

Supporting Information

Can Silaborane Serve as an Effective Bridging Unit for Lewis Pairs? A Comparative Discourse with Carborane

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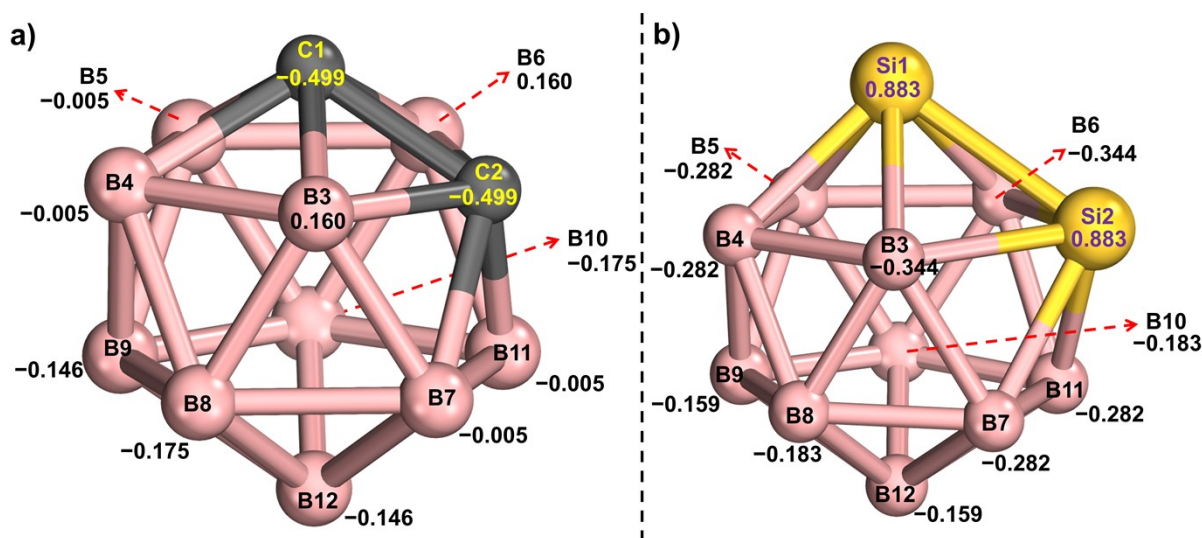


Figure S1. NBO charges of the a) *o*-carborane and b) *o*-silaborane.

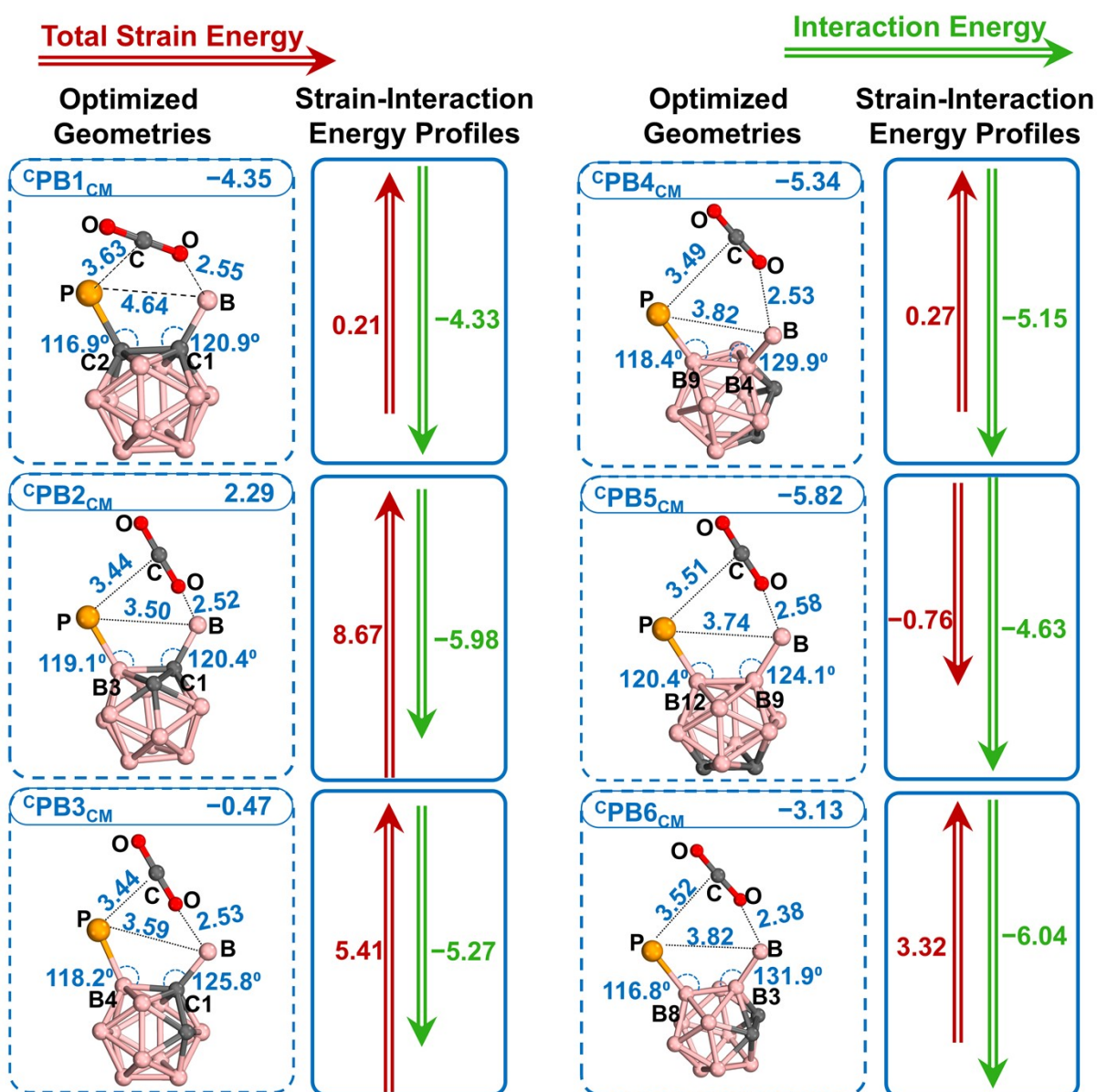


Figure S2. Optimized geometries of the reactant complexes (CMs) formed by the interaction of CO₂ with carborane supported IFLPs along with corresponding strain and interaction profiles. (the distances are in angstroms, ΔE is the zero-point corrected relative energy in kcal/mol, the number in red in the strain-interaction profile represents the strain induced (in kcal/mol) while the number in green shows the interaction energy (in kcal/mol) between CO₂ and the IFLP)

Reaction of CO₂ substituted o-carborane (^CPB₃: 1st and 4th) and o-silaborane IFLPs (^{Si}PB₄: 4th and 9th)

From Table S1, it is evident that the activation energies computed for the substituted IFLP systems give CO₂ activation energies similar to the corresponding unsubstituted o-carborane- and silaborane-based IFLPs. For the o-carborane IFLPs, substitution results in activation barriers of 9.12 kcal/mol for IFLP-PH₂/B(CF₃)₂ and 13.37 kcal/mol for IFLP-P(CH₃)₂/B(CF₃)₂. Further, for the silaborane-based systems, the substituted derivatives exhibit activation energies of 10.35 kcal/mol for IFLP-PH₂/B(CF₃)₂ and 15.27 kcal/mol for IFLP-P(CH₃)₂/B(CF₃)₂, which are again comparable to the unsubstituted analogues. However, in the case of ^CPB₃, the activation barrier is lower than those of both substituted systems, IFLP-P(CH₃)₂/B(CF₃)₂ and IFLP-PH₂/B(CF₃)₂. A similar observation holds for the silaborane series, where the unsubstituted ^{Si}PB₄ exhibits a lower activation barrier than its substituted counterparts.

In terms of adduct stability, the substituted systems form comparatively more stable adducts. This behaviour can be attributed to the stronger electron-withdrawing nature of the substituents, which enhances the acidity of the Lewis acid component and stabilizes the system, consequently increasing the stability of the adducts. Thus, substitution may impart additional electronic and steric effects that further influence the reactivity of the IFLPs. Therefore, endeavours to find suitable substituents complementing the electronic effects of the cages could provide new directions and avenues.

TableS1. Relative energies of the CMs, TSs, and ADs obtained in the reaction of CO₂ with substituted o-carborane (^CPB₃: 1st and 4th) and o-silaborane IFLPs (^{Si}PB₄: 4th and 9th). (E_a is the CO₂ activation energy; all values are in kcal/mol.)

IFLP System	CM	TS	AD	E _a
o-carborane				
IFLP-PH ₂ /B(CF ₃) ₂	8.41	9.12	-8.16	9.12
IFLP-P(CH ₃) ₂ /B(CF ₃) ₂	-4.23	9.14	-13.98	13.37
o-Silaborane				
IFLP-PH ₂ /B(CF ₃) ₂	9.23	10.35	-5.02	10.35
IFLP-P(CH ₃) ₂ /B(CF ₃) ₂	-3.73	11.54	-10.26	15.27

Comparison of CO₂ activation with H₂ activation:

In case of Carborane, for CO₂ activation, the activation energy decreases progressively as we move from ^oPB1 to ^oPB3, indicating the catalysts become increasingly efficient in stabilizing the CO₂ transition state. ^oPB1 shows the highest energy barrier of value 14.18 kcal/mol, which slightly decreases in ^oPB2 and reaches a minimum in ^oPB3 (i.e. 11.37 and 7.79 kcal/mol respectively). Although, a slight increase is observed in energy barrier of ^oPB4 and ^oPB5 showing value of 11.10 and 13.18 kcal/mol respectively, the barrier drops again in ^oPB6 to 9.04 kcal/mol, confirming that ^oPB3 provides highly favorable environment for CO₂ bending and activation. A very similar pattern is observed in H₂ activation. The barrier is high for ^oPB1 (i.e. 17.93 kcal/mol) and reduces significantly for ^oPB2 and ^oPB3 of value 14.23 and 10.49 kcal/mol respectively, showing the same enhancement in catalytic efficiency. While ^oPB4 with energy barrier of 15.13 kcal/mol and ^oPB5 with highest barrier of 24.64 kcal/mol for H₂ activation has been observed whereas the value drops sharply for ^oPB6 becoming 12.65 kcal/mol. Thus, in both CO₂ and H₂ activation, overall trend shows an initial decrease up to ^oPB3, a significant rise around ^oPB4 and ^oPB5 and a final sharp decrease for ^oPB6. This consistent pattern across each substrate suggests that the electronic and steric features of the catalysts that improve CO₂ activation similarly enhance H₂ activation, with **^oPB3** emerging as the most effective system for both.

A clear comparative trend emerges for both CO₂ and H₂ activation energies in the CM pathway. Beginning with CBPB1, the zero-point corrected CM energies are -4.35 kcal/mol for CO₂ and -0.57 kcal/mol for H₂. In both cases, these energies increase as we move to ^oPB2, reaching 2.28 kcal/mol for CO₂ and 3.60 kcal/mol for H₂. Upon further progression to ^oPB3, the CM energies for the two molecules begin to stabilize, resulting in -0.47 kcal/mol for CO₂ and 2.91 kcal/mol for H₂. The trend then shifts markedly for ^oPB4 and ^oPB5, where both CO₂ and H₂ exhibit significant decreases in CM energy. For ^oPB4, the values drop to -5.34 kcal/mol (CO₂) and -4.08 kcal/mol (H₂), and decline further in ^oPB5 to -5.81 kcal/mol and -4.59 kcal/mol, respectively. In the final case, the CM energies of both species increase again, reaching -3.13 kcal/mol for CO₂ and -3.58 kcal/mol for H₂. Overall, CO₂ and H₂ follow closely parallel trends across the series, an initial increase from ^oPB1 to ^oPB2, slight stabilization at ^oPB3, a pronounced decrease at ^oPB4 and ^oPB5, and a modest rise at the final point. This comparative progression highlights the consistent and correlated energetic behaviour of both molecules within the CM pathway.

Considering the stability of the adducts, the trend mirrors that observed for the corresponding activation energy barriers. For both the CO₂ and H₂ adducts, there is a progressive stabilization

from ^cPB1 to ^cPB3. Specifically, the adduct stability values for CBPB1 are 8.76 and 15.90 kcal/mol for CO₂ and H₂, respectively. These values decrease to 5.44 kcal/mol and 9.49 kcal/mol in ^cPB2, and further decline to 0.42 kcal/mol (CO₂) and 4.03 kcal/mol (H₂) in ^cPB3. Subsequently, a slight destabilization is observed in ^cPB4, with adduct stabilities of 1.87 and 8.97 kcal/mol for CO₂ and H₂, respectively, which continues to destabilize in ^cPB5, where the values increase to 4.75 and 15.03 kcal/mol. Finally, in the last case, the adducts regain some stability, exhibiting values of 1.45 kcal/mol for CO₂ and 5.67 kcal/mol for H₂. Overall, this pattern demonstrates a consistent and comparable trend in adduct stabilization for both molecules across the ^cPB series.

