H	2.84494	-3.75955	1.47045
H	3.26500	-2.23433	2.25078
H	1.84064	-2.30696	1.22643
H	4.27834	-4.32112	-0.38231
H	5.52780	-3.41316	0.43497
C	-0.74594	-3.22220	0.21430
C	-0.00711	-4.49448	-0.25383
O	0.56224	-4.11576	-1.52737
C	0.53837	-2.76011	-1.58280
H	-0.64585	-5.36143	-0.42630
C	1.09579	-0.83030	-3.18867
C	1.18440	-2.18854	-2.78086
H	0.81320	-4.76959	0.41496
C	-2.30217	-3.26997	0.07068

C	-2.83241	-4.39425	0.98513
H	-2.49434	-5.38788	0.67208
H	-2.51644	-4.24374	2.02424
H	-3.92726	-4.40646	0.97055
C	-2.72547	-3.53410	-1.38697
H	-2.31795	-4.47383	-1.77574
H	-3.81677	-3.59816	-1.45588
H	-2.39948	-2.72376	-2.04573
C	-2.91333	-1.93595	0.54032
H	-4.00646	-1.97890	0.47164
H	-2.65336	-1.72609	1.58446
H	-2.56367	-1.09847	-0.06901
H	-0.51339	-3.00955	1.26151
C	2.36624	4.42958	-3.24261
C	1.15861	4.14400	-3.88050
C	0.48242	2.95302	-3.60508
C	1.01412	2.04066	-2.68189
C	2.22621	2.33233	-2.03100
C	2.89512	3.52149	-2.32137
H	2.89059	5.35640	-3.45974
H	0.73911	4.84641	-4.59603
H	-0.45559	2.74034	-4.10886
H	2.62588	1.61651	-1.30763
H	3.83437	3.74047	-1.82017
C	-4.01346	0.80216	-4.22392
C	-2.99222	0.14710	-4.91193
C	-1.72316	0.02718	-4.34160
C	-1.46444	0.55816	-3.06942
C	-2.50380	1.20304	-2.37910
C	-3.76618	1.33194	-2.95555
H	-4.99969	0.89441	-4.67050
H	-3.18026	-0.27246	-5.89659
H	-0.93655	-0.48153	-4.88954
H	-2.31890	1.59642	-1.38279
H	-4.55896	1.83814	-2.41160
C	1.71594	-0.45006	-4.39051
H	1.67029	0.58914	-4.69975
C	1.88056	-3.09801	-3.60419
H	1.95007	-4.13101	-3.28795
C	2.39520	-1.36448	-5.19124
H	2.86215	-1.03200	-6.11410
C	2.47891	-2.69916	-4.79202
H	3.01120	-3.42575	-5.39847
C	5.78048	-1.50670	-1.72191
H	6.48602	-1.30076	-0.90412
H	6.30833	-1.26796	-2.65539
C	5.38547	-2.98460	-1.67777
H	6.25728	-3.63029	-1.84854
H	4.67500	-3.18731	-2.49087

Re-INT-1

	A	B	C
	-1275177.837	-1274951.899	-1275255.136
Pd	-0.47764	-0.16768	0.11037
C	-0.53580	-1.49659	1.91147
C	2.25809	2.75539	2.16584
O	1.50721	1.09026	0.64468
P	-0.80050	1.23977	-1.72985
C	2.16841	1.46094	1.71867
C	-1.80921	-1.42557	1.31547
C	-2.39416	-0.14433	1.15150
N	1.23949	-0.89970	-1.35839

C	2.93492	0.34298	2.42918
C	1.51963	3.87653	1.49118
C	3.10967	3.16687	3.34792
H	-3.30856	-0.03446	0.56135
H	0.02192	-2.43762	1.90393
H	-2.23191	0.62956	1.91054
H	-0.23411	-0.76458	2.66705
H	-2.21928	-2.29122	0.78357
H	2.27279	-0.53639	2.49668
H	3.77903	0.04026	1.78216
H	0.86395	4.42043	2.20077
H	2.21438	4.63346	1.07653
H	0.90865	3.49857	0.66289
H	2.47174	3.41059	4.22333
H	3.64333	4.10650	3.10947
C	1.89668	-2.20206	-1.09768
C	3.37488	-1.79832	-0.82061
O	3.46217	-0.42935	-1.32761
C	2.17016	-0.00525	-1.49342
H	4.12333	-2.39242	-1.35223
C	0.79424	2.02787	-2.19430
C	2.03541	1.37862	-1.97605
H	3.60582	-1.77650	0.25076
C	1.70061	-3.19466	-2.28992
C	2.43969	-4.51893	-1.97466
H	3.52978	-4.38224	-1.92181
H	2.09671	-4.94400	-1.01811
H	2.23715	-5.25705	-2.76508
C	2.23579	-2.59235	-3.60820
H	3.29413	-2.30344	-3.52414
H	2.15038	-3.33139	-4.41937
H	1.65392	-1.70441	-3.88973
C	0.19136	-3.49687	-2.44056
H	0.02863	-4.20325	-3.26918
H	-0.20571	-3.95507	-1.52062
H	-0.37337	-2.57891	-2.64464
H	1.45521	-2.66500	-0.20582
C	-3.72603	4.79952	-1.11416
C	-3.70460	4.14647	-2.34589
C	-2.83131	3.07853	-2.56159
C	-1.97077	2.64982	-1.53909
C	-2.00656	3.30848	-0.29757
C	-2.87299	4.38026	-0.09166
H	-4.40677	5.63211	-0.94977
H	-4.36946	4.46882	-3.14463
H	-2.82533	2.57704	-3.52587
H	-1.34726	2.98281	0.50408
H	-2.88461	4.88726	0.87072
C	-2.35901	-0.86162	-5.57322
C	-1.29193	0.03092	-5.66629
C	-0.80496	0.66888	-4.52342
C	-1.38137	0.41421	-3.26965
C	-2.44673	-0.49775	-3.18476
C	-2.93684	-1.12390	-4.32969
H	-2.73751	-1.35522	-6.46568
H	-0.83565	0.23533	-6.63268
H	0.02426	1.36638	-4.60774
H	-2.88882	-0.72125	-2.21586
H	-3.76609	-1.82373	-4.25095
C	0.79307	3.33733	-2.69617
H	-0.15155	3.85384	-2.84044
C	3.21983	2.06649	-2.28232

H	4.16446	1.56492	-2.10446
C	1.98069	4.00181	-2.99891
H	1.95025	5.01645	-3.38949
C	3.19824	3.36013	-2.78744
C	3.46829	0.71683	3.83061
H	4.17347	-0.04824	4.19065
H	2.63407	0.75448	4.55052
C	4.14434	2.09939	3.77359
H	4.96745	2.06928	3.04124
H	4.58152	2.36198	4.74881
H	4.13377	3.86894	-3.00873

Si-INT-1

	A	B	C
	-1275180.351	-1274954.451	-1275257.653
Pd	-0.25038	-0.15303	0.13072
C	-0.11488	-1.43802	1.94911
C	2.93559	0.71365	2.82047
O	1.92275	0.64237	0.66734
P	-0.71867	1.26181	-1.66432
C	2.20207	1.25978	1.79492
C	-1.46122	-1.33280	1.55739
C	-2.01300	-0.03517	1.40640
N	1.30090	-0.91719	-1.55140
C	1.65466	2.68479	1.91529
C	3.55927	-0.64985	2.69744
C	3.27777	1.46676	4.08862
H	-2.99824	0.08559	0.94582
H	0.39459	-2.40421	1.88588
H	-1.71911	0.76478	2.09560
H	0.36150	-0.68746	2.59140
H	-1.98016	-2.19981	1.13299
H	1.77540	3.16991	0.93360
H	0.56418	2.63618	2.10221
H	4.66655	-0.59368	2.71864
H	3.27142	-1.31925	3.53124
H	3.26162	-1.11901	1.75038
H	4.34448	1.77679	4.08007
H	3.18001	0.79330	4.96136
C	1.95126	-2.23919	-1.37457
C	3.46439	-1.87726	-1.32350
O	3.51295	-0.53156	-1.89350
C	2.22707	-0.06253	-1.83934
H	4.11504	-2.51337	-1.92942
C	0.83907	2.03866	-2.26614
C	2.07684	1.34858	-2.23120
H	3.83903	-1.81919	-0.29582
C	1.55436	-3.23760	-2.50903
C	2.29570	-4.57889	-2.28244
H	3.38472	-4.47391	-2.39373
H	2.08709	-4.97965	-1.27797
H	1.95787	-5.32148	-3.02061
C	1.90954	-2.66712	-3.90055
H	2.97460	-2.40082	-3.97060
H	1.69471	-3.41548	-4.67847
H	1.31284	-1.76987	-4.11345
C	0.03231	-3.49883	-2.43381
H	-0.26606	-4.21651	-3.21352
H	-0.23925	-3.92664	-1.45571
H	-0.53235	-2.56980	-2.57734
H	1.63179	-2.67262	-0.41876
C	-3.55288	4.86661	-0.87608

