Electronic Supplementary Material (ESI) for ChemComm.

Can Silylenes Rival Transition Metal Systems in Bond-Strengthening π-Back Donation? A Computational Investigation

Electronic Supporting Information

Amrita Pal and Kumar Vanka*
Physical Chemistry Division, National Chemical Laboratory, Dr. HomiBhabha Road, Pashan,Pune-411008, India.

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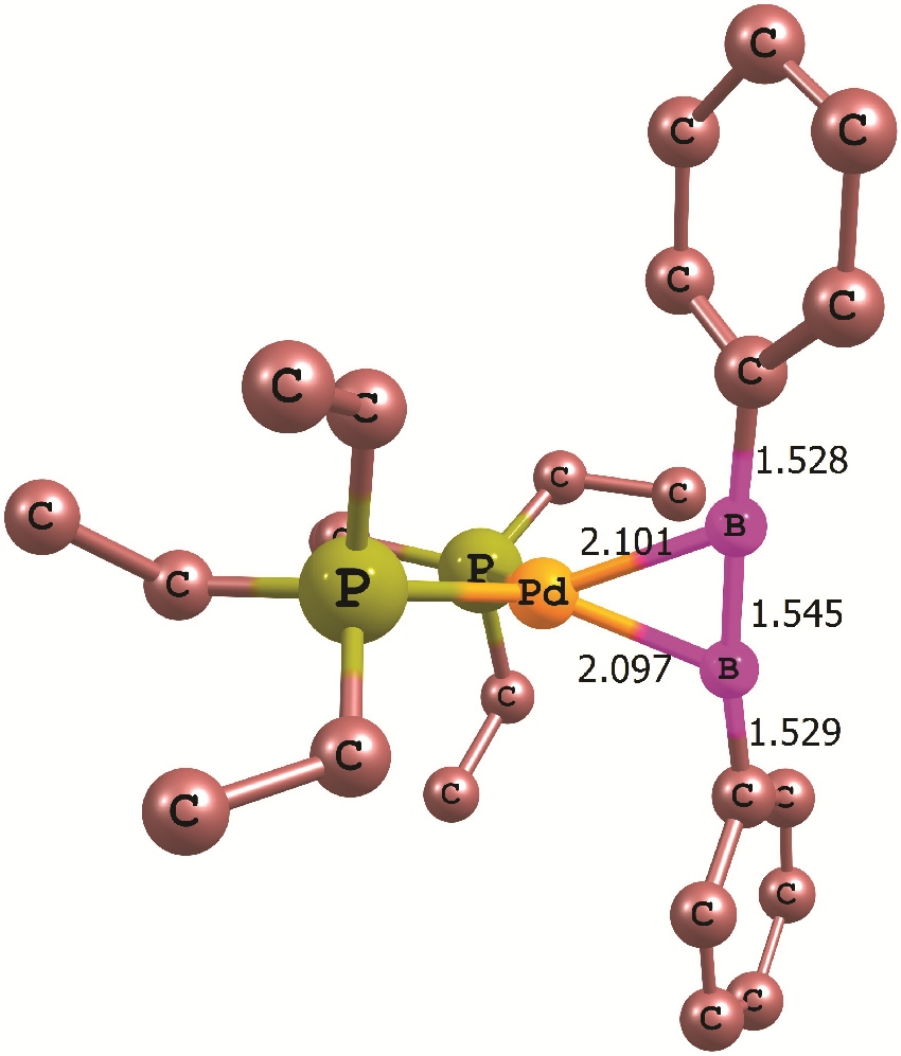


Fig. S1 The optimized structure of $Pd(PEt_3)_2$complexed to the π-diborene; hydrogen atoms have not been shown for the purpose of clarity.

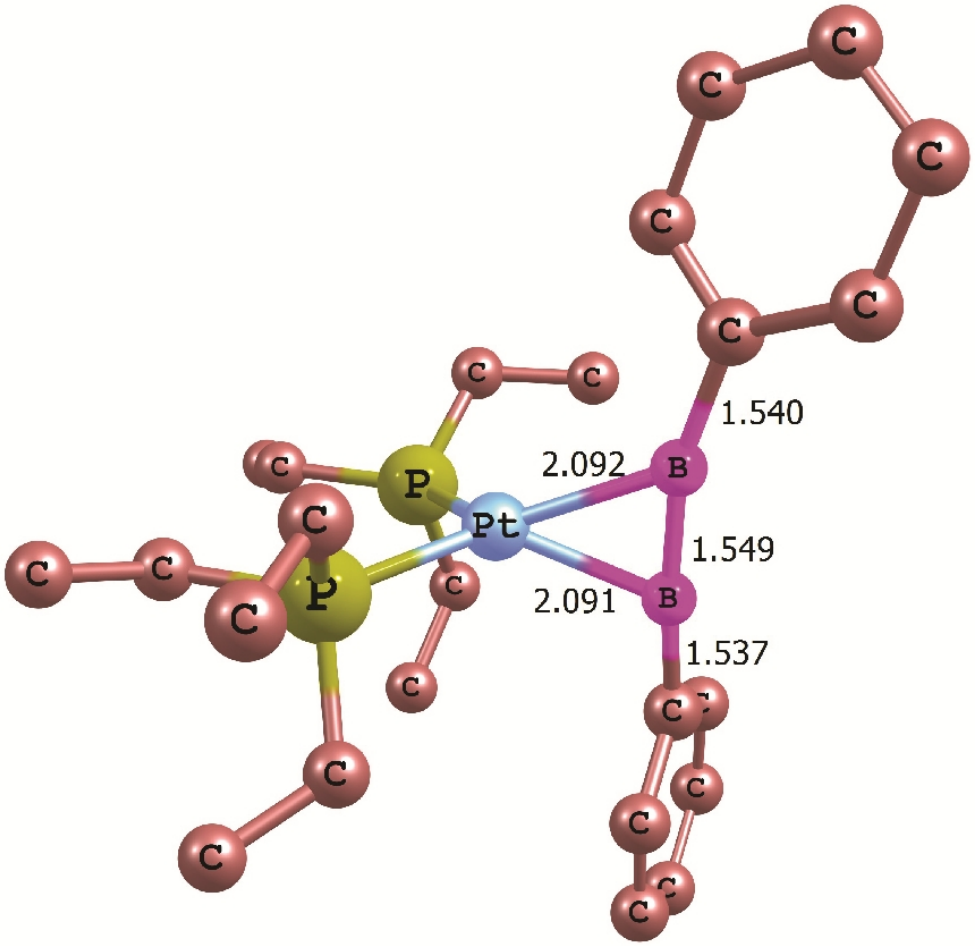


Fig. S2 The optimized structure of $Pt(PEt_3)_2$complexed to the π-diborene; hydrogen atoms have not been shown for the purpose of clarity.

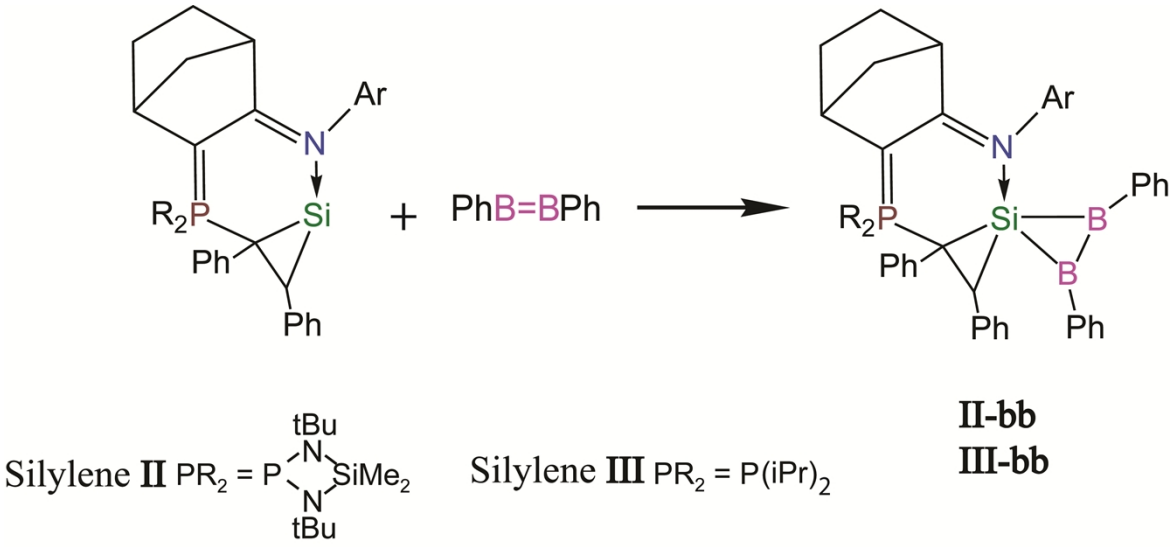


Fig. S3 The schematic representation of silylene **II** and **III** complexed with π-diborene.

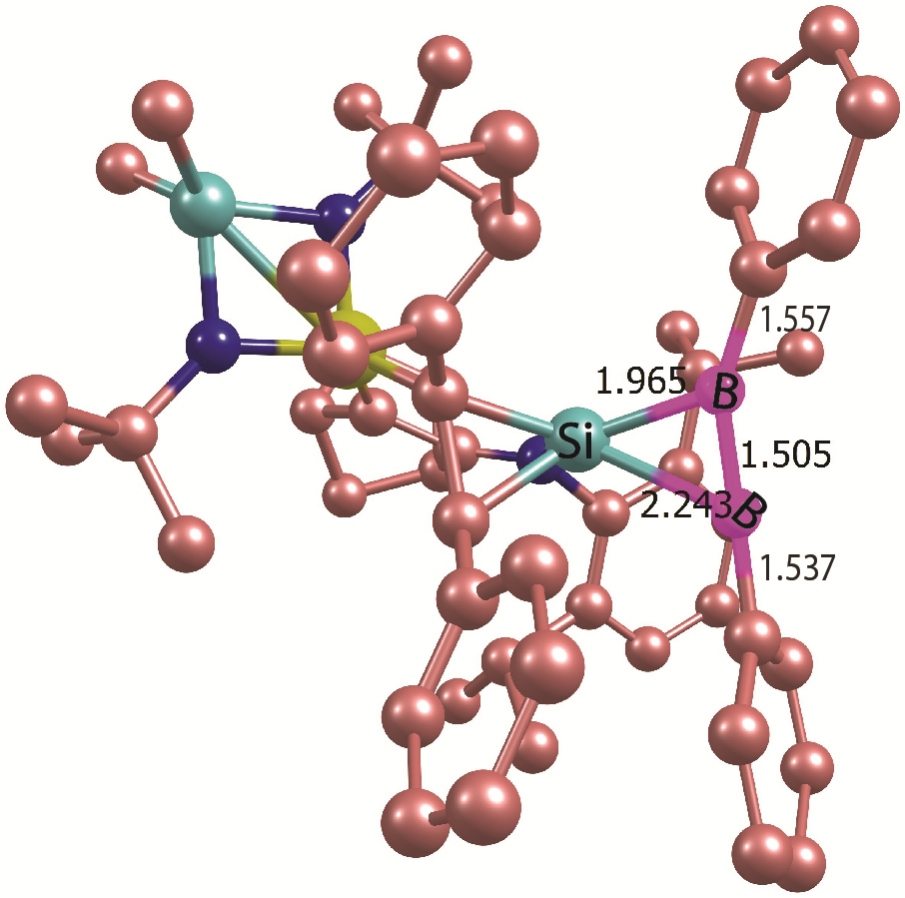


Fig. S4 The optimized structure for silylene **II** complexed to the π-diborene; hydrogen atoms have not been shown for the purpose of clarity.

