Supporting Information for

Theoretical Prediction of Metallomimetic Stable Cyclic Group 13 Carbenoids

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Computational details

All the calculations were performed using DFT method employing Gaussian 09 suite of programs. All ground states and transition states were optimized using M06 functional in conjunction with Def2-TZVP basis set.[1, 2] Frequency calculations were also performed to characterize the nature of the stationary points, using the same level of theory. All the ground state structures were verified as minima with real vibrational frequencies whereas transition states were characterized by the presence of only one imaginary frequency, which was further confirmed by performing intrinsic reaction coordinate (IRC) analysis.[3] Natural bond orbital (NBO) analysis[4] was performed to examine the bonding conditions in the optimized molecules. Dispersion effects were incorporated by using the D3 version of Grimme's dispersion correction in combination with the original D3 damping function using the keyword Empiricaldispersion=GD3.[5] The ultrafine integration grid was used for all the calculations. Solvent effects (benzene) were further incorporated throughout the calculations using the the polarizable continuum model.[6] The reliability of the calculated singlet-triplet energy separation i.e. $\Delta E_{S\text{-}T}$ values were checked by recalculating them with two other widely used density functionals such as B3LYP[7] and ωB97XD[8] (Table S1). Further, to check the presence of any internal stability in **1**-**3**, we performed stability tests on the single-determinant wave functions of the optimized geometries of **1**-**3** (both singlet and triplet states).[9,10] Furthermore, to check the reliability of the results predicted by the M06 functional, we have performed a few calculations using functionals B3LYP and ωB97XD and the results were found to be comparable (Table S2).

References:

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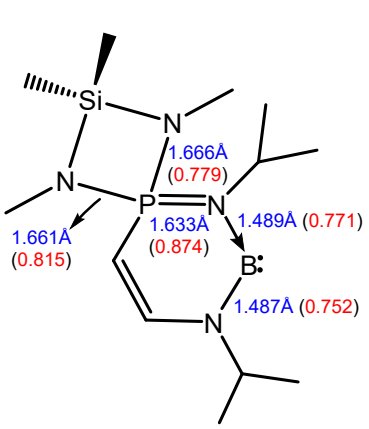
Difference between the present and our previous works

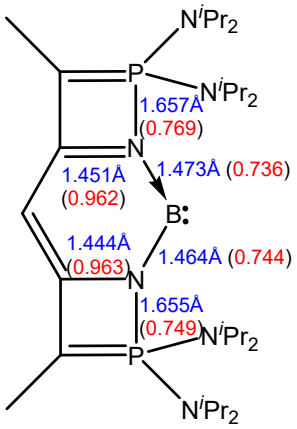
The systems considered in the present work (for example, **A**) are different from the one considered in our first publication (*Inorg. Chem.* **2019**, *58*, 5428) in 2019 (**B**) as evident from the structures given below. In the structure **B**, two strongly electron donating cyclic ylidic moieties were installed on both side of the NacNac framework. It may be emphasized that **B** owe its stability not only to the substantial transfer of electron density from the α-nitrogen to boron but also to the presence of thermodynamically robust ylidic bonds. The presence of ylidic groups makes the α-nitrogen atoms highly electron-rich, thereby enabling enhanced charge transfer to the boron atom compared to that in **A**. This is evident from the calculated values of natural charge at the N-atoms attached to the central boron atom. While both the N-atoms of compound **B** carry negative charges of -1.112 and -1.122, that of **A** carry charges of -1.093 and -0.687. Further, both the B─N bonds of **B** are shorter and stronger than those of **A** as shown below.



A

ΔE_{S-T} = 14.7 kcal mol^{-1}

Present Work



B

ΔE_{S-T} = 30.0 kcal mol^{-1}

Inorg. Chem. **2019**, *58*, 5428

Scheme: Schematic representation of the structures considered in the present work (**A**) and in 2019 (**B**). The bond lengths are given in *blue* while the Wiberg Bond Indices (WBI) are given within parenthesis in *red*.

Mechanism of activation of E−H bonds by V'

The activation of E−H (E = H, C, N, P and Si) bonds by **V'** (truncated version of **V** where the bulky Dipp group is replaced by the smaller phenyl group) is predicted to proceed via a two-step mechanism which involves participation of both the boron atom and carbenic carbon (C_c) resulting in cooperative splitting of the bonds of interest. For example, for H−H bond activation of H_2, the first step involves interaction of σ_{H-H} orbital with vacant p-orbital of boron as well as backdonation from filled p-orbital to σ^*_{H-H}, leading to the formation of 1,1-product (i.e. both the hydrogens are attached to the boron center). The reaction proceeds via a transition state (**V′_TS$_1^{H-H}$**, please see the Figure below) featuring an elongated H−H bond.