C	-3.68061	4.15025	-2.06505
C	-2.83648	3.07002	-2.33065
C	-1.85443	2.69151	-1.40176
C	-1.73948	3.41536	-0.20143
C	-2.57810	4.49851	0.05351
H	-4.21165	5.70811	-0.67220
H	-4.43996	4.43175	-2.79186
H	-2.94676	2.52122	-3.26210
H	-0.98595	3.13190	0.53048
H	-2.47431	5.05476	0.98276
C	-2.61161	-0.80960	-5.37171
C	-1.58790	0.11950	-5.55626
C	-0.99889	0.74680	-4.45647
C	-1.42653	0.44299	-3.15461
C	-2.44837	-0.50462	-2.97881
C	-3.04247	-1.11917	-4.08062
H	-3.06992	-1.29469	-6.23092
H	-1.24630	0.36072	-6.56085
H	-0.20595	1.47347	-4.61338
H	-2.77337	-0.76446	-1.97312
H	-3.83663	-1.84764	-3.93089
C	0.82064	3.37220	-2.70367
H	-0.11907	3.91620	-2.71883
C	3.23969	2.02416	-2.63458
H	4.18225	1.49036	-2.58950
C	1.98501	4.02112	-3.11038
H	1.93954	5.05368	-3.44996
C	3.20045	3.34231	-3.07084
C	2.32020	3.53826	3.01926
H	1.75785	4.47165	3.17763
H	3.33791	3.82241	2.70465
C	2.40692	2.72257	4.32306
H	1.39212	2.41907	4.63056
H	2.82909	3.33049	5.13815
H	4.11916	3.83984	-3.37377

Re-6

	A	B	C
	-1275193.8	-1274967.457	-1275269.017
Ni	-0.50344	0.06302	0.57958
C	-0.69528	-1.16612	2.42351
C	0.97536	2.43915	3.51675
O	0.44154	1.78262	1.30131
P	-0.57648	1.17181	-1.55162
C	1.26549	1.78573	2.36054
C	-0.72624	-1.99983	1.29287
C	-1.68792	-1.77399	0.27972
N	1.17725	-1.32731	-2.07617
C	2.59875	1.08894	2.13922
C	-0.36468	3.08611	3.74635
C	1.98938	2.59972	4.63221
H	-1.60382	-2.29784	-0.66622
H	0.14985	-1.18915	3.10300
H	-2.68548	-1.43239	0.55007
H	-1.61029	-0.72556	2.81306
H	0.13949	-2.62208	1.07355
H	2.39857	0.10685	1.68689
H	3.16207	1.65056	1.37842
H	-0.75505	2.84786	4.74713
H	-0.30733	4.18529	3.69624
H	-1.09493	2.75668	3.00324
H	1.69603	1.98327	5.50074

H	1.96240	3.63702	5.00209
C	1.61866	-2.72081	-1.89824
C	3.13229	-2.58957	-1.55824
O	3.38997	-1.16965	-1.61455
C	2.19711	-0.57325	-1.91953
H	3.79394	-3.08148	-2.27706
C	1.11841	1.74257	-2.05628
C	2.25619	0.89273	-2.09123
H	3.38146	-2.94077	-0.55280
C	1.27645	-3.61098	-3.13163
C	1.79545	-5.03872	-2.87084
H	2.88737	-5.07654	-2.78437
H	1.37046	-5.45416	-1.94912
H	1.51240	-5.70323	-3.69431
C	1.90595	-3.04459	-4.41814
H	2.99936	-2.99140	-4.35939
H	1.65772	-3.68329	-5.27307
H	1.52691	-2.03997	-4.62611
C	-0.25477	-3.65552	-3.29672
H	-0.53056	-4.28307	-4.15214
H	-0.73478	-4.08247	-2.40716
H	-0.66361	-2.65568	-3.45794
H	1.07625	-3.14861	-1.04388
C	-3.07686	5.09881	-1.21805
C	-3.09770	4.37341	-2.40995
C	-2.34919	3.20152	-2.53439
C	-1.56884	2.73796	-1.46218
C	-1.55131	3.47275	-0.26328
C	-2.29983	4.64541	-0.15029
H	-3.66166	6.00996	-1.12309
H	-3.69822	4.71698	-3.24839
H	-2.37900	2.65177	-3.46909
H	-0.93471	3.12332	0.56301
H	-2.27456	5.20442	0.78144
C	-2.55170	-0.70378	-5.31752
C	-1.32902	-0.04281	-5.44356
C	-0.70459	0.50117	-4.32005
C	-1.29368	0.38390	-3.05410
C	-2.52010	-0.28469	-2.93568
C	-3.14640	-0.82290	-4.06015
H	-3.03818	-1.12382	-6.19350
H	-0.86032	0.05518	-6.41914
H	0.24268	1.01944	-4.43100
H	-2.98999	-0.37900	-1.96065
H	-4.09867	-1.33525	-3.95320
C	1.31166	3.10900	-2.30234
H	0.46179	3.77970	-2.27104
C	3.52249	1.44364	-2.34407
H	4.38058	0.78200	-2.35511
C	2.57363	3.63807	-2.57118
H	2.67946	4.70318	-2.75816
C	3.68632	2.80398	-2.58453
C	3.43601	0.93625	3.41616
H	4.46229	0.63698	3.16687
H	3.01739	0.13290	4.04000
C	3.42289	2.24389	4.21445
H	3.82983	3.04871	3.58614
H	4.07122	2.17277	5.09726
H	4.67674	3.20469	-2.78004

Si-6

A

B

C

	-1275193.4	-1274966.865	-1275268.219
Pd	-0.32293	-0.03096	0.55703
C	-0.45739	-1.30003	2.38321
C	2.67862	1.37969	2.71788
O	0.87429	1.56785	1.18195
P	-0.54161	1.14470	-1.53747
C	1.37722	1.64491	2.42614
C	-0.57963	-2.09557	1.23135
C	-1.59972	-1.81688	0.29178
N	1.25665	-1.24940	-2.16643
C	0.39913	2.12709	3.48923
C	3.65269	0.94735	1.65596
C	3.24886	1.55402	4.11138
H	-1.59276	-2.31695	-0.67048
H	0.43272	-1.35884	3.00070
H	-2.56655	-1.45558	0.63680
H	-1.33880	-0.86254	2.84598
H	0.25248	-2.73336	0.93974
H	-0.21548	2.92237	3.04743
H	-0.30245	1.31142	3.72633
H	4.49569	1.65142	1.57420
H	4.09829	-0.03315	1.88677
H	3.16705	0.88774	0.68109
H	3.89340	2.45075	4.14145
H	3.92515	0.71477	4.33676
C	1.75475	-2.62502	-1.99947
C	3.26998	-2.43396	-1.69569
O	3.48680	-1.01277	-1.83959
C	2.26010	-0.46193	-2.08121
H	3.93607	-2.94928	-2.39303
C	1.08311	1.79768	-2.16415
C	2.25223	1.00065	-2.27647
H	3.54086	-2.71541	-0.67363
C	1.41506	-3.52231	-3.22864
C	1.97399	-4.93682	-2.97926
H	3.06749	-4.94688	-2.90705
H	1.57237	-5.36489	-2.05296
H	1.69730	-5.60656	-3.80055
C	2.00947	-2.93815	-4.52367
H	3.10185	-2.85829	-4.48172
H	1.76304	-3.58032	-5.37624
H	1.60313	-1.94238	-4.72310
C	-0.11716	-3.60476	-3.36860
H	-0.39110	-4.24273	-4.21682
H	-0.57213	-4.03883	-2.46946
H	-0.55291	-2.61557	-3.52631
H	1.25092	-3.07441	-1.13338
C	-3.06457	4.98635	-0.74617
C	-3.25424	4.28376	-1.93641
C	-2.50322	3.13730	-2.20600
C	-1.55377	2.67700	-1.28052
C	-1.36693	3.38858	-0.08237
C	-2.11648	4.53643	0.17561
H	-3.65116	5.87740	-0.53876
H	-3.98855	4.62601	-2.66115
H	-2.66305	2.60509	-3.13783
H	-0.62307	3.03155	0.62774
H	-1.96022	5.07903	1.10438
C	-2.75572	-0.68486	-5.20153
C	-1.55925	0.00688	-5.39718
C	-0.86941	0.54533	-4.30886
C	-1.36468	0.39274	-3.00659

C	-2.56713	-0.30475	-2.81855
C	-3.25881	-0.83686	-3.90754
H	-3.29225	-1.10116	-6.04954
H	-1.16018	0.13293	-6.40020
H	0.05697	1.08582	-4.47590
H	-2.96716	-0.42727	-1.81601
H	-4.19059	-1.37146	-3.74342
C	1.19645	3.16783	-2.43885
H	0.32228	3.80207	-2.35256
C	3.47224	1.60053	-2.62697
H	4.35532	0.97540	-2.69040
C	2.41116	3.74690	-2.80680
H	2.45451	4.81298	-3.01269
C	3.55812	2.96351	-2.89372
C	1.07399	2.62824	4.77325
H	0.33047	2.76037	5.56986
H	1.51566	3.61790	4.58977
C	2.18070	1.66323	5.20738
H	1.74166	0.67239	5.39292
H	2.63486	1.98818	6.15220
H	4.51236	3.40560	-3.16462