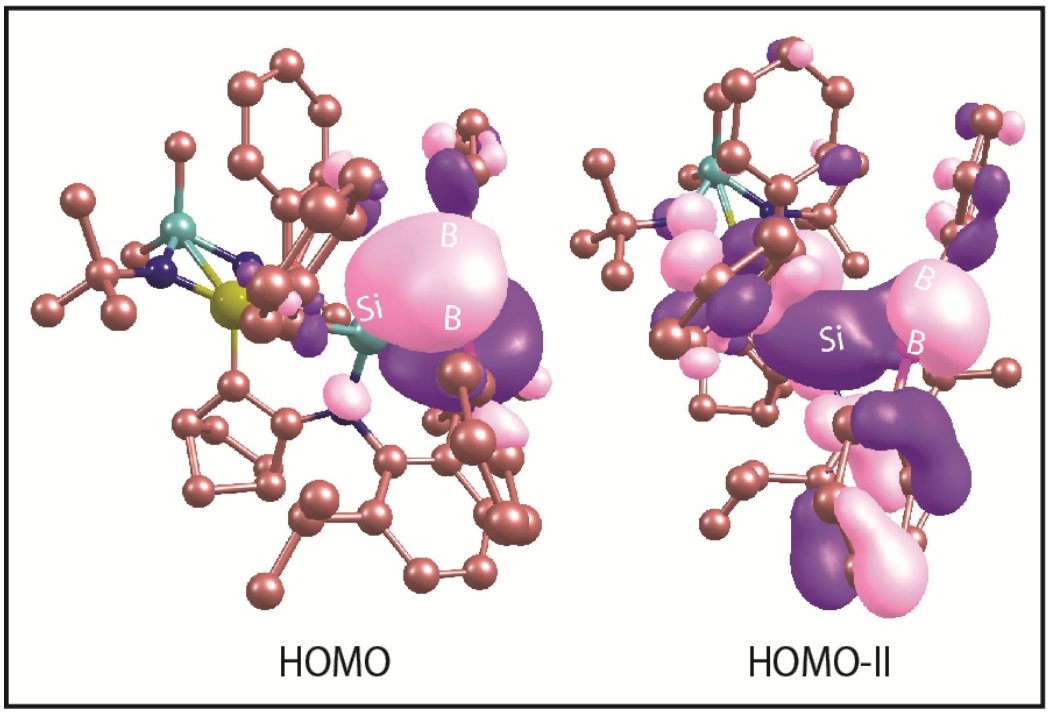


Fig. S5 The HOMO (-0.12 Ha) and the HOMO-II (-0.165 Ha) for the complex shown in Figure S4 above.

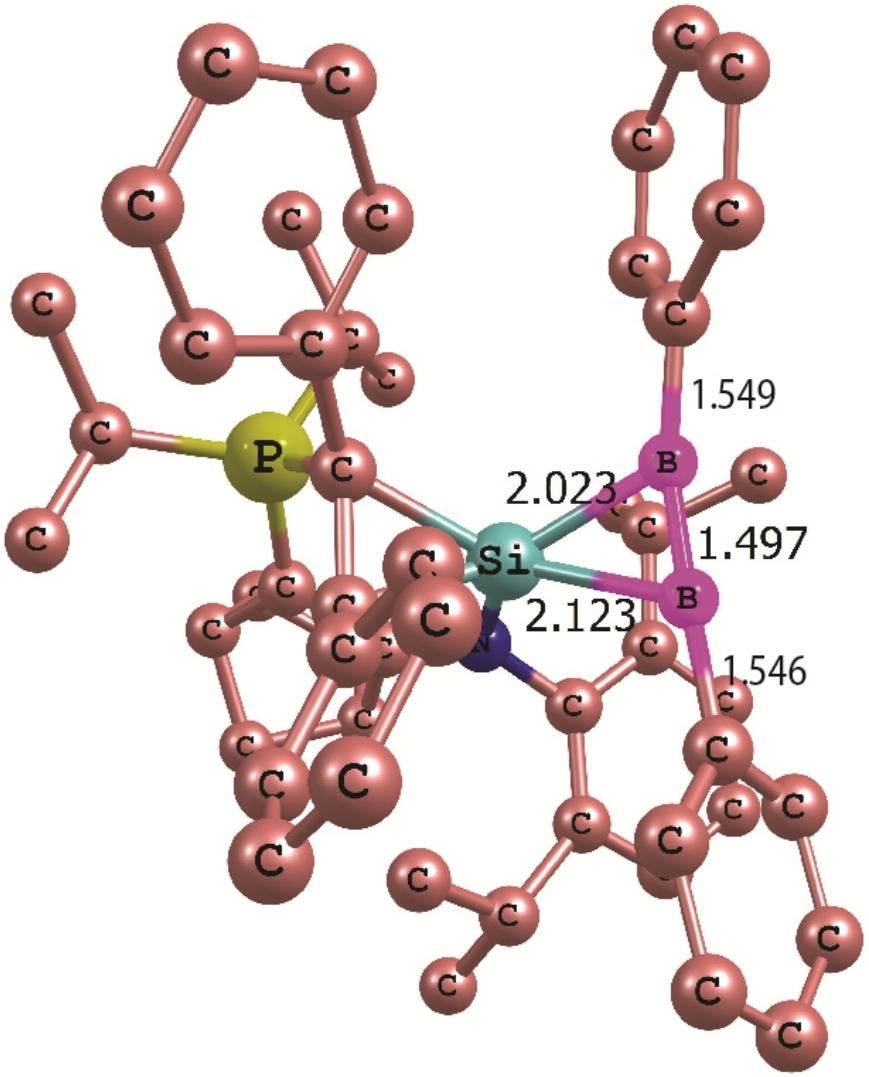


Fig. S6 The optimized structure of silylene **III** complexed to the π-diborene; hydrogen atoms have not been shown for the purpose of clarity.

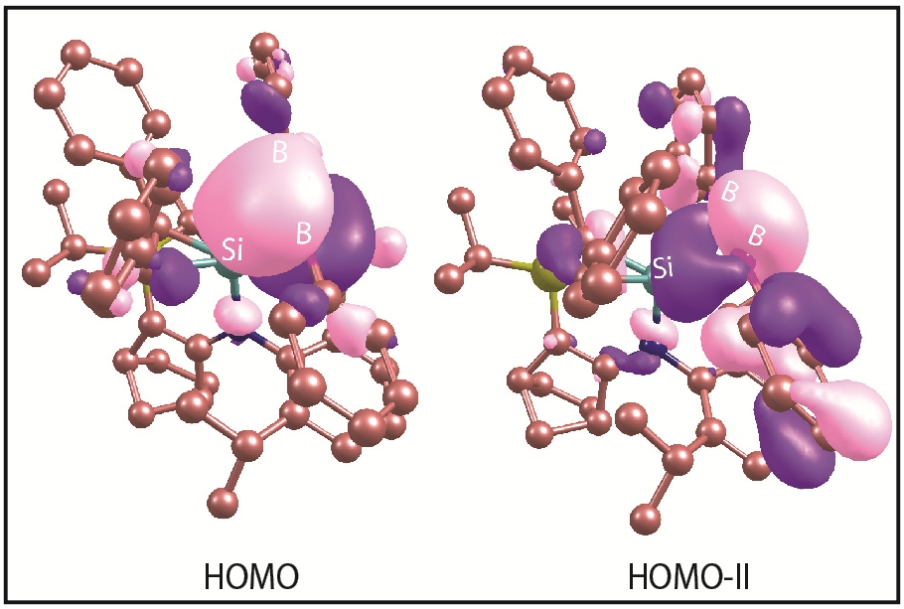
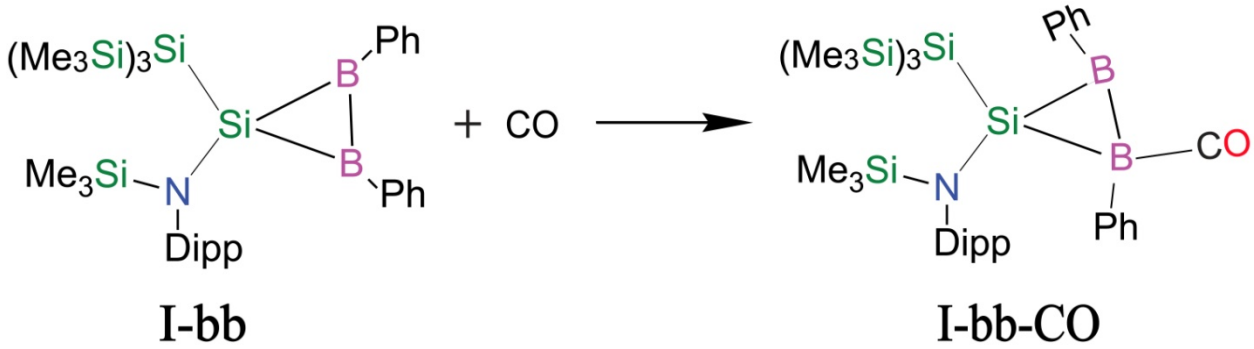


Fig. S7 The HOMO (-0.125 Ha) and the HOMO-II (-0.161 Ha)for the complex shown in Figure S6 above.



I-bb I-bb-CO

Fig. S8 The schematic representation of silylene **I-bb** complexed with carbon monoxide.

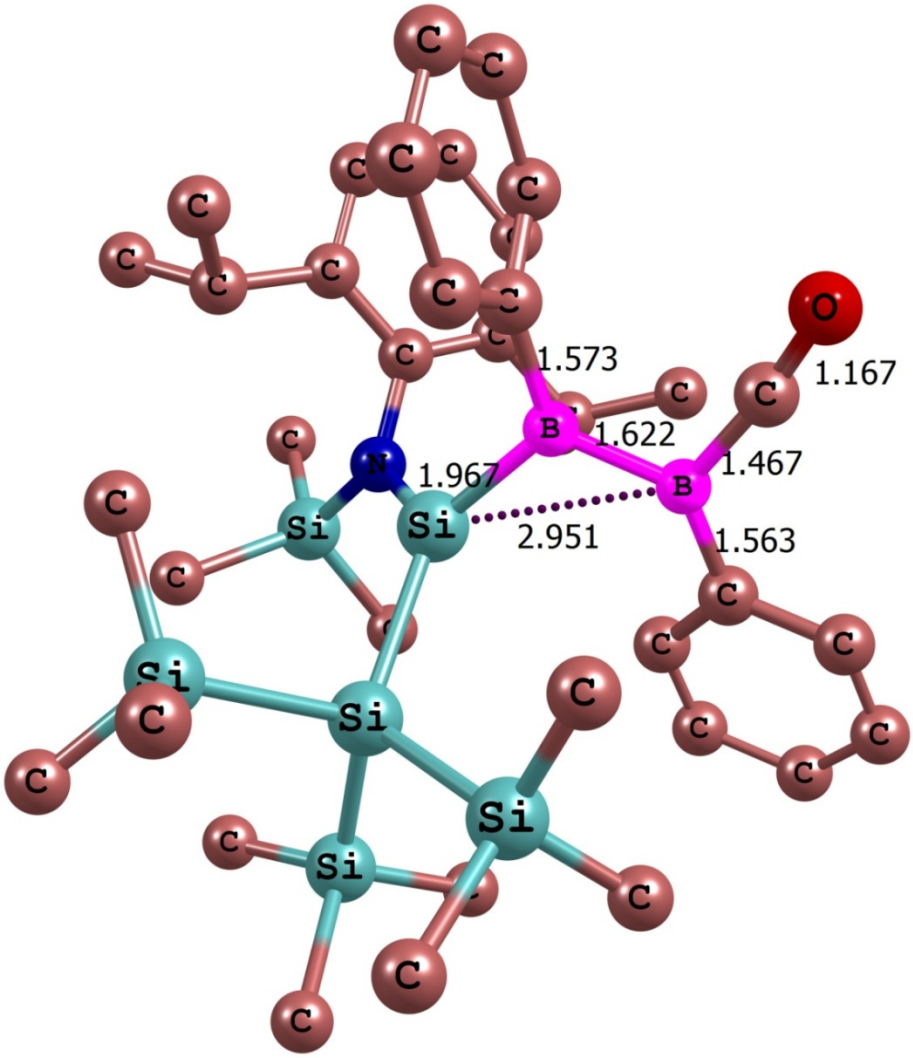


Fig. S9 The optimized structure for **I-bb** complexed to carbon monoxide; hydrogen atoms have not been shown for the purpose of clarity.

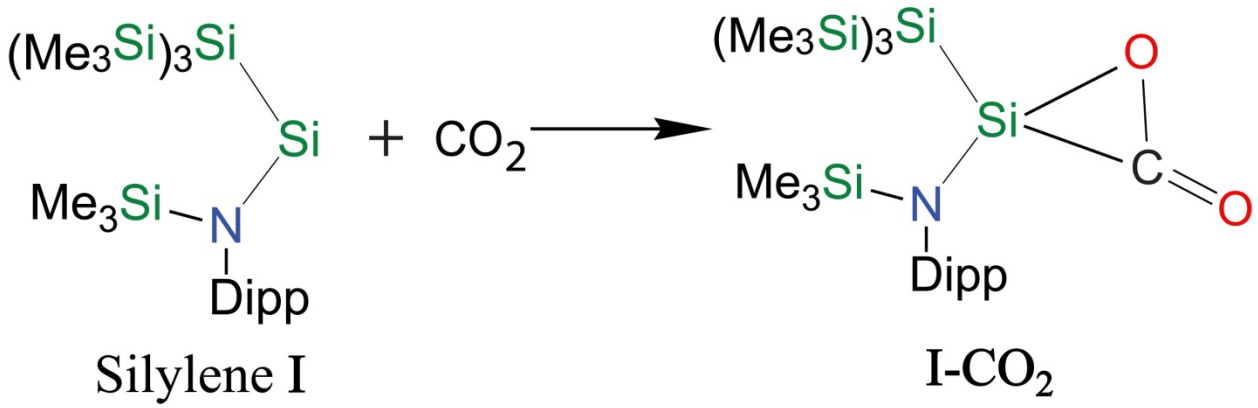


Fig. S10 The schematic representation of silylene **I** complexed with carbon dioxide.