On comparing CM relative energies, activation energies and adduct stabilities for both CO₂ and H₂ molecule, it was clearly seen that both follows the similar trend of activation for the investigated IFLPs

TableS2. Relative energies of the CMs, TSs and ADs obtained in the reaction of CO₂ and H₂ with the considered o-carborane based IFLPs. (E_a is the activation energy, all the energies are in kcal/mol)

	CO ₂				H ₂			
	CM	TS	AD	E _a	CM	TS	AD	E _a
^c PB1	-4.35	9.83	8.76	14.18	-0.57	17.36	15.90	17.93
^c PB2	2.28	11.37	5.44	11.37	3.60	14.29	9.49	14.29
^c PB3	-0.47	7.31	0.42	7.79	2.91	10.49	4.03	10.49
^c PB4	-5.34	5.75	1.87	11.10	-4.08	11.05	8.97	15.13
^c PB5	-5.81	7.37	4.75	13.18	-4.59	20.04	15.03	24.64
^c PB6	-3.13	5.90	1.45	9.04	-3.58	9.07	5.67	12.65

Cartesian coordinates of the optimized geometries

^cPB1

C	-0.42290500	1.01392000	0.00006300
C	-0.63418200	-0.62344500	0.00009200
B	-0.09245800	0.11775200	-1.44448700
H	-0.87065000	0.21749800	-2.32933900
B	0.97112600	1.41211700	-0.88734300
H	0.98089200	2.42542500	-1.49653000
B	0.97114100	1.41200500	0.88731900
H	0.98116200	2.42513800	1.49678900
B	-0.09221800	0.11731400	1.44456100
H	-0.87011100	0.21789200	2.32957400
B	0.54296200	-1.45642800	-0.89210000
H	0.21654600	-2.42420300	-1.49041800
B	1.63470200	-0.15837200	-1.44491500
H	2.21174200	-0.25003800	-2.47577000
B	2.30763500	0.64314300	-0.00007200
H	3.39527900	1.11419000	0.00012400
B	1.63490900	-0.15851100	1.44476900
H	2.21211800	-0.25003800	2.47554000
B	0.54321100	-1.45666700	0.89215300
H	0.21672100	-2.42448600	1.49034600
B	2.04277800	-1.12377800	-0.00016400
H	2.93207900	-1.90743900	-0.00061600
B	-1.98696000	1.54617900	0.00022900
H	-2.38320900	2.01895000	-1.02514700
H	-2.38306300	2.01875600	1.02575900
P	-2.45512900	-0.50028900	-0.00003100
H	-2.92697400	-1.24670100	-1.09509000
H	-2.92721900	-1.24723200	1.09456600

^cPB1_{CM}

C	-0.25048100	-0.70186400	-0.68410800
C	-0.29209000	0.86242300	-0.11151000
B	-1.31802300	0.45455500	-1.41740800
H	-1.03797800	0.85946100	-2.49186600
B	-1.82665000	-1.22387500	-1.08599600
H	-1.93653300	-1.95574000	-2.00982800
B	-1.03261300	-1.77045600	0.39742100
H	-0.60107600	-2.86911800	0.46947800
B	-0.01074300	-0.44410300	0.98826900
H	1.07113700	-0.56679100	1.44322500
B	-1.88728300	1.47059100	-0.07832800
H	-2.02774400	2.62702700	-0.28572200
B	-2.89305900	0.13906900	-0.68669400
H	-3.87659300	0.35031300	-1.31264300
B	-2.72145600	-1.23075100	0.44834600
H	-3.59820500	-2.00605800	0.63432000
B	-1.58477100	-0.74836200	1.73412300
H	-1.63148200	-1.15788800	2.84494200

B	-1.07655900	0.92160900	1.39840300
H	-0.67645000	1.70789600	2.18699200
B	-2.75029600	0.43067700	1.06993400
H	-3.64396400	0.86646600	1.71522400
B	0.87194100	-1.16762800	-1.68051900
H	1.48530600	-0.35912900	-2.29941600
H	0.95801400	-2.32850100	-1.90784900
P	1.20999800	1.91913300	-0.43498800
H	0.66353400	2.66197000	-1.50924200
H	0.88874300	2.88345900	0.54853000
C	3.64400200	-0.65757000	0.35557400
O	3.02099000	-1.37444600	-0.31127300
O	4.27304800	0.04008100	1.02392100

^cPB1_{TS}

C	0.18486400	0.90260900	-0.34473900
C	0.10839600	-0.73287300	-0.15034600
B	0.93500700	-0.14671600	-1.52193300
H	0.40793600	-0.25525600	-2.57246100
B	1.72827400	1.31974500	-0.93399600
H	1.80207300	2.24236500	-1.66957400
B	1.30334400	1.56086600	0.76872600
H	1.08136000	2.64569200	1.18183800
B	0.22362500	0.25551000	1.25353100
H	-0.73656000	0.36785900	1.93258400
B	1.54902600	-1.53439700	-0.58988100
H	1.44719200	-2.60947600	-1.07678600
B	2.63236100	-0.21425500	-1.07316500
H	3.44879800	-0.37428200	-1.91668900
B	2.87012100	0.83999100	0.34532900
H	3.87979900	1.43617800	0.51686800
B	1.92324900	0.17533000	1.70107800
H	2.22853000	0.28322900	2.84071200
B	1.10592600	-1.28913700	1.11538400
H	0.71243000	-2.20230800	1.75907700
B	2.75025900	-0.92263100	0.56196300
H	3.66184300	-1.60350000	0.89396600
B	-1.13743900	1.65772500	-0.91395800
H	-1.51745100	1.19006200	-1.95542600
H	-1.04111000	2.84498700	-0.87227800
P	-1.58206300	-1.35994000	-0.41709800
H	-1.55188700	-1.91035500	-1.71178700
H	-1.62386400	-2.51655900	0.38217200
C	-3.04077700	0.32183600	0.27245100
O	-2.40607400	1.34712500	0.11714300
O	-4.01915200	-0.17201400	0.66969100

^cPB1_{AD}

C	0.18982200	0.94621000	-0.28890700
C	0.08044900	-0.68790600	-0.17602800
B	0.90150800	-0.06173700	-1.53345900
H	0.35392700	-0.10765300	-2.57765200
B	1.74034400	1.34298400	-0.87641200
H	1.83863200	2.30031600	-1.56206900
B	1.34381000	1.50435400	0.84357100
H	1.16583100	2.57007600	1.32109100
B	0.23553700	0.21047100	1.28172100
H	-0.71615300	0.30994600	1.97369100
B	1.47646200	-1.52346400	-0.68314400
H	1.32603900	-2.56612800	-1.22582000
B	2.59595700	-0.21227300	-1.10909000
H	3.39635800	-0.35506800	-1.97053900
B	2.88200500	0.75599100	0.35981200
H	3.91388900	1.30633400	0.54972100
B	1.93518900	0.04859200	1.69315000
H	2.25959100	0.08487500	2.83168300
B	1.06331200	-1.35756800	1.04471300
H	0.64060800	-2.29230400	1.63742400
B	2.70977800	-1.01352200	0.48429200
H	3.60317300	-1.73947800	0.76517700
B	-1.18249600	1.70537000	-0.78469400
H	-1.49675300	1.27660500	-1.87531900
H	-1.05965300	2.89229400	-0.74156100
P	-1.62893800	-1.19549200	-0.45084100
H	-1.80748600	-1.51833400	-1.80360000
H	-1.84952100	-2.38246400	0.25995300
C	-2.86827800	0.17883300	0.24271800
O	-2.37991900	1.33731100	0.17486100
O	-3.87675600	-0.27049300	0.68907000

^cPB2

C	0.43069500	0.94853200	0.09406000
C	0.01805400	0.11960900	-1.26061600
B	0.70641100	-0.75658500	0.01752100
B	0.04468700	-0.00502300	1.46660200
H	0.76161800	0.09616600	2.40448300
B	-0.96678400	1.35849500	0.96589300
H	-0.96695200	2.36015500	1.59347700
B	-0.93945600	1.45698200	-0.80050900
H	-0.86242100	2.44507100	-1.44075400
B	-0.60675300	-1.43892800	-0.94393300
H	-0.36762600	-2.30327500	-1.71618100
B	-0.64133200	-1.52887800	0.83571900
H	-0.49134700	-2.55530000	1.40935900
B	-1.70269300	-0.20998500	1.42191500
H	-2.32861300	-0.31961300	2.42242000
B	-2.31645600	0.69413700	0.01130500
H	-3.38276000	1.21004300	-0.01009700

B	-1.63634200	-0.06603300	-1.44481100
H	-2.08131400	-0.04856000	-2.54031200
B	-2.11548100	-1.08595900	-0.07162700
H	-3.04688900	-1.81420100	-0.15393900
H	0.65779400	0.30254200	-2.11298000
P	2.61534200	-0.47868100	-0.01138500
H	3.22395400	-1.08246700	1.09936300
H	3.26770800	-1.09057300	-1.09628100
B	1.98148400	1.49215600	0.01124900
H	2.27488300	1.99514900	-1.04023700
H	2.38291500	2.02433300	1.00516600

^cPB2_{CM}

C	0.29867800	-0.68182600	0.64888100
C	0.33946400	-0.43536700	-0.95035600
B	0.19964700	0.95284500	0.08358400
B	1.21781300	0.51454500	1.46197300
H	0.84950900	0.84436400	2.53775700
B	1.84539900	-1.13261600	1.21150200
H	1.89915700	-1.88861400	2.12193700
B	1.25485400	-1.74424900	-0.34394800
H	0.83928600	-2.83531000	-0.51319600
B	1.23117800	0.94755200	-1.36386500
H	0.86694900	1.58633900	-2.29140300
B	1.86171000	1.55773400	0.17967100
H	2.03572100	2.71669500	0.35641700
B	2.87956600	0.27755800	0.89145100
H	3.80028000	0.52535900	1.59538500
B	2.89403800	-1.11320900	-0.22966900
H	3.81139100	-1.85577700	-0.33227600
B	1.87640900	-0.69212400	-1.62220100
H	1.93324400	-1.13009300	-2.71914700
B	2.89392400	0.55325400	-0.86685100
H	3.82359200	1.00608000	-1.44590800
H	-0.55731300	-0.70071600	-1.49018600
P	-1.50668700	1.88094500	0.16871200
H	-1.33390600	2.41386100	1.46885400
H	-1.07705400	3.04732500	-0.50770400
B	-0.92562200	-1.34409100	1.40424500
H	-1.05817600	-2.52282000	1.36926000
H	-1.58756700	-0.66004400	2.11947300
C	-3.70821800	-0.71201400	-0.31594200
O	-2.69914100	-1.28702800	-0.38840900
O	-4.72197300	-0.17191900	-0.25220200

^cPB2_{TS}

C	0.22771200	0.80908700	-0.45996300
C	0.38275000	0.29568700	1.08078900

B	0.06224000	-0.87001800	-0.13010000
B	0.98439600	-0.31575700	-1.51893500
H	0.50202300	-0.45642700	-2.59032800
B	1.76201300	1.21366200	-1.08011200
H	1.82076700	2.09473500	-1.86692700
B	1.34537200	1.61335400	0.59312100
H	1.04895200	2.68893900	0.97524600
B	1.17957900	-1.20426600	1.20254400
H	0.82562600	-1.95313200	2.04876700
B	1.62762400	-1.60313200	-0.47142500
H	1.67464800	-2.72908900	-0.84043200
B	2.69567600	-0.30514400	-1.06738600
H	3.53554700	-0.51089400	-1.87786900
B	2.91412800	0.88592800	0.24135100
H	3.90071900	1.52777700	0.37591300
B	1.97792900	0.32554800	1.64201300
H	2.15748100	0.57851800	2.78315000
B	2.82242100	-0.85774300	0.62053000
H	3.75143400	-1.46324100	1.03875800
H	-0.43747000	0.54192100	1.73914700
P	-1.75088700	-1.50963100	-0.27727000
H	-1.78928800	-2.08879400	-1.55956700
H	-1.79589600	-2.67149300	0.51835600
B	-1.08237100	1.62594100	-0.95641000
H	-0.99949100	2.81085600	-0.86624500
H	-1.56099300	1.17292200	-1.95696900
C	-3.16426800	0.45574900	0.26095100
O	-2.31937200	1.31607200	0.23296200
O	-4.24224800	0.08353500	0.46346700

^CPB2_{AD}

C	0.22479600	0.84598500	-0.45530400
C	0.32734900	0.26082100	1.08241100
B	0.02888500	-0.81919400	-0.18528000
B	0.98887100	-0.26566100	-1.53535200
H	0.52287900	-0.36052200	-2.61871700
B	1.79117700	1.21772500	-1.01197600
H	1.90887300	2.12409300	-1.76068800
B	1.33085800	1.56504500	0.66199100
H	1.06275700	2.63197600	1.08501100
B	1.06726700	-1.27743400	1.16463500
H	0.65823900	-2.04792400	1.96515900
B	1.54984300	-1.62273800	-0.51917100
H	1.56218900	-2.73397300	-0.93307700
B	2.67793000	-0.33523600	-1.03051600
H	3.53592600	-0.54176900	-1.82106200
B	2.89023600	0.79600400	0.32917300
H	3.89557300	1.39234800	0.51927200
B	1.89936600	0.21333600	1.68208200
H	2.05697700	0.41454200	2.83609600

B	2.73361800	-0.95991800	0.63806700
H	3.63084000	-1.61110000	1.05590400
H	-0.50568000	0.51273100	1.72376700
P	-1.82566900	-1.24399900	-0.46510000
H	-2.09280300	-1.43075800	-1.82727900
H	-2.27360800	-2.41067600	0.16820800
B	-1.15619700	1.62219100	-0.92554700
H	-1.00815600	2.80843900	-0.96088000
H	-1.51261000	1.13636500	-1.97928800
C	-2.86432000	0.22029100	0.26874400
O	-2.28514200	1.34576000	0.12494100
O	-3.86393100	-0.07788100	0.85111400

^cPB3

C	-0.89152600	1.25991800	-0.79945000
C	0.45660900	0.90184000	0.02554100
B	-0.92066300	1.40096900	0.90322200
H	-0.93079000	2.47565800	1.38976700
B	-2.28710100	0.71131000	-0.00886700
H	-3.27890700	1.34842000	-0.10005500
B	-1.65277800	-0.13684800	-1.43904700
H	-2.21056900	-0.04336900	-2.47746800
B	0.09611700	0.02359900	-1.42451400
H	0.76455500	0.25060100	-2.37131400
B	0.06887600	0.04232600	1.45011800
H	0.77690700	0.20669700	2.38525400
B	-1.68310600	-0.11975600	1.44239400
H	-2.30745400	-0.13938900	2.44898500
B	-2.13177300	-1.06487700	-0.00368900
H	-3.09572000	-1.75402000	-0.02644800
B	-0.63909500	-1.49704900	-0.88622400
H	-0.50988600	-2.47471700	-1.54376000
B	0.69750500	-0.77779400	0.02297200
B	-0.66117100	-1.49122700	0.90404800
H	-0.54689300	-2.48170800	1.54564400
H	-0.88387200	2.18786900	-1.35246900
B	1.99957100	1.48541300	-0.03503000
H	2.36082200	2.04304100	0.96291800
H	2.31826600	1.97933200	-1.08154700
P	2.61183200	-0.48798900	0.01137100
H	3.26309600	-1.03188100	1.13042400
H	3.28056700	-1.09758500	-1.06395500

^cPB3_{CM}

C	-1.33454800	-1.53460800	0.42951300
C	-0.28351100	-0.72091800	-0.53339200
B	-1.81671500	-1.17821200	-1.17039600
H	-1.84425500	-2.05796300	-1.95988500
B	-2.93621300	-1.04622500	0.20884800