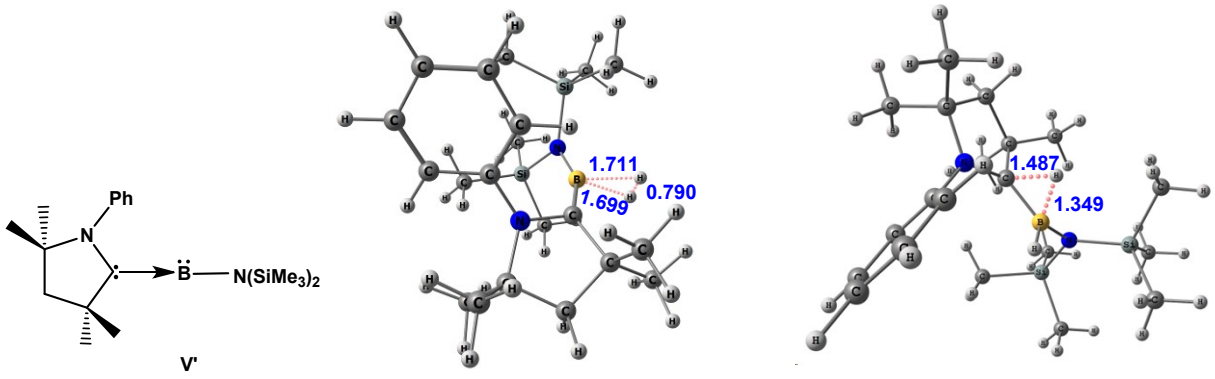


Figure: The transition states obtained for the activation of H_2 by **V'**.

In the second step, the 1,1-product rearranges to the more stable 1,2-product via 1,2-hydride shift thus indicating the cooperative nature of splitting. The process proceeds via a transition state (**V'_TS$_2^{H-H}$**) featuring an elongated and polarized B–H bond. The same mechanism is followed for activation of C−H and Si−H bond of CH_4 and SiH_3Ph respectively.

The calculated the barrier heights and reaction free energies for activation of the substrates considered in this work (i.e. H_2, CH_4, NH_3, PH_3 and SiH_3Ph) by **V′** are given in the Tables below.

Table: PCM(Benzene)-M06-D3/Def2-TZVP calculated reaction free energies ($\Delta G^{\circ}_{\text{Total (1,1)}}{}^{\text{E–H}}$ and $\Delta G^{\circ}_{\text{Total (1,2)}}{}^{\text{E–H}}$) and activation energy barriers ($\Delta G^{\circ}_{\text{TS1}}{}^{\text{E–H‡}}$ and $\Delta G^{\circ}_{\text{TS2}}{}^{\text{E–H‡}}$) for the activation of E−H (E = H, C and Si) bonds by **V'**. The energies are given in kcal mol^{-1}.

Molecules	$\Delta G^{\circ}_{\text{TS}_1}{}^{\text{E–H‡}}$	$\Delta G^{\circ}_{\text{Total (1,1)}}{}^{\text{E–H}}$	$\Delta G^{\circ}_{\text{TS}_2}{}^{\text{E–H‡}}$	$\Delta G^{\circ}_{\text{Total (1,2)}}{}^{\text{E–H}}$
V'H–H	20.1	-14.2	3.1	-25.1
V'C–H	37.1	2.9	-1.8	-12.1
V'Si–H	18.0	-5.3	12.0	-4.2

The first step in NH_3 activation is the formation of borylene-NH_3 adduct (**V'_Int^{N-H}**) via interaction of the amine lone pair with the vacant p-orbital of boron. In the second step, the boronic lone pair polarizes one of the N–H bonds of the NH_3-borylene adduct resulting in the formation of a positively polarized hydrogen atom ($H^{\delta+}$) and a pseudoamide fragment ($NH_2^{\delta-}$). While $NH_2^{\delta-}$ remains attached to the boron center, $H^{\delta+}$ migrates to the electron rich carbene carbon giving rise to the N–H splitting 1,2-product (**V'_P$_{1,2}^{N–H}$**). The complete reaction profile diagram for activation of NH_3 by **V'** is given in the Figure below. The same mechanistic pathway is expected to be followed for activation of P−H bond of PH_3. For both NH_3 and PH_3, the 1,2−products are preferred over 1,1−products owing to the more exergonic reaction free energies associated with the formation of 1,2−products (please refer to the Table below).

Table: PCM(Benzene)-M06-D3/Def2-TZVP calculated reaction free energies ($\Delta G^{\circ}_{Int}{}^{E-H}$, $\Delta G^{\circ}_{Total(1,1)}{}^{E-H}$ and $\Delta G^{\circ}_{Total(1,2)}{}^{E-H}$) and activation energy barriers ($\Delta G^{\circ}_{TS_{1,1}}{}^{E-H\ddagger}$ and $\Delta G^{\circ}_{TS_{1,2}}{}^{E-H\ddagger}$) associated with the activation of E−H bonds (E = N and P).

Molecules	$\Delta G^{\circ}_{Int}{}^{E-H}$	$\Delta G^{\circ}_{TS_{1,1}}{}^{E-H\ddagger}$	$\Delta G^{\circ}_{Total\ (1,1)}{}^{E-H}$	$\Delta G^{\circ}_{TS_{1,2}}{}^{E-H\ddagger}$	$\Delta G^{\circ}_{Total\ (1,2)}{}^{E-H\ddagger}$
V'$^{N-H}$	-6.6	[a]	-11.0	35.0	-38.9
V'$^{P-H}$	4.4	[a]	-5.3-	[a]	-11.1

[a]Despite our best efforts, we could not obtain these transition state (TS).