Re-INT-2

	A	B	C
	-1275177.313	-1274950.159	-1275254.49
Pd	0.00000	0.00000	0.00000
O	0.00000	0.00000	2.31838
C	2.62959	0.00000	0.59530
C	1.03815	1.82617	0.10674
C	2.17871	1.00143	-0.22364
C	-0.08994	0.99824	3.18302
C	-1.04724	1.97549	3.18637
N	-1.60259	0.50400	-1.50745
P	-1.01013	-2.15887	-0.07798
C	1.01574	0.98580	4.24060
C	-2.18347	1.96981	2.20066
C	-1.07153	3.09889	4.20250
H	3.39409	-0.69218	0.25294
H	0.75491	2.58363	-0.62338
H	2.25764	-0.10205	1.61002
H	0.86448	2.11992	1.14069
H	2.58321	1.06710	-1.23339
C	0.73275	1.87709	5.45559
C	0.23392	3.24869	4.99405
C	-1.50693	1.55094	-2.55608
C	-2.96144	2.06667	-2.63053
O	-3.73378	1.01422	-2.00940
C	-2.85374	0.24743	-1.31244
C	-2.81951	-1.84722	0.18248
C	-3.49197	-0.74902	-0.42128
C	-0.92495	1.02851	-3.90933
C	-0.87060	2.21555	-4.89459
C	-1.79073	-0.10128	-4.49879
C	0.50983	0.51222	-3.69270
C	0.22511	-5.38191	3.01987
C	-0.27746	-5.79195	1.78368
C	-0.66908	-4.84347	0.83936
C	-0.55968	-3.47333	1.12887
C	-0.04591	-3.06133	2.37003
C	0.33771	-4.02129	3.30835
C	-0.71760	-4.46029	-4.11111
C	-1.96978	-4.29210	-3.52016

C	-2.09100	-3.59625	-2.31467
C	-0.95863	-3.05305	-1.69033
C	0.29611	-3.22028	-2.29908
C	0.41632	-3.92426	-3.49607
C	-3.55008	-2.68868	1.02911
C	-4.86321	-0.56439	-0.16946
C	-4.90751	-2.48134	1.27921
C	-5.56929	-1.41817	0.67292
H	1.63130	1.97248	6.07944
H	-0.03752	1.40758	6.08376
H	0.99975	3.71037	4.35440
H	0.08753	3.92276	5.84803
H	1.16355	-0.05673	4.55114
H	1.96205	1.29034	3.76502
H	-3.15357	2.07693	2.71146
H	-2.12499	2.80563	1.48170
H	-2.20261	1.03771	1.63341
H	-1.90701	2.94709	4.91087
H	-1.30483	4.05055	3.69727
H	-3.34932	2.20806	-3.63966
H	-3.11310	2.98459	-2.05221
H	-1.86474	2.59864	-5.15002
H	-0.28411	3.04702	-4.48582
H	-0.39524	1.90440	-5.83070
H	-2.82446	0.21607	-4.67720
H	-1.37939	-0.42444	-5.46110
H	-1.81114	-0.97316	-3.83943
H	0.93324	0.16827	-4.64333
H	1.16077	1.30526	-3.30660
H	0.53387	-0.32051	-2.98622
H	-0.84072	2.33788	-2.19172
H	0.53314	-6.12290	3.75313
H	-0.36106	-6.85044	1.55138
H	-1.05071	-5.17181	-0.12248
H	0.05247	-1.99457	2.58373
H	0.73464	-3.69986	4.26758
H	-0.62513	-5.00395	-5.04730
H	-2.85621	-4.70633	-3.99340
H	-3.06972	-3.48306	-1.85829
H	1.17985	-2.79455	-1.83002
H	1.39460	-4.04935	-3.95222
H	-3.04638	-3.52225	1.50580
H	-5.36973	0.27142	-0.63613
H	-5.43921	-3.15349	1.94695
H	-6.62493	-1.24410	0.85782

Si-INT-2

	A	B	C
	-1275177.986	---	-1275254.881
Pd	0.00000	0.00000	0.00000
O	0.00000	0.00000	2.31213
C	2.58595	0.00000	0.56106
C	1.00188	1.84982	0.20379
C	2.12413	1.03984	-0.20641
C	-0.70854	0.84861	3.04414
C	-0.19291	1.54636	4.10270
N	-1.61592	0.49888	-1.53962
P	-0.91747	-2.18516	-0.19039
C	-2.18295	0.96633	2.67140
C	1.26294	1.45922	4.47430
C	-1.05494	2.38713	5.02393
H	3.32792	-0.69132	0.17161

H	0.68890	2.64674	-0.46951
H	2.25653	-0.11896	1.58864
H	0.86753	2.06592	1.26069
H	2.49627	1.14477	-1.22492
C	-2.92536	2.11328	3.36844
C	-2.56117	2.14397	4.85527
C	-1.55399	1.62267	-2.50846
C	-3.02243	2.09972	-2.54556
O	-3.76201	0.97607	-2.01772
C	-2.85834	0.18613	-1.37540
C	-2.75119	-1.98566	0.00273
C	-3.46556	-0.89695	-0.56966
C	-0.96300	1.21450	-3.89676
C	-0.93457	2.47208	-4.79137
C	-1.80544	0.11344	-4.56903
C	0.48135	0.71135	-3.71671
C	0.31942	-5.40770	2.91421
C	-0.06439	-5.81527	1.63470
C	-0.44914	-4.86949	0.68401
C	-0.45281	-3.50304	1.00947
C	-0.05637	-3.09222	2.29406
C	0.32186	-4.04954	3.23780
C	-0.37429	-4.33399	-4.28306
C	-1.65152	-4.24722	-3.72957
C	-1.84534	-3.60219	-2.50568
C	-0.76189	-3.02800	-1.82433
C	0.51827	-3.11228	-2.39591
C	0.71125	-3.76650	-3.61174
C	-3.46319	-2.91838	0.76664
C	-4.85442	-0.80960	-0.36674
C	-4.84002	-2.81003	0.96548
C	-5.53932	-1.75321	0.39201
H	-4.00985	2.00895	3.22828
H	-2.64008	3.07178	2.91051
H	-2.82965	1.17879	5.30846
H	-3.13539	2.91415	5.38679
H	-2.23544	1.07900	1.57927
H	-2.67580	0.00678	2.89358
H	1.70792	2.45751	4.60570
H	1.41252	0.93255	5.43094
H	1.83247	0.92587	3.71083
H	-0.84154	3.46100	4.87034
H	-0.76876	2.19240	6.07036
H	-3.41315	2.31422	-3.54061
H	-3.20238	2.96152	-1.89324
H	-1.93676	2.85428	-5.01469
H	-0.36241	3.28190	-4.32335
H	-0.45745	2.24093	-5.74947
H	-2.84549	0.42106	-4.72509
H	-1.38764	-0.12876	-5.55205
H	-1.80704	-0.80538	-3.97591
H	0.91239	0.44780	-4.68934
H	1.11607	1.48583	-3.27090
H	0.52021	-0.17123	-3.07429
H	-0.90817	2.39937	-2.08945
H	0.62093	-6.14641	3.65215
H	-0.06203	-6.87035	1.37323
H	-0.74006	-5.19680	-0.30973
H	-0.03708	-2.02699	2.53525
H	0.62761	-3.72667	4.22939
H	-0.22495	-4.83772	-5.23416
H	-2.50116	-4.68518	-4.24680

H	-2.84293	-3.55249	-2.08028
H	1.36391	-2.65980	-1.88384
H	1.70846	-3.82753	-4.03899
H	-2.92913	-3.74696	1.21795
H	-5.39344	0.02014	-0.80664
H	-5.35699	-3.55281	1.56676
H	-6.61091	-1.65416	0.53774