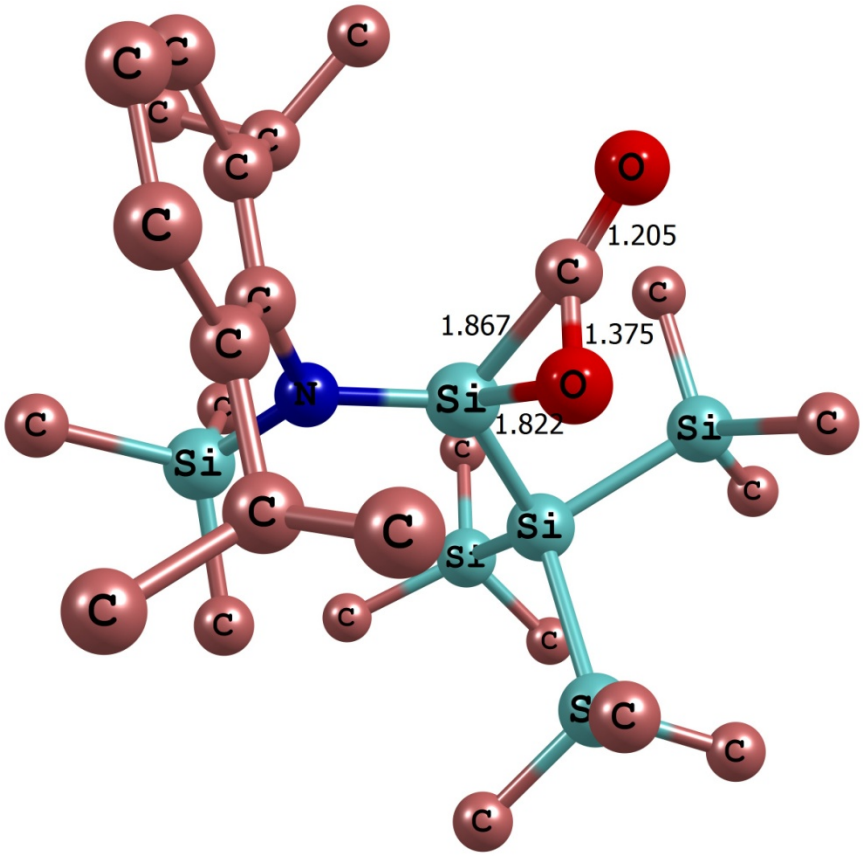


Fig. S11 The optimized structure for silylene **I** complexed to carbon dioxide; hydrogen atoms have not been shown for the purpose of clarity.

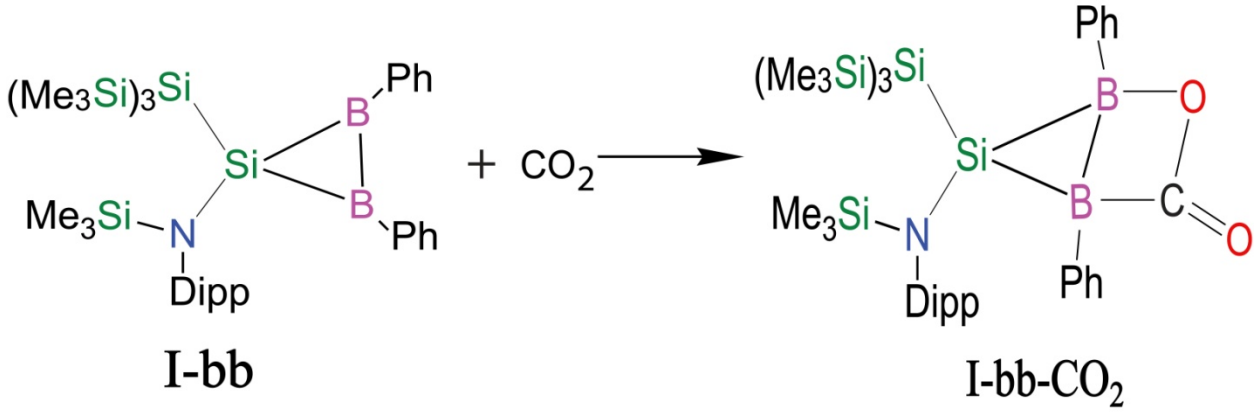


Fig. S12 The schematic representation of silylene **I-bb** complexed with carbon dioxide.

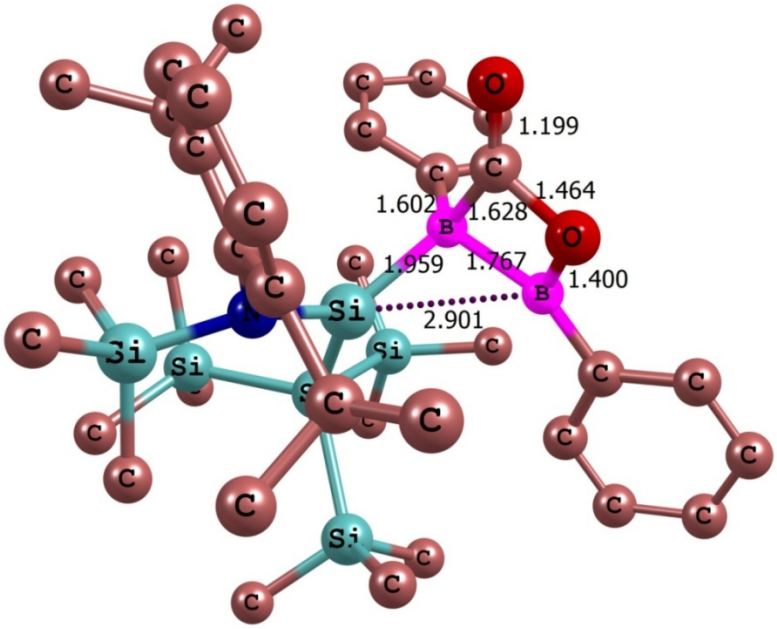


Fig. S13 The optimized structure of **I-bb** complexed to carbon dioxide; hydrogen atoms have not been shown for the purpose of clarity.

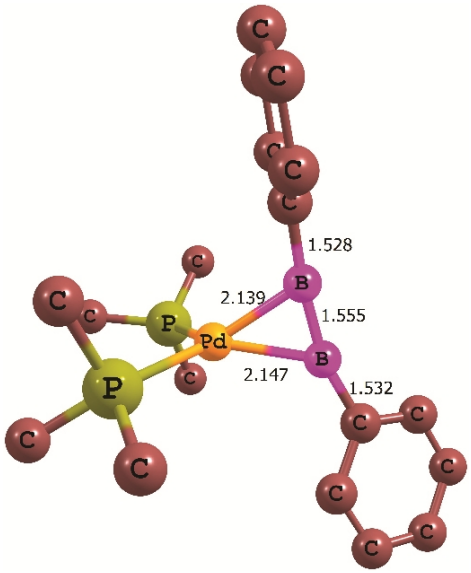


Fig. S14 The optimized structure for $Pd(PMe_3)_2$ complexed to the π-diborene where the basis set for the palladium atom is DGDZVP ; hydrogen atoms have not been shown for the purpose of clarity.

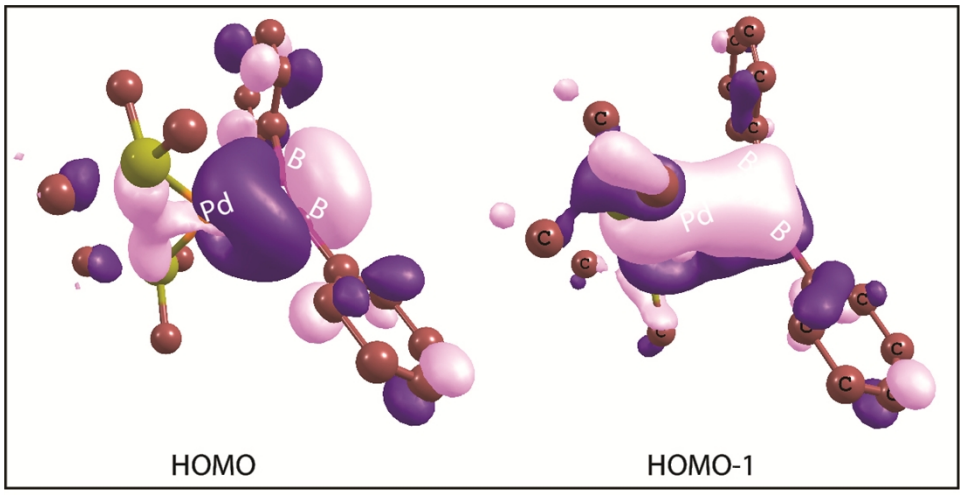


Fig. S15 The HOMO (-0.11 Ha) and the HOMO-I (-0.17 Ha) for the complex shown in Fig. S14 above.

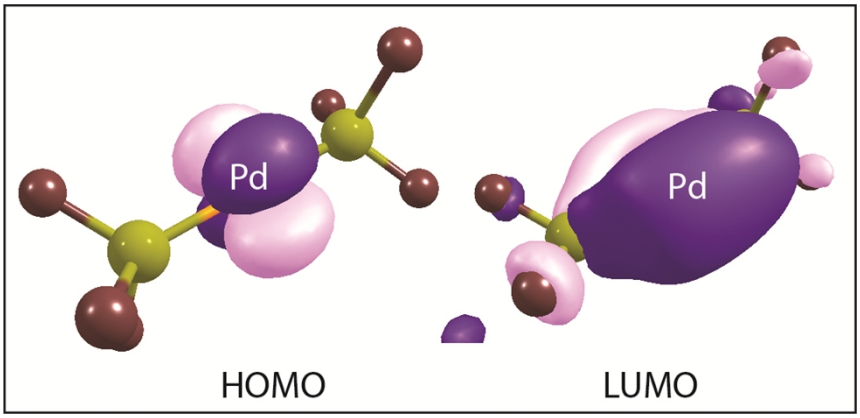


Fig. S16 The HOMO (-0.124 Ha) and the LUMO (-0.016Ha) for the bare $Pd(Me3)_2$ complex.

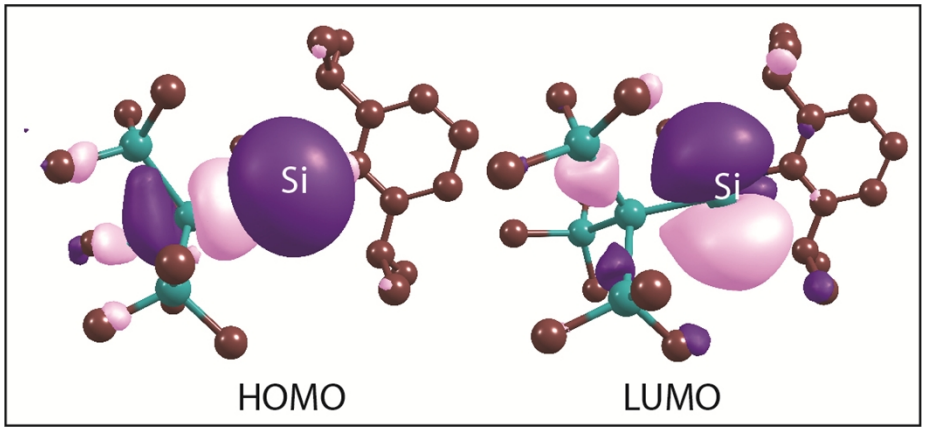


Fig. S17 The HOMO (-0.157 Ha) and LUMO (-0.085 Ha) for silylene I.