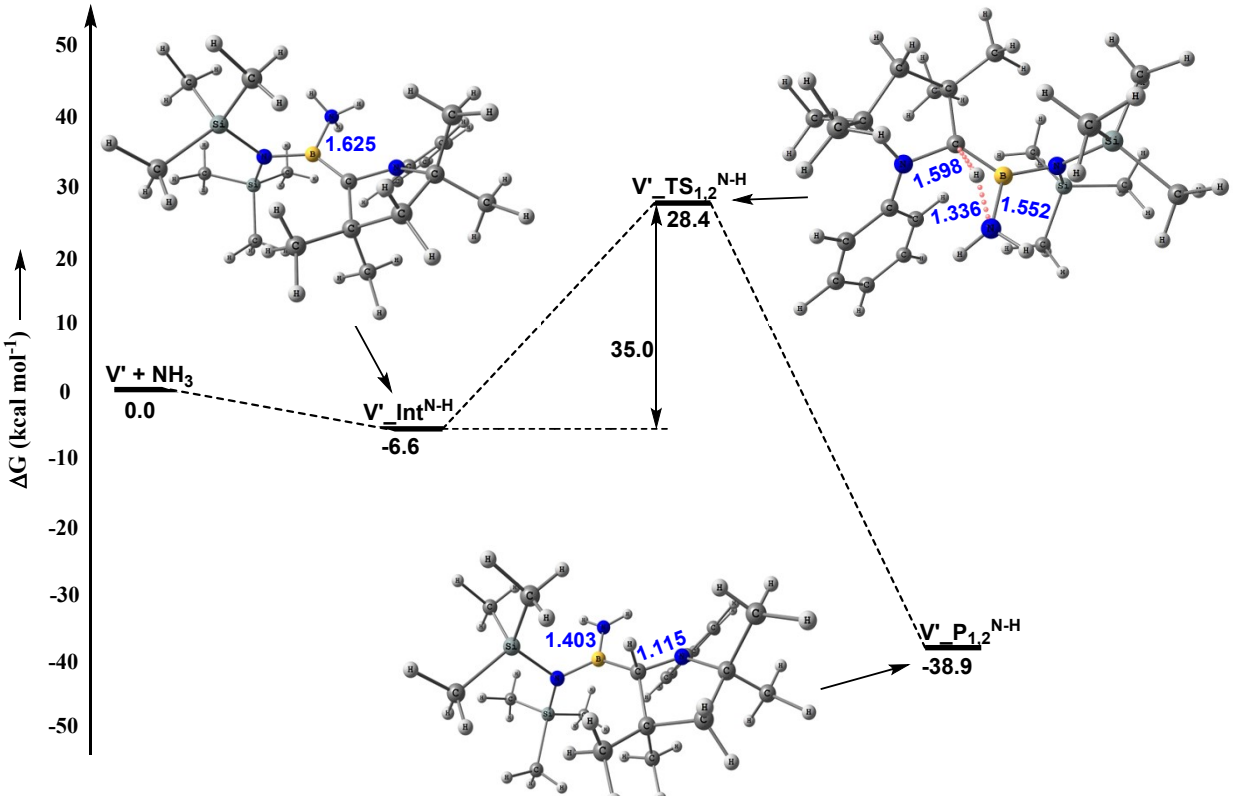


Figure: Reaction profile diagram for activation of N–H bond by V′. The reaction free energies and bond lengths are given in kcal mol^{-1} and Å respectively.

The in depth mechanistic analyses and electron transfer processes for these bond activation reactions by the base-stabilized borylene **V'** have already been discussed in one of our prior works (*Inorg. Chem.* **2023**, *62*, 9063-9076).

However, in contrast to **V'**, a single step mechanism is envisioned for the activation of E−H bonds by our proposed group 13 carbenoids **1**−**3**. In addition, as mentioned above, **V'** exhibit π-symmetric lone pair (**b** and **c**, Figure S2) and two reactive centers (boron and carbenic carbon) whereas the proposed group 13 carbenoids **1**−**3** exhibit σ-symmetric lone pair (**a**, Figure S2) and only one reactive center (i.e., B/Al/Ga).

Table S1: Calculated singlet-triplet energy separations (ΔE_{S-T} in kcal mol^{-1}) of the proposed carbenoids **1**, **2** and **3** using different functionals.

Molecules	ΔE_{S-T}		
	M06	**B3LYP**	**ωB97XD**
1	14.7	14.6	15.5
2	40.8	41.5	42.9
3	59.5	56.3	60.0

Table S2: Calculated reaction free energies (ΔG°_{Pro}) and activation barriers (ΔG°_{TS}) associated with activation of H_2 and NH_3 by **1-3** using different functionals.