Re-7

	A	B	C
	-1275187.684	-1274959.15	-1275263.393
Pd	-0.72194	0.22606	0.45845
O	0.39954	-0.05593	2.15160
C	1.42802	3.44554	1.01799
C	-0.78594	2.28500	0.83918
C	0.39502	2.98012	0.29732
C	0.14795	0.47898	3.35494
C	1.14314	0.98986	4.13011
N	-1.92839	0.43007	-1.31722
P	-1.19772	-2.21905	0.08000
C	-1.28339	0.35598	3.85949
C	2.56183	1.08793	3.63350
C	0.90775	1.42423	5.56343
H	2.27596	3.93627	0.54836
H	-1.72460	2.61294	0.37768
H	1.45519	3.33275	2.09775
H	-0.84552	2.36776	1.92523
H	0.42457	3.12836	-0.78440
C	-1.56042	1.16942	5.13011
C	-0.43361	0.95693	6.14556
C	-1.75000	1.41419	-2.41655
C	-3.20653	1.62093	-2.89022
O	-3.91571	0.47217	-2.35868
C	-3.12073	-0.06009	-1.40044
C	-3.05239	-2.09727	0.16022
C	-3.76152	-1.09332	-0.55636
C	-0.75492	0.95704	-3.53179
C	-0.61409	2.12267	-4.53435
C	-1.25735	-0.30062	-4.26576
C	0.62776	0.66989	-2.91647
C	0.11019	-5.45614	3.13789
C	-0.57434	-5.85499	1.98640
C	-0.99032	-4.90384	1.05736
C	-0.73459	-3.53912	1.27952
C	-0.03185	-3.14460	2.42789
C	0.38333	-4.10627	3.35280
C	-0.29877	-4.48063	-3.89001
C	-1.62202	-4.37906	-3.46169
C	-1.93016	-3.69191	-2.28507
C	-0.91514	-3.09235	-1.52553
C	0.41332	-3.19168	-1.97192
C	0.71902	-3.88553	-3.14115
C	-3.78791	-2.96710	0.97279
C	-5.16130	-1.03378	-0.46531
C	-5.17766	-2.87740	1.07602
C	-5.86890	-1.91490	0.34768
H	-2.53284	0.89092	5.55663
H	-1.62115	2.23770	4.87748
H	-0.37295	-0.11316	6.39083
H	-0.64521	1.48413	7.08476
H	-1.96171	0.65496	3.04900
H	-1.49611	-0.70976	4.04151

H	2.99333	2.07743	3.84612
H	3.21598	0.35641	4.13406
H	2.61235	0.90783	2.55842
H	0.97309	2.52462	5.63186
H	1.73070	1.05525	6.19557
H	-3.34223	1.61930	-3.97159
H	-3.66542	2.52163	-2.46853
H	-1.55773	2.36128	-5.03841
H	-0.25633	3.03355	-4.04050
H	0.11032	1.86188	-5.31271
H	-2.22238	-0.14088	-4.75972
H	-0.54141	-0.58749	-5.04303
H	-1.35840	-1.14982	-3.58586
H	1.33633	0.39501	-3.70590
H	1.02833	1.54621	-2.39726
H	0.58561	-0.15120	-2.19709
H	-1.35600	2.33486	-1.97924
H	0.43860	-6.20088	3.85827
H	-0.77587	-6.90819	1.80876
H	-1.50350	-5.22391	0.15497
H	0.20499	-2.09093	2.56505
H	0.93104	-3.79413	4.23771
H	-0.06074	-5.01917	-4.80308
H	-2.41895	-4.84017	-4.03904
H	-2.96363	-3.63089	-1.95808
H	1.21100	-2.72808	-1.39674
H	1.75205	-3.95880	-3.46963
H	-3.26600	-3.73093	1.53781
H	-5.68915	-0.27470	-1.03085
H	-5.71287	-3.56674	1.72335
H	-6.95021	-1.84067	0.41435

Si-7

	A	B	C
	-1275189.407	-1274961.01	-1275266.081
Pd	-1.18906	0.38971	0.66211
O	-0.46099	0.27490	2.58217
C	0.35943	3.86990	1.65663
C	-1.58701	2.41705	1.02968
C	-0.44609	3.29745	0.74302
C	0.76894	0.69419	2.89635
C	1.02277	1.37858	4.04693
N	-2.12459	0.45339	-1.27792
P	-1.33637	-2.08771	0.29769
C	1.87924	0.30934	1.92826
C	-0.07782	1.72597	5.01368
C	2.42872	1.75850	4.46445
H	1.19811	4.49523	1.36131
H	-2.45781	2.61683	0.39512
H	0.20479	3.72100	2.72008
H	-1.86566	2.40983	2.08486
H	-0.23777	3.49812	-0.31078
C	3.29017	0.40850	2.52541
C	3.44535	1.71095	3.31623
C	-1.87036	1.47116	-2.33036
C	-3.22811	1.50445	-3.06631
O	-3.86709	0.26192	-2.67852
C	-3.20300	-0.18825	-1.58599
C	-3.15888	-2.24205	-0.04677
C	-3.84345	-1.33041	-0.89702
C	-0.63829	1.15352	-3.23930
C	-0.47070	2.33041	-4.22451

C	-0.83098	-0.15843	-4.02337
C	0.63599	1.05098	-2.38027
C	-0.51278	-4.96494	3.84414
C	-0.56271	-5.48823	2.54987
C	-0.81335	-4.64815	1.46611
C	-1.02014	-3.27294	1.67008
C	-0.95216	-2.74767	2.97146
C	-0.70542	-3.59913	4.05047
C	0.76331	-4.21981	-3.26882
C	-0.62016	-4.33798	-3.13767
C	-1.28396	-3.70604	-2.08344
C	-0.56875	-2.94140	-1.15000
C	0.82349	-2.82014	-1.29814
C	1.48424	-3.46004	-2.34506
C	-3.90654	-3.25593	0.56455
C	-5.22147	-1.49254	-1.12185
C	-5.27951	-3.39166	0.34818
C	-5.94083	-2.51139	-0.50340
H	4.04551	0.33754	1.73154
H	3.46219	-0.44291	3.19904
H	3.27285	2.56156	2.64301
H	4.46648	1.81231	3.70577
H	1.68169	-0.71571	1.58723
H	1.79707	0.95186	1.03844
H	0.04246	1.19959	5.97361
H	-0.07886	2.79971	5.25526
H	-1.05346	1.45775	4.60361
H	2.77210	1.10107	5.28328
H	2.41390	2.76827	4.90234
H	-3.16112	1.51373	-4.15420
H	-3.86899	2.32897	-2.73532
H	-1.32589	2.43975	-4.90118
H	-0.33777	3.27975	-3.69284
H	0.41564	2.17370	-4.84803
H	-1.70853	-0.13042	-4.67914
H	0.04144	-0.34283	-4.65928
H	-0.93307	-1.01572	-3.35287
H	1.50609	0.87682	-3.02350
H	0.81589	1.97108	-1.81531
H	0.57275	0.22871	-1.66369
H	-1.67856	2.42605	-1.83466
H	-0.31301	-5.62152	4.68701
H	-0.40182	-6.55022	2.38362
H	-0.84135	-5.06178	0.46228
H	-1.04503	-1.67420	3.12161
H	-0.64829	-3.18602	5.05363
H	1.27781	-4.71487	-4.08778
H	-1.18697	-4.92819	-3.85284
H	-2.35973	-3.81663	-1.98677
H	1.39046	-2.22314	-0.58818
H	2.56191	-3.36139	-2.44221
H	-3.40551	-3.95676	1.22309
H	-5.72611	-0.79866	-1.78383
H	-5.82371	-4.19058	0.84462
H	-7.00711	-2.60933	-0.68358

Re-INT-3

	A	B	C
	-1275183.336	-1274958.003	-1275264.986
Pd	0.02029	-0.01478	-0.00635

C	0.00480	-0.01128	2.07554
C	1.43854	0.00281	1.88449
C	-0.98490	3.07281	-0.68047
C	-2.32371	3.08126	-0.99374
O	-0.43733	2.33296	0.25366
C	2.04561	1.05355	1.24660
P	-1.56548	-1.60007	-0.48618
N	0.27357	0.16522	-2.17691
C	-0.01674	4.00706	-1.41191
C	-3.30377	2.31949	-0.14723
C	-2.90821	3.90344	-2.11938
H	-0.43322	-0.87058	2.57796
H	3.08908	0.98747	0.95016
H	-0.48965	0.94132	2.26126
H	1.50390	1.98107	1.06853
H	2.00229	-0.90986	2.07541
C	-0.69725	5.09017	-2.25990
C	-1.84974	4.48414	-3.06712
C	1.52614	0.58305	-2.85114
C	0.99067	1.30657	-4.10952
O	-0.39380	0.89379	-4.19273
C	-0.71056	0.33229	-2.99867
C	-2.62667	-0.93311	-1.85143
C	-2.12458	-0.06640	-2.86158
C	2.49773	-0.60547	-3.14246
C	3.75317	-0.03586	-3.83608
C	1.83484	-1.66716	-4.04088
C	2.93029	-1.26134	-1.81809
C	-4.57261	-2.77189	2.86018
C	-4.05155	-3.76795	2.03533
C	-3.15487	-3.44041	1.01633
C	-2.76589	-2.10722	0.81659
C	-3.28815	-1.11093	1.65864
C	-4.19080	-1.44242	2.66703
C	0.01487	-5.69880	-2.02099
C	-1.04138	-5.08408	-2.69347
C	-1.52917	-3.84971	-2.25892
C	-0.95680	-3.21219	-1.14820
C	0.11529	-3.83280	-0.48679
C	0.59176	-5.07094	-0.91463
C	-3.98217	-1.29119	-1.89067
C	-3.00603	0.40206	-3.85413
C	-4.83877	-0.82048	-2.88436
C	-4.34685	0.03692	-3.86652
H	0.03127	5.58368	-2.91773
H	-1.09929	5.87119	-1.59937
H	-1.45657	3.68299	-3.71056
H	-2.30021	5.23189	-3.73315
H	0.62916	4.45967	-0.64799
H	0.65748	3.40210	-2.03886
H	-4.18025	2.93816	0.10274
H	-3.69981	1.41608	-0.63966
H	-2.82327	2.01347	0.78636
H	-3.52400	4.72943	-1.71581
H	-3.61783	3.28703	-2.69942
H	1.47397	1.01636	-5.04325
H	1.01266	2.39546	-4.01178
H	3.53287	0.39812	-4.81753
H	4.22697	0.74064	-3.22404
H	4.49042	-0.83037	-3.99245
H	1.51457	-1.25715	-5.00531
H	2.54269	-2.47623	-4.25085