Computational Details:

The DFT calculations have been done with the Turbomole suite of programs, using Turbomole 6.0. The TZVP basis set (triple-z basis set augmented by a polarization function) and the PBE[1-7]functional have been employed in all the calculations. The dispersion correction[8] was used to incorporate dispersion effects. The resolution of identity (RI), along with the multipole accelerated resolution of identity (marij) approximations were employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Furthermore, solvent effects have been included for the solvent benzene ($\varepsilon = 2.3$) through single point calculations with the Conductor Like Screening Model – COSMO[9]. For the case of silylene **III-bb** the geometry optimization has also been done with the B3LYP hybrid functional. Frequency calculations have been done at the DFT level in order to obtain the zero point energy, the internal energy and entropic contributions (calculated at 298.15 K). All the numbers reported are ΔG values. The molecular orbital (MO) diagrams have been generated for all the proposed complexes by the Gaussian 09[10] program with PBEPBE functional and 6-31g* basis set. Only the transition metal atom in the geometries has been treated with the 3-21g* basis set. It is to be noted that full geometry calculations done with a higher basis set (DGDZVP) for the palladium atom in the **Pd-Me-bb** complex leads to no change in the results, indicating the reliability of the calculations. All the bond lengths and the nature of the HOMO and HOMO-1 orbitals for **Pd-Me-bb** (Pd with DGDZVP) are shown in the fig.S14 and fig.S15 below. The Wiberg bond indices[11] and NBO analysis were also calculated with Gaussian 09.

References

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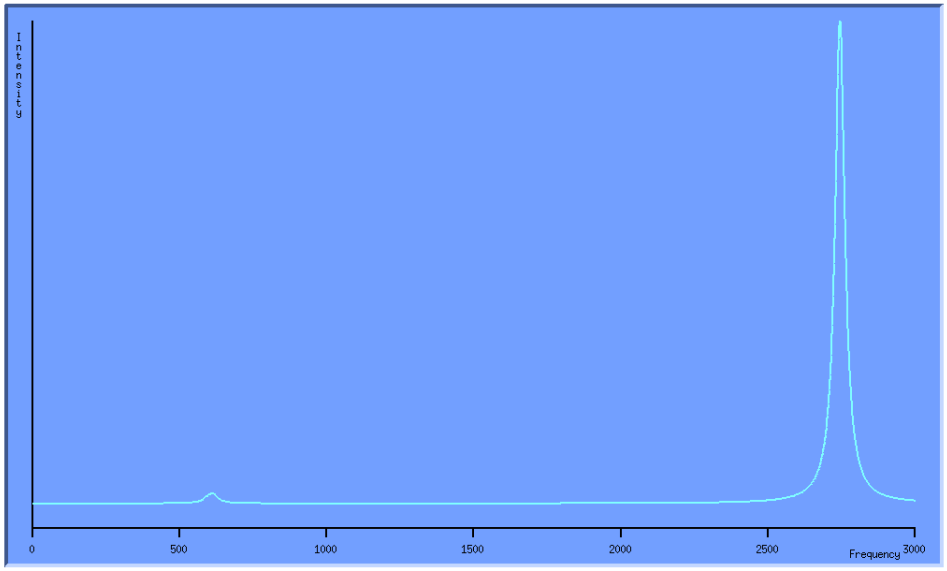
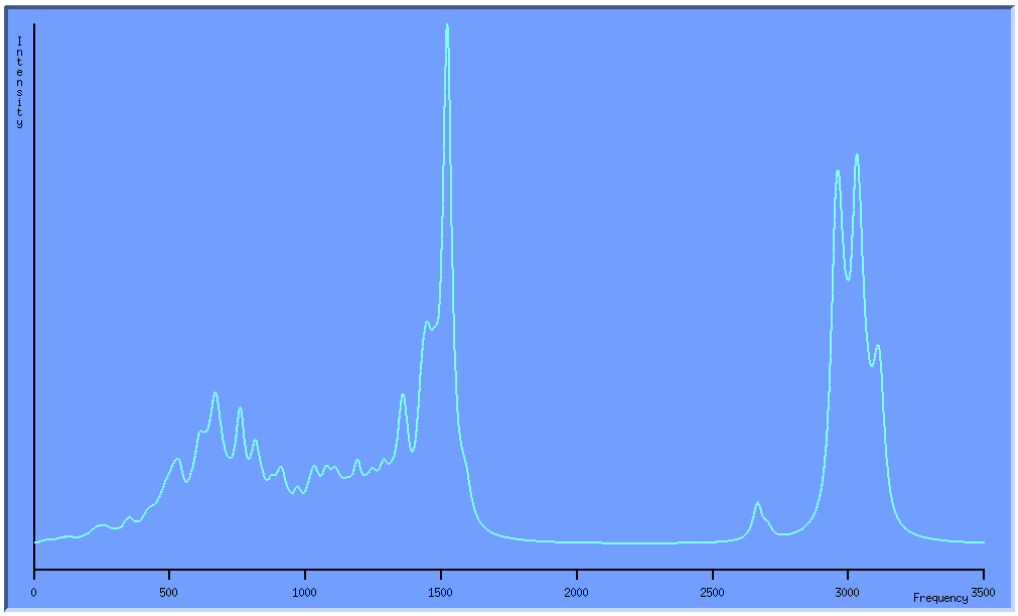
Vibrational Spectra:



Vibrational Spectra for the HBBH complex.



Vibrational Spectra for the I-HBBH complex.

We have also investigated whether the analysis of the vibrational frequencies provides corroboration of the strengthening of the B-B bond upon complexation with the silylene complex. Since it was found that B-B stretching mode is coupled with other normal modes in the diborene complex RBBR, where R is the phenyl group, we decided to do the vibrational frequency analysis with the diborene complex HBBH, since this would allow a "clean" comparison. For this case, we find a clear change in the B-B stretching frequency before and after complexation to silylene **I**: the stretching frequency is increased from 1242.43 cm^{-1} in the free HBBH molecule to 1290.14 cm^{-1} in **I-HBBH**. Furthermore, two other stretching motions are observed in the **I-HBBH** complexed case, both being seen to have stretching frequencies higher than 1290.14 cm^{-1}: 1291.09 cm^{-1} and 1294.16 cm^{-1}. Hence, the complexation of

the diborene to the silylene is seen to lead to an increase in the stretching frequency of the bond, which suggests that there is a clear correlation between the stretching frequency and the strengthening of the bond.

B-B (in free HBBH) : 1242.43 cm^{-1}
B-H : 2744.08 cm^{-1} and 2768.19 cm^{-1}.

B-B (in I-HBBH) : 1290.14 cm^{-1}: 1291.09 cm^{-1} and 1294.16 cm^{-1}.
B-H : 2664.48 cm^{-1} and 2700.68 cm^{-1}.

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Table S1. All the relative bond length and bond angle values for both the transition metal and silylene structures.

No	Name of the complexes	d(B-B)	d(C-B)	d(M/Si-B)	angle(C-B-B)
1.	Free π-diborene	1.526	1.510 1.510		
2.	**Pd-me-bb**	1.544	1.528 1.530	2.102 2.107	169.2 174.0
3.	**Pd-et-bb**	1.545	1.528 1.529	2.101 2.097	171.4 177.3
4.	**Pt-et-bb**	1.549	1.540 1.537	2.092 2.091	164.4 172.4
5.	**I-bb**	1.516	1.546 1.531	2.047 2.116	156.3 166.2

6.	**II-bb**	1.505	1.557 1.537	1.965 2.243	152.2 171.7
7.	**III-bb**	1.496	1.549 1.546	2.023 2.123	169.2 162.0

Table S2. The SOMO and HOMO energy values for model free diborene, transition metal and silylene systems; the energy values are in hartree.

Orbital name	Diborene	Silylene **I**	Silylene **II**	Silylene **III**
SOMO	-0.1532 -0.1696			
HOMO		-0.1571	-0.1630	-0.1632

Table S3. The binding energy values for both the transition metal and silylenediborene complexes.

No	Name of the complexes	Binding energy (Gas phase in kcal/mol)	Binding energy (benzene solvent in kcal/mol)
1.	**Pd-me-bb**	-39.5	-39.2
2.	**Pd-et-bb**	-34.0	-34.6
3.	**Pt-et-bb**	-39.8	-40.3
4.	**I-bb**	-41.1	-39.8
5.	**II-bb**	-40.4	-39.3
6.	**III-bb**	-38.9	-37.7

Table S4. The Wiberg Bond Indices (WBI) for the palladium and all the silylenediborene complexes.

No	Name of the complexes	WBI of first Metal/Si-B bond	WBI of second Metal/Si-B bond	WBI of B-B bond in the complexes
1.	**Pd-me-bb**	0.60	0.62	1.43
2.	**Pd-et-bb**	0.60	0.60	1.50
3.	**I-bb**	0.82	0.68	1.63
4.	**II-bb**	0.93	0.44	1.70
5.	**III-bb**	0.78	0.58	1.78

NBO analysis data:

Pd-me-bb

(1.91300) BD (1) B 28 - B 29
(50.43%) 0.7102* B 28 s(49.23%)p 1.03(50.75%)d 0.00(0.02%)
0.0011 -0.7016 -0.0018 0.6767 0.0000
0.2224 0.0122 -0.0064 0.0046 0.0055
0.0044 0.0010 -0.0099 0.0032
(49.57%) 0.7040* B 29 s(46.62%)p 1.14(53.37%)d 0.00(0.01%)
0.0011 -0.6828 -0.0027 -0.6088 0.0031
0.3839 0.0195 0.1235 0.0035 0.0015
0.0020 0.0004 -0.0109 0.0038
26. (1.52281) BD (2) B 28 - B 29
(49.34%) 0.7024* B 28 s(6.84%)p13.60(93.11%)d 0.01(0.05%)
-0.0027 0.2600 -0.0291 -0.0419 0.0166
0.9528 -0.0221 0.1440 0.0013 -0.0125
-0.0012 0.0090 -0.0126 -0.0103
(50.66%) 0.7118* B 29 s(9.04%)p10.06(90.92%)d 0.00(0.04%)
-0.0021 0.2992 -0.0294 0.2545 -0.0278
0.9158 -0.0214 0.0658 -0.0106 0.0173
0.0023 0.0042 -0.0027 -0.0097

I-bb

(1.90394) BD (1) B 16 - B 44
(49.14%) 0.7010* B 16 s(53.05%)p 0.88(46.92%)d 0.00(0.02%)
-0.0004 0.7283 0.0071 -0.0011 0.4436
-0.0118 -0.2298 0.0039 0.4684 0.0101
-0.0136 -0.0005 -0.0011 -0.0010 -0.0075
(50.86%) 0.7131* B 44 s(46.56%)p 1.15(53.41%)d 0.00(0.03%)
-0.0007 0.6823 0.0055 0.0012 -0.5101
0.0134 0.5220 0.0122 0.0174 0.0287
-0.0066 0.0116 -0.0081 0.0024 0.0026
39. (1.59332) BD (2) B 16 - B 44
(45.46%) 0.6743* B 16 s(0.65%)p99.99(99.27%)d 0.12(0.08%)
0.0007 0.0802 0.0045 0.0005 0.6177
0.0040 0.6870 0.0029 -0.3729 0.0085
-0.0074 -0.0121 0.0017 0.0232 0.0073
(54.54%) 0.7385* B 44 s(0.16%)p99.99(99.77%)d 0.46(0.07%)
-0.0009 -0.0399 -0.0029 -0.0007 0.6188
0.0124 0.6703 -0.0142 -0.4063 0.0006
-0.0035 -0.0133 -0.0194 -0.0065 0.0113

XYZ Coordinates of the optimized structures.