H	-3.78516700	-1.86346400	0.30536600
B	-1.99598800	-0.56087600	1.63671700
H	-2.21784900	-1.05144700	2.68938100
B	-0.28963400	-0.39097300	1.15388600
H	0.61364400	-0.78147700	1.80381700
B	-1.13061000	0.43898800	-1.46991600
H	-0.71565100	0.66579100	-2.55505400
B	-2.83187900	0.26028500	-0.99779500
H	-3.70696400	0.45385200	-1.77244000
B	-2.94678900	0.64453700	0.74464800
H	-3.91920800	1.12417500	1.22294300
B	-1.30378700	1.04786300	1.32804300
H	-1.08758800	1.80701900	2.21219000
B	-0.18811300	0.92630900	-0.05272800
B	-1.83654900	1.56082300	-0.29275500
H	-1.99564500	2.70257600	-0.56940800
H	-1.07683000	-2.56788100	0.61134000
B	0.86645900	-1.54829400	-1.21058800
H	1.53305600	-1.01629900	-2.03643100
H	0.92988300	-2.71728100	-1.00198900
P	1.51978100	1.84325200	-0.24082900
H	1.12875900	2.74713500	-1.25784900
H	1.32396900	2.75843300	0.82187400
C	3.80324900	-0.67220300	0.28273700
O	4.76815200	-0.04517000	0.23445000
O	2.85198400	-1.33691800	0.34500200

^cPB3_{TS}

C	-1.36704300	1.40991600	-0.61042800
C	-0.18627800	0.79765000	0.34801800
B	-1.67948100	1.25476000	1.06022800
H	-1.69631100	2.22980500	1.72530500
B	-2.91120300	0.87801400	-0.17246100
H	-3.81728700	1.62755400	-0.29495500
B	-2.08264100	0.24412700	-1.61155200
H	-2.43098200	0.57116000	-2.69306300
B	-0.34176000	0.23248000	-1.27784300
H	0.48146800	0.55820900	-2.05846600
B	-0.88527700	-0.26288500	1.50538100
H	-0.35718100	-0.33139400	2.56195500
B	-2.62556700	-0.24274700	1.17688600
H	-3.41645300	-0.37334400	2.04913100
B	-2.87219900	-0.87118700	-0.47760400
H	-3.85232900	-1.45895400	-0.79115500
B	-1.27012100	-1.27149800	-1.16224000
H	-1.07908600	-2.13581300	-1.95128200
B	-0.06402300	-0.87758100	0.07524100
B	-1.61869100	-1.57882100	0.56186300
H	-1.67200100	-2.67856500	1.00295700
H	-1.19273500	2.41990400	-0.95168500

B	1.05492200	1.74076200	0.76348600
H	1.48231700	1.49798200	1.85376300
H	0.91575300	2.88938200	0.46451800
P	1.74000200	-1.54089000	0.23683000
H	1.74646500	-2.27532700	1.43897900
H	1.80947200	-2.60386800	-0.68562900
C	3.21836800	0.45464700	-0.20773700
O	4.29893400	0.05364200	-0.31655700
O	2.38466500	1.31838500	-0.25955000

^CPB3_{AD}

C	1.34137000	1.36009300	0.67371800
C	0.18581300	0.82269900	-0.35251600
B	1.71621900	1.25838700	-0.98854500
H	1.79403500	2.25317700	-1.61641600
B	2.88735600	0.79367700	0.27646900
H	3.81400600	1.50308200	0.46305800
B	1.99159700	0.13285600	1.66093700
H	2.31104600	0.40573600	2.76547900
B	0.27270600	0.19257400	1.26917400
H	-0.58061700	0.50038800	2.02267900
B	0.90983100	-0.21646600	-1.52378700
H	0.41300200	-0.24441300	-2.59649600
B	2.62771000	-0.26717800	-1.12330800
H	3.44970000	-0.39420800	-1.96625300
B	2.78739800	-0.96656800	0.51414800
H	3.73624900	-1.59589100	0.84113900
B	1.15161300	-1.34358800	1.12704500
H	0.89714300	-2.23127100	1.87046800
B	0.03555300	-0.83632400	-0.14041100
B	1.55817800	-1.59847500	-0.60148200
H	1.58889500	-2.68253500	-1.08165800
H	1.18252000	2.36186400	1.04621400
B	-1.12852300	1.72218100	-0.76319100
H	-1.41542500	1.44357600	-1.90601400
H	-0.92253100	2.89049100	-0.57713700
P	-1.81630100	-1.26215600	-0.41791700
H	-2.10963900	-1.49373500	-1.76976600
H	-2.28111700	-2.40166800	0.25070700
C	-2.90396400	0.20833400	0.22586300
O	-3.95502100	-0.10804500	0.70271900
O	-2.34751100	1.34749600	0.13542000

^CPB₄

C	0.89841800	1.29566100	-0.77680100
C	2.15278900	0.63608800	0.00570000
B	0.91957900	1.40933700	0.92859600
H	1.18746600	2.44557900	1.42660000
B	-0.58007700	1.02721200	0.03986900

B	-0.08714800	0.09118800	-1.41318900
H	-0.66818700	0.29028800	-2.42435200
B	1.65374100	-0.12269600	-1.44941200
H	2.33026000	0.01519100	-2.40653300
B	1.67894700	-0.13692300	1.43488900
H	2.41926900	-0.11136700	2.35628000
B	-0.06776300	0.05333400	1.45781000
H	-0.69193400	0.12362300	2.46418600
B	-0.69877400	-0.74517100	0.01196400
B	0.63234200	-1.46664600	-0.90932600
H	0.54536000	-2.43475900	-1.58717100
B	2.12030400	-1.06705100	-0.01981800
H	3.15704000	-1.63452400	-0.05551000
B	0.64845200	-1.48862500	0.88259200
H	0.57833600	-2.49067100	1.51197400
H	3.09108000	1.16763300	-0.05383500
H	1.10884100	2.20454600	-1.32244000
P	-2.62303100	-0.53423000	0.00967200
H	-3.25131100	-1.20652000	-1.05713600
H	-3.22487200	-1.15933800	1.11818800
B	-2.24659700	1.50516100	-0.03477200
H	-2.73616400	1.99792100	0.94981800
H	-2.67198200	1.91975300	-1.08454900

CPB4_{CM}

C	1.34022100	-1.53623600	0.43680600
C	2.81629300	-0.93394900	0.19392000
B	1.80307100	-1.20643600	-1.17592600
H	2.07169900	-2.11921200	-1.87578000
B	0.16840900	-0.82721000	-0.59120000
B	0.30072700	-0.40575700	1.13626100
H	-0.51834000	-0.78149300	1.90060800
B	2.00269500	-0.51597100	1.64259600
H	2.36734100	-1.01336800	2.64865900
B	2.81749900	0.24986300	-1.01886000
H	3.77120300	0.33566600	-1.71242700
B	1.11494000	0.38641900	-1.50706900
H	0.81241300	0.67407200	-2.61666900
B	0.17483600	0.89112500	-0.08433400
B	1.29692500	1.06422300	1.29171100
H	1.11968800	1.83586800	2.17368500
B	2.93479700	0.67485500	0.70827300
H	3.96428200	1.04265700	1.15876400
B	1.81238200	1.54927100	-0.34674300
H	2.00400400	2.68335100	-0.63346100
H	3.63801600	-1.62598200	0.30425300
H	1.28486700	-2.58449800	0.69258700
P	-1.48896800	1.90672400	-0.22047900
H	-1.08790900	3.02735100	0.54911900
H	-1.22535000	2.52439600	-1.46849900

B	-1.08757200	-1.76765600	-1.20441000
H	-1.84262800	-1.32024700	-2.01651400
H	-1.17072900	-2.93707400	-0.96037000
C	-3.83393300	-0.62241200	0.31899400
O	-4.78287400	0.01009000	0.15034500
O	-2.90250900	-1.29139200	0.50133000

^cPB4_{TS}

C	1.42492000	1.39955000	-0.63052000
C	2.82362500	0.73005900	-0.18152200
B	1.73682700	1.27267400	1.04536700
H	2.03504200	2.25006300	1.63589200
B	0.12180800	0.93843600	0.37983700
B	0.36925600	0.25772700	-1.26148600
H	-0.37462200	0.56584400	-2.12762500
B	2.09888500	0.16499200	-1.62819600
H	2.58274700	0.48360300	-2.65595700
B	2.64003500	-0.26599700	1.17428800
H	3.52883600	-0.32362200	1.95141200
B	0.90564800	-0.20102500	1.52935400
H	0.48410800	-0.31559400	2.63124000
B	0.05982900	-0.81947400	0.10739300
B	1.24079400	-1.29530500	-1.12967100
H	1.05854900	-2.17067700	-1.90767400
B	2.85248800	-0.94299800	-0.46090800
H	3.88038500	-1.44261500	-0.76300800
B	1.58455900	-1.57580800	0.60509900
H	1.65151000	-2.66771200	1.06195000
H	3.70865900	1.33473300	-0.31399100
H	1.47944100	2.39962900	-1.03592700
P	-1.74871200	-1.46362000	0.28562000
H	-1.87866800	-2.60545300	-0.53022700
H	-1.81525100	-2.06975700	1.55557300
B	-1.20635100	1.95370900	0.71190200
H	-1.67472800	1.85940200	1.81532900
H	-1.17131500	3.06761700	0.26322300
C	-3.27352700	0.34002600	-0.22204600
O	-4.32831000	-0.14238500	-0.36259500
O	-2.56331800	1.30943200	-0.26551600

^cPB4_{AD}

C	-1.36492700	1.35963100	0.70112300
C	-2.77578400	0.68390600	0.29405800
B	-1.75661700	1.29734800	-0.96133500
H	-2.10312100	2.28933000	-1.49724800
B	-0.10347900	0.95841000	-0.38984800
B	-0.27906200	0.20796700	1.24114500
H	0.51681100	0.47864700	2.07176700
B	-1.98134800	0.07171300	1.68167000

H	-2.42152500	0.33862800	2.74269900
B	-2.65052700	-0.25202000	-1.10770200
H	-3.57634600	-0.29429500	-1.84075500
B	-0.94323600	-0.14546300	-1.54480400
H	-0.56021000	-0.21988700	-2.66368600
B	-0.03885000	-0.79583500	-0.18462900
B	-1.12790900	-1.35898700	1.08701400
H	-0.89333900	-2.26191600	1.81719300
B	-2.77128900	-1.00275600	0.50600900
H	-3.77699400	-1.52908500	0.83460900
B	-1.55218600	-1.57481300	-0.64777600
H	-1.62420300	-2.64780500	-1.14610100
H	-3.66321100	1.26649900	0.49353100
H	-1.41560000	2.33985900	1.15335100
P	1.80582400	-1.21880500	-0.51290900
H	2.28139900	-2.44080300	-0.01735400
H	2.04342000	-1.28530900	-1.89395300
B	1.32553700	1.84402000	-0.75638400
H	1.66427900	1.61202700	-1.90302100
H	1.25766300	3.02715600	-0.53360300
C	2.95730800	0.14537100	0.27322200
O	3.93391100	-0.29677500	0.81504000
O	2.52594800	1.32523500	0.16608400

^cPB5

C	1.95983000	-0.97833400	0.00055100
C	2.15349100	0.64028600	-0.00070900
B	1.64656200	-0.11714200	-1.45378600
H	2.43326200	-0.21626300	-2.32812000
B	0.60307200	-1.45307200	-0.89459200
H	0.64695700	-2.47360400	-1.49084200
B	0.60341800	-1.45167100	0.89692400
H	0.64757200	-2.47127400	1.49474000
B	1.64702600	-0.11483900	1.45369600
H	2.43402500	-0.21251400	2.32792200
B	0.94454300	1.43542900	-0.88985100
H	1.26166500	2.39993800	-1.49704200
B	-0.08401000	0.10166500	-1.44437600
H	-0.69982500	0.15564700	-2.45684200
B	-0.71882000	-0.69933300	0.00089900
B	-0.08356800	0.10396800	1.44451000
H	-0.69903200	0.15962600	2.45708700
B	0.94481200	1.43687700	0.88747600
H	1.26214000	2.40237600	1.49298000
B	-0.56417700	1.07449400	-0.00067600
H	3.17812300	0.98235500	-0.00113900
H	2.86950800	-1.56031900	0.00088000
B	-2.24692100	1.52388300	-0.00034800
H	-2.72170600	1.96617800	-1.01768900
H	-2.72022600	1.96578800	1.01788400

P	-2.63819300	-0.52449600	0.00017200
H	-3.22862600	-1.20162000	-1.08576300
H	-3.23054000	-1.20187500	1.08493700

^cPB5_{CM}

C	2.80270400	0.59056000	0.61705400
C	2.82102100	-0.96082300	0.16877800
B	2.01846300	-0.55574400	1.62927700
H	2.54286500	-0.84015000	2.64755800
B	1.30402300	1.03356100	1.27738000
H	1.28932500	1.83632800	2.14589600
B	1.78841100	1.52184800	-0.36254400
H	2.08999300	2.64542700	-0.57522100
B	2.79212600	0.23676500	-1.06478500
H	3.78530600	0.42343000	-1.67441000
B	1.34408100	-1.72538400	0.47925200
H	1.36073000	-2.86909200	0.77880600
B	0.31921700	-0.44635700	1.16010200
H	-0.52042800	-0.67667700	1.96270000
B	0.16461700	0.84979200	-0.07011300
B	1.08969600	0.35324200	-1.50702200
H	0.79265300	0.67468600	-2.60896700
B	1.80737100	-1.24042500	-1.16503800
H	2.13973200	-2.06112500	-1.94965000
B	0.17171100	-0.87532900	-0.56981100
H	3.76146800	-1.47943400	0.28321000
H	3.73004600	0.98753000	1.00326400
B	-1.15644900	-1.66979000	-1.25230400
H	-1.31735300	-2.84994200	-1.13156900
H	-1.91187600	-1.09331900	-1.98436200
P	-1.47715200	1.90392300	-0.18199300
H	-1.06966600	2.97941200	0.64900500
H	-1.18218800	2.58164500	-1.39198100
C	-3.87106900	-0.62572900	0.31753300
O	-2.94543700	-1.27675700	0.57322300
O	-4.81276200	-0.00480600	0.07470800

^cPB5_{TS}

C	-2.66851400	-0.87141800	0.47337400
C	-2.81004100	0.73037900	0.26498000
B	-2.01496900	0.17009500	1.67601700
H	-2.58774600	0.24622200	2.70483900
B	-1.15676700	-1.28348600	1.11640400
H	-1.08350300	-2.20994400	1.84791500
B	-1.55963300	-1.54783600	-0.60648100
H	-1.74816100	-2.64672900	-1.00086600
B	-2.65605200	-0.25397600	-1.13250200
H	-3.61728600	-0.42826100	-1.79445500
B	-1.41229700	1.56315000	0.74057600