H	0.96171	-2.11010	-3.55300
H	3.64214	-2.07147	-2.01426
H	3.41947	-0.53681	-1.15782
H	2.07483	-1.67929	-1.28177
H	2.04519	1.28838	-2.19531
H	-5.27063	-3.02949	3.65206
H	-4.34294	-4.80472	2.18066
H	-2.76093	-4.22546	0.37937
H	-2.99030	-0.07651	1.51759
H	-4.59115	-0.66058	3.30641
H	0.39129	-6.65984	-2.36035
H	-1.49121	-5.56527	-3.55779
H	-2.35750	-3.38597	-2.78522
H	0.57791	-3.33592	0.36227
H	1.41835	-5.54177	-0.38971
H	-4.37793	-1.94699	-1.12262
H	-2.62042	1.06460	-4.61892
H	-5.88385	-1.11696	-2.88130
H	-5.00261	0.42279	-4.64140

Si-INT-3

	A	B	C
	-1275184.325	-1274959.627	-1275263.541
Pd	0.08535	0.05117	0.00298
C	0.09905	0.06630	2.12076
C	1.48942	0.13089	1.78790
C	-1.42495	3.10808	-0.53258
C	-0.91858	4.08963	-1.35444
O	-0.71681	2.36694	0.28576
C	1.92390	1.17983	0.98917
P	-1.60766	-1.43391	-0.46327
N	0.34103	0.27224	-2.15791
C	-2.93605	2.84339	-0.50375
C	0.53364	4.48344	-1.28550
C	-1.78586	4.94148	-2.25793
C	-3.80185	3.92088	-1.17195
C	-3.18091	4.35314	-2.50240
H	-3.87082	4.79804	-0.51269
H	-4.82872	3.55665	-1.31348
H	-3.82108	5.08258	-3.01670
H	-3.10060	3.47792	-3.16332
H	-3.13422	1.86433	-0.96643
H	-3.21752	2.73666	0.55278
H	1.00273	4.56421	-2.28068
H	0.67202	5.47331	-0.81737
H	1.10154	3.76148	-0.69358
H	-1.27976	5.09386	-3.22664
H	-1.89844	5.96206	-1.84297
H	-0.27688	-0.80281	2.65380
H	2.91978	1.16169	0.55618
H	-0.44505	0.99777	2.26891
H	1.32831	2.08975	0.90922
H	2.12774	-0.73549	1.95224
C	1.57175	0.86070	-2.74977
C	0.98354	1.72953	-3.87576
O	-0.29666	1.10526	-4.14078
C	-0.61646	0.42027	-3.01571
H	1.54808	1.73493	-4.80830
C	-2.56658	-0.87400	-1.94438
C	-2.00831	-0.07455	-2.97701
H	0.78733	2.75223	-3.54253
C	2.59684	-0.22657	-3.21180

C	3.84790	0.49768	-3.75167
H	3.63408	1.09375	-4.64553
H	4.27654	1.16768	-2.99708
H	4.61848	-0.23110	-4.02461
C	2.00781	-1.13724	-4.30758
H	1.70704	-0.57747	-5.19945
H	2.75379	-1.87600	-4.62082
H	1.13529	-1.68653	-3.94042
C	3.01368	-1.09656	-2.01034
H	3.74932	-1.84492	-2.32672
H	3.47242	-0.49133	-1.22082
H	2.15659	-1.61890	-1.57735
H	2.05160	1.48543	-1.99317
C	-4.85208	-1.79931	2.83354
C	-4.42168	-2.95571	2.18328
C	-3.44895	-2.87918	1.18383
C	-2.89531	-1.63952	0.83356
C	-3.32224	-0.47933	1.50191
C	-4.30117	-0.56218	2.49004
H	-5.61021	-1.86144	3.60967
H	-4.84331	-3.92101	2.45080
H	-3.12341	-3.78451	0.68062
H	-2.87930	0.48080	1.24951
H	-4.62862	0.34112	2.99739
C	-0.24286	-5.78245	-1.38631
C	-1.26719	-5.22032	-2.14821
C	-1.69493	-3.91491	-1.89869
C	-1.09560	-3.15424	-0.88395
C	-0.05365	-3.72329	-0.13408
C	0.36325	-5.03079	-0.37735
H	0.08735	-6.79885	-1.58227
H	-1.73732	-5.79736	-2.94002
H	-2.49504	-3.49179	-2.49747
H	0.43530	-3.12943	0.63376
H	1.16713	-5.45960	0.21465
C	-3.91549	-1.24700	-2.04294
H	-4.35990	-1.83662	-1.24813
C	-2.82448	0.29872	-4.06207
H	-2.39765	0.91528	-4.84279
C	-4.70710	-0.86917	-3.12564
H	-5.74904	-1.17435	-3.16554
C	-4.15512	-0.09424	-4.14268
H	-4.75818	0.21621	-4.99081

Re-8

	A	B	C
	-1275184.085	-1274956.607	-1275260.646
Pd	-0.02259	-0.00870	-0.01304
C	-0.07424	-0.04352	2.07155
C	1.28406	-0.04577	2.64928
C	1.74372	0.81524	3.57264
C	2.74014	-2.58802	0.35869
O	0.45076	-2.04464	-0.07760
C	1.39923	-2.74673	0.54783
N	-0.06303	-0.09244	-2.27796
P	-0.64102	2.17299	-0.30837
C	0.84743	-3.82459	1.47432
C	3.30085	-1.56822	-0.59698
C	3.76837	-3.45722	1.05620
H	-0.69356	0.76709	2.46605
H	-0.57998	-1.00667	2.19664
H	1.94699	-0.83490	2.29139

H	2.75720	0.74520	3.95921
H	1.11621	1.60159	3.98537
H	3.92265	-0.81965	-0.08148
H	3.95459	-2.04118	-1.34714
H	2.50609	-1.03544	-1.12363
H	0.47314	-3.34433	2.39213
H	-0.03413	-4.25816	0.98546
H	4.23196	-4.14111	0.32239
H	4.59805	-2.82778	1.41517
C	-0.15303	-1.40611	-2.96314
C	0.69470	-1.16240	-4.23116
O	0.81214	0.28518	-4.31023
C	0.43663	0.76201	-3.09746
C	0.66553	2.21139	-2.89817
C	0.25425	2.94170	-1.75085
H	0.23888	-1.50370	-5.16136
H	1.70702	-1.57194	-4.15107
H	0.30839	-2.13581	-2.29259
C	-1.62468	-1.86057	-3.22362
C	-1.57258	-3.25623	-3.88125
H	-1.07505	-3.24377	-4.85819
H	-1.04477	-3.97350	-3.24271
H	-2.58750	-3.63615	-4.04100
C	-2.37881	-0.87745	-4.13928
H	-1.91322	-0.77915	-5.12693
H	-3.40554	-1.22494	-4.29907
H	-2.43582	0.11860	-3.68872
C	-2.36873	-1.98241	-1.87912
H	-3.35279	-2.44023	-2.03591
H	-1.80022	-2.58868	-1.16808
H	-2.52317	-1.00043	-1.42346
C	0.07215	5.27782	3.07584
C	-1.18424	5.20641	2.47336
C	-1.42504	4.28429	1.45341
C	-0.40815	3.41496	1.02981
C	0.84783	3.47732	1.65593
C	1.08647	4.41058	2.66439
H	0.25751	5.99822	3.86750
H	-1.98161	5.87143	2.79359
H	-2.40428	4.24578	0.98717
H	1.63119	2.78196	1.36997
H	2.06299	4.44701	3.13889
C	-5.16660	2.51787	-1.31416
C	-4.25878	3.32747	-1.99753
C	-2.89328	3.24211	-1.72085
C	-2.42081	2.33580	-0.76029
C	-3.34120	1.51689	-0.08487
C	-4.70572	1.61390	-0.35574
H	-6.22882	2.58664	-1.53196
H	-4.61227	4.02938	-2.74792
H	-2.19859	3.88161	-2.25642
H	-2.98116	0.79589	0.64411
H	-5.40639	0.97525	0.17482
C	0.53705	4.31430	-1.70759
H	0.23630	4.88962	-0.83949
C	1.33002	2.88334	-3.93855
H	1.63851	2.31412	-4.80673
C	1.19794	4.96600	-2.74960
H	1.39683	6.03152	-2.67544
C	1.59674	4.24778	-3.87202
H	2.11412	4.73928	-4.69038
C	3.20267	-4.27623	2.22450