II-bb

C	-4.626092	17.917138	8.677215
C	-3.429652	17.218977	8.873271
C	-3.411292	15.835190	8.626711
C	-4.552451	15.173195	8.170987
C	-5.737659	15.886700	7.960730
C	-5.772380	17.260154	8.222504
C	-2.183648	17.901769	9.357299
C	-1.530099	17.425513	10.680524
C	-2.035796	16.258729	11.436299
C	-1.106409	15.375143	12.015969

C	-1.522258	14.279001	12.775885
C	-2.886313	14.030640	12.958417
C	-3.822823	14.900474	12.387158
C	-3.407854	16.007623	11.645591
Si	-2.250317	19.211885	10.841066
B	-3.956683	19.871265	11.557758
N	-0.655964	20.188583	10.660746
C	0.289715	19.982761	9.720545
C	0.267889	19.176601	8.581044
C	1.555147	19.463225	7.809680
C	1.477228	20.902731	7.223494
C	1.454321	21.784868	8.505187
C	1.612650	20.744842	9.662607
C	2.521417	19.693424	8.993340
P	-1.084558	18.267825	7.969726
N	-1.904354	18.906091	6.604067
C	-2.515582	20.230003	6.343867
C	-1.873781	20.834740	5.083200
C	-0.275450	20.921688	11.849351
C	-0.880404	22.167451	12.120370
C	-0.474075	22.865284	13.266866
C	0.496650	22.351703	14.123665
C	1.073649	21.114746	13.844872
C	0.702348	20.375192	12.715661
C	-1.899849	22.806034	11.196002
C	-1.278400	24.002605	10.455855
C	1.360057	19.022752	12.485232
C	2.893942	19.115585	12.524167
N	-0.666980	16.937878	6.968296
Si	-1.571949	17.514614	5.544467
C	-3.094476	16.537116	5.044317
C	0.164200	15.741022	7.210143
C	-0.578148	14.514043	6.658182
C	0.441695	15.560920	8.706055
C	1.506274	15.878607	6.468145
C	0.864726	17.992164	13.510382
C	-3.165517	23.235764	11.948482
B	-3.343860	19.278968	12.798012
C	-0.470561	17.856264	4.050965
C	-2.292483	21.160794	7.539079
C	-4.021056	20.074784	6.079363
H	1.940679	21.177424	10.611605
H	0.526333	22.363133	8.607812
H	2.296258	22.491952	8.527689
H	0.586737	21.039163	6.599935
H	2.363387	21.117161	6.606392
H	1.830150	18.696280	7.077411
H	3.494846	20.108818	8.687689
H	3.334963	18.137604	12.274586
H	0.382838	18.489853	4.333357
H	-1.028390	18.356424	3.244188
H	-0.082081	16.908499	3.643376
H	-2.820226	15.571407	4.591527
H	-3.676617	17.102362	4.298242
H	-3.732196	16.349767	5.920577
H	-4.194735	19.360059	5.260052
H	-4.449583	21.046497	5.788183
H	-4.546785	19.714404	6.969265
H	-0.781964	20.901911	5.179858
H	-2.277663	21.842969	4.905046
H	-2.103088	20.219258	4.199183
H	-2.712151	20.718023	8.453263
H	-2.803983	22.117542	7.359566
H	-1.224063	21.353027	7.703679
H	1.820929	20.699680	14.524770
H	0.797575	22.911366	15.012039
H	-0.932000	23.832333	13.484303
H	1.078881	18.660074	11.486370
H	1.091110	18.327508	14.533727
H	1.365512	17.024264	13.345778
H	-0.219890	17.840876	13.442047
H	2.666368	18.798201	9.614367
H	3.245902	19.390854	13.530134
H	3.277198	19.861237	11.812340
H	-2.190308	22.051322	10.450448
H	-3.624339	22.365652	12.440254
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H	-2.934978	24.003746	12.703166
H	-1.012216	24.797388	11.170589
H	-1.997729	24.420119	9.733408
H	-0.363403	23.717535	9.915345
H	-0.434927	17.444945	10.633511
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H	-4.890937	14.726894	12.535698
H	-3.217244	13.170959	13.544753
H	-0.777938	13.616854	13.223813
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H	-0.718935	14.605988	5.568609
H	-1.567152	14.412953	7.124419
H	0.006440	13.600914	6.846591
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H	2.081560	14.943682	6.551278
H	1.341193	16.092011	5.401509
H	-4.667695	18.974895	8.929222
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C	-5.161391	20.449714	10.757453
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C	-1.248237	19.535191	16.002212
C	-1.282245	18.227968	16.500193
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H	-0.712588	20.317063	16.545690
H	-0.778475	17.985247	17.439125
H	-1.991651	16.208619	16.172755

H	-3.135177	16.755626	14.049307
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C	-7.569576	20.345597	10.278090
C	-7.440567	21.320645	9.280021
C	-6.180028	21.874331	9.032557
C	-5.067359	21.449777	9.764179
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H	-8.549232	19.909712	10.491222
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H	-6.063173	22.646921	8.267591
H	-4.098396	21.906667	9.562441

III-bb

C	-1.433337	21.837412	13.313182
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C	-1.061464	21.574520	15.697824
C	-1.567366	22.308993	14.622627
C	-0.694295	19.996085	11.679101
C	0.589609	19.278393	11.266622
C	1.855593	19.334319	12.023723
C	2.703528	18.210459	12.007115
C	3.957402	18.239714	12.622909
C	4.387430	19.395033	13.284508
C	3.551209	20.517925	13.316037
C	2.303425	20.494592	12.692445
Si	0.161029	20.755533	10.052016
B	1.747223	22.114048	9.672650
C	2.953895	21.483751	8.938311
C	3.116464	21.731986	7.554497
C	4.218322	21.240040	6.853449
C	5.184941	20.471864	7.513179
C	5.044182	20.209843	8.881361
C	3.947561	20.710801	9.585054
N	-0.485676	19.817711	8.554585
C	-1.279977	18.726067	8.644282
C	-1.989350	18.258692	9.745018
C	-2.704677	16.976869	9.301844
C	-3.863727	17.348247	8.332557
C	-3.094499	17.959191	7.123317
C	-1.589459	17.763302	7.503412
C	-1.668345	16.434874	8.290390
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C	-0.147825	21.657873	5.313156
C	0.844952	20.937052	4.657086
C	1.442357	19.869150	5.312143
C	1.072117	19.470700	6.609861
C	-1.659265	22.154977	7.230320
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C	1.705895	17.020267	6.323448
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B	0.471318	22.753773	10.123582
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C	-0.073086	24.574309	11.830448
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H	-3.309845	17.416289	6.191749
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H	-0.617479	22.510929	4.820407
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H	0.746066	16.549296	6.585743
H	2.503104	16.297316	6.556444
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H	3.881262	21.429814	13.818299
H	5.366112	19.422575	13.767674
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H	0.985741	24.544675	12.096408
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C	-3.369045	18.360301	13.809371
H	-3.695887	17.392205	11.902891
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H	-2.086937	15.999555	13.194231
H	-1.346030	16.494679	11.643045
H	-0.882146	17.312019	13.153920
H	-3.516212	17.477275	14.452202
H	-2.641917	19.017499	14.304199
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H	-3.920720	20.996578	13.112214
H	-4.604503	21.573185	9.450189
H	-3.522282	20.301532	8.828964
H	-5.026952	19.864164	9.689174

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C	1.480824	11.094123	14.541474
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C	3.133608	12.058919	16.083025
C	3.417242	10.770894	16.551704
C	2.757459	9.654427	16.043141
C	1.789964	9.826431	15.055709
N	1.982154	13.533210	14.475009
Si	3.032517	13.873168	13.048998
C	4.216793	12.421608	12.797268
C	3.847872	13.246232	16.700385
C	5.304697	13.369246	16.225306
C	0.427881	11.178603	13.449292
C	0.879701	10.462294	12.165961
C	3.813448	13.207452	18.233831
C	-0.912714	10.598305	13.924305
Si	0.492864	14.423755	14.819157
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Si	0.494492	17.499245	11.898383
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C	-1.762971	19.417697	14.968927
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H	-1.243774	11.092891	14.850109
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H	1.820558	10.874602	11.774080
H	3.309025	14.141639	16.373367
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H	2.794595	13.054404	18.607880
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C	0.342291	11.713329	17.874145
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H	-5.328552	14.089944	11.354131
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H	-1.152944	13.734311	12.363459

Silylene-II

C	-1.513928	14.937537	12.047686
C	-2.321637	15.978303	11.544706
C	-3.718837	15.847897	11.693554
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C	1.777106	20.226696	10.618817
C	2.675425	19.196530	9.903595
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C	-1.273250	21.035981	5.719618
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Si	-1.088056	17.657145	5.863630
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C	0.328774	15.283781	9.048539
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C	-2.155196	17.793354	9.622659
C	-3.418331	17.279950	8.994457
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C	-3.536073	20.181111	6.310787
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H	2.700594	22.034382	9.780973
H	1.044050	20.966212	7.564575
H	2.819251	20.924815	7.698664
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H	-2.463395	22.103875	7.942131
H	-1.000093	21.214067	8.457795
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H	0.082781	22.473668	15.815682
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H	-1.295775	17.646314	13.917120
H	2.820655	18.915230	13.341246
H	2.447599	17.230287	13.801184
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H	-1.463844	21.934198	10.544211
H	-3.530489	21.793289	11.909925
H	-3.555246	23.245185	10.863866
H	-3.194693	23.406214	12.605110
H	-1.010672	24.640554	11.932154
H	-1.374047	24.378912	10.211037
H	0.178850	23.816761	10.894968
H	-0.585659	17.109815	11.005701
H	-4.371868	16.646225	11.337129
H	-5.361450	14.653390	12.406662
H	-3.898017	12.824032	13.277064

H	-1.416322	13.031008	13.053145
H	-0.428161	15.021222	11.950308
H	-2.618769	15.308603	8.660483
H	-4.689507	14.415688	7.611437
H	-6.703335	15.875735	7.393081
H	-0.679979	15.145432	9.458973
H	0.896603	14.353015	9.195587
H	0.820786	16.087744	9.617551
H	-0.379178	14.721987	5.692136
H	-1.451297	14.417381	7.085445
H	0.111140	13.553285	6.943530
H	2.307785	16.484403	7.655425
H	2.260619	14.785841	7.118403
H	1.765435	16.087211	5.999760
H	-4.526205	19.097474	9.280699
H	-6.619780	18.224141	8.233787

Silylene-III

C	-1.100884	22.009952	12.776452
C	-0.784752	20.642379	12.834658
C	-0.507027	20.077382	14.093233
C	-0.589224	20.842719	15.258425
C	-0.941963	22.195282	15.187100
C	-1.191653	22.778346	13.940176
C	-0.730951	19.801320	11.590541
C	0.546814	19.034782	11.231732
C	1.698286	18.901682	12.143706
C	2.271910	17.630475	12.353961
C	3.381588	17.460519	13.185605
C	3.945231	18.561470	13.839421
C	3.393030	19.832323	13.637013
C	2.290396	20.002349	12.799201
Si	0.273309	20.603022	10.045150
N	-0.496984	19.662539	8.571774
C	-1.329083	18.605166	8.616253
C	-2.062023	18.109519	9.690086
C	-2.759653	16.835739	9.194373
C	-3.911430	17.216995	8.219159
C	-3.139276	17.911586	7.056230
C	-1.637323	17.694483	7.434732
C	-1.707712	16.337609	8.172957
P	-2.280593	18.948904	11.227135
C	-0.145674	20.212920	7.288361
C	-1.014334	21.208805	6.767096
C	-0.674218	21.854166	5.574999
C	0.500289	21.527755	4.898060
C	1.326129	20.532165	5.406426
C	1.029998	19.841911	6.597340
C	-2.283493	21.612903	7.503184
C	-3.487889	21.777287	6.565723
C	2.019947	18.722346	6.939929
C	1.833635	17.537653	5.968005
H	3.011958	19.153079	6.715021
C	-2.057257	22.900109	8.313649
H	-0.946149	17.792480	6.592533
H	-3.376057	18.980407	6.967301
H	-3.354593	17.436966	6.087814
H	-4.663046	17.863672	8.685445
H	-4.421839	16.307793	7.863570
H	-3.046492	16.121412	9.976975
H	-2.076445	15.519947	7.532534
H	-0.752703	16.055279	8.640165
H	2.243482	20.267915	4.871951
H	0.769440	22.047012	3.975727
H	-1.333595	22.628120	5.176708
C	2.091483	18.192456	8.372122
H	0.900667	16.996061	6.186467
H	2.666104	16.825995	6.085082
H	1.802068	17.871251	4.920501
H	-2.523477	20.813613	8.217863
H	-1.225637	22.773641	9.025102
H	-2.969076	23.166732	8.874320
H	-1.810089	23.736439	7.640216
H	-3.363111	22.646853	5.902257
H	-4.402822	21.941220	7.156490
H	-3.635284	20.888772	5.932886
H	0.322867	18.093644	10.716623
H	1.883822	21.001818	12.633456
H	3.832846	20.702438	14.130032
H	4.810254	18.432664	14.492953
H	3.805755	16.463345	13.326377
H	1.832591	16.766620	11.846544
H	-0.207139	19.029623	14.145172
H	-0.367197	20.384730	16.224775
H	-1.004232	22.795314	16.097316
H	-1.260549	22.462692	11.794984
H	-1.447267	23.837930	13.872333
H	2.931885	17.483500	8.442197
H	2.254772	18.988715	9.110334
H	1.173634	17.657398	8.654575
C	-2.784840	17.564369	12.395728
C	-3.554505	20.335738	11.153825
C	-4.170247	20.757515	12.494201
H	-2.906723	21.152493	10.790522
C	-4.645165	20.081068	10.113582
C	-3.258195	17.957443	13.799152
H	-3.613939	17.064439	11.864676
C	-1.592416	16.597224	12.470798
H	-1.884250	15.705759	13.048559
H	-1.259887	16.278755	11.472713
H	-0.735493	17.071304	12.972748
H	-3.341543	17.041997	14.407169
H	-2.545140	18.628026	14.297003
H	-4.239093	18.445135	13.789999
H	-4.599509	21.765753	12.379935
H	-4.990355	20.080782	12.775598
H	-3.439581	20.795682	13.311403
H	-5.288947	20.972464	10.038191
H	-4.219652	19.875375	9.122434
H	-5.284713	19.232053	10.403920