H	-1.54617200	2.63488400	1.22096900
B	-0.31062200	0.27962100	1.25940700
H	0.50288200	0.43900600	2.10709500
B	-0.03587800	-0.76955100	-0.14833200
B	-0.94726500	-0.15167700	-1.52989400
H	-0.58300400	-0.28296400	-2.65012700
B	-1.79571300	1.30266000	-0.97449400
H	-2.19274100	2.19933300	-1.63528600
B	-0.14194400	0.99231000	-0.38383500
H	-3.79623800	1.14097600	0.42536900
H	-3.56710700	-1.39730700	0.76032700
B	1.23601000	1.88087500	-0.88243000
H	1.27550000	3.05116900	-0.62064200
H	1.68378800	1.58874800	-1.96421200
P	1.76519800	-1.40135000	-0.40849200
H	1.92197300	-2.62389100	0.27513100
H	1.82204400	-1.85252800	-1.74147600
C	3.23105700	0.32252600	0.28441600
O	2.58330700	1.33036000	0.16730100
O	4.22899800	-0.18514900	0.63069900

^CPB5_{AD}

C	-2.62070900	-0.91924800	0.44529200
C	-2.77459200	0.69394000	0.31559800
B	-1.96558500	0.07216500	1.69100100
H	-2.53017000	0.09309300	2.72655700
B	-1.10414700	-1.35086300	1.05774600
H	-1.01368700	-2.31297400	1.73889500
B	-1.52345400	-1.53286000	-0.68178000
H	-1.70341200	-2.61285900	-1.12831700
B	-2.63438800	-0.21898800	-1.12856200
H	-3.60262300	-0.36976700	-1.78566200
B	-1.37648800	1.51684500	0.81648300
H	-1.51914200	2.55868400	1.35581300
B	-0.27012300	0.21439900	1.26707200
H	0.56149600	0.32939100	2.10339500
B	-0.02121600	-0.74880000	-0.19332600
B	-0.93578200	-0.08170700	-1.54021100
H	-0.56914900	-0.16521700	-2.66413200
B	-1.77900400	1.33786000	-0.90516600
H	-2.19560700	2.25949700	-1.51700900
B	-0.11183800	1.01149500	-0.34863200
H	-3.76287600	1.08625300	0.50714100
H	-3.51322900	-1.46419300	0.71484500
B	1.35727900	1.79886900	-0.81898300
H	1.34937700	2.99914000	-0.72457200
H	1.69870900	1.43559100	-1.93471300
P	1.81369100	-1.19514400	-0.53692400
H	2.26402500	-2.43405200	-0.05762100
H	2.03972500	-1.25313800	-1.91966200

C	2.96674700	0.14913600	0.29286900
O	2.54803400	1.32672700	0.15580100
O	3.91274900	-0.30889300	0.87396700

^cPB6

C	-0.91522600	1.27415200	0.80246900
C	-0.91460700	1.27297300	-0.80451100
B	0.59582000	1.00150600	-0.00047900
B	0.06775400	0.05877000	1.42757300
H	0.66616700	0.25866400	2.42864500
B	-1.68163400	-0.12176300	1.43614200
H	-2.28380600	-0.01657800	2.44814500
B	-2.32287100	0.70166700	-0.00094500
H	-3.28589200	1.38371700	-0.00126200
B	0.06833400	0.05655800	-1.42720500
H	0.66757300	0.25505300	-2.42808000
B	0.69533000	-0.76291300	0.00100700
B	-0.65913500	-1.48120100	0.89307400
H	-0.56692600	-2.46042300	1.55490400
B	-2.14997600	-1.06192300	0.00049300
H	-3.12492200	-1.73504800	0.00048300
B	-1.68100100	-0.12382100	-1.43642000
H	-2.28240300	-0.01998300	-2.44902200
B	-0.65871500	-1.48256500	-0.89076100
H	-0.56566700	-2.46285700	-1.55089200
H	-1.02474900	2.22770500	-1.29816000
H	-1.02544900	2.22967900	1.29455500
P	2.62116000	-0.53179800	0.00009700
H	3.24690000	-1.16767500	1.08911700
H	3.24473500	-1.16869000	-1.08954600
B	2.24730800	1.50372500	-0.00020500
H	2.69544500	1.96579700	-1.01872200
H	2.69452900	1.96465500	1.01926400

^cPB6_{CM}

C	1.28914900	-1.52907200	0.47787000
C	1.74139300	-1.12201100	-1.00880000
B	0.10809100	-0.78411400	-0.56148200
B	0.28242600	-0.35867100	1.16076200
H	-0.56994800	-0.70488500	1.90255200
B	1.98624000	-0.52802400	1.65082100
H	2.24476600	-0.99962600	2.70374800
B	2.92284700	-1.06454800	0.24475200
H	3.74474700	-1.91127100	0.26398500
B	1.10620600	0.37760700	-1.48087300
H	0.83253000	0.53727400	-2.62117100
B	0.17899200	0.92506900	-0.07327200
B	1.32102200	1.07965100	1.28925600
H	1.15006300	1.87306700	2.15376100

B	2.95538300	0.63493600	0.71571800
H	3.95174800	1.10160600	1.15493900
B	2.81099400	0.19675800	-1.00291800
H	3.65560200	0.23200100	-1.82964700
B	1.84165500	1.53135200	-0.34883600
H	2.04490400	2.65240500	-0.67627200
H	1.87175000	-1.93232000	-1.71159700
H	1.12482700	-2.58168900	0.65603400
P	-1.46995100	1.95832900	-0.24261800
H	-1.07000400	3.07632800	0.53005000
H	-1.18290600	2.56938100	-1.48905900
B	-1.12180300	-1.70908300	-1.26132400
H	-1.84311900	-1.22900200	-2.08373800
H	-1.16982900	-2.89543300	-1.10759600
C	-3.76152700	-0.65600500	0.32682200
O	-2.82303000	-1.34079200	0.36904800
O	-4.71574700	-0.01232100	0.30031600

^cPB6_{TS}

C	-1.44197000	1.37977600	0.67537500
C	-1.67923100	1.17271200	-0.90240200
B	-0.08448600	0.91470100	-0.30339000
B	-0.42174500	0.20456800	1.30717700
H	0.32153300	0.49034300	2.18202600
B	-2.17152800	0.15190600	1.59712900
H	-2.59796400	0.43064900	2.66377300
B	-2.98328500	0.82562100	0.17094600
H	-3.88678600	1.58355800	0.20850400
B	-0.86358700	-0.17647300	-1.49828800
H	-0.43306600	-0.14833400	-2.59935500
B	-0.06977100	-0.84291600	-0.07415000
B	-1.31524000	-1.32296100	1.09837400
H	-1.15722000	-2.22427000	1.85266100
B	-2.90715400	-0.92605500	0.38825800
H	-3.89705300	-1.53201500	0.62468100
B	-2.61375400	-0.21886500	-1.21795800
H	-3.35527900	-0.19847700	-2.13838400
B	-1.59722600	-1.55643100	-0.64561300
H	-1.64265300	-2.62597600	-1.15540700
H	-1.80660200	2.06799600	-1.49380400
H	-1.40427500	2.40119700	1.02481000
P	1.73744400	-1.49781200	-0.22909700
H	1.84707100	-2.60379900	0.63747400
H	1.79365500	-2.16821300	-1.46747400
B	1.21538300	1.95500700	-0.65670400
H	1.64434500	1.89196500	-1.77854900
H	1.16236800	3.06273300	-0.19399400
C	3.29492500	0.35850100	0.19640500

O	2.56810200	1.31235000	0.27018200
O	4.35313300	-0.12067800	0.28285800

C^{PB6}_{AD}

C	-1.38862700	1.33848900	0.73899000
C	-1.70368200	1.17890200	-0.83092500
B	-0.07316200	0.93588500	-0.32351000
B	-0.32726300	0.16364400	1.28441200
H	0.46901200	0.42267800	2.11889500
B	-2.05199600	0.06244100	1.65710600
H	-2.43094200	0.29382200	2.75200400
B	-2.94385700	0.76657400	0.29576000
H	-3.86221100	1.49829900	0.40676600
B	-0.90834900	-0.13252100	-1.51372600
H	-0.51980500	-0.07115900	-2.62824800
B	-0.04454800	-0.81657600	-0.14968100
B	-1.19368400	-1.38203100	1.06890000
H	-0.97647300	-2.30457000	1.78079600
B	-2.82466500	-0.99284900	0.44981400
H	-3.78911300	-1.62647500	0.71499300
B	-2.63279900	-0.22366300	-1.14443800
H	-3.42344500	-0.19145500	-2.02206400
B	-1.56187700	-1.56314300	-0.67376900
H	-1.60978400	-2.61523300	-1.21801600
H	-1.87724900	2.09029300	-1.38493100
H	-1.35343000	2.34766700	1.12307500
P	1.80153400	-1.24302700	-0.45206700
H	2.27559200	-2.43578200	0.11047300
H	2.05448300	-1.38594900	-1.82511200
B	1.30958700	1.86606600	-0.71614400
H	1.61149300	1.69956500	-1.88291300
H	1.21331600	3.03592900	-0.43474700
C	2.97492600	0.15271800	0.24691000
O	2.53612700	1.33156400	0.14773200
O	3.98423500	-0.27556400	0.73558800

Si^{PB1}

B	0.20597400	0.04375400	-1.55641100
H	-0.38983600	0.06543800	-2.58713400
B	1.22893300	1.45724900	-0.94183800
H	1.35966000	2.44296100	-1.59230200
B	1.23015600	1.46103700	0.93530200
H	1.36185800	2.44944700	1.58147500
B	0.20789000	0.05012200	1.55724600
H	-0.38625300	0.07612800	2.58876500
B	1.05199700	-1.53919900	-0.95779900
H	1.02892900	-2.53820900	-1.59847400
B	1.95793000	-0.08939600	-1.45341100
H	2.57811400	-0.13685000	-2.46366300

B	2.56211600	0.76395500	-0.00275800
H	3.62576800	1.28875900	-0.00436000
B	1.95973400	-0.08352600	1.45217300
H	2.58117100	-0.12693400	2.46183400
B	1.05340000	-1.53548200	0.96371500
H	1.03117400	-2.53183000	1.60852800
B	2.44979300	-1.01739700	0.00090100
H	3.42350300	-1.69487500	0.00150200
Si	-0.57098100	1.28787900	-0.00171200
Si	-0.63536400	-1.01664000	0.00333800
B	-2.61269900	1.41394600	0.00212300
H	-3.06871700	1.82657500	1.03024000
H	-3.07715300	1.83273300	-1.01956000
P	-2.84699000	-0.59660900	-0.00101200
H	-3.46999400	-1.21117100	-1.10171500
H	-3.48068300	-1.21570200	1.09106700

^{Si}PB1_{CM}

B	-1.47777300	0.41834400	-1.49663900
H	-1.39731300	0.78578400	-2.62462500
B	-2.08882400	-1.26726700	-1.02115500
H	-2.41108700	-2.04277600	-1.86304300
B	-1.29289600	-1.81717400	0.58342400
H	-1.07094700	-2.96379000	0.80809600
B	-0.13531600	-0.51606900	1.18942900
H	0.83124000	-0.75317400	1.84359600
B	-2.00164200	1.53221200	-0.10727100
H	-2.24542600	2.67674100	-0.31959700
B	-3.02584300	0.19443500	-0.65230100
H	-4.01610700	0.42443000	-1.26386700
B	-2.92390300	-1.13242600	0.53945200
H	-3.85372500	-1.83609500	0.75650300
B	-1.78751700	-0.65981100	1.82932000
H	-1.91019600	-1.01811700	2.95364300
B	-1.19159800	0.97725100	1.49323100
H	-0.89677900	1.75104500	2.34731500
B	-2.86747000	0.55436200	1.08955300
H	-3.75240500	1.05037000	1.70412800
Si	-0.08007100	-1.06808100	-0.86110800
Si	-0.02466600	1.12662800	-0.14582200
B	1.41866100	-1.94883400	-1.86172200
H	1.71044600	-3.06595300	-1.58141700
H	1.89316500	-1.40289600	-2.80408800
P	1.74932800	2.45742600	-0.43885000
H	1.41887500	2.71375800	-1.79487900
H	1.06068100	3.59163100	0.06256500
C	3.48274700	-0.87633200	0.66749300
O	3.87556500	-0.68730600	1.73156600
O	3.10444800	-1.06383700	-0.41608000

SiPB1_{TS}

B	1.22663400	-0.08984900	-1.60575100
H	0.88985100	-0.15671600	-2.74458000
B	2.07733700	1.37344900	-0.87152300
H	2.34143700	2.31433600	-1.54772900
B	1.65197200	1.52757400	0.94692100
H	1.62015200	2.57570300	1.50622200
B	0.50467000	0.17212300	1.43599000
H	-0.31058700	0.26812400	2.29854500
B	1.89751900	-1.59329000	-0.68244800
H	1.99771700	-2.64694600	-1.22155900
B	2.91036000	-0.18873300	-1.07392400
H	3.74585900	-0.30501800	-1.90802900
B	3.16424700	0.78542800	0.40193900
H	4.19393200	1.34122600	0.59451300
B	2.24253700	0.05121300	1.74330800
H	2.61235800	0.09610900	2.86951800
B	1.45194600	-1.43222000	1.16393200
H	1.25570400	-2.38030200	1.85247200
B	3.04568600	-0.98570200	0.52399900
H	3.98255700	-1.65659200	0.80478800
Si	0.11122000	1.27707500	-0.36094700
Si	0.03712600	-1.01840100	-0.19681800
B	-1.74940600	1.89836400	-0.90511700
H	-1.91504300	3.07844600	-0.89402100
H	-2.04042100	1.33276000	-1.92693400
P	-2.13067700	-1.42555500	-0.54314100
H	-2.22826900	-1.67161600	-1.92557200
H	-2.47253800	-2.67423000	0.00744000
C	-3.33651000	0.28500900	0.45598900
O	-4.22232500	-0.21973600	1.02368400
O	-2.76365400	1.33783200	0.23483900

SiPB1_{AD}

B	1.20113000	0.01219600	-1.61505400
H	0.84671600	0.01833100	-2.75021200
B	2.08066800	1.40309800	-0.79665800
H	2.36176400	2.37843300	-1.41443000
B	1.67596700	1.45165800	1.03178300
H	1.67669200	2.46161000	1.65768400
B	0.51081700	0.09548200	1.45516200
H	-0.29714100	0.14797200	2.32692900
B	1.85250400	-1.57070300	-0.79547900
H	1.92395200	-2.59027200	-1.39960200
B	2.88409700	-0.15904100	-1.10647900
H	3.71054000	-0.24036700	-1.95339900
B	3.16810200	0.71573700	0.42504500
H	4.21119200	1.23643000	0.64098300