H	3.04310	-3.61840	3.09037
H	3.92609	-5.03988	2.53751
C	1.86672	-4.91378	1.83051
H	1.48140	-5.55128	2.63658
H	2.02299	-5.56726	0.96022

Si-8

	A	B	C
	-1275184.085	-1274956.607	-1275260.646
Pd	0.05289	-0.06571	-0.05798
C	0.12060	-0.24448	2.03440
C	1.48547	-0.18110	2.56694
C	2.02381	0.87491	3.20164
C	3.59040	2.18205	0.72037
O	1.89867	0.89796	-0.30070
C	2.30542	2.01485	0.28778
N	-0.14979	0.13423	-2.36423
P	-1.97782	-1.11236	-0.28813
C	1.27726	3.13298	0.39193
C	4.58626	1.05642	0.65513
C	4.11759	3.51849	1.20097
H	-0.51581	0.56663	2.40272
H	-0.35918	-1.20662	2.23397
H	2.10635	-1.06456	2.41367
H	3.04296	0.86043	3.57473
H	1.44980	1.78048	3.38321
H	5.30900	1.19344	-0.16518
H	5.17987	0.99635	1.57900
H	4.08033	0.10136	0.50018
H	1.01998	3.46557	-0.62662
H	0.35400	2.69961	0.80131
H	4.31034	3.47498	2.28715
H	5.10385	3.70666	0.74749
C	1.05470	0.41855	-3.18000
C	0.50446	1.38674	-4.25288
O	-0.93897	1.26853	-4.13821
C	-1.17620	0.60356	-2.97819
C	-2.60319	0.51895	-2.59181
C	-3.08813	-0.19628	-1.46348
H	0.77216	1.13263	-5.27966
H	0.76845	2.43155	-4.05930
H	1.77006	0.91007	-2.51535
C	1.72650	-0.87734	-3.73088
C	2.97485	-0.45787	-4.53556
H	2.72499	0.14597	-5.41589
H	3.66844	0.12043	-3.91484
H	3.50863	-1.34483	-4.89384
C	0.76789	-1.68245	-4.62870
H	0.43657	-1.11277	-5.50510
H	1.26575	-2.58547	-4.99906
H	-0.12061	-1.99960	-4.07369
C	2.17970	-1.75188	-2.54526
H	2.76689	-2.60378	-2.90847
H	2.78960	-1.17627	-1.84253
H	1.32128	-2.14408	-1.99408
C	-4.51728	-1.64084	3.56987
C	-4.25153	-2.75431	2.77403
C	-3.51676	-2.61764	1.59410
C	-3.03504	-1.36094	1.20039
C	-3.29943	-0.24657	2.01517
C	-4.04226	-0.38478	3.18526
H	-5.08630	-1.75066	4.48898

H	-4.61509	-3.73504	3.06904
H	-3.31925	-3.49250	0.98346
H	-2.91811	0.73078	1.73185
H	-4.23924	0.48617	3.80408
C	-1.59671	-5.41750	-1.99980
C	-2.67354	-4.62354	-2.39679
C	-2.80553	-3.32282	-1.90823
C	-1.85329	-2.79892	-1.02116
C	-0.76725	-3.60143	-0.63553
C	-0.64441	-4.90470	-1.11734
H	-1.49710	-6.43010	-2.38109
H	-3.41543	-5.01673	-3.08663
H	-3.65138	-2.71776	-2.22000
H	-0.01498	-3.19513	0.03531
H	0.20054	-5.51461	-0.80994
C	-4.47011	-0.19432	-1.22414
H	-4.85936	-0.73132	-0.36648
C	-3.51630	1.19459	-3.41945
H	-3.13366	1.73721	-4.27513
C	-5.36249	0.48169	-2.05677
H	-6.42619	0.45694	-1.83632
C	-4.88385	1.18072	-3.16069
H	-5.56486	1.71445	-3.81673
C	3.18138	4.69631	0.89661
H	3.24323	4.94572	-0.17206
H	3.50081	5.58971	1.44818
C	1.73451	4.32805	1.23864
H	1.06298	5.18280	1.08549
H	1.67454	4.06816	2.30452

Re-INT4

	A	B	C
	-1275174.727	-1274949.011	-1275255.984
Pd	0.00000	0.00000	0.00000
O	0.00000	0.00000	2.56617
C	2.23258	0.00000	1.68232
C	-1.73080	3.26479	0.21685
P	-0.55409	-0.59314	-2.13430
N	-0.64698	-2.17231	0.42667
C	0.33222	2.00290	-0.43906
C	-0.97089	2.63984	-0.70014
C	1.15191	0.56461	2.37736
C	1.30411	1.94848	3.02263
C	2.38305	-1.50015	1.54935
C	3.52934	0.75874	1.45676
C	2.74275	2.47328	3.11178
C	3.46707	2.25816	1.77948
H	3.28362	1.93226	3.90130
H	2.74842	3.53252	3.39976
H	4.48193	2.67519	1.81249
H	2.93559	2.79760	0.98377
H	0.66783	2.66915	2.48793
H	0.85083	1.85301	4.01710
H	2.55045	-1.84884	0.52000
H	3.26029	-1.83872	2.12857
H	1.50756	-2.01533	1.94624
H	3.87753	0.61768	0.42021
H	4.32326	0.30300	2.07959
H	1.02155	2.06193	-1.28136
H	-2.68529	3.71335	-0.04442
H	0.80351	2.36444	0.47055
H	-1.42125	3.33973	1.25588

H	-1.33655	2.59236	-1.72747
C	-1.20682	-2.61551	1.73069
C	-0.74239	-4.09000	1.79412
O	-0.31749	-4.39531	0.43587
C	-0.22772	-3.20656	-0.20603
H	-1.52164	-4.80589	2.05827
C	0.29425	-2.20919	-2.50095
C	0.36284	-3.26918	-1.56020
H	0.12149	-4.23697	2.45006
C	-2.74792	-2.40332	1.85137
C	-3.17273	-2.87562	3.25870
H	-3.00452	-3.94816	3.41325
H	-2.62744	-2.33090	4.03736
H	-4.24233	-2.69293	3.40951
C	-3.52576	-3.18920	0.77874
H	-3.35776	-4.27095	0.84561
H	-4.60225	-3.02217	0.89626
H	-3.25182	-2.86558	-0.22990
C	-3.06498	-0.90042	1.72920
H	-4.12963	-0.72438	1.92611
H	-2.46638	-0.31344	2.43141
H	-2.84239	-0.53205	0.72465
H	-0.72513	-1.99392	2.49057
C	0.97011	2.19750	-5.52817
C	-0.37262	1.82352	-5.50450
C	-0.85072	0.97322	-4.50442
C	0.01340	0.49348	-3.50965
C	1.36479	0.88397	-3.53689
C	1.83938	1.72199	-4.54321
H	1.33905	2.85790	-6.30798
H	-1.05437	2.18935	-6.26740
H	-1.89608	0.68285	-4.50433
H	2.04528	0.52423	-2.76937
H	2.88669	2.01056	-4.55321
C	-5.02845	-1.33012	-3.19354
C	-4.05592	-2.20123	-3.68737
C	-2.71002	-2.00461	-3.37390
C	-2.32093	-0.93478	-2.55225
C	-3.30629	-0.06920	-2.05013
C	-4.64932	-0.26373	-2.37586
H	-6.07521	-1.48504	-3.43950
H	-4.34253	-3.03615	-4.32123
H	-1.96495	-2.68667	-3.77134
H	-3.02081	0.75210	-1.39887
H	-5.40034	0.41455	-1.98049
C	0.87955	-2.40420	-3.75968
H	0.83277	-1.61297	-4.49857
C	1.00997	-4.46374	-1.91106
H	1.05200	-5.26295	-1.18085
C	1.52669	-3.59556	-4.09165
H	1.97229	-3.70738	-5.07644
C	1.59423	-4.62919	-3.16354
H	2.09687	-5.56033	-3.40800

Re-9

	A	B	C
	-1275184.231	-1274957.92	-1275265.951
Pd	-0.01139	0.06715	-0.02488
C	-0.07679	-0.05451	2.20284
C	2.09228	0.13323	-0.07999
C	2.88206	-1.09344	0.13805
C	3.82939	-1.27328	1.07488