Silylene-I

C	2.029788	11.750051	14.617721

C	3.174182	11.470268	15.397902
C	3.938015	10.338951	15.084890
C	3.595020	9.508319	14.018579
C	2.471840	9.805731	13.248185
C	1.677391	10.925927	13.525601
C	3.555527	12.334116	16.587282
C	3.157883	11.633717	17.896834
C	0.445596	11.204505	12.682329
C	-0.677614	10.216589	13.036095
N	1.216107	12.904100	14.930511
Si	-0.097466	12.564073	16.051162
Si	-1.423345	14.537500	16.459899
Si	-3.460228	13.321139	16.539929
C	-4.959963	14.423831	16.959276
C	0.750607	11.184222	11.178486
Si	1.699337	14.450340	14.119905
C	0.305283	14.968060	12.949013
C	2.068343	15.734650	15.457930
C	3.267675	14.107230	13.119720
C	5.042703	12.711542	16.591581
Si	-0.930923	14.931197	18.745047
C	-2.510730	15.297302	19.750158
Si	-2.030142	16.640167	15.543375
C	-3.046708	17.577561	16.861680
C	-0.060619	13.429475	19.534984
C	0.227474	16.442842	18.891135
C	-0.586943	17.791070	15.069479
C	-3.146337	16.391862	14.013999
C	-3.752638	12.530329	14.826041
C	-3.360456	11.928438	17.839955
H	2.202386	9.157103	12.411650
H	4.203221	8.631079	13.788510
H	4.817857	10.108360	15.689938
H	0.086219	12.211163	12.936316
H	-0.361921	9.182444	12.825070
H	-1.584368	10.430829	12.447927
H	-0.926890	10.280719	14.107755
H	1.067596	10.183734	10.846222
H	-0.148705	11.457415	10.604676
H	1.553856	11.893764	10.925752
H	2.974405	13.265055	16.523929
H	3.400757	12.264705	18.767011
H	2.078033	11.414233	17.909858
H	3.697533	10.678597	17.998350
H	5.259351	13.389856	17.431395
H	5.329249	13.215008	15.655265
H	5.683080	11.823415	16.706806
H	4.087845	13.764380	13.768563
H	3.095106	13.327458	12.362571
H	3.593959	15.025852	12.605488
H	-0.658585	14.968152	13.478405
H	0.239166	14.261793	12.106772
H	0.474446	15.975157	12.536340
H	1.217464	15.841074	16.145844
H	2.953142	15.426179	16.037316
H	2.273626	16.722121	15.017252
H	-4.694809	11.957662	14.809769
H	-3.805497	13.300683	14.040350
H	-2.931711	11.840945	14.568871
H	-5.877141	13.811530	16.980604
H	-4.839980	14.895628	17.946312
H	-5.101160	15.220965	16.213816
H	-4.287413	11.330853	17.830598
H	-2.512355	11.258990	17.628993
H	-3.227233	12.334969	18.854583
H	0.127620	13.620306	20.605198
H	-0.676747	12.521376	19.449766
H	0.907477	13.221367	19.051619
H	0.435559	16.659255	19.952491
H	1.187956	16.262447	18.384311
H	-0.226357	17.341252	18.444146
H	-2.249577	15.507884	20.801166
H	-3.047900	16.168492	19.346997
H	-3.198252	14.437748	19.736291
H	-3.515338	17.368585	13.658291
H	-2.608514	15.910138	13.183777
H	-4.019058	15.767480	14.259657
H	-1.000106	18.748363	14.709470
H	0.057426	18.000069	15.936555
H	0.040049	17.364673	14.275091
H	-3.401103	18.534667	16.442702
H	-3.921641	16.999081	17.191326
H	-2.432460	17.801727	17.747301

Pd-Me

Pd	-0.528613	0.033768	-0.623102
P	-0.274343	1.330846	1.311429
P	1.350333	-1.315165	-0.828158
C	1.017047	-2.982433	-1.567305
C	2.447409	-0.531164	-2.097535
C	2.562857	-1.751338	0.516923
C	-1.721745	1.088019	2.443106
C	1.150786	1.212545	2.506897
C	-0.321634	3.158818	0.999897
H	1.954360	-3.521653	-1.780439
H	0.402431	-3.575398	-0.875079
H	0.445144	-2.840694	-2.494547
H	3.401666	-2.347328	0.121494
H	2.951062	-0.826199	0.965780
H	2.047111	-2.326507	1.299537
H	3.277584	-1.201371	-2.372435
H	1.843625	-0.285779	-2.983474
H	2.849913	0.409581	-1.696722
H	1.017219	1.890351	3.365909
H	1.232495	0.177563	2.868298
H	2.082970	1.471799	1.983796
H	-0.314183	3.725789	1.944524
H	0.548081	3.445429	0.391914
H	-1.232442	3.391887	0.431505
H	-1.660877	1.754578	3.318255
H	-2.642218	1.288329	1.878122
H	-1.749397	0.041565	2.777174

B	-1.411231	0.559439	-2.457072
B	-2.305030	-0.417509	-1.662718
C	-0.551094	1.432650	-3.371031
C	-3.353441	-1.386805	-1.111969
C	-4.740532	-1.124751	-1.238890
C	-5.694619	-1.986720	-0.695781
C	-5.297310	-3.159972	-0.041741
C	-3.932890	-3.453837	0.078605
C	-2.979013	-2.572693	-0.431282
H	-5.063061	-0.229418	-1.775779
H	-6.757446	-1.754617	-0.799822
H	-6.045640	-3.842616	0.366553
H	-3.615089	-4.368168	0.586150
H	-1.913596	-2.786467	-0.310207
C	-0.096744	0.941247	-4.622284
C	0.770875	1.685311	-5.423650
C	1.186556	2.961682	-5.023129
C	0.732070	3.479817	-3.803201
C	-0.104740	2.721881	-2.983720
H	-0.439704	-0.038647	-4.963869
H	1.109969	1.277051	-6.378952
H	1.851188	3.549998	-5.659089
H	1.046540	4.476810	-3.484346
H	-0.428443	3.120498	-2.019595

Pd-Me-bb

Pd	0.122626	5.217209	-0.735872
P	1.422244	5.558552	1.098812
C	1.396730	7.256156	1.856584
P	-1.190018	4.881954	-2.562224
C	-1.421454	3.129752	-3.140601
C	-2.960068	5.440984	-2.441492
C	-0.676257	5.704230	-4.149162
C	1.073239	4.507147	2.592376
C	3.252866	5.293079	0.907162
H	1.755353	4.751715	3.423387
H	0.033442	4.668294	2.909809
H	1.188316	3.448260	2.321398
H	2.050264	7.308269	2.742771
H	1.730705	7.988135	1.107960
H	0.365703	7.505965	2.143287
H	3.787290	5.483483	1.852523
H	3.433891	4.258383	0.584035
H	3.632547	5.967192	0.126564
H	-1.380678	5.471435	-4.964555
H	-0.637741	6.791643	-3.994738
H	0.331081	5.360949	-4.422996
H	-2.077827	3.084309	-4.025161
H	-0.440712	2.699286	-3.386670
H	-1.860871	2.538685	-2.324791
H	-3.509408	5.241022	-3.376394
H	-3.445681	4.913613	-1.608583
H	-2.981936	6.518160	-2.224768

Pd-Et-bb

C	0.221831	2.780700	-3.328461
C	-0.121269	1.422906	-3.549242
C	0.460104	0.787507	-4.676704
C	1.350107	1.462319	-5.514117
C	1.667583	2.805679	-5.276772
C	1.085830	3.463253	-4.184996
B	-1.003328	0.637241	-2.577858
B	-2.010252	-0.225852	-1.785779
C	-3.043194	-1.089653	-1.064341
C	-4.388578	-0.663685	-0.917237
C	-5.304675	-1.399948	-0.164839
C	-4.922009	-2.602036	0.444752
C	-3.604528	-3.055129	0.297214
C	-2.679990	-2.307413	-0.431659
Pd	-0.282299	0.182387	-0.662472
P	1.515289	-1.260518	-0.772262
C	2.616701	-1.681481	0.683351
P	-0.369184	1.237546	1.436408
C	-0.623153	3.078334	1.216660
C	-1.932384	0.581054	2.231186
C	0.942035	1.088892	2.773475
C	1.127165	-2.931139	-1.503691
C	2.686173	-0.517770	-2.010635
H	2.077407	-3.467301	-1.662025
H	0.558197	-3.485685	-0.739302
C	0.334459	-2.837015	-2.807706
C	3.832905	-2.564624	0.394510
H	2.927678	-0.710673	1.101533
H	1.958922	-2.146146	1.436385
H	3.563859	-1.174022	-2.133398
H	2.136957	-0.495921	-2.964329
C	3.083774	0.909572	-1.626066
C	0.517749	1.280920	4.233343
H	1.366227	0.081959	2.636426
H	1.740192	1.798055	2.494869
C	-0.439989	4.002104	2.423529
H	0.073969	3.359200	0.411708
H	-1.631742	3.173661	0.782759
C	-2.735195	1.536617	3.117752
H	-2.548400	0.227875	1.389351
H	-1.633442	-0.320698	2.790444
H	-4.709547	0.261914	-1.401304
H	-6.332284	-1.041783	-0.064357
H	-5.644260	-3.182268	1.022585
H	-3.295371	-3.993853	0.764193
H	-1.647000	-2.653387	-0.519104
H	0.198602	-0.251284	-4.894125
H	1.786766	0.942442	-6.370712
H	2.352753	3.336834	-5.940554
H	1.321961	4.512884	-3.992323
H	-0.201502	3.296076	-2.462295
H	0.041650	-3.839160	-3.155222
H	-0.576890	-2.231642	-2.674978
H	0.931271	-2.361761	-3.600260
H	3.741289	1.347642	-2.392071
H	2.182757	1.538054	-1.553121
H	3.613660	0.940619	-0.660448
H	4.428482	-2.717061	1.308477
H	3.533038	-3.555444	0.023400

H	4.491383	-2.106180	-0.358318
H	1.372290	1.107020	4.906926
H	0.139455	2.294336	4.421266
H	-0.273835	0.568700	4.509434
H	-3.663885	1.046532	3.449659
H	-2.173665	1.844975	4.010750
H	-3.021150	2.444263	2.565203
H	-0.570291	5.052769	2.118997
H	-1.167170	3.786354	3.217723
H	0.569702	3.905302	2.850658

Pd-Et

C	1.249782	7.102617	2.082818
P	1.329567	5.445813	1.224107
C	3.177307	5.180779	1.110564
Pd	0.135120	5.188932	-0.700580
P	-1.132698	4.852751	-2.566197
C	-0.651450	5.724404	-4.146650
C	0.816220	4.301649	2.610258
C	-1.266380	3.086800	-3.158873
C	-2.920870	5.378678	-2.390077
H	1.512749	4.428836	3.457329
H	-0.174156	4.655721	2.937552
C	0.726107	2.838396	2.168687
H	1.799902	7.049413	3.037793
H	1.783473	7.810130	1.428590
C	-0.195528	7.561280	2.293047
H	3.581114	4.994917	2.120722
C	3.553635	4.062011	0.133977
H	3.594167	6.139136	0.760270
H	-1.433033	5.557818	-4.907776
C	-0.403231	7.217051	-3.915586
H	0.268730	5.233527	-4.501066
H	-1.991029	3.036778	-3.989966
H	-0.274199	2.831614	-3.564769
C	-1.637914	2.120523	-2.030596
H	-3.526185	4.852626	-3.148481
C	-3.466239	5.163320	-0.975560
H	-2.942680	6.452140	-2.638940
H	-1.576065	1.074419	-2.369128
H	-0.954888	2.259739	-1.176676
H	-2.662523	2.298007	-1.671077
H	-4.473145	5.597930	-0.869291
H	-3.527018	4.094446	-0.724124
H	-2.790572	5.631117	-0.241382
H	-0.045519	7.706513	-4.834864
H	-1.323180	7.732295	-3.597683
H	0.346802	7.357727	-3.121336
H	4.645154	4.011156	-0.005271
H	3.209751	3.080594	0.490884
H	3.073635	4.240666	-0.841369
H	0.288105	2.212480	2.962131
H	0.100554	2.757997	1.264959
H	1.717776	2.429137	1.926121
H	-0.231811	8.581479	2.705919
H	-0.739154	7.545577	1.334931
H	-0.729485	6.898449	2.991367