B	2.24815300	-0.08304800	1.72977700
H	2.63152700	-0.11589700	2.85158200
B	1.42524400	-1.51676300	1.07410100
H	1.21594000	-2.50256200	1.70196600
B	3.01790100	-1.05808500	0.43880100
H	3.94354800	-1.76344900	0.66680000
Si	0.10835900	1.33811200	-0.27382000
Si	0.02468500	-0.96134900	-0.24542400
B	-1.81090700	1.86969900	-0.79668500
H	-1.97909300	3.04931700	-0.85741300
H	-1.98965900	1.28894500	-1.84647200
P	-2.17161900	-1.26781200	-0.59359100
H	-2.42035400	-1.26065100	-1.97499300
H	-2.67548200	-2.49360300	-0.13515700
C	-3.18966400	0.12166600	0.42028900
O	-4.04765900	-0.35418900	1.09140700
O	-2.77469900	1.30382800	0.27305600

SiPB2

B	1.28316200	1.62115600	0.25001400
H	1.54853500	2.74625900	0.52159000
B	2.00517400	0.17685000	1.23326700
H	2.70830700	0.39315900	2.16622700
B	0.84308700	-1.30719100	1.19518300
H	0.76620100	-2.06218500	2.10979800
B	-0.61015900	-0.83438400	0.17734900
B	1.11531700	0.97376800	-1.48126500
H	1.25722900	1.69158300	-2.41741700
B	2.48131100	0.50530200	-0.44596200
H	3.56181400	0.94379700	-0.66337100
B	2.25366400	-1.18249100	0.12038300
H	3.18740500	-1.89291600	0.29274300
B	0.70186500	-1.79420800	-0.50760200
H	0.51240400	-2.93116700	-0.79214000
B	-0.01560400	-0.49330200	-1.49366500
H	-0.73124100	-0.73576700	-2.41595500
B	1.72032500	-0.71156900	-1.50777800
H	2.26304900	-1.10764800	-2.48471500
H	-0.61068000	0.95821800	2.80195800
Si	0.07200100	0.54679800	1.56945700
Si	-0.68848700	1.19107200	-0.53765900
B	-2.75612300	1.09803600	-0.41440100
H	-3.17331200	1.71719000	0.52550900
H	-3.31351000	1.24675400	-1.46228600
P	-2.54763500	-0.83698600	0.08959800
H	-3.01630300	-1.76455000	-0.85622000
H	-3.22466800	-1.23795100	1.25752100

SiPB2CM

B	1.96401100	-1.45146100	-0.77649500
H	2.22603900	-2.36809400	-1.48581200
B	2.95741500	0.12941400	-0.77954000
H	3.86989100	0.25339700	-1.53087600
B	1.86726300	1.57846900	-0.30077400
H	2.04164900	2.67295700	-0.73147000
B	0.12811000	0.98078500	0.01555300
B	1.37956700	-1.64451700	0.96800200
H	1.21637000	-2.73031600	1.42392100
B	2.97944000	-0.97657800	0.60797500
H	3.94897700	-1.62702500	0.81716100
B	2.94247400	0.78935400	0.86518900
H	3.89273700	1.37875700	1.26009100
B	1.28607600	1.25913200	1.33964900
H	1.06026700	2.16911500	2.06817600
B	0.28642700	-0.20330800	1.43447200
H	-0.61578900	-0.31197100	2.20290600
B	1.98858600	-0.27684700	1.91598100
H	2.25956100	-0.44048300	3.05886600
H	0.84323600	0.52953800	-3.08224800
Si	1.15853600	0.27972100	-1.67097900
Si	-0.09266200	-1.12710200	-0.32642800
B	-1.76410600	-2.04819700	-0.95735500
H	-2.29875700	-1.61851900	-1.93069800
H	-1.95249700	-3.16519600	-0.60119300
P	-1.52526600	2.00561100	-0.19989500
H	-1.20060700	3.08327500	0.65796800
H	-1.21552900	2.69970200	-1.39720500
C	-3.91057600	-0.40786400	0.37843200
O	-4.80114000	0.31362200	0.37978500
O	-3.04031500	-1.18612600	0.40754700

^{Si}PB2_{TS}

B	1.99828300	1.43262100	0.71907400
H	2.29188000	2.38884900	1.35965000
B	2.85544400	-0.21927100	0.95222800
H	3.69584600	-0.33786400	1.78389200
B	1.68884700	-1.62161000	0.52064200
H	1.73538900	-2.67758400	1.06542900
B	0.06055000	-0.90209800	0.00063500
B	1.56530000	1.49196700	-1.08000300
H	1.53939000	2.53179200	-1.65498500
B	3.07201500	0.74241500	-0.52406000
H	4.10642000	1.29211900	-0.70972900
B	2.91265600	-1.03532100	-0.62056600
H	3.84208500	-1.72547100	-0.87757200
B	1.26735600	-1.42534500	-1.18937000
H	1.01643000	-2.38313700	-1.84535700
B	0.40537000	0.09869900	-1.49437100
H	-0.43252100	0.19248000	-2.33576300

B	2.13361800	-0.00851700	-1.84267600
H	2.50630500	0.02106500	-2.96794100
H	0.53626400	-0.22941800	3.08780700
Si	0.99221400	-0.12555700	1.69675500
Si	-0.04729000	1.23872600	0.12978800
B	-1.84759600	2.06552800	0.53744400
H	-2.20394900	1.84308200	1.65843600
H	-1.99502000	3.16936200	0.11512300
P	-1.72594400	-1.63862800	0.15596700
H	-1.73218600	-2.72610000	-0.74253600
H	-1.73536400	-2.36944500	1.36423000
C	-3.57343000	0.18009500	-0.26841900
O	-4.55301300	-0.42890800	-0.24950500
O	-2.90066000	1.15758400	-0.43751500

SiPB2_{AD}

B	2.11478300	1.46969800	0.25389200
H	2.54629300	2.51945200	0.60241900
B	2.85932900	-0.15316200	0.85492200
H	3.76240800	-0.14504700	1.62641800
B	1.55091600	-1.49136600	0.88351200
H	1.55272500	-2.37635300	1.67761000
B	-0.01452700	-0.73638800	0.28549300
B	1.52194500	1.11371900	-1.46213400
H	1.53872300	1.96430600	-2.29122500
B	3.01195800	0.38011900	-0.83299500
H	4.06567200	0.75839200	-1.22344200
B	2.70688700	-1.34204000	-0.45449300
H	3.55192000	-2.16298400	-0.58546300
B	0.99386500	-1.69700400	-0.79555900
H	0.60108900	-2.75895300	-1.15502600
B	0.23875500	-0.21068500	-1.42459800
H	-0.67376000	-0.25825600	-2.18834200
B	1.90715300	-0.58163100	-1.84930300
H	2.18195500	-0.87402600	-2.96440400
H	0.72829000	0.60083600	3.05978800
Si	1.09208600	0.33722300	1.66294300
Si	-0.01058100	1.37849500	-0.13071400
B	-1.93728300	1.97579200	0.38649800
H	-1.97926300	1.67193100	1.56172900
H	-2.15177300	3.12694300	0.15818200
P	-1.83553000	-1.19438100	0.68422300
H	-2.19705500	-2.51055200	0.36630200
H	-2.17683000	-1.06950400	2.04107700
C	-3.11040300	-0.14703500	-0.31276000
O	-4.01180500	-0.77660200	-0.78254100
O	-2.87132100	1.10865700	-0.43618400

SiPB3

B	-1.15095000	0.80393100	1.43939400
H	-1.40604700	1.52960400	2.34421300
B	-2.46855000	0.10645300	0.33281100
H	-3.60408600	0.41603900	0.49732300
B	-1.78741600	-0.23614800	-1.38546800
H	-2.47102500	-0.13781200	-2.35280400
B	-0.01653300	0.23176800	-1.44362700
H	0.53887900	0.59518800	-2.43161500
B	0.13299100	-0.49361500	1.47967800
H	0.84187500	-0.62756900	2.42741000
B	-1.56890800	-0.93435900	1.45437800
H	-2.09937700	-1.35193900	2.42956400
B	-1.98443900	-1.52616600	-0.18086100
H	-2.83079100	-2.34153800	-0.33991100
B	-0.52504000	-1.46843300	-1.20678700
H	-0.30977000	-2.23779200	-2.08450100
B	0.76248700	-0.80995400	-0.20951000
B	-0.39734900	-1.90549700	0.52053100
H	-0.07407000	-2.99298600	0.86861400
H	-1.84241600	2.86488400	-0.99025900
Si	-1.35934500	1.55828300	-0.53044700
Si	0.71553700	1.15924000	0.39883000
P	2.69462600	-0.65507500	-0.25591200
H	3.34883300	-1.55638900	0.60149700
H	3.25788600	-0.95304900	-1.50887900
B	2.76816800	1.27074400	0.29231500
H	3.28162400	1.41266000	1.36418000
H	3.14010600	1.96789500	-0.60778300

^{Si}PB₃CM

B	1.47125200	-1.27261600	1.21481900
H	1.43847000	-2.25627100	1.88068200
B	3.05802300	-0.50940200	0.62648300
H	4.09808200	-1.02264100	0.88592800
B	2.77876100	0.38397300	-1.00534000
H	3.63026600	0.46137100	-1.83097600
B	0.99952500	0.22784400	-1.51713500
H	0.65266800	0.23193900	-2.65456600
B	0.31408500	0.14494200	1.44491700
H	-0.53824100	0.10120700	2.27443300
B	2.03689200	0.29734700	1.82903100
H	2.38576900	0.34627300	2.96174300
B	2.83247600	1.24644200	0.54280400
H	3.75135700	1.95861900	0.77711200
B	1.61436800	1.67665000	-0.68661800
H	1.66007500	2.68444400	-1.31213000
B	0.03789700	1.03788100	-0.18031900
B	1.17427300	1.64340800	1.03879400
H	0.90401300	2.63839200	1.62668100
H	2.40253900	-2.68887800	-1.54461300

Si	2.02344500	-1.47757900	-0.80888000
Si	-0.13511600	-0.99559500	-0.16887400
P	-1.69904700	1.86378900	-0.55274600
H	-1.51415300	3.06088400	0.17865800
H	-1.39860600	2.42253800	-1.81785700
B	-1.77364100	-2.08620500	-0.57320700
H	-1.86272900	-3.15417300	-0.05931400
H	-2.30052300	-1.87262200	-1.62013800
C	-3.94324600	-0.43865400	0.36956100
O	-3.04509700	-1.15749700	0.58865900
O	-4.86989900	0.21213700	0.20454000

^{Si}PB3_{TS}

B	-1.61197100	1.15534900	1.26347400
H	-1.68796000	2.09200500	1.99017600
B	-3.10622000	0.34740700	0.51385100
H	-4.18981700	0.78591400	0.72797200
B	-2.66729400	-0.42391900	-1.14332700
H	-3.45617200	-0.49269000	-2.02958100
B	-0.87469200	-0.13646500	-1.51277000
H	-0.44425000	-0.05251300	-2.61832400
B	-0.39806500	-0.20637100	1.48325100
H	0.39904300	-0.17642900	2.36719700
B	-2.12760400	-0.48152500	1.73765700
H	-2.55056800	-0.62267500	2.83675400
B	-2.77809700	-1.38726100	0.34212400
H	-3.67018800	-2.15843500	0.46765300
B	-1.45722000	-1.67236700	-0.82160700
H	-1.39565700	-2.63873200	-1.50853900
B	0.02196100	-0.96114300	-0.16106500
B	-1.13795100	-1.72578800	0.93158000
H	-0.84321500	-2.73959000	1.47433000
H	-2.44490100	2.68940800	-1.47044500
Si	-2.03271700	1.46170500	-0.78190500
Si	0.10446600	1.07572200	-0.01652400
P	1.84011600	-1.58423400	-0.45575000
H	1.88840000	-2.79526200	0.26728400
H	1.78903400	-2.12492900	-1.75818500
B	1.82461200	2.10140800	-0.26569300
H	1.87950800	3.13002500	0.33288600
H	2.18704900	2.09089900	-1.40535700
C	3.70127000	0.25927900	0.22920500
O	2.97538000	1.14877400	0.55909600
O	4.68569100	-0.31749400	0.08188400

^{Si}PB3_{AD}

B	-1.59619700	0.90001800	1.44517400
H	-1.73921300	1.71384500	2.29780100
B	-3.03396400	0.01981500	0.66542100

H	-4.14342500	0.28868500	0.99430300
B	-2.63287300	-0.46713600	-1.10304700
H	-3.47354500	-0.51676000	-1.94097800
B	-0.92884200	0.09083800	-1.52382500
H	-0.56955300	0.36302500	-2.62406700
B	-0.23298500	-0.30481100	1.40441200
H	0.63375500	-0.30566800	2.21977300
B	-1.88949000	-0.83796000	1.71324200
H	-2.21686600	-1.17800100	2.80060500
B	-2.52471900	-1.62695000	0.23942000
H	-3.31051000	-2.51200000	0.30583400
B	-1.26956800	-1.58893500	-1.02612300
H	-1.12758700	-2.44322800	-1.83887600
B	0.11249600	-0.74789400	-0.33535800
B	-0.81963200	-1.82943300	0.69022700
H	-0.35439100	-2.85707400	1.06045100
H	-2.80369600	2.65754400	-1.00614000
Si	-2.18262100	1.42299100	-0.51649200
Si	0.04507500	1.26360200	0.08682100
P	1.95145300	-1.08618000	-0.78813800
H	2.38276100	-2.40411600	-0.58746600
H	2.22455300	-0.82752100	-2.14018700
B	1.93265300	2.02304100	-0.33265400
H	2.05185800	3.16995100	-0.02496400
H	1.99021700	1.79880500	-1.52324500
C	3.19948600	-0.06489600	0.25535000
O	2.91505300	1.17627000	0.44589000
O	4.12597000	-0.68010600	0.69511900

SiPB4

B	1.40409100	-0.07224700	-1.53810500
H	2.01945300	0.08702200	-2.54168100
B	1.64123100	-1.54598400	-0.43181500
H	2.46333900	-2.36157100	-0.69821700
B	1.27204600	-1.08076100	1.34855600
H	1.83246900	-1.60094300	2.25780600
B	0.78232900	0.73003200	1.47053200
H	1.00193700	1.37907800	2.44038800
B	-0.35112800	0.38041400	-1.36113900
H	-0.96022800	0.87227100	-2.25719400
B	0.14561800	-1.32591700	-1.35676200
H	-0.09035500	-2.01170100	-2.29531900
B	0.08369400	-1.92565200	0.32940100
H	-0.19812300	-3.04868500	0.58531900
B	-0.40838000	-0.57504100	1.40388400
H	-1.07184100	-0.77875400	2.36803700
B	-0.77894700	0.88880800	0.44274700
B	-1.08759600	-0.73276400	-0.22683200
H	1.20342800	3.06040200	-0.77105800
H	3.87035400	0.45692200	0.47509300