C	-1.09407	0.96154	2.55567
O	-2.30653	0.71329	2.60144
N	-2.27435	0.67042	-0.43300
P	-0.39505	-0.94824	-2.22886
C	-0.61790	2.38336	2.88687
C	-0.61958	-1.48533	2.30556
C	1.21296	0.08483	3.02664
H	2.20311	0.47863	-1.11619
H	2.39102	0.93303	0.59960
H	2.69907	-1.91333	-0.55350
H	4.37680	-2.20899	1.15623
H	4.10514	-0.48746	1.77383
H	1.01605	-0.36607	4.01669
H	2.00529	-0.52750	2.58856
H	0.13364	-2.21179	1.98284
H	-0.88261	-1.72430	3.34926
H	-1.52842	-1.63066	1.71691
H	-0.32647	2.88074	1.95138
H	-1.47478	2.92521	3.30006
C	-2.94559	1.93374	-0.02020
C	-4.37031	1.44685	0.31038
O	-4.46734	0.16883	-0.37666
C	-3.19634	-0.19406	-0.66578
C	-3.06650	-1.54259	-1.26445
C	-1.94633	-1.97312	-2.02326
H	-5.17920	2.07576	-0.06313
H	-4.48530	1.26257	1.38109
H	-2.47374	2.29558	0.89138
C	-2.84149	3.05814	-1.09678
C	-1.35725	3.40755	-1.31385
H	-0.78758	2.53526	-1.64238
H	-1.25492	4.19131	-2.07332
H	-0.90009	3.77689	-0.38873
C	-3.47694	2.63669	-2.43499
H	-2.95323	1.78491	-2.87733
H	-4.53281	2.36556	-2.32209
H	-3.42748	3.46225	-3.15346
C	-3.56335	4.30883	-0.55213
H	-3.43246	5.14981	-1.24168
H	-4.64110	4.15199	-0.43363
H	-3.15879	4.61005	0.42109
C	2.69807	-4.20071	-3.49379
C	2.41888	-3.14949	-4.36481
C	1.47993	-2.17417	-4.01782
C	0.81532	-2.23278	-2.78538
C	1.11802	-3.28863	-1.90628
C	2.04132	-4.26887	-2.26235
H	3.42349	-4.96143	-3.76884
H	2.92541	-3.08747	-5.32436
H	1.26405	-1.37283	-4.71658
H	0.62334	-3.34518	-0.94028
H	2.25447	-5.08202	-1.57382
C	-1.01761	1.47320	-6.16409
C	-1.81885	0.35555	-5.92263
C	-1.66469	-0.38148	-4.74727
C	-0.71039	-0.00340	-3.78989
C	0.08193	1.12945	-4.03643
C	-0.06548	1.85730	-5.21815
H	-1.13748	2.04286	-7.08125
H	-2.56403	0.05130	-6.65284
H	-2.28836	-1.25384	-4.57853
H	0.81628	1.44298	-3.29887

H	0.55963	2.72819	-5.39475
C	-2.01416	-3.23894	-2.62449
H	-1.18299	-3.58743	-3.22553
C	-4.17084	-2.39685	-1.11189
C	-4.19896	-3.65902	-1.69634
H	-5.01420	-2.05061	-0.52678
C	-3.11951	-4.07582	-2.46753
H	-3.12698	-5.05014	-2.94879
H	-5.06150	-4.30363	-1.55498
C	1.70487	1.51802	3.26802
H	2.56579	1.50001	3.94869
H	2.05511	1.96635	2.32934
C	0.58439	2.38898	3.84343
H	0.92757	3.41667	4.01628
H	0.27475	1.99222	4.82070

Si-9

	A	B	C
	-1275186.417	-1274961.07	-1275270.598
Pd	-0.01139	0.06715	-0.02488
C	-0.07679	-0.05451	2.20284
C	2.09228	0.13323	-0.07999
C	2.88206	-1.09344	0.13805
C	3.82939	-1.27328	1.07488
C	-1.09407	0.96154	2.55567
O	-2.30653	0.71329	2.60144
N	-2.27435	0.67042	-0.43300
P	-0.39505	-0.94824	-2.22886
C	-0.61790	2.38336	2.88687
C	-0.61958	-1.48533	2.30556
C	1.21296	0.08483	3.02664
H	2.20311	0.47863	-1.11619
H	2.39102	0.93303	0.59960
H	2.69907	-1.91333	-0.55350
H	4.37680	-2.20899	1.15623
H	4.10514	-0.48746	1.77383
H	1.01605	-0.36607	4.01669
H	2.00529	-0.52750	2.58856
H	0.13364	-2.21179	1.98284
H	-0.88261	-1.72430	3.34926
H	-1.52842	-1.63066	1.71691
H	-0.32647	2.88074	1.95138
H	-1.47478	2.92521	3.30006
C	-2.94559	1.93374	-0.02020
C	-4.37031	1.44685	0.31038
O	-4.46734	0.16883	-0.37666
C	-3.19634	-0.19406	-0.66578
C	-3.06650	-1.54259	-1.26445
C	-1.94633	-1.97312	-2.02326
H	-5.17920	2.07576	-0.06313
H	-4.48530	1.26257	1.38109
H	-2.47374	2.29558	0.89138
C	-2.84149	3.05814	-1.09678
C	-1.35725	3.40755	-1.31385
H	-0.78758	2.53526	-1.64238
H	-1.25492	4.19131	-2.07332
H	-0.90009	3.77689	-0.38873
C	-3.47694	2.63669	-2.43499
H	-2.95323	1.78491	-2.87733
H	-4.53281	2.36556	-2.32209
H	-3.42748	3.46225	-3.15346
C	-3.56335	4.30883	-0.55213

H	-3.43246	5.14981	-1.24168
H	-4.64110	4.15199	-0.43363
H	-3.15879	4.61005	0.42109
C	2.69807	-4.20071	-3.49379
C	2.41888	-3.14949	-4.36481
C	1.47993	-2.17417	-4.01782
C	0.81532	-2.23278	-2.78538
C	1.11802	-3.28863	-1.90628
C	2.04132	-4.26887	-2.26235
H	3.42349	-4.96143	-3.76884
H	2.92541	-3.08747	-5.32436
H	1.26405	-1.37283	-4.71658
H	0.62334	-3.34518	-0.94028
H	2.25447	-5.08202	-1.57382
C	-1.01761	1.47320	-6.16409
C	-1.81885	0.35555	-5.92263
C	-1.66469	-0.38148	-4.74727
C	-0.71039	-0.00340	-3.78989
C	0.08193	1.12945	-4.03643
C	-0.06548	1.85730	-5.21815
H	-1.13748	2.04286	-7.08125
H	-2.56403	0.05130	-6.65284
H	-2.28836	-1.25384	-4.57853
H	0.81628	1.44298	-3.29887
H	0.55963	2.72819	-5.39475
C	-2.01416	-3.23894	-2.62449
H	-1.18299	-3.58743	-3.22553
C	-4.17084	-2.39685	-1.11189
C	-4.19896	-3.65902	-1.69634
H	-5.01420	-2.05061	-0.52678
C	-3.11951	-4.07582	-2.46753
H	-3.12698	-5.05014	-2.94879
H	-5.06150	-4.30363	-1.55498
C	1.70487	1.51802	3.26802
H	2.56579	1.50001	3.94869
H	2.05511	1.96635	2.32934
C	0.58439	2.38898	3.84343
H	0.92757	3.41667	4.01628
H	0.27475	1.99222	4.82070

Si-INT-5

	A	B	C
	-1275148.111	-1274921.705	-1275222.638
Pd	0.46367	-0.34557	-0.19517
C	1.29512	0.80497	1.80093
C	2.06948	-1.18125	1.15757
C	1.64226	-2.08689	2.23574
C	2.38520	-2.46096	3.29141
C	-0.01098	0.62841	2.56332
O	-0.94545	-0.02200	2.11528
N	-2.53152	0.80536	-1.00818
P	-0.38362	-0.97856	-2.27186
C	-0.19987	1.39300	3.87644
C	1.19487	2.04194	0.87286
C	2.50329	1.00495	2.74052
H	2.00675	-1.68187	0.17427
H	3.07188	-0.77762	1.26842
H	0.64088	-2.50229	2.13029
H	2.00854	-3.16744	4.02566
H	3.40379	-2.10747	3.43427
H	2.78285	0.05649	3.20712
H	3.36187	1.33737	2.14443

H	2.08772	2.11162	0.24436
H	0.31619	2.03846	0.21906
H	1.15110	2.96489	1.47443
H	-0.52862	2.40394	3.58716
H	-1.03674	0.93086	4.40902
C	-3.00252	1.83442	-0.06364
C	-3.91920	1.04131	0.90864
O	-4.07688	-0.24857	0.27274
C	-3.18394	-0.26604	-0.76018
C	-3.12370	-1.52682	-1.52395
C	-2.00609	-1.90488	-2.31472
H	-4.91448	1.46989	1.05036
H	-3.44351	0.87581	1.87846
H	-2.13717	2.23093	0.48086
C	-3.66391	3.03631	-0.80762
C	-2.61100	3.68338	-1.72805
H	-2.23842	2.96828	-2.46477
H	-3.04068	4.54029	-2.26059
H	-1.75389	4.04896	-1.14895
C	-4.86330	2.57376	-1.65655
H	-4.54702	1.85559	-2.41871
H	-5.64467	2.10288	-1.04887
H	-5.31839	3.42948	-2.16827
C	-4.12676	4.07551	0.23206
H	-4.53670	4.95959	-0.26896
H	-4.90914	3.68471	0.89249
H	-3.29151	4.40815	0.86028
C	2.56850	-3.97615	-4.30932
C	2.05032	-2.92156	-5.05908
C	1.14373	-2.02578	-4.48612
C	0.75153	-2.16484	-3.14686
C	1.28769	-3.22831	-2.40015
C	2.17890	-4.13057	-2.97635
H	3.27361	-4.67135	-4.75705
H	2.34884	-2.79219	-6.09636
H	0.74589	-1.21505	-5.08730
H	1.00185	-3.34465	-1.35757
H	2.57743	-4.94876	-2.38218
C	-0.74999	2.35490	-5.50225
C	-1.66089	1.29756	-5.51191
C	-1.58141	0.29156	-4.54694
C	-0.59395	0.33584	-3.55294
C	0.30973	1.40800	-3.54545
C	0.23719	2.40699	-4.51624
H	-0.81227	3.13616	-6.25522
H	-2.43476	1.25253	-6.27410
H	-2.29290	-0.52855	-4.56794
H	1.06800	1.45500	-2.76751
H	0.94722	3.22980	-4.49823
C	-2.11053	-3.09135	-3.05908
H	-1.27637	-3.40693	-3.67515
C	-4.26007	-2.35049	-1.47838
C	-4.33481	-3.52254	-2.22431
H	-5.09161	-2.04733	-0.85216
C	-3.25609	-3.88655	-3.02677
H	-3.29607	-4.79237	-3.62619
C	2.24012	1.99533	3.89172
H	3.14645	2.07606	4.50387
H	2.03336	3.00444	3.51058
C	1.06293	1.50845	4.74043
H	0.87457	2.18278	5.58412
H	1.30437	0.52607	5.16760