Pt-Et

C	1.285186	7.120502	1.995737
C	-0.136364	7.561242	2.352657
P	1.341381	5.424339	1.211264
C	0.866599	4.357214	2.671526
C	0.923280	2.854458	2.385119
C	3.192710	5.177315	1.083448
C	3.606462	4.006709	0.186544
Pt	0.103029	5.133166	-0.679998
P	-1.171310	4.848555	-2.549162
C	-2.956656	5.400832	-2.428584
C	-3.620691	5.081845	-1.086163
C	-0.629537	5.751408	-4.094551
C	-0.401006	7.246499	-3.860622
C	-1.306297	3.109864	-3.223458
C	-1.837564	2.091805	-2.210849
H	1.519001	4.630115	3.519463
H	-0.160918	4.652775	2.934746
H	1.938835	7.115043	2.884947
H	1.727661	7.810764	1.260427
H	3.596971	5.069754	2.104920
H	3.587772	6.121469	0.674348
H	-1.386381	5.578459	-4.879215
H	0.304034	5.266883	-4.421742
H	-1.937332	3.140522	-4.128266
H	-0.286403	2.836558	-3.538416
H	-3.510646	4.956279	-3.273746
H	-2.939480	6.491437	-2.586387
H	-1.768402	1.069017	-2.613460
H	-1.257626	2.142171	-1.276373
H	-2.892400	2.283058	-1.964813
H	-4.627800	5.525443	-1.035469
H	-3.717455	3.998097	-0.928534
H	-3.011900	5.480374	-0.260142
H	-0.033639	7.733803	-4.777306
H	-1.331322	7.754096	-3.561603
H	0.335508	7.398393	-3.056925
H	4.702148	3.968991	0.078219
H	3.272020	3.043048	0.596207
H	3.152196	4.115099	-0.809842
H	0.504782	2.280943	3.227124
H	0.347018	2.616282	1.477497
H	1.957169	2.513830	2.228668
H	-0.141598	8.592254	2.739395
H	-0.783339	7.514223	1.463055
H	-0.576989	6.912389	3.125028

Pt-Et-bb

C	-3.058019	-2.736374	-0.618852
C	-3.331937	-1.515270	-1.280854
C	-4.678251	-1.263876	-1.640277
C	-5.694979	-2.171380	-1.336398
C	-5.393700	-3.377205	-0.691302

C	-4.067449	-3.659630	-0.341391
B	-2.229570	-0.489227	-1.603055
Pt	-0.533849	-0.047066	-0.460829
P	-0.263006	1.224041	1.531803
C	1.063493	0.882959	2.823240
C	0.852753	1.393858	4.251983
B	-1.338858	0.577894	-2.286297
C	-0.487858	1.533940	-3.136507
C	-0.299318	2.896980	-2.799822
C	0.538637	3.725084	-3.548599
C	1.237000	3.216086	-4.650567
C	1.063597	1.873184	-5.008741
C	0.207309	1.051350	-4.273743
P	1.423009	-1.335878	-0.612638
C	2.462580	-0.597914	-1.970407
C	2.918305	0.829684	-1.661218
C	2.675340	-1.634599	0.758347
C	3.984222	-2.322049	0.360828
C	1.102359	-3.066849	-1.240224
C	0.325174	-3.099163	-2.557928
C	0.008748	3.008715	1.028098
C	0.597579	3.975945	2.057875
C	-1.858182	1.205779	2.514970
C	-2.235498	2.476119	3.282511
H	2.074550	-3.575197	-1.348250
H	0.542884	-3.587370	-0.446073
H	2.876228	-0.644981	1.196630
H	2.143662	-2.213308	1.531793
H	3.317377	-1.267877	-2.162838
H	1.826090	-0.591905	-2.867675
H	1.167601	-0.213085	2.830394
H	2.002111	1.274966	2.396125
H	0.654150	2.957763	0.138130
H	-0.971431	3.356776	0.665495
H	-2.634976	0.958181	1.777096
H	-1.788024	0.339814	3.194284
H	-4.917905	-0.339259	-2.170935
H	-6.726498	-1.947406	-1.619544
H	-6.186237	-4.095085	-0.468093
H	-3.824784	-4.599989	0.160178
H	-2.026960	-2.950378	-0.324093
H	0.065185	0.011477	-4.580630
H	1.590951	1.467795	-5.876076
H	1.899351	3.861436	-5.231349
H	0.656476	4.774656	-3.266987
H	-0.822561	3.303562	-1.931363
H	0.073018	-4.135811	-2.828037
H	-0.608542	-2.521381	-2.478576
H	0.919094	-2.670253	-3.378938
H	3.521831	1.227729	-2.490786
H	2.044149	1.486613	-1.538841
H	3.526879	0.874948	-0.743463
H	4.631329	-2.460310	1.241567
H	3.808454	-3.315047	-0.078875
H	4.543124	-1.721430	-0.371809
H	1.679281	1.062817	4.901359
H	0.807645	2.490010	4.295108
H	-0.081259	0.998683	4.678041
H	-3.223778	2.350072	3.752467
H	-1.511484	2.713164	4.073038
H	-2.299833	3.342817	2.607957
H	0.755147	4.963824	1.596646
H	-0.064954	4.108256	2.923508
H	1.572731	3.623563	2.425227

I-bb-co2

C	2.630316	11.572050	15.541102
C	2.113273	11.942412	14.273893
C	1.692477	10.961013	13.346760
C	1.860250	9.611748	13.680487
C	2.411280	9.232144	14.899193
C	2.779208	10.209257	15.822274
N	2.047494	13.358340	13.929512
Si	3.384144	13.897601	12.815491
C	2.753298	14.120534	11.040739
C	1.031555	11.294564	12.020999
C	1.829956	10.724151	10.836515
C	3.013446	12.603577	16.593181
C	4.444355	13.119876	16.376859
Si	0.561253	14.131701	14.429409
Si	0.397440	16.510926	14.337022
Si	-1.748626	17.329066	15.017164
C	-1.552353	19.238367	15.132337
B	-0.875866	13.091831	15.259876
C	-0.677919	11.511649	15.598215
C	-2.327347	13.468192	14.697148
C	-2.582168	13.446409	13.309166
C	-3.873636	13.583171	12.791227
C	-4.955743	13.767796	13.657390
C	-4.731769	13.804815	15.038305
C	-3.438521	13.649333	15.545013
B	-0.381983	13.063437	16.956676
C	-0.151622	13.873385	18.259023
C	0.112963	15.254850	18.250648
C	0.394727	15.947154	19.430781
C	0.388654	15.267038	20.653119
C	0.112186	13.894183	20.690267
C	-0.145635	13.206063	19.504854
Si	1.982382	17.591131	15.768070
C	1.068779	18.624400	17.086333
Si	0.441991	17.286577	12.085119
C	-0.406668	18.991394	11.967501
C	3.089822	16.348742	16.685972
C	3.046132	18.825252	14.774807
C	4.098038	15.550435	13.387801
C	4.712272	12.554598	12.791992
C	-0.412623	10.768857	11.969721
C	2.874715	12.090518	18.031657
C	2.170322	17.580271	11.339266
C	-0.578912	16.058315	11.041381
C	-3.092418	16.980933	13.724066
C	-2.377379	16.736096	16.709031
H	1.526396	8.849317	12.973768

H	2.527497	8.175045	15.145870
H	3.166747	9.906900	16.795599
H	0.994477	12.388657	11.921375
H	-0.420713	9.668557	12.010685
H	-0.892247	11.079162	11.027148
H	-1.007901	11.127547	12.817873
H	1.820632	9.623733	10.867260
H	1.377262	11.037229	9.882080
H	2.880754	11.048827	10.848911
H	2.331361	13.466007	16.485350
H	2.953391	12.936112	18.731222
H	1.907653	11.595336	18.186725
H	3.680462	11.379774	18.275696
H	4.717024	13.832472	17.169962
H	4.554855	13.625638	15.409882
H	5.153367	12.276686	16.406425
H	5.160568	12.382754	13.779540
H	4.296476	11.598239	12.444453
H	5.508618	12.862912	12.094466
H	1.846945	14.737214	10.990587
H	2.543217	13.157782	10.557767
H	3.534369	14.629089	10.451351
H	3.296599	16.272295	13.595303
H	4.722009	15.455029	14.286672
H	4.720978	15.969921	12.581570
H	-4.009467	17.508024	14.037851
H	-2.816047	17.349901	12.725838
H	-3.322754	15.910965	13.651432
H	-2.405810	19.721220	14.629669
H	-1.549447	19.554441	16.185530
H	-0.634449	19.615577	14.661319
H	-3.431197	17.047521	16.804580
H	-2.334030	15.645298	16.810264
H	-1.811849	17.183431	17.538761
H	3.921535	16.889430	17.168082
H	2.519310	15.830204	17.470000
H	3.514357	15.591873	16.017502
H	3.664561	19.411869	15.474908
H	3.717416	18.329472	14.059716
H	2.407207	19.528156	14.217576
H	1.779392	18.865552	17.894523
H	0.695389	19.566474	16.662764
H	0.215982	18.089341	17.525374
H	-0.586397	16.368411	9.983382
H	-0.193706	15.029230	11.092835
H	-1.617782	16.034077	11.403883
H	2.042643	17.947709	10.306990
H	2.694462	18.358951	11.913716
H	2.806242	16.689830	11.309430
H	-0.447192	19.278820	10.903236
H	-1.429373	18.995919	12.366106
H	0.169704	19.762778	12.500939
H	0.098672	15.786841	17.296004
H	0.615828	17.015755	19.402026
H	0.598346	15.807787	21.578786
H	0.109070	13.363407	21.644994
H	-0.339317	12.131135	19.525219
H	-3.285106	13.649953	16.627404
H	-5.571368	13.942177	15.723785
H	-5.966628	13.880251	13.260194
H	-4.034029	13.553792	11.710805
H	-1.746778	13.290751	12.620567
O	-0.186949	11.677080	16.967896
O	-0.961042	10.425669	15.175828

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C	-2.041333	13.728363	13.022030
C	-2.755657	13.541047	14.225028
C	-4.167712	13.580959	14.120822
C	-4.814076	13.794139	12.903536
C	-4.071192	13.976883	11.729432
C	-2.675539	13.946433	11.796335
B	-2.053653	13.291613	15.598623
B	-0.589171	13.589852	16.229248
C	-0.006499	13.267816	17.654550
C	0.134278	14.286181	18.622509
C	0.601469	14.008495	19.910245
C	0.960391	12.702232	20.259662
C	0.842297	11.681003	19.311359
C	0.363824	11.959698	18.028562
Si	0.570723	14.437784	14.885810
Si	0.307251	16.701947	14.231903
Si	1.845866	17.821688	15.695805
C	2.989037	16.625204	16.630302
N	1.907971	13.473028	14.313768
Si	2.958445	13.832472	12.879955
C	3.928001	15.414907	13.235811
C	2.134107	12.178135	14.939024
C	1.419490	11.036090	14.500741
C	1.705865	9.799693	15.096883
C	2.676057	9.674917	16.088603
C	3.380680	10.803981	16.497578
C	3.130392	12.062576	15.937834
C	0.387993	11.072298	13.386964
C	-0.951491	10.455335	13.813722
C	3.928586	13.251174	16.441449
C	3.678335	13.493131	17.937118
C	4.146193	12.392389	12.607024
C	1.794446	13.989096	11.399245
C	5.437224	13.094657	16.193015
C	0.903540	10.361080	12.123122
Si	0.475170	17.570105	12.015233
C	2.212728	17.575085	11.238087
Si	-1.852228	17.460494	14.944322
C	-3.169940	17.128745	13.617209
C	-0.734514	16.715737	10.816460
C	-0.084671	19.391457	12.127928
C	-2.396674	16.743893	16.613727
C	-1.773134	19.369507	15.151859
C	2.939773	19.013073	14.685633
C	0.934887	18.825952	17.032805
H	1.152461	8.918762	14.764613
H	2.882146	8.701407	16.538259