Si	2.44497900	0.16789700	0.28339200
Si	0.84735900	1.68324800	-0.41373300
B	-2.41480100	1.49037200	0.58236100
H	-2.77095800	2.31541500	-0.22372500
H	-2.86431700	1.62671200	1.69169100
P	-2.97761200	-0.35125100	-0.12397700
H	-3.64382600	-0.52625000	-1.35281600
H	-3.66067300	-1.27347800	0.69197100

SiPB₄CM

B	-1.77346800	-0.25918200	-1.67754500
H	-2.09969600	-0.58919600	-2.77075200
B	-2.56487000	1.16017600	-0.77032600
H	-3.45997800	1.75956000	-1.27157100
B	-2.48061400	0.86349000	1.08387400
H	-3.31891500	1.26410300	1.82443800
B	-1.62877600	-0.75307200	1.43252700
H	-1.86965000	-1.41110300	2.39247400
B	-0.00586800	-0.26605600	-1.10768500
H	0.84960100	-0.63725000	-1.84257100
B	-0.88893900	1.25177900	-1.34518100
H	-0.62166500	1.94059700	-2.27348400
B	-1.33384100	1.92293100	0.24606200
H	-1.38014300	3.09294200	0.43283600
B	-0.76056500	0.80144200	1.50887200
H	-0.40913500	1.17699800	2.57865200
B	0.09596300	-0.56610000	0.74976900
B	0.21577500	1.07130800	0.04524800
H	-1.00315200	-3.20735700	-0.57421600
H	-4.42063500	-1.30501900	-0.13238300
Si	-3.10633400	-0.65552700	-0.08688900
Si	-1.10578600	-1.76389500	-0.33988200
B	1.34502700	-1.38153800	1.55715100
H	1.40044800	-2.57637100	1.63443200
H	2.13290200	-0.76257500	2.21232800
P	1.97009100	1.93332100	0.09218800
H	1.65489300	3.04610100	-0.72751000
H	1.80102500	2.63578600	1.31175700
C	4.04263600	-0.83760200	-0.30593900
O	3.05929900	-1.45520500	-0.27727500
O	5.04163700	-0.26422000	-0.34530800

SiPB₄TS

B	1.83617900	-0.01189900	-1.66124300
H	2.25547000	0.17226400	-2.75693500
B	2.44690100	-1.38635000	-0.56615300
H	3.31556800	-2.10435200	-0.94194700
B	2.28625400	-0.89037100	1.23930300
H	3.04588100	-1.28087900	2.06496500

B	1.55665000	0.82242000	1.37486600
H	1.80736100	1.55489100	2.27568600
B	0.06021000	0.20222200	-1.21504900
H	-0.73082000	0.55324400	-2.03035400
B	0.80845200	-1.40459800	-1.24125500
H	0.52398200	-2.16703600	-2.10480000
B	1.09852900	-1.93482700	0.44223900
H	1.02054400	-3.07755900	0.75000500
B	0.56305500	-0.63535500	1.54785800
H	0.10661100	-0.87522100	2.61678800
B	-0.13816800	0.71461800	0.60510800
B	-0.32813800	-0.96155600	0.05408600
H	1.26915200	3.09301300	-0.91914000
H	4.47034000	0.96422700	-0.06100000
Si	3.09788000	0.44779900	-0.03327300
Si	1.21465200	1.68524200	-0.51596000
B	-1.44836300	1.67429200	1.16850300
H	-1.38020000	2.87011200	1.06810800
H	-1.97199000	1.28028000	2.17700300
P	-2.18018500	-1.49911600	0.14812000
H	-2.33733400	-2.56042800	-0.76741000
H	-2.28073800	-2.22180200	1.35433300
C	-3.56326100	0.52155300	-0.22673600
O	-2.77623100	1.40160600	-0.02005100
O	-4.61311000	0.14228400	-0.55979200

^{Si}PB4_{AD}

B	-1.76341600	0.01586500	-1.67847600
H	-2.16661500	-0.17632800	-2.77841200
B	-2.37750700	1.41078300	-0.61112100
H	-3.23295200	2.13214700	-1.00886100
B	-2.26516700	0.93263700	1.20273400
H	-3.03917400	1.34601800	2.00296500
B	-1.55550000	-0.78924000	1.37877000
H	-1.83830100	-1.50776500	2.28041600
B	-0.01344500	-0.21348300	-1.20382100
H	0.80505400	-0.57409200	-1.98594500
B	-0.73070800	1.40744500	-1.26013500
H	-0.41222700	2.16068800	-2.11920900
B	-1.04553700	1.95763800	0.42179900
H	-0.95111900	3.10140500	0.72062500
B	-0.55918500	0.65670200	1.55557100
H	-0.10341700	0.91543800	2.62036200
B	0.15912700	-0.71393500	0.64636100
B	0.34385500	0.93704900	0.06848000
H	-1.24715500	-3.09159800	-0.89403900
H	-4.43793400	-0.90057700	-0.12494000
Si	-3.05417300	-0.41765000	-0.07261700
Si	-1.16668500	-1.68626100	-0.48884400
B	1.57914500	-1.56821600	1.18898800

H	1.44473500	-2.76205900	1.30415000
H	1.97455700	-1.05980500	2.22350500
P	2.22147700	1.27428500	0.27220400
H	2.76802500	2.33148900	-0.46883300
H	2.51902100	1.58765100	1.60656800
C	3.23133400	-0.28949500	-0.26208500
O	2.73322300	-1.38993700	0.11700700
O	4.19690900	-0.05898600	-0.93878300

SiPB5

B	1.21202900	-0.20463100	-1.57942300
H	1.76116600	-0.37608400	-2.61836000
B	-0.12092600	-1.32421800	-0.93836800
H	-0.44245700	-2.28213800	-1.56355700
B	-0.12087000	-1.32435100	0.93848000
H	-0.44256500	-2.28225900	1.56359300
B	1.21191600	-0.20466800	1.57949700
H	1.76118600	-0.37581800	2.61841500
B	0.75740300	1.49067200	-0.94255800
H	1.05262400	2.45349200	-1.57442900
B	-0.47761700	0.33293700	-1.44940000
H	-1.07130200	0.51653700	-2.46045300
B	-1.27365500	-0.34294800	0.00006100
B	-0.47772800	0.33272100	1.44942400
H	-1.07143700	0.51643900	2.46043900
B	0.75715700	1.49074000	0.94247900
H	1.05276800	2.45335600	1.57450800
B	-0.74012200	1.35945800	-0.00001400
H	3.73924700	1.07443700	0.00047900
H	2.57125500	-2.68169400	-0.00014800
Si	1.65112500	-1.53915700	0.00002200
Si	2.33209600	0.66103800	0.00007600
P	-3.19698200	-0.70881000	-0.00094700
H	-3.20598000	-1.67928500	-1.03552100
H	-3.20944200	-1.66624300	1.04572800
B	-1.87304000	2.61302800	0.00014500
H	-2.28519100	3.08442100	-1.02152600
H	-2.29297900	3.07695200	1.02205400

SiPB5_{CM}

B	2.47030900	0.36050800	1.11878600
H	3.39053500	0.62604100	1.82089500
B	1.27548700	1.63867800	0.49293500
H	1.42783200	2.78468200	0.76717000
B	0.56056500	1.10053800	-1.15913500
H	0.23991800	1.88627800	-1.99141900
B	1.28886200	-0.53723000	-1.66642600
H	1.42570400	-0.85438500	-2.80252200
B	1.45306000	-1.18888800	1.31883500

H	1.75076100	-1.97382100	2.16132900
B	0.78112100	0.41404200	1.67089100
H	0.58935500	0.73355300	2.79726800
B	-0.32772900	0.87906500	0.35764300
B	-0.30207500	-0.42230200	-0.87745100
H	-1.24256600	-0.66974300	-1.55730500
B	0.76165800	-1.72309000	-0.33747700
H	0.57926400	-2.86711600	-0.60108400
B	-0.22525500	-0.83502100	0.85893000
H	3.89170500	-2.06439800	-0.49402000
H	3.62940800	1.70110700	-1.60047300
Si	2.55925700	0.97657500	-0.90635600
Si	2.70931000	-1.22848400	-0.26184400
P	-1.97829400	1.88454000	0.66184400
H	-1.75792900	2.18268100	2.03006500
H	-1.52574100	3.14523400	0.19508300
B	-1.42805900	-1.64074500	1.73646100
H	-2.05674600	-1.07328600	2.58341800
H	-1.59553700	-2.82171400	1.63391000
C	-3.82751500	-0.70215100	-0.72815500
O	-3.50874600	-1.32392400	0.19656700
O	-4.16701900	-0.11249400	-1.66109100

^{Si}PB5_{TS}

B	-2.24895900	-0.18346900	1.39756300
H	-3.01093600	-0.32018400	2.29798100
B	-1.10608400	-1.53590800	0.83674800
H	-1.11861700	-2.59894000	1.36771200
B	-0.73772500	-1.34574700	-1.00396900
H	-0.50847300	-2.28316500	-1.69772800
B	-1.64620300	0.12899300	-1.68469300
H	-2.00827300	0.19126900	-2.81379400
B	-1.30859300	1.40969400	1.08404600
H	-1.51027500	2.34263800	1.79217200
B	-0.49455700	-0.06306700	1.62104900
H	-0.07137800	-0.14253700	2.72664300
B	0.36316700	-0.75480500	0.24007300
B	0.05813400	0.23106400	-1.20595100
H	0.86563200	0.34292100	-2.06849900
B	-0.95814200	1.59576600	-0.74740700
H	-0.91180500	2.65588900	-1.28096800
B	0.28297500	1.01300600	0.39690100
H	-4.09435600	1.78707100	-0.37781300
H	-3.79099300	-2.09919300	-0.71760600
Si	-2.66088000	-1.21789000	-0.40392400
Si	-2.82441100	1.07444200	-0.20448500
P	2.17228700	-1.37862200	0.47338500
H	2.27081200	-1.73705400	1.83221000
H	2.28554800	-2.65108500	-0.12285300
B	1.68538500	1.90213100	0.82465400

H	2.17660400	1.62182100	1.89068800
H	1.72654400	3.06657500	0.53916600
C	3.62716300	0.30571500	-0.39296800
O	2.99422900	1.32033100	-0.27232700
O	4.59324200	-0.23420800	-0.77612600

SiPB5_{AD}

B	-2.21906300	-0.12709800	1.40895000
H	-2.98017100	-0.22582300	2.31477200
B	-1.06830400	-1.50293800	0.92018400
H	-1.06543600	-2.53607000	1.50696100
B	-0.70384500	-1.40525500	-0.93912900
H	-0.46133700	-2.37436600	-1.58206400
B	-1.62168100	0.03230800	-1.68616400
H	-1.98736800	0.03391800	-2.81546000
B	-1.28174700	1.46045600	1.01690300
H	-1.49549300	2.42262800	1.67992800
B	-0.47102000	0.01995400	1.62557400
H	-0.03398100	-0.01206400	2.72809600
B	0.37059900	-0.72559300	0.27311400
B	0.07770600	0.17092800	-1.21941800
H	0.89329500	0.23496800	-2.07841700
B	-0.93197800	1.55605500	-0.82233700
H	-0.89937600	2.58326600	-1.41700400
B	0.31538400	1.03757300	0.34843800
H	-4.07863600	1.72696200	-0.46046800
H	-3.75166400	-2.15767600	-0.60223100
Si	-2.62529900	-1.25579900	-0.33767700
Si	-2.79557900	1.04821400	-0.25209400
P	2.21560400	-1.16695900	0.56156900
H	2.50227000	-1.16016000	1.93416400
H	2.63576500	-2.43250000	0.12615900
B	1.81398100	1.82762000	0.72278100
H	2.19507500	1.51027900	1.84004400
H	1.80731300	3.02301000	0.57729300
C	3.35350200	0.11357100	-0.37249300
O	2.95881000	1.30465900	-0.27581200
O	4.27329100	-0.38306800	-0.96519200

SiPB6

B	-2.35575600	-0.04838400	-0.00035200
H	-3.52387200	0.16633100	-0.00035000
B	-1.46744900	-0.74494200	-1.47460100
H	-2.06229500	-0.95508100	-2.48155800
B	0.28923900	-0.16841300	-1.47508300
H	0.92307800	0.00404300	-2.46683500
B	0.65627500	0.96788100	0.00045800
B	-1.46781100	-0.74524800	1.47402200

H	-2.06363000	-0.95473000	2.48055400
B	-1.69775700	-1.70658400	-0.00040000
H	-2.48196100	-2.59592700	-0.00028900
B	-0.15186700	-1.78862500	-0.88969300
H	0.17081600	-2.73571700	-1.52623000
B	1.01286600	-0.78936900	0.00047800
B	0.28872400	-0.16838800	1.47576800
H	0.92214000	0.00335700	2.46789400
B	-0.15204800	-1.78871000	0.88971800
H	0.16915800	-2.73630900	1.52624100
H	-1.53748200	2.35407300	1.98124800
H	-1.53430700	2.35535200	-1.98122900
Si	-1.10508100	1.22850100	-1.14677900
Si	-1.10534600	1.22844600	1.14664300
P	2.88959900	-0.33194800	0.00000400
H	3.58328600	-0.89245400	1.09004300
H	3.58250100	-0.89200600	-1.09076000
B	2.27202700	1.61860000	0.00024900
H	2.66125300	2.13612300	1.01782500
H	2.66110400	2.13581300	-1.01754200

^{Si}PB6_{CM}

B	-2.97165400	-0.47196200	0.51542300
H	-4.03193400	-0.96527600	0.72256700
B	-1.76305400	-0.05171700	1.85708800
H	-2.01806300	-0.29750400	2.99128300
B	-0.00417600	-0.15476000	1.19724100
H	0.90475600	-0.46296600	1.89604800
B	0.00441300	-0.65134800	-0.60268500
B	-2.69995400	0.81948100	-0.79854000
H	-3.60300100	1.16081100	-1.49127000
B	-2.58391600	1.21484100	0.92614700
H	-3.43713600	1.85826200	1.44000000
B	-0.85817200	1.39075000	1.35608000
H	-0.49621200	2.15975600	2.18358900
B	0.13695700	1.06797000	-0.09085500
B	-0.94087500	0.73042400	-1.44868800
H	-0.67504700	1.00606300	-2.57425600
B	-1.43200600	1.92097000	-0.23450700
H	-1.47712100	3.06599100	-0.53945300
H	-2.41268100	-1.91244500	-2.33944200
H	-1.17566200	-3.08056900	1.20070500
Si	-1.25039600	-1.67623800	0.78570500
Si	-1.97044700	-0.99700800	-1.28212800
P	1.88616200	1.90643100	-0.35321000
H	1.65087700	2.44345900	-1.64394000
H	1.60934900	3.11767100	0.32864300
B	1.23143200	-1.51222000	-1.39261100
H	1.96537200	-0.94739400	-2.15047700
H	1.30462300	-2.70768400	-1.35965200