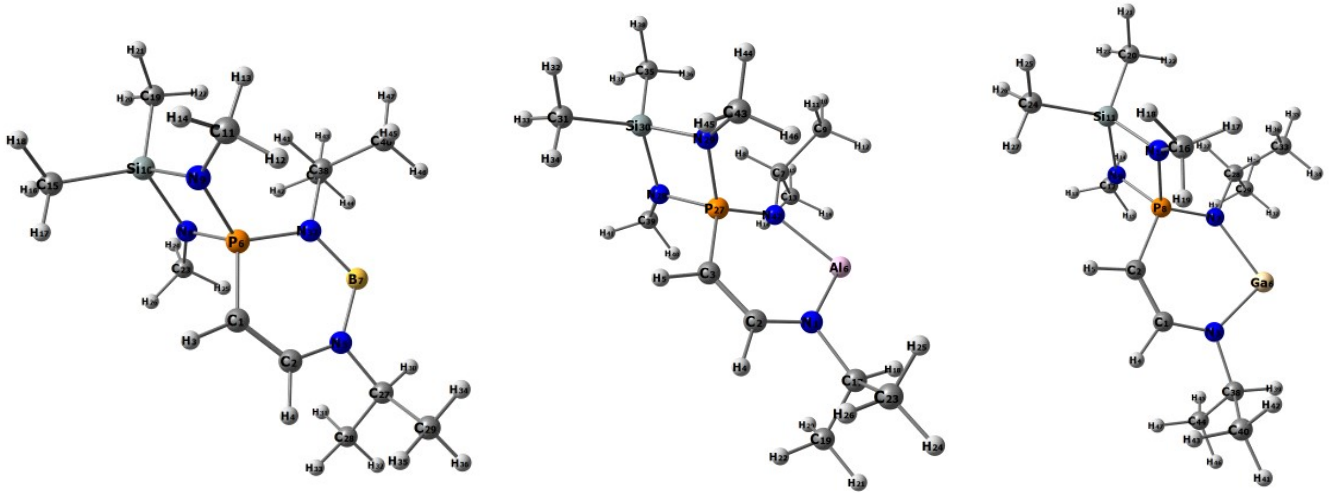
Molecules	Functional	$\Delta G^{\circ}_{TS}{}^{H-H\ddagger}$	$\Delta G^{\circ}_{Pro}{}^{H-H}$	$\Delta G^{\circ}_{TS}{}^{N-H\ddagger}$	$\Delta G^{\circ}_{Pro}{}^{N-H}$
1	M06	14.1	-54.7	15.0	-61.0
	B3LYP	13.4	-54.1	15.7	-56.2
	ωB97XD	15.8	-56.8	18.1	-60.5
2	M06	36.2	-31.2	29.2	-43.6
	B3LYP	36.2	-29.9	28.6	-42.4
	ωB97XD	38.7	-32.2	30.6	-44.0
3	M06	52.6	-7.7	47.9	-8.9
	B3LYP	56.7	-6.3	48.6	-7.0
	ωB97XD	54.7	-11.9	48.7	-12.4

Table S3: Calculated Mulliken spin densities at the central atom (E =B/Al/Ga), two α-nitrogens (N_1 and N_2) with respect to the central atom for 1-3.

Molecules	E	N_1	N_2
1	1.137	-0.048	-0.098
2	1.154	-0.013	-0.001
3	1.328	0.100	0.148

Table S4: Calculated percentage of atomic contribution (% Atomic contrib.) (only those atoms were considered which have contributed more than 10% to the MOs) to the frontier orbitals (HOMO and LUMO) of **1-3**.

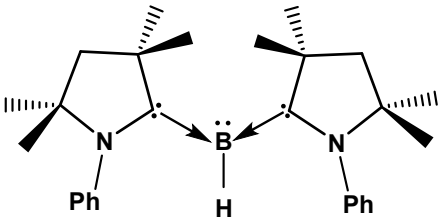
1				**2**				**3**			
HOMO		**LUMO**		**HOMO**		**LUMO**		**HOMO**		**LUMO**	
Center	% Atomic contrib.	Center	% Atomic contrib.	Center	% Atomic contrib.	Center	% Atomic contrib.	Center	% Atomic contrib.	Center	% Atomic contrib.
B(7)	86.19	B(7)	11.40	Al(6)	83.95	Al(6)	57.06	Ga(6)	71.44	Ga(6)	75.79
		P(6)	10.72			C(2)	18.18	N(7)	9.09	C(1)	10.16
		C(2)	37.84					N(3)	10.45		
		C(1)	11.77								



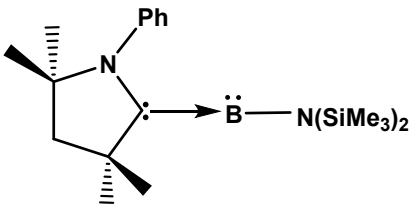
1 **2** **3**

Table S5: PCM(Benzene)-M06-D3/Def2-TZVP calculated energies (in eV) of the π-symmetric lone pair (E_{π}) and π-symmetric unoccupied orbitals (E_{π^*}), HOMO-LUMO gaps ($\Delta E_{H\text{-}L}$ in eV), singlet-triplet energy separations ($\Delta E_{S\text{-}T}$ in kcal mol^{-1}) of **IV'** and **V'** (truncated versions of **IV** and **V;** the bulky Dipp group attached to the amino groups were replaced by the smaller phenyl group).

Molecules	E_{π}	E_{π^*}	$\Delta E_{H\text{-}L}$	$\Delta E_{S\text{-}T}$
IV'	-4.06	-0.98	3.08	14.5
V'	-4.56	0.39	4.44	25.9



IV'



V'

Table S6: PCM(Benzene)-M06-D3/Def2-TZVP calculated H–H, E(I)–$H^{\delta+}$ and E(I)–$H^{\delta-}$ bond lengths (in Å) and their corresponding Wiberg Bond Index (WBI) values (given within parentheses), occupancy of the formally vacant p-orbital at the E(I) center ($Occ_{E(I)}$), natural charges at E(I) center ($q_{E(I)}$) and hydrogen atoms of dihydrogen molecule ($q_{H^{\delta+}}$ & $q_{H^{\delta-}}$) in the transition states (**$TS^{H–H}$**) for H_2 activation by **1-3** and **I-III**.