H	4.140415	10.719046	17.277970
H	0.209128	12.122992	13.127669
H	-0.844961	9.373733	13.992969
H	-1.699150	10.598980	13.019241
H	-1.327824	10.934822	14.727857
H	1.123621	9.304334	12.342216
H	0.135313	10.392998	11.334109
H	1.820399	10.822926	11.730059
H	3.584023	14.135328	15.892645
H	4.212267	14.398334	18.266027
H	2.610034	13.614249	18.155334
H	4.047157	12.642803	18.532009
H	5.972557	13.975627	16.581713
H	5.677454	12.991878	15.125495
H	5.827554	12.206803	16.714842
H	4.893342	12.315516	13.407561
H	3.615932	11.431515	12.560655
H	4.676832	12.544825	11.652563
H	0.993516	14.707894	11.621413
H	1.328683	13.012811	11.192937
H	2.315508	14.323897	10.488837
H	3.253953	16.242383	13.502089
H	4.618865	15.241549	14.075355
H	4.519379	15.727163	12.360731
H	-4.145627	17.467444	14.004955
H	-2.957258	17.703417	12.702354
H	-3.255378	16.067203	13.353488
H	-2.664835	19.812787	14.679156
H	-1.787034	19.631581	16.219770
H	-0.889286	19.835057	14.696735
H	-3.368538	17.188025	16.888259
H	-2.494392	15.649875	16.572170
H	-1.674554	16.990856	17.407320
H	3.533417	17.194201	17.402396
H	2.435680	15.820810	17.138447
H	3.730842	16.169642	15.960430
H	3.597261	19.575987	15.369008
H	3.577996	18.462337	13.978244
H	2.340194	19.737573	14.114846
H	1.683543	19.180955	17.760740
H	0.412618	19.698432	16.619856
H	0.200398	18.211210	17.573829
H	-0.885514	17.382180	9.950337
H	-0.353279	15.756396	10.438946
H	-1.709832	16.531022	11.287029
H	2.145341	18.071989	10.255585
H	2.930604	18.135395	11.854454
H	2.604052	16.561465	11.085050
H	0.014959	19.847138	11.128039
H	-1.135891	19.475428	12.438123
H	0.526475	19.977748	12.829762
H	-0.147952	15.310874	18.363404
H	0.689402	14.814912	20.642383
H	1.330780	12.483383	21.263478
H	1.127154	10.658409	19.570584
H	0.287804	11.154074	17.294255
H	-4.767301	13.447141	15.025076
H	-5.905675	13.818552	12.866200
H	-4.575101	14.135288	10.773893
H	-2.080183	14.082485	10.891653
H	-0.946740	13.670288	13.030114
C	-2.705760	12.663391	16.752654
O	-3.090288	12.200600	17.752896

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B	0.525902	-0.000527	-0.013117
B	0.525914	-0.000521	1.513121
C	0.540234	-0.000342	-1.522773
C	0.540322	-0.000330	3.022743
C	-0.664236	-0.000119	-2.274867
C	-0.642469	0.000032	-3.668477
C	0.579154	0.000346	-4.353888
C	1.781464	0.000247	-3.635531
C	1.765015	-0.000261	-2.241934
H	-1.621847	0.000419	-1.749441
H	-1.581136	0.000389	-4.226578
H	0.594062	0.000692	-5.445871
H	2.735326	0.000080	-4.167520
H	2.707713	-0.000991	-1.690358
C	-0.664292	-0.000306	3.774917
C	-0.642411	-0.000161	5.168408
C	0.579056	0.000346	5.853974
C	1.781559	0.000448	5.135457
C	1.764957	-0.000054	3.742002
H	-1.621817	0.000078	3.249426
H	-1.581163	0.000039	5.726575
H	0.594051	0.000685	6.945834
H	2.735305	0.000434	5.667533
H	2.707756	-0.000624	3.190357

Ts-I-bb-Co_2

C	0.397115	15.586808	18.077601
C	-0.498020	14.549877	17.740416
C	-1.473794	14.190376	18.699791
C	-1.545055	14.845265	19.928289
C	-0.664976	15.895084	20.225181
C	0.308932	16.267428	19.292905
B	-0.461003	13.901263	16.332240
O	0.022916	11.506426	16.689851
C	-1.199168	11.801157	16.566587
O	-2.218973	11.379173	17.154970
Si	0.665075	14.440518	14.810225
B	-1.569903	13.014381	15.521840
C	-2.484110	12.835081	14.303291
C	-2.244439	13.492634	13.073963
C	-3.003852	13.213793	11.937930
C	-4.076667	12.318538	12.021842
C	-4.367152	11.691429	13.240511
C	-3.570931	11.927816	14.359574
N	1.599704	13.321463	13.870095
Si	2.512051	13.722266	12.350209

C	1.255582	13.847275	10.947788
C	1.995026	12.046373	14.445687
C	1.457882	10.854110	13.912133
C	1.962981	9.633282	14.372626
C	2.958882	9.580341	15.345126
C	3.446965	10.765178	15.888682
C	2.978733	12.012104	15.457513
C	0.325697	10.841714	12.898369
C	-0.867639	10.022675	13.418607
C	3.526438	13.258565	16.126235
C	3.164668	13.272523	17.619229
C	3.471567	15.330022	12.630030
C	3.803858	12.380281	12.050046
C	5.039953	13.410697	15.918866
C	0.763822	10.273258	11.537665
Si	0.210955	16.657106	14.119867
Si	-1.961359	17.331360	14.912534
C	-1.911263	19.217400	15.224411
Si	1.934048	17.915337	15.228991
C	1.208411	18.934635	16.662304
Si	0.035701	17.381367	11.839614
C	-0.580693	19.186868	11.944727
C	3.356245	16.858362	15.937185
C	2.754861	19.110260	13.989292
C	1.639936	17.431324	10.817854
C	-1.270767	16.414959	10.824422
C	-3.242281	16.989531	13.542946
C	-2.652490	16.545018	16.488968
H	1.548831	8.706989	13.968315
H	3.335868	8.617529	15.695698
H	4.204499	10.730902	16.675361
H	-0.014349	11.877683	12.751881
H	-0.615340	8.950586	13.443124
H	-1.734759	10.158097	12.755130
H	-1.151247	10.324981	14.433205
H	1.117207	9.236848	11.656700
H	-0.090217	10.261745	10.841451
H	1.575125	10.854393	11.077483
H	3.053371	14.140130	15.664736
H	3.475387	14.223584	18.081888
H	2.082997	13.138786	17.761026
H	3.679022	12.453977	18.146193
H	5.399496	14.340584	16.387313
H	5.298247	13.435887	14.848436
H	5.580437	12.566760	16.375469
H	3.376093	11.371662	11.994031
H	4.333478	12.597093	11.107460
H	4.541089	12.378527	12.867719
H	0.439224	14.524230	11.232461
H	0.814772	12.861135	10.742846
H	1.710272	14.226780	10.019524
H	2.832800	16.163874	12.953111
H	4.236474	15.147976	13.400875
H	3.988172	15.638750	11.707200
H	-4.220451	17.348334	13.905460
H	-3.018583	17.506369	12.599618
H	-3.333113	15.912500	13.336424
H	-2.936397	19.611757	15.122523
H	-1.570809	19.421625	16.249566
H	-1.265075	19.768064	14.528157
H	-2.784026	15.459914	16.380280
H	-2.023587	16.725769	17.370508
H	-3.642581	17.000840	16.663647
H	4.088694	17.553839	16.382182
H	3.050702	16.152666	16.721982
H	3.869418	16.289083	15.151125
H	3.458815	19.761080	14.534507
H	3.325772	18.558427	13.227422
H	2.027178	19.753937	13.473727
H	2.038886	19.355809	17.253461
H	0.594375	19.766591	16.290353
H	0.587546	18.318149	17.328929
H	-1.934376	17.140800	10.327052
H	-0.790732	15.807330	10.043038
H	-1.901193	15.760390	11.438605
H	1.399271	17.905152	9.850775
H	2.422791	18.029169	11.304736
H	2.037509	16.428933	10.618313
H	-0.602319	19.597697	10.921113
H	-1.595664	19.250173	12.360505
H	0.078123	19.825752	12.550761
H	1.167006	15.865309	17.356792
H	1.008049	17.075762	19.519610
H	-0.732642	16.413272	21.184208
H	-2.299501	14.544818	20.658497
H	-2.170277	13.381045	18.474981
H	-3.758740	11.406883	15.300797
H	-5.206357	10.995622	13.308363
H	-4.690738	12.117529	11.141226
H	-2.779003	13.715545	10.994076
H	-1.436688	14.229789	13.009438

III-bb-b3lyp

C	-0.831164	21.915025	13.263547
C	-0.834781	20.536949	13.052871
C	-0.686223	19.703229	14.166530
C	-0.603915	20.221694	15.453142
C	-0.636393	21.600048	15.649844
C	-0.739212	22.443520	14.548100
C	-0.851068	19.922296	11.673607
C	0.503159	19.265652	11.235609
C	1.639511	19.091133	12.171431
C	2.219988	17.823550	12.294439
C	3.322441	17.611546	13.118849
C	3.860073	18.669373	13.846636
C	3.290038	19.937460	13.733893
C	2.196363	20.148907	12.903780
Si	0.092415	20.783782	10.172135
B	1.960380	22.192381	9.722631
C	3.221827	21.525155	9.175572
C	3.610295	21.827935	7.853502

C	4.763561	21.287432	7.297601
C	5.542451	20.396839	8.035486
C	5.170856	20.070114	9.339328
C	4.037974	20.640370	9.907698
N	-0.489813	19.957915	8.625407
C	-1.261022	18.850765	8.605471
C	-2.063235	18.330056	9.597647
C	-2.730850	17.085131	9.001429
C	-3.736288	17.533854	7.889860
C	-2.791944	18.070178	6.773127
C	-1.380601	17.913949	7.405778
C	-1.566009	16.562549	8.133295
P	-2.352488	19.031839	11.193317
C	0.001686	20.474868	7.362043
C	-0.701329	21.580108	6.822710
C	-0.308389	22.091324	5.590632
C	0.775008	21.552663	4.907443
C	1.471608	20.500053	5.465750
C	1.110505	19.923903	6.693496
C	-1.826114	22.252465	7.596444
C	-3.158246	21.492215	7.538399
C	2.046812	18.781785	7.119101
C	2.028965	17.615872	6.106776
H	3.042196	19.230257	7.057071
C	-2.048032	23.716172	7.206529
B	0.605218	22.674303	10.135444
C	-0.363955	23.882394	10.301519
C	0.139850	25.194790	10.176407
C	-0.678030	26.311646	10.296464
C	-2.042833	26.168268	10.552473
C	-2.570393	24.886549	10.686586
C	-1.744950	23.774843	10.560306
H	-0.573092	18.000718	6.692255
H	-3.007423	19.092184	6.475284
H	-2.842779	17.441734	5.881984
H	-4.423105	18.303032	8.237463
H	-4.326412	16.684363	7.537471
H	-3.146220	16.382721	9.721647
H	-1.851856	15.757848	7.449336
H	-0.698597	16.263061	8.723320
H	2.341536	20.107972	4.952402
H	1.084340	21.969459	3.955605
H	-0.833752	22.937168	5.169868
C	1.941856	18.202268	8.524897
H	1.120448	17.015995	6.203748
H	2.878418	16.956365	6.305875
H	2.098703	17.960814	5.074304
H	-1.512560	22.267554	8.635237
H	-1.109657	24.272062	7.226403
H	-2.724785	24.177958	7.927238
H	-2.493970	23.806360	6.210868
H	-3.492653	21.364123	6.504417
H	-3.924469	22.062556	8.073036
H	-3.082396	20.510272	8.003564
H	0.333207	18.360095	10.662731
H	1.786121	21.143298	12.790843
H	3.708171	20.771433	14.285566
H	4.717909	18.510783	14.489489
H	3.760533	16.622255	13.190994
H	1.805819	16.999223	11.723508
H	-0.595375	18.636354	14.019046
H	-0.490264	19.551098	16.296905
H	-0.561053	22.011234	16.649831
H	2.981527	22.478033	7.257596
H	5.042411	21.540210	6.280876
H	6.432389	19.959672	7.597101
H	5.772539	19.379310	9.918817
H	3.769092	20.390815	10.925166
H	-2.184257	22.787718	10.651274
H	-3.628579	24.751736	10.886500
H	-2.680092	27.039776	10.646773
H	-0.250051	27.302914	10.190164
H	1.197436	25.327459	9.979039
H	-0.878970	22.583246	12.420290
H	-0.738095	23.519276	14.678591
H	2.755125	17.484198	8.660703
H	2.053310	18.965174	9.286339
H	1.002654	17.672013	8.682064
C	-2.889333	17.577627	12.231298
C	-3.786544	20.218893	11.105006
C	-3.951028	21.183334	12.283917
H	-3.546343	20.796637	10.208365
C	-5.088197	19.443766	10.853880
C	-3.479986	17.907385	13.605862
H	-3.690912	17.145522	11.625048
C	-1.743502	16.561294	12.306935
H	-2.079794	15.674603	12.851680
H	-1.421834	16.255318	11.309689
H	-0.874750	16.970541	12.825488
H	-3.790346	16.973045	14.083397
H	-2.760869	18.399761	14.256842
H	-4.357009	18.549045	13.527087
H	-4.867814	21.760047	12.127743
H	-4.041485	20.656563	13.234683
H	-3.121146	21.878232	12.364226
H	-5.865700	20.144697	10.539883
H	-4.983147	18.684140	10.080483
H	-5.432451	18.954655	11.766851