C	3.99820700	-0.76208900	0.32012100
O	4.98237800	-0.16308700	0.34175000
O	3.03100000	-1.40551200	0.31356600

^{Si}PB6_{TS}

B	-2.97612100	-0.22654300	0.39491800
H	-4.08655200	-0.60887000	0.57144100
B	-1.86204300	0.31663300	1.77473600
H	-2.23443600	0.26676600	2.90180100
B	-0.07717500	-0.00245900	1.31100700
H	0.75665900	-0.24898700	2.12198200
B	0.05770700	-0.78164700	-0.39390800
B	-2.50005200	0.83021500	-1.05843300
H	-3.31416600	1.12421200	-1.87226700
B	-2.49959700	1.47732300	0.59367700
H	-3.34066300	2.24500200	0.92381100
B	-0.81025100	1.60621200	1.15905100
H	-0.45045200	2.46934100	1.88913700
B	0.24910200	0.97479300	-0.12409700
B	-0.71434200	0.52367600	-1.51997000
H	-0.31725200	0.61372300	-2.63674100
B	-1.20226900	1.92147600	-0.54472500
H	-1.11989900	3.00639900	-1.01696000
H	-2.31198300	-2.11742600	-2.14862700
H	-1.46756000	-2.80760300	1.63130600
Si	-1.38330100	-1.48728200	1.00023600
Si	-1.86923300	-1.08730100	-1.20409900
P	2.09862700	1.47881600	-0.38357200
H	2.13824000	2.02482900	-1.68297200
H	2.28150600	2.66190400	0.36250500
B	1.35562200	-1.77919400	-0.91104500
H	1.82589400	-1.49548600	-1.98250400
H	1.28991100	-2.95902800	-0.69099000
C	3.51161100	-0.49494600	0.24373100
O	4.56105400	-0.06674900	0.50310500
O	2.71822600	-1.38895100	0.16793300

^{Si}PB6_{AD}

B	-2.93372200	-0.14125300	0.42762900
H	-4.05206100	-0.48069300	0.63697400
B	-1.79684400	0.44404400	1.76804700
H	-2.16008600	0.46476300	2.89847200
B	-0.03512000	0.05684500	1.31271800
H	0.81583200	-0.16035600	2.11282000
B	0.07031000	-0.82485500	-0.36465700
B	-2.45604900	0.82672500	-1.08290500
H	-3.27409500	1.10466600	-1.89787900
B	-2.41607900	1.56128100	0.53418100
H	-3.23371700	2.36598300	0.83179000

B	-0.72056300	1.67846100	1.07947100
H	-0.32225400	2.57007600	1.75238400
B	0.27321600	0.92407100	-0.17919700
B	-0.69736600	0.44872500	-1.54987400
H	-0.29162500	0.47971000	-2.66617600
B	-1.12401400	1.91373400	-0.64225500
H	-1.00919900	2.96913800	-1.17112800
H	-2.36343200	-2.17763100	-2.02006200
H	-1.48652500	-2.69246800	1.78671600
Si	-1.36275100	-1.41526700	1.07977400
Si	-1.87011300	-1.11747800	-1.13694100
P	2.14595800	1.19677400	-0.51925000
H	2.39970500	1.27158900	-1.89664600
H	2.71244400	2.36704600	0.00559000
B	1.46116000	-1.75111100	-0.84631300
H	1.78693500	-1.42776700	-1.97726900
H	1.32809000	-2.94730900	-0.75431400
C	3.19017000	-0.24773600	0.23986900
O	4.19259600	0.09752500	0.80360400
O	2.67678700	-1.39713000	0.09944400

o-Carborane

IFLP-PH₂/B(CF₃)₂

CM

C	-1.57078000	1.42617400	-0.67190500
C	-0.66002000	0.25111400	0.04670900
B	-1.50819900	1.38965000	1.03756900
H	-0.86876400	2.20885200	1.60036300
B	-3.00796100	1.75086800	0.14870000
H	-3.39137300	2.87359900	0.16282100
B	-2.98849700	0.83435600	-1.37440900
H	-3.35860300	1.34025800	-2.38195800
B	-1.47605900	-0.09627300	-1.43916700
H	-0.81428500	-0.20120600	-2.41567300
B	-1.51481200	-0.34137800	1.42422700
H	-0.88673400	-0.70719400	2.35793600
B	-3.02041400	0.59332200	1.49451800
H	-3.52690600	0.85638000	2.53751500
B	-3.94128200	0.24946900	0.00397700
H	-5.13040000	0.26469000	-0.02578200
B	-2.98409600	-0.89389800	-0.98058500
H	-3.46071500	-1.70310500	-1.71167400
B	-1.48886000	-1.26262800	-0.09025200
B	-3.01543400	-1.04117000	0.79325100
H	-3.51502200	-1.97354700	1.33924500

H	-1.02226500	2.22558100	-1.14929000
B	0.94865200	0.42329700	0.02462400
P	-0.49218900	-2.92592000	-0.28753400
H	-0.75579600	-3.48426600	0.98254200
H	-1.48627500	-3.64681900	-0.98615000
C	2.17408700	-1.71197800	-1.15079000
O	2.85566200	-2.62872100	-1.24826000
O	1.56412800	-0.69364800	-1.15034900
C	1.54896000	1.78309300	-0.65779800
F	2.89080200	1.78436300	-0.76687100
F	1.07909700	1.97434200	-1.92141100
F	1.20829100	2.88201300	0.05031200
C	1.75019900	-0.04801500	1.36678000
F	3.09628500	-0.01884300	1.21276600
F	1.45515800	0.73087600	2.41976100
F	1.46723100	-1.33229300	1.71452600

TS

C	1.56778100	-1.42385800	-0.66952500
C	0.64945200	-0.25646100	0.04907500
B	1.49566600	-1.39538900	1.03934800
H	0.85746200	-2.22004800	1.59472800
B	3.00242900	-1.74639400	0.15752200
H	3.39140800	-2.86714800	0.16910500
B	2.98948000	-0.82449800	-1.36222700
H	3.36792300	-1.32499900	-2.36926400
B	1.47505700	0.09910800	-1.43223800
H	0.81741100	0.21038200	-2.41075300
B	1.49553300	0.33285800	1.43416800
H	0.86189900	0.69809900	2.36405600
B	3.00403900	-0.59503300	1.50806800
H	3.50658900	-0.85979400	2.55244600
B	3.93230300	-0.24132500	0.02410700
H	5.12156000	-0.25267300	0.00125300
B	2.97756700	0.90241300	-0.96176900
H	3.45298000	1.71812900	-1.68653500
B	1.47719900	1.25213300	-0.07764100
B	2.99756300	1.04291900	0.81372500
H	3.48873400	1.97609000	1.36614700
H	1.02463500	-2.22344200	-1.15286600
B	-0.96825200	-0.40662600	-0.00026300
P	0.43895100	2.88071200	-0.27552600
H	0.66021400	3.48928000	0.97694300
H	1.35466400	3.65027400	-1.02373000
C	-2.02703100	1.81006500	-1.09962600
O	-2.70532600	2.72777700	-1.24015800
O	-1.56238200	0.70759500	-1.11312500
C	-1.55240600	-1.76463300	-0.70141700
F	-1.20863100	-2.87063000	-0.00349700
F	-2.89228000	-1.77651800	-0.82305500

F	-1.06849600	-1.93915900	-1.96342200
C	-1.76425800	0.00895400	1.36531200
F	-3.10916500	-0.04907800	1.23104400
F	-1.43674600	-0.77664900	2.40397700
F	-1.50492800	1.29725500	1.73281000

AD

C	1.52294600	-1.40334900	-0.72513300
C	0.59582600	-0.29310900	0.05996600
B	1.44022900	-1.48440600	0.98187100
H	0.81505200	-2.34328500	1.48392900
B	2.95857500	-1.76679500	0.08796700
H	3.36204000	-2.87557900	0.03608900
B	2.95699300	-0.75935500	-1.37498800
H	3.34777700	-1.19204400	-2.40214200
B	1.44285600	0.14782900	-1.40755200
H	0.78809300	0.34132900	-2.36833900
B	1.44025400	0.20894100	1.49175600
H	0.80650200	0.53828100	2.42709000
B	2.95170100	-0.70342100	1.50686400
H	3.45266600	-1.02421700	2.52983000
B	3.88734500	-0.25145800	0.05199300
H	5.07129800	-0.25522100	0.03710200
B	2.93743800	0.94324600	-0.87332800
H	3.39475200	1.81126000	-1.53880100
B	1.43942100	1.16962900	0.02714800
B	2.94388700	0.97820700	0.91691000
H	3.41325100	1.88371300	1.52165200
H	0.98062200	-2.16946900	-1.25646500
B	-1.06174500	-0.29880100	-0.08129800
P	0.24608300	2.65558700	-0.12697900
H	-0.08282100	3.28450000	1.07953300
H	0.73567700	3.67411600	-0.95491400
C	-1.36981800	2.08398600	-0.96595100
O	-2.02487000	2.93923700	-1.47870500
O	-1.57028900	0.81237300	-0.97654900
C	-1.60951800	-1.65487200	-0.81373800
F	-1.24653700	-2.78347200	-0.15167500
F	-2.93891000	-1.70069000	-0.95202600
F	-1.09788900	-1.79001400	-2.07298300
C	-1.78882200	-0.05692400	1.36815100
F	-3.12546100	-0.10880900	1.31624800
F	-1.40187100	-0.89220600	2.34599600
F	-1.50081400	1.22046600	1.82284500

IFLP-P(CH₃)₂/B(CF₃)₂**CM**

C	-2.38660100	1.27200600	-0.80977700
C	-1.29265100	0.43920000	0.05878400
B	-2.44626600	1.39556700	0.89335200
H	-2.08570000	2.39716700	1.40922900
B	-3.92309900	1.25428300	-0.09621600
H	-4.61183900	2.21311600	-0.21421000
B	-3.56627800	0.24858800	-1.51747300
H	-3.99246300	0.54700700	-2.58378100
B	-1.88711700	-0.24021500	-1.42037300
H	-1.16147700	-0.26455900	-2.35026500
B	-2.05361400	-0.24240200	1.44376400
H	-1.42496100	-0.37427900	2.43423400
B	-3.73545800	0.24884900	1.35340400
H	-4.37116800	0.44496400	2.33881900
B	-4.42152200	-0.45910100	-0.13415500
H	-5.57125000	-0.75294800	-0.21845800
B	-3.13970700	-1.39416200	-0.95772700
H	-3.33874200	-2.34808900	-1.64102600
B	-1.67714300	-1.21704300	0.03091300
B	-3.25217600	-1.39581800	0.82308400
H	-3.53375200	-2.36827900	1.44950900
H	-2.01511800	2.13882400	-1.34130800
B	0.36960600	0.39011100	0.05284100
P	0.21627300	-1.63891300	0.11102100
C	1.08687300	0.98849100	-1.30294500
C	1.09844100	1.05933600	1.35718500
F	2.37064900	1.37488000	-1.11435800
F	0.43427600	2.08971500	-1.76811100
F	1.14194200	0.12643200	-2.35769600
F	1.09796200	2.41199100	1.27958000
F	2.40217700	0.67921300	1.47807200
F	0.54718800	0.76497100	2.56174000
C	0.78428500	-2.44805200	1.63910400
H	0.40602400	-3.47337800	1.68173500
H	1.87753800	-2.45874100	1.64982600
H	0.42479100	-1.89242800	2.50707900
C	0.81656700	-2.65917300	-1.27291700
H	1.90540600	-2.60867700	-1.33376900
H	0.50359400	-3.69457200	-1.10667300
H	0.38680700	-2.29881000	-2.20862000
C	4.51353600	-0.55909700	-0.14566500
O	5.29741000	0.29593000	-0.10612400
O	3.74654500	-1.43930200	-0.18767200

TS

C	0.66921000	-2.17799100	-0.71609300
C	0.26767300	-0.78269900	0.06549000
B	0.55217400	-2.21626200	0.99138400
H	-0.38007000	-2.74623200	1.48517000
B	1.82749100	-3.09180200	0.10817100
H	1.74087100	-4.27340000	0.05605800
B	2.24021300	-2.16745100	-1.35176600
H	2.42788200	-2.72461000	-2.38180300
B	1.22233300	-0.71593500	-1.38856700
H	0.70476000	-0.28083600	-2.35909800
B	1.22926400	-0.65959000	1.49828700
H	0.76348700	-0.11237600	2.43762400
B	2.24016600	-2.11214200	1.52946400
H	2.55945000	-2.61011400	2.56027300
B	3.28712900	-2.08230800	0.08167200
H	4.37307300	-2.56698000	0.07359500
B	2.90473900	-0.60573900	-0.84449600
H	3.69077400	-0.00623800	-1.50806500
B	1.63089400	0.24221200	0.04136100
B	2.91405200	-0.57424800	0.93915600
H	3.71442500	0.06109600	1.55212300
H	-0.13313500	-2.66501700	-1.25278000
B	-1.26636300	-0.24578100	-0.01418000
P	1.29073400	2.11792900	-0.10459500
C	-0.78396500	2.36800400	-1.02017000
O	-0.96654600	3.48174100	-1.39411600
O	-1.38000800	1.27175200	-1.07508200
C	-2.29735000	-1.16217100	-0.88107700
F	-2.45072600	-2.38081300	-0.28833300
F	-3.52272600	-0.64568800	-1.02379200
F	-1.84241300	-1.41603100	-2.13894000
C	-1.89627400	0.33583600	1.37098300
F	-3.15748200	0.77837500	1.25525500
F	-1.89819000	-0.59907300	2.34909600
F	-1.17924800	1.39599800	1.85483300
C	2.44060900	2.85959400	-1.30616200
H	2.16712400	3.90645300	-1.46608100
H	3.47103600	2.79747300	-0.94357200
H	2.36696100	2.32627000	-2.25737200
C	1.54842900	2.98635400	1.47444400
H	1.27291600	4.03845800	1.36080200
H	0.92756400	2.53474500	2.24968900
H	2.60091100	2.91318800	1.76596400