Molecules	**H–H**	**E(I)–$H^{\delta+}$**	**E(I)–$H^{\delta-}$**	**$Occ_{E(I)}$**	**$q_{E(I)}$**	**$q_{H^{\delta+}}$**	**$q_{H^{\delta-}}$**
$1TS^{H–H}$	0.923	1.408	1.898	0.407	0.266	-0.003	-0.079
	(0.452)	(0.524)	(0.439)				
$2TS^{H–H}$	1.233	1.605	1.954	0.258	0.939	-0.172	-0.235
	(0.248)	(0.689)	(0.675)				
$3TS^{H–H}$	1.370	1.571	1.992	0.376	0.830	-0.115	-0.266
	(0.181)	(0.751)	(0.718)				
$ITS^{H–H}$	1.073	1.214	1.944	0.757	0.065	0.185	-0.191
	(0.315)	(0.621)	(0.467)				
$IITS^{H–H}$	1.267	1.591	1.972	0.513	0.967	-0.159	-0.249
	(0.228)	(0.722)	(0.690)				
$IIITS^{H–H}$	1.399	1.557	2.001	0.535	0.833	-0.099	-0.278
	(0.166)	(0.772)	(0.730)				

Table S7: PCM(Benzene)-M06-D3/Def2-TZVP calculated activated C–H, E(I)–H and E(I)–C bond lengths (in Å) and their corresponding Wiberg Bond Index (WBI) values (given within parentheses), occupancy of the formally vacant p-orbital at the E(I) center ($Occ_{E(I)}$), natural charges at E(I) center ($q_{E(I)}$), and carbon (q_C) and hydrogen atoms (q_H) of methane in the transition states ($\mathbf{TS^{C-H}}$) for CH_4 activation by **1-3**.

Molecules	C–H	E(I)–H	E(I)–C	$Occ_{E(I)}$	$q_{E(I)}$	q_C	q_H
$\mathbf{1TS^{C-H}}$	1.460	1.358	2.484	0.400	0.383	-0.881	0.094
	(0.337)	(0.629)	(0.422)				
$\mathbf{2TS^{C-H}}$	1.658	1.593	2.404	0.267	1.094	-1.017	-0.109
	(0.246)	(0.713)	(0.560)				
$\mathbf{3TS^{C-H}}$	1.791	1.559	2.451	0.328	0.966	-0.991	-0.078
	(0.183)	(0.757)	(0.608)				
$\mathbf{ITS^{C-H}}$	1.610	1.156	2.458	0.786	0.102	-0.853	0.272
	(0.202)	(0.697)	(0.503)				
$\mathbf{IITS^{C-H}}$	1.680	1.581	2.374	0.444	1.081	-1.017	-0.089
	(0.235)	(0.733)	(0.584)				
$\mathbf{IIITS^{C-H}}$	1.818	1.547	2.413	0.475	0.960	-0.989	-0.055
	(0.174)	(0.772)	(0.630)				

Table S8: PCM(Benzene)-M06-D3/Def2-TZVP calculated activated N–H, E(I)–H and E(I)–N bond lengths (in Å) and their corresponding Wiberg Bond Index (WBI) values (given within parentheses), occupancy of the formally vacant p-orbital at the E(I) center ($Occ_{E(I)}$), natural charges at E(I) center ($q_{E(I)}$), nitrogen (q_N) and hydrogen atoms (q_H) of ammonia in the transition states ($\mathbf{TS^{N–H}}$) for NH_3 activation by **1-3** and **I-III**.

Molecules	N–H	E(I)–H	E(I)–N	$Occ_{E(I)}$	$q_{E(I)}$	q_N	q_H
$\mathbf{1TS^{N–H}}$	1.386	1.403	2.513	0.325	0.466	-1.202	0.169
	(0.306)	(0.638)	(0.294)				
$\mathbf{2TS^{N–H}}$	1.407	1.714	1.969	0.176	1.087	-1.324	0.068
	(0.294)	(0.671)	(0.501)				
$\mathbf{3TS^{N–H}}$	1.551	1.646	2.101	0.194	1.041	-1.296	0.034
	(0.230)	(0.719)	(0.511)				
$\mathbf{ITS^{N–H}}$	1.539	1.156	2.423	0.794	0.192	-1.161	0.325
	(0.178)	(0.694)	(0.404)				
$\mathbf{IITS^{N–H}}$	1.408	1.716	1.935	0.507	1.075	-1.319	0.081
	(0.300)	(0.662)	(0.538)				
$\mathbf{IIITS^{N–H}}$	1.547	1.653	2.046	0.411	1.042	-1.291	0.051
	(0.240)	(0.707)	(0.553)				

Table S9: PCM(Benzene)-M06-D3/Def2-TZVP calculated activated P–H, E(I)–H and E(I)–P bond lengths (in Å) and their corresponding Wiberg Bond Index (WBI) values (given within parentheses), occupancy of the formally vacant p-orbital at the E(I) center ($Occ_{E(I)}$), natural charges at E(I) center ($q_{E(I)}$), and phosphorus (q_P) and hydrogen atoms (q_H) of phosphine in the transition states ($\mathbf{TS^{P-H}}$) for PH_3 activation by **1-3** and **I-III**.