H -5.22737 -4.13993 -2.18101

Re-INT-6

	A	B	C
	-1275185.937	-1274958.968	-1275261.796
Pd	0.08183	0.03521	0.00932
C	0.10557	0.09571	2.15852
C	1.48044	0.01558	2.51926
C	2.14057	-1.15028	2.89924
C	3.07702	-2.24491	1.23232
C	1.85283	-2.55743	0.60382
O	1.30015	-1.75693	-0.23019
N	0.26666	0.14443	-2.45252
P	-1.30127	1.82615	-0.46366
C	1.07632	-3.80282	1.01077
C	3.92466	-1.14066	0.64306
C	3.85538	-3.33575	1.95538
H	-0.38756	1.04502	2.35655
H	-0.51028	-0.76620	2.43264
H	2.06975	0.92898	2.43804
H	3.11901	-1.06427	3.36345
H	1.54512	-1.98765	3.25036
H	4.64598	-0.75915	1.37604
H	4.50275	-1.50954	-0.21687
H	3.30319	-0.31304	0.29616
H	0.38702	-3.53436	1.82863
H	0.44303	-4.09095	0.16466
H	4.59549	-3.75279	1.25153
H	4.45093	-2.89201	2.76617
C	0.86469	-1.01182	-3.15804
C	1.97407	-0.35456	-4.01296
O	1.66497	1.06043	-3.97102
C	0.72822	1.21515	-2.99248
C	0.34989	2.61703	-2.71304
C	-0.54974	3.01500	-1.68585
H	1.98837	-0.65854	-5.06146
H	2.97265	-0.49219	-3.58494
H	1.29260	-1.67129	-2.39945
C	-0.20415	-1.82331	-3.95371
C	0.50056	-3.02204	-4.62157
H	1.24574	-2.71047	-5.36286
H	1.00758	-3.64694	-3.87717
H	-0.23028	-3.65071	-5.14205
C	-0.89886	-0.95952	-5.02330
H	-0.19373	-0.56537	-5.76451
H	-1.64268	-1.55364	-5.56586
H	-1.42029	-0.11292	-4.56625
C	-1.25881	-2.35746	-2.96555
H	-1.97521	-3.00331	-3.48671
H	-0.78790	-2.93861	-2.16595
H	-1.81228	-1.53933	-2.49912
C	-2.48044	4.56526	3.11424
C	-3.48786	3.99205	2.33937
C	-3.16520	3.19262	1.24007
C	-1.82533	2.95282	0.90313
C	-0.81743	3.52406	1.70142
C	-1.14204	4.33100	2.78992
H	-2.73466	5.18643	3.96875
H	-4.53159	4.16797	2.58649
H	-3.96139	2.75971	0.64333
H	0.22696	3.33622	1.46405
H	-0.34973	4.76829	3.39143

C	-5.40020	0.55550	-2.27924
C	-4.80657	1.74274	-2.71131
C	-3.57142	2.14172	-2.19628
C	-2.90745	1.35129	-1.24596
C	-3.50616	0.15171	-0.82877
C	-4.74635	-0.23884	-1.33578
H	-6.36246	0.24885	-2.67982
H	-5.30646	2.36420	-3.44958
H	-3.12616	3.07172	-2.53668
H	-2.98581	-0.47755	-0.11121
H	-5.19589	-1.16908	-0.99949
C	-0.83950	4.38396	-1.56451
H	-1.52136	4.71273	-0.78846
C	0.91750	3.59634	-3.54845
H	1.60579	3.27813	-4.32183
C	-0.27642	5.34025	-2.40867
H	-0.53486	6.38811	-2.28089
C	0.61215	4.94561	-3.40515
C	2.99025	-4.47947	2.50474
H	2.44713	-4.14076	3.39703
H	3.63374	-5.30585	2.83108
C	1.98183	-4.96043	1.45519
H	1.37851	-5.78876	1.84691
H	2.52443	-5.35293	0.58346
H	1.06484	5.67786	-4.06713

Si-INT-6

	A	B	C
	-1275185.824	-1274959.209	-1275261.586
Pd	0.03155	-0.04492	-0.00455
C	0.03852	-0.08605	2.14545
C	1.40666	-0.02991	2.52764
C	2.08370	1.13642	2.89626
C	3.19810	2.12429	1.32446
C	2.06174	2.29905	0.50027
O	1.68507	1.38730	-0.30995
N	0.09250	-0.16166	-2.45114
P	-1.86893	-1.26730	-0.45925
C	1.16090	3.52095	0.65126
C	4.16440	1.01604	0.96659
C	3.81648	3.33090	2.03006
H	-0.56877	0.78317	2.41353
H	-0.47660	-1.02753	2.33344
H	1.97488	-0.95897	2.49336
H	3.01847	1.03601	3.44052
H	1.49198	2.00113	3.18688
H	4.83230	1.33384	0.15319
H	4.80024	0.75166	1.82019
H	3.63077	0.12518	0.63119
H	1.10191	3.99645	-0.33821
H	0.14563	3.16078	0.86572
H	3.78482	3.18877	3.12158
H	4.88472	3.37761	1.77611
C	1.36291	0.17780	-3.13098
C	0.92814	1.26538	-4.14368
O	-0.51865	1.18392	-4.15789
C	-0.86601	0.39661	-3.10093
C	-2.31908	0.28433	-2.85613
C	-2.89212	-0.43537	-1.76932
H	1.27693	1.10856	-5.16632
H	1.20429	2.27357	-3.81840
H	2.03481	0.59892	-2.37870

C	2.04879	-1.07937	-3.74964
C	3.36013	-0.63205	-4.42789
H	3.18592	0.03942	-5.27657
H	4.01582	-0.11421	-3.71824
H	3.90526	-1.50182	-4.81088
C	1.13700	-1.77671	-4.77718
H	0.86200	-1.11457	-5.60685
H	1.64702	-2.64505	-5.20941
H	0.21564	-2.13297	-4.30673
C	2.39161	-2.06834	-2.61866
H	2.91830	-2.94107	-3.02309
H	3.03940	-1.60050	-1.86874
H	1.48947	-2.41831	-2.11244
C	-4.83272	-2.06407	3.04381
C	-4.51801	-3.10928	2.17549
C	-3.65595	-2.89494	1.09862
C	-3.09226	-1.62855	0.87905
C	-3.40779	-0.58607	1.76736
C	-4.27823	-0.79963	2.83462
H	-5.50119	-2.23499	3.88324
H	-4.94384	-4.09663	2.33421
H	-3.42208	-3.71722	0.43023
H	-2.96076	0.39375	1.62103
H	-4.51278	0.01765	3.51119
C	-1.00609	-5.54278	-2.08427
C	-2.00492	-4.77855	-2.68819
C	-2.27806	-3.48812	-2.22917
C	-1.54539	-2.94226	-1.16509
C	-0.53322	-3.71493	-0.57320
C	-0.27137	-5.00843	-1.02405
H	-0.79718	-6.54754	-2.44147
H	-2.57783	-5.18731	-3.51644
H	-3.06583	-2.90827	-2.70048
H	0.05540	-3.29151	0.23646
H	0.51364	-5.59449	-0.55396
C	-4.29157	-0.45877	-1.66203
H	-4.74921	-0.99692	-0.83951
C	-3.16537	0.93394	-3.77223
H	-2.71523	1.48008	-4.59240
C	-5.11507	0.18671	-2.58367
H	-6.19432	0.13598	-2.46670
C	-4.54997	0.88799	-3.64585
C	3.15078	4.67100	1.67549
H	3.46634	4.98208	0.66957
H	3.49007	5.45226	2.36678
C	1.62435	4.54289	1.70128
H	1.14617	5.51307	1.51906
H	1.30614	4.22859	2.70453
H	-5.17811	1.39774	-4.37027