AD

C	0.80002400	-2.13359600	-0.66686400
C	0.30412900	-0.74794400	0.07406600
B	0.64516000	-2.14207600	1.03527400
H	-0.25682400	-2.71561100	1.52288700
B	1.98924800	-2.96382400	0.20057800
H	1.97396500	-4.14473400	0.17633200
B	2.38639900	-2.05504100	-1.27235900
H	2.62853000	-2.62148300	-2.28040400
B	1.29317500	-0.66846500	-1.36504300
H	0.78164900	-0.27467400	-2.35160300
B	1.22801200	-0.54493200	1.52303800
H	0.72278300	0.00603200	2.43340600
B	2.31771800	-1.93365100	1.60647400
H	2.64237500	-2.38785300	2.65019500
B	3.39519000	-1.87768400	0.18076300
H	4.50092400	-2.30140600	0.20804900
B	2.95636800	-0.44753400	-0.78963300
H	3.71359800	0.18465900	-1.44885700
B	1.61178000	0.32354900	0.05061600
B	2.92203400	-0.37319900	0.99577300
H	3.66600700	0.32107900	1.60691300
H	0.03689500	-2.67125100	-1.20690200
B	-1.24553900	-0.17154300	-0.11781900
P	1.10384700	2.14889700	-0.15750900
C	-0.65641700	2.20589000	-0.83967300
O	-1.02058900	3.27995600	-1.22997400
O	-1.30295700	1.08986100	-0.94011600
C	-2.18140100	-1.22534100	-0.95190600
F	-2.27429900	-2.43267200	-0.33214800
F	-3.43363000	-0.80380400	-1.15846600
F	-1.67145300	-1.49332500	-2.19092700
C	-1.93480300	0.21630000	1.32208200
F	-3.22472300	0.56587200	1.22261900
F	-1.86459700	-0.73844700	2.26756100
F	-1.30857000	1.32415200	1.86078400
C	1.17927100	3.13144800	1.35540500
H	0.74327700	4.11299600	1.16315200
H	0.62253200	2.62417000	2.14134500
H	2.22479300	3.23572900	1.65160300
C	2.09700000	2.97327500	-1.42283000
H	1.69051900	3.96945000	-1.60123400
H	3.13195300	3.03659800	-1.08256100
H	2.05857900	2.39014700	-2.34376400

Silaborane

IFLP-PH₂/B(CF₃)₂

CM

B	-3.15271500	-0.13545800	-1.40612000
H	-3.79182600	-0.38244700	-2.38139400
B	-3.86971800	0.69934400	0.09302800
H	-5.02528000	0.99169800	0.12003800
B	-2.94068900	0.15759000	1.63322700
H	-3.46827500	0.08237500	2.69953800
B	-1.59099300	-1.04591000	1.17811800
H	-1.20664300	-1.89527000	1.91845000
B	-1.38512800	0.43841600	-1.48608500
H	-0.84009500	0.55661600	-2.54076000
B	-2.68939200	1.51546600	-0.94841600
H	-3.03823700	2.40584000	-1.65833100
B	-2.60191100	1.69224800	0.82337500
H	-2.88937800	2.71556100	1.35927900
B	-1.26189000	0.68181000	1.42639200
H	-0.63188000	0.98563200	2.38707700
B	-0.43366900	-0.10863100	0.05123300
B	-1.10468600	1.54424100	-0.12430400
H	-1.27374900	-2.72869100	-1.57426300
H	-4.47460900	-2.37035600	0.52613000
Si	-3.52435600	-1.27111900	0.33927400
Si	-1.60097100	-1.47705700	-0.89539000
B	1.24995800	-0.48484900	0.07795100
P	0.11597500	3.05381100	-0.37360700
H	-0.78827400	3.94370700	-1.00024300
H	0.00853600	3.62731900	0.91458400
C	2.73174500	1.53748400	-1.19581200
O	2.04683200	0.57475600	-1.17435300
O	3.47110600	2.41255300	-1.29414000
C	1.72111100	-1.89790900	-0.57455900
C	2.09200800	-0.05198100	1.39852600
F	1.92746900	1.25945800	1.71865700
F	1.69395800	-0.77555800	2.46531400
F	3.43646200	-0.21681400	1.29326400
F	3.04526500	-2.12445000	-0.64039000
F	1.26218800	-2.04140600	-1.85488100
F	1.18200700	-2.93012300	0.12988600

TS

B	-3.14562400	-0.12212900	-1.39031500
H	-3.79176900	-0.36538300	-2.36180900
B	-3.84968300	0.72061000	0.11105600
H	-5.00303100	1.02070400	0.14411700
B	-2.91788100	0.17214200	1.64771200
H	-3.44241100	0.10334500	2.71582800
B	-1.57838600	-1.04442100	1.18855900
H	-1.20163100	-1.89708200	1.92840800
B	-1.37850500	0.43506800	-1.47928500
H	-0.83409600	0.55276900	-2.53444200
B	-2.66997700	1.52678900	-0.93726600
H	-3.01046400	2.42172700	-1.64569200
B	-2.57045000	1.70391500	0.83539000
H	-2.84280400	2.73127500	1.37172300
B	-1.23602300	0.67921500	1.43373700
H	-0.59787000	0.98564100	2.38800000
B	-0.41696800	-0.11849800	0.05561000
B	-1.08589900	1.52934100	-0.11910600
H	-1.29101500	-2.73248600	-1.56675600
H	-4.47880700	-2.34008200	0.54923600
Si	-3.51593600	-1.25300600	0.35674200
Si	-1.59622600	-1.47784800	-0.88367100
B	1.28239000	-0.45687600	0.03635300
P	0.19725400	2.96935000	-0.36974500
H	-0.56086800	3.88800500	-1.12864000
H	0.11312600	3.64044000	0.86857400
C	2.53450000	1.67736000	-1.11316300
O	2.03570100	0.59174900	-1.09647100
O	3.27973300	2.54302900	-1.27998500
C	2.09637300	-0.11175200	1.40271200
C	1.72586600	-1.86892900	-0.64018200
F	1.97858300	1.20543300	1.74566200
F	1.63480300	-0.83102900	2.44646100
F	3.43309300	-0.33365400	1.33978800
F	1.19660500	-2.91238600	0.05698400
F	3.04610900	-2.10342300	-0.74154200
F	1.23572100	-1.99174600	-1.91425900

AD

B	-3.08610700	-0.06736100	-1.38315900
H	-3.72754500	-0.26133600	-2.36801800
B	-3.79974300	0.71044100	0.15123900
H	-4.95214000	1.01063000	0.19282600
B	-2.88722500	0.07864500	1.66901100
H	-3.42760700	-0.03459300	2.72456400
B	-1.54181100	-1.12348800	1.16650500
H	-1.18388200	-2.01484400	1.86718700
B	-1.33374200	0.47730500	-1.43669300

H	-0.76393100	0.66302400	-2.46755200
B	-2.61727500	1.56109100	-0.85141800
H	-2.93043100	2.50151900	-1.51178300
B	-2.52450300	1.65100600	0.93954300
H	-2.78286000	2.65840300	1.51915400
B	-1.20265000	0.57682500	1.50419000
H	-0.56680800	0.86079400	2.46553400
B	-0.35927100	-0.15177100	0.09112200
B	-1.06033300	1.46056400	-0.01321000
H	-1.25037700	-2.68295400	-1.67382600
H	-4.45186000	-2.35242400	0.43306200
Si	-3.46574900	-1.27842000	0.29779700
Si	-1.51869500	-1.45982900	-0.92422800
B	1.38366700	-0.34138200	-0.03287300
P	0.35591600	2.73044600	-0.20879000
H	0.05330800	3.82405400	-1.02667600
H	0.78201200	3.30092500	0.99444400
C	1.88770200	1.96313800	-1.04730100
O	2.03762100	0.69139700	-0.95246300
O	2.57755900	2.74728800	-1.64873300
C	2.11398500	-0.16413300	1.41968200
C	1.77602500	-1.76131900	-0.73478000
F	1.97242100	1.14101900	1.86439900
F	1.59516100	-0.93979300	2.40013600
F	3.44532400	-0.38351800	1.42867100
F	1.23650600	-2.82950100	-0.06649400
F	3.08326800	-2.02932100	-0.87578500
F	1.24541600	-1.84659400	-2.00474500

IFLP-P(CH₃)₂/B(CF₃)₂

CM

B	-3.57234100	0.02983400	-1.48861500
H	-4.18528500	-0.18033100	-2.48904200
B	-4.18326100	1.15061200	-0.14068100
H	-5.25577900	1.66391900	-0.23177100
B	-3.51346400	0.57682400	1.51404900
H	-4.11947800	0.73070000	2.52881800
B	-2.43180600	-0.94818800	1.30384500
H	-2.31889900	-1.76838800	2.15961700
B	-1.76344900	0.19340400	-1.46049600
H	-1.13439300	0.08780600	-2.46415200
B	-2.79312200	1.60206000	-1.14384300
H	-2.88843800	2.45961900	-1.96473900
B	-2.77824300	1.92676700	0.61380700
H	-2.86588200	3.02908200	1.05532900
B	-1.76788400	0.68874800	1.41748500
H	-1.14730000	0.97198800	2.38854200
B	-1.02489600	-0.39436600	0.20190700

B	-1.32825000	1.31206200	-0.18046100
H	-2.26390500	-2.92044500	-1.29208300
H	-5.51128800	-1.62061700	0.48839900
Si	-4.29465000	-0.82685100	0.29731100
Si	-2.36295700	-1.57860700	-0.71644400
B	0.72670900	-0.39743300	0.15534400
P	0.58833800	1.58702700	-0.22296900
C	1.49837900	-0.74071200	1.54619400
C	1.38003300	-1.26405500	-1.06367400
F	2.81524500	-0.36608900	1.56411000
F	1.49409700	-2.07287700	1.80912000
F	0.97073700	-0.15271700	2.65609800
F	0.86029600	-2.52750600	-1.12212300
F	2.72699200	-1.43458700	-0.99354500
F	1.16531900	-0.74533800	-2.31120900
C	1.21089500	2.69442300	1.08532800
H	2.30356500	2.65979400	1.09661600
H	0.87491500	3.71838600	0.89688300
H	0.83517600	2.36203900	2.05474000
C	1.20576200	2.27639100	-1.79509900
H	0.92718800	3.33308000	-1.85594900
H	2.29255100	2.17877400	-1.84386700
H	0.75981000	1.73735100	-2.63225200
C	4.90717700	0.47321600	-0.25609800
O	5.62344400	-0.41435000	-0.03759900
O	4.21671300	1.38723500	-0.48319700

TS

B	-3.11932200	-0.31314600	-1.36945800
H	-3.76468900	-0.47384400	-2.35807000
B	-3.82756300	0.40702400	0.19532600
H	-4.98040000	0.70462500	0.25109200
B	-2.90132300	-0.26995200	1.68383200
H	-3.43095000	-0.42459300	2.74000400
B	-1.55964300	-1.44795100	1.12933800
H	-1.19129400	-2.36055900	1.79704900
B	-1.35789900	0.24450400	-1.41116800
H	-0.80399100	0.46100200	-2.44464900
B	-2.64799000	1.29242900	-0.78175500
H	-2.97848400	2.24860400	-1.41106400
B	-2.54850000	1.32421100	1.00372200
H	-2.81398500	2.30897300	1.61999400
B	-1.21833900	0.24493600	1.52046900
H	-0.58078900	0.47935200	2.49499500
B	-0.38660700	-0.43262700	0.08175800
B	-1.07630100	1.19988200	0.03952700
H	-1.27443600	-2.90436400	-1.76183900
H	-4.46383300	-2.67143800	0.37686500
Si	-3.49048400	-1.58201000	0.27368300
Si	-1.55909500	-1.70971400	-0.97260000

B	1.31611200	-0.75411900	0.02892700
P	0.23663900	2.58207700	-0.11808400
C	2.13714600	1.73381100	-1.05833900
O	2.23172500	0.49784500	-0.93950400
O	2.76288700	2.60675700	-1.57744000
C	2.10198200	-0.65073200	1.44676100
C	1.74213100	-2.04433800	-0.86066700
F	2.01847600	0.60395900	1.98831900
F	1.56345900	-1.49110400	2.36873400
F	3.41940300	-0.93174300	1.40442700
F	1.19400300	-3.17923000	-0.31573300
F	3.04856100	-2.29084000	-1.01019300
F	1.22514100	-1.97978400	-2.12944000
C	0.53451700	3.41929300	1.47234300
H	1.33567100	4.15441700	1.35637200
H	-0.38064300	3.92259600	1.80019100
H	0.82870600	2.68321000	2.22221300
C	-0.29807400	3.86809000	-1.29053700
H	0.53126400	4.55863100	-1.46850100
H	-0.57428100	3.40040100	-2.23920800
H	-1.16096000	4.41514600	-0.89875400

AD

B	-3.14363700	-0.21973900	-1.32126100
H	-3.81303200	-0.37660800	-2.29443200
B	-3.79504300	0.56513100	0.23755100
H	-4.93395600	0.90944700	0.30745500
B	-2.87379300	-0.11808600	1.72642200
H	-3.39472400	-0.22458100	2.79271500
B	-1.58700400	-1.36329700	1.18007300
H	-1.25172500	-2.27697200	1.86293700
B	-1.37166100	0.26302900	-1.40513800
H	-0.82085400	0.44032200	-2.44808000
B	-2.60217100	1.38064000	-0.77964200
H	-2.89791800	2.33978200	-1.42253900
B	-2.46567900	1.44667800	1.00581300
H	-2.67495600	2.45682000	1.60285400
B	-1.17454100	0.31898300	1.52802900
H	-0.51118300	0.56147100	2.48311200
B	-0.38811000	-0.42057000	0.09226600
B	-1.02708000	1.21951900	0.01964500
H	-1.41679200	-2.89395900	-1.68567400
H	-4.55397700	-2.47403600	0.49792300
Si	-3.53112300	-1.43604400	0.35191200
Si	-1.61644300	-1.67182000	-0.91321300
B	1.34143500	-0.68251900	-0.06289500
P	0.37278900	2.49847300	-0.19037600
C	1.95190600	1.68664500	-0.84630100
O	2.06379700	0.40331300	-0.84927600
O	2.75824300	2.47553500	-1.28734000

C	2.07976100	-0.72993200	1.39822000
C	1.65384700	-2.03709800	-0.92077500
F	2.06900400	0.52142100	1.98397800
F	1.48323500	-1.55342700	2.29586700
F	3.38292100	-1.08500000	1.37549100
F	1.09377100	-3.14871900	-0.34194300
F	2.94289300	-2.33915900	-1.13771700
F	1.07778200	-1.97873600	-2.17362200
C	0.80590000	3.37162900	1.33816000
H	1.03820800	2.64479100	2.11817800
H	1.67607100	4.00782300	1.15562100
H	-0.04629300	3.98204200	1.65038600
C	-0.02373200	3.74740700	-1.44365500
H	-0.28954300	3.24929000	-2.37958900
H	-0.87552600	4.34298800	-1.10354000
H	0.84784400	4.38541800	-1.60723000