Molecules	P–H	E(I)–H	E(I)–P	$Occ_{E(I)}$	$q_{E(I)}$	q_P	q_H
$\mathbf{1TS^{P-H}}$	1.555	1.730	3.110	0.362	0.374	-0.131	-0.023
	(0.650)	(0.329)	(0.267)				
$\mathbf{2TS^{P-H}}$	1.954	1.643	2.951	0.317	1.107	-0.261	-0.238
	(0.265)	(0.635)	(0.645)				
$\mathbf{3TS^{P-H}}$	1.761	1.786	2.688	0.260	1.057	-0.386	-0.104
	(0.462)	(0.467)	(0.661)				
$\mathbf{ITS^{P-H}}$	1.734	1.373	3.027	0.834	0.165	-0.230	0.132
	(0.478)	(0.482)	(0.333)				
$\mathbf{IITS^{P-H}}$	1.617	1.956	2.492	0.422	1.013	-0.288	-0.036
	(0.462)	(0.464)	(0.661)				
$\mathbf{IIITS^{P-H}}$	1.726	1.837	2.537	0.353	0.990	-0.309	-0.067
	(0.527)	(0.411)	(0.787)				

Table S10: PCM(Benzene)-M06-D3/Def2-TZVP calculated activated Si–H, E(I)–Si and E(I)–H bond lengths (in Å) and their corresponding Wiberg Bond Index (WBI) values (given within parentheses), occupancy of the formally vacant p-orbital at the E(I) center ($Occ_{E(I)}$), natural charges at E(I) center ($q_{E(I)}$), silicon(q_{Si}) and hydrogen atoms (q_H) of phenylsilane in the transition states (**TS$^{Si–H}$**) for SiH_3Ph activation by **1-3** and **I-III**.

Molecules	**Si–H**	**E(I)–Si**	**E(I)–H**	**$Occ_{E(I)}$**	**$q_{E(I)}$**	**q_{Si}**	**q_H**
1TS$^{Si–H}$	1.670 (0.507)	3.021 (0.331)	1.535 (0.437)	0.374	0.362	0.827	-0.146
2TS$^{Si–H}$	2.053 (0.209)	3.007 (0.624)	1.610 (0.650)	0.523	1.065	0.659	-0.301
3TS$^{Si–H}$	2.211 (0.146)	2.975 (0.662)	1.572 (0.740)	0.569	0.888	0.636	-0.213
ITS$^{Si–H}$	1.861 (0.370)	2.982 (0.365)	1.281 (0.575)	0.826	0.080	0.707	0.095
IITS$^{Si–H}$	2.071 (0.196)	3.025 (0.659)	1.593 (0.671)	0.718	1.085	0.627	-0.294
IIITS$^{Si–H}$	2.256 (0.136)	2.951 (0.701)	1.559 (0.760)	0.652	0.885	0.618	-0.193

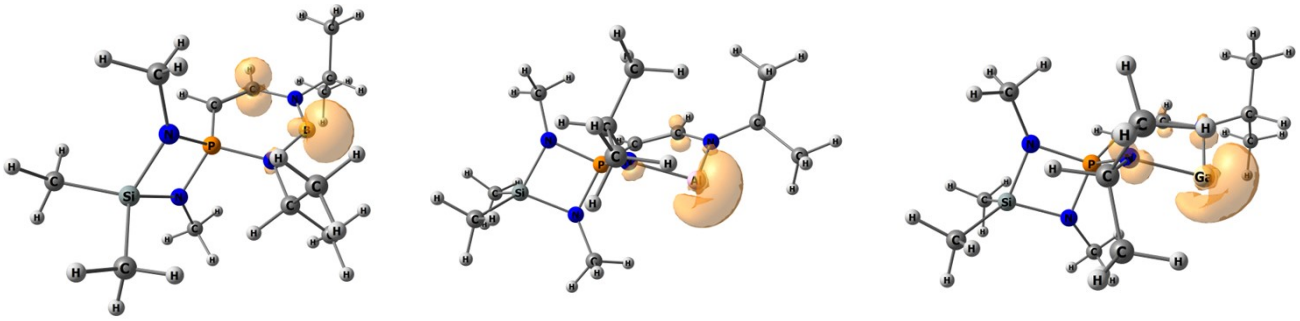


Fig. S1: Mulliken spin density plots for the triplet states of **1**-**3**.

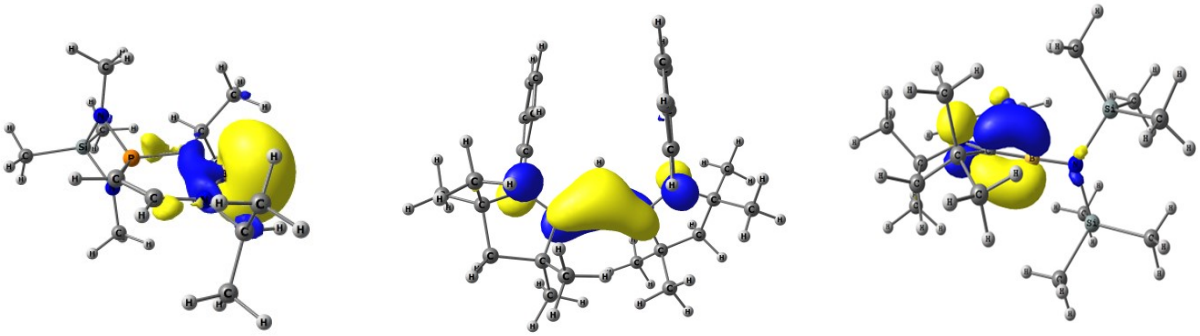


Fig. S2: Contour plots of a representative σ-symmetric lone pair in our proposed Group 13 carbenoids (**a**), and π-symmetric lone pairs in **IV'** (**b**) and **V'** (**c**).

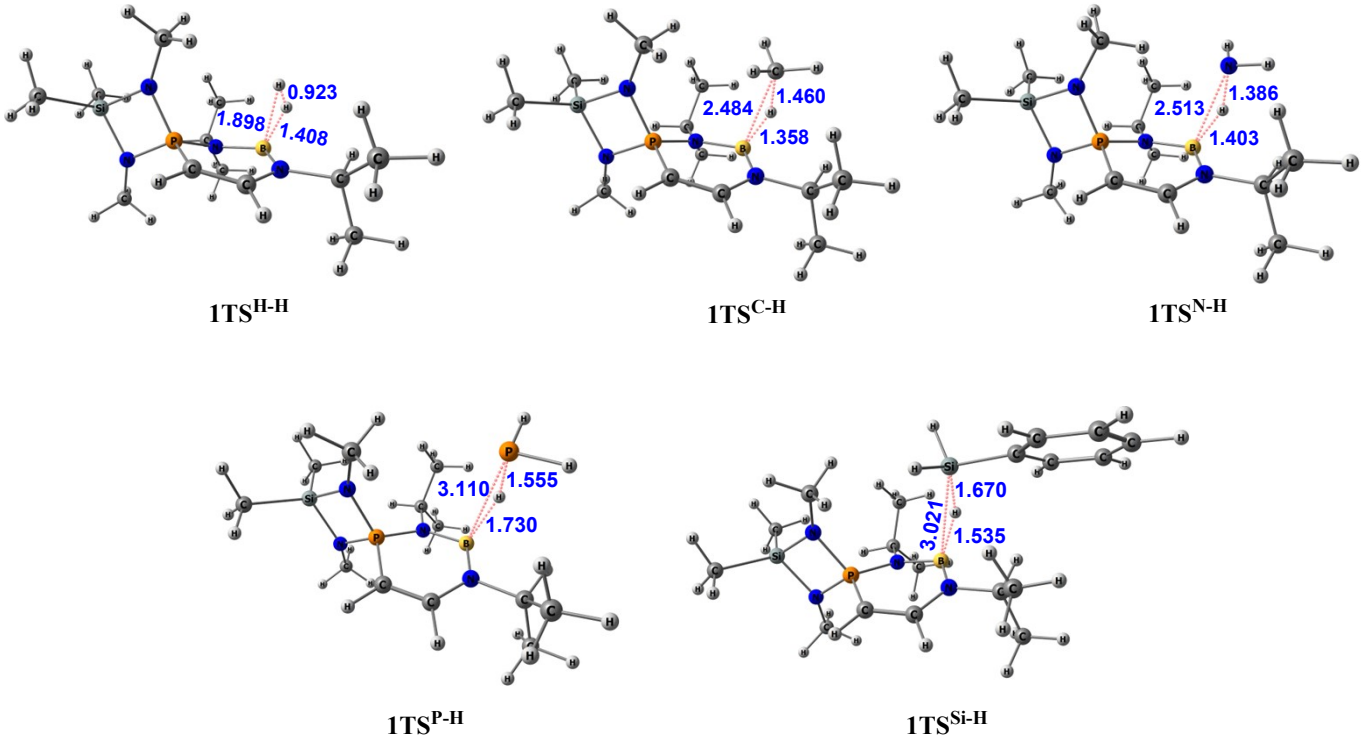


Fig. S3: Pictorial representation of the transition states involved in the activation of X–H (X = H, C, N, P and Si) bonds by **1**. The bond lengths are given in Å.

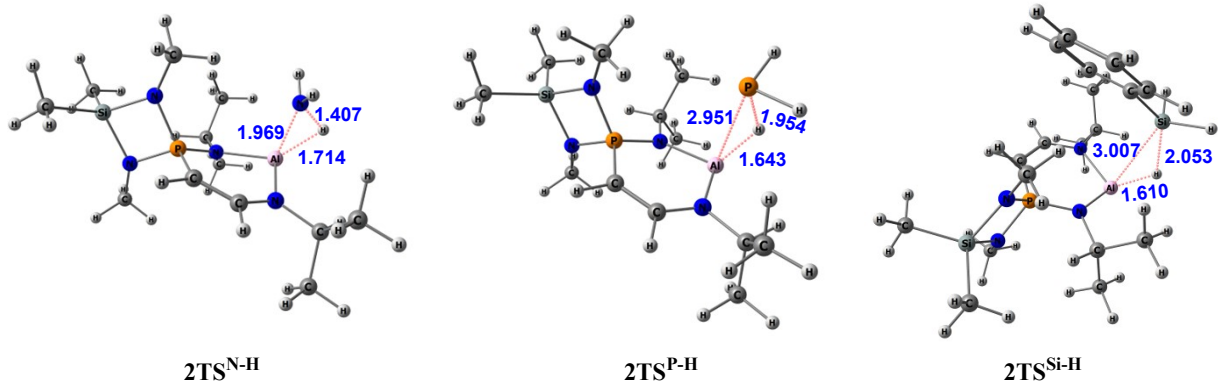
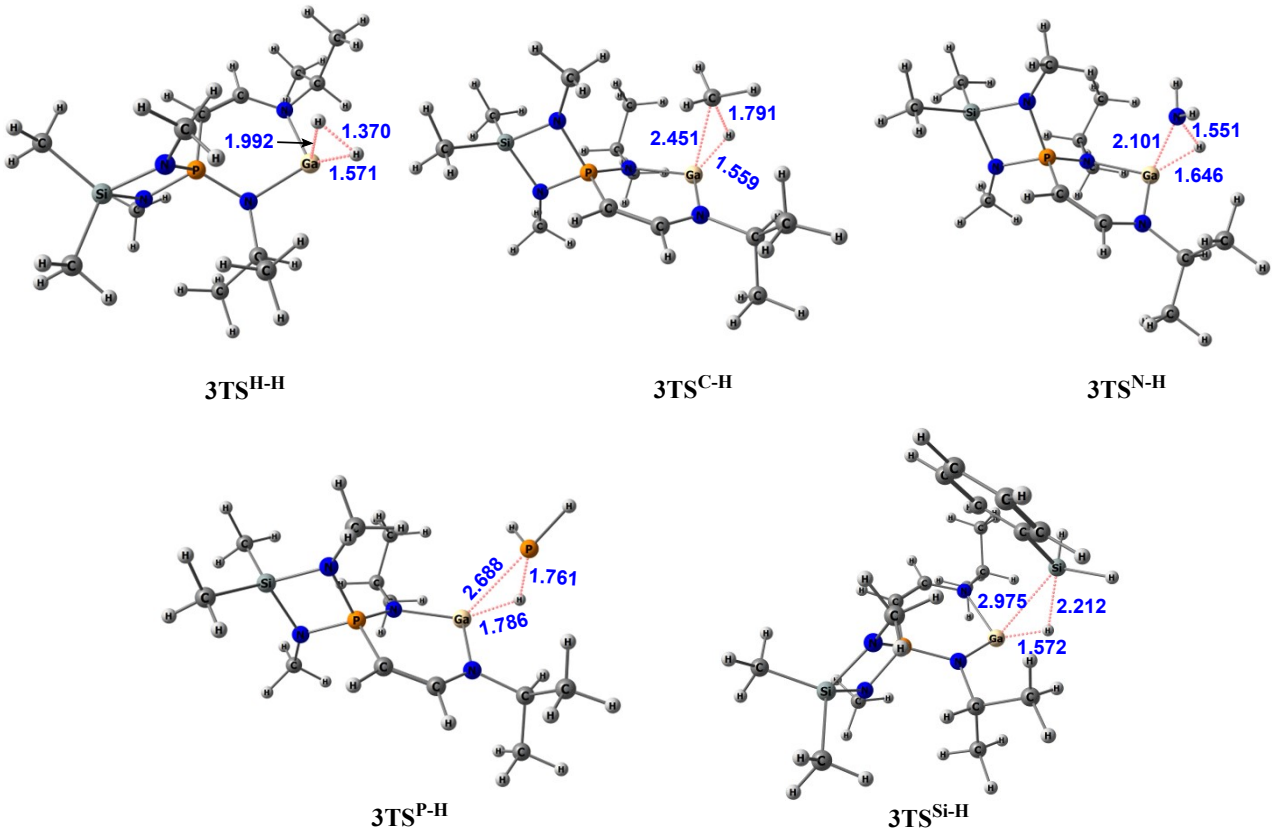


Fig. S4: Pictorial representation of the transition states involved in the activation of X–H (X = N, P and Si) bonds by **2**. The bond lengths are given in Å.



3TS^{H-H} **3TS^{C-H}** **3TS^{N-H}**

3TS^{P-H} **3TS^{Si-H}**

Fig. S5: Pictorial representation of the transition states involved in the activation of X–H (X = H, C, N, P and Si) bonds by **3**. The bond lengths are given in Å.

Cartesian coordinates of the optimized geometries of the proposed intramolecular base stabilized group 13 carbenoids **1**, **2** and **3** and the experimentally known boron carbenoid **I**, aluminium carbenoid **II** and gallium carbenoid **III** in both singlet (s) and triplet (t) spin states along with their total energies (in hartrees) including zero point vibrational correction.

1_s (TE = -1348.253681)

6	-0.796729000	-1.488926000	-0.810150000
6	-2.124170000	-1.256236000	-0.626896000
1	-0.455751000	-2.408276000	-1.267317000
1	-2.818826000	-2.021122000	-0.979318000
7	-2.660477000	-0.163494000	-0.061000000
15	0.368773000	-0.344384000	-0.281611000
5	-1.955420000	1.112650000	0.234565000
7	1.363961000	-0.840933000	0.959492000
7	1.725205000	-0.206907000	-1.230497000

14	2.833927000	-0.708540000	0.031443000
6	1.821387000	0.508038000	-2.480234000
1	0.822091000	0.752628000	-2.850658000
1	2.371814000	1.449140000	-2.367567000
1	2.319424000	-0.090785000	-3.245626000
6	3.702263000	-2.313764000	-0.274532000
1	4.165137000	-2.683655000	0.643484000
1	2.999653000	-3.067945000	-0.633231000
1	4.495044000	-2.198330000	-1.016844000
6	4.018789000	0.612616000	0.562427000
1	4.625195000	0.281082000	1.408071000
1	4.704668000	0.858428000	-0.252620000
1	3.492955000	1.523972000	0.854217000
6	0.898020000	-1.372708000	2.216528000
1	1.566784000	-1.086218000	3.030592000
1	-0.091810000	-0.965033000	2.451491000
1	0.815246000	-2.463899000	2.205212000
6	-4.114496000	-0.196415000	0.195806000
6	-4.493379000	-1.334299000	1.120266000
6	-4.909865000	-0.196710000	-1.090943000
1	-4.290537000	0.752593000	0.711390000
1	-3.889006000	-1.305822000	2.030408000
1	-5.544751000	-1.254058000	1.404192000
1	-4.356624000	-2.313053000	0.649995000
1	-4.630175000	0.661928000	-1.705479000
1	-4.741195000	-1.107816000	-1.674021000
1	-5.979626000	-0.137155000	-0.879125000
7	-0.485008000	1.014656000	0.022349000
6	0.344777000	2.226610000	0.293779000
6	0.379545000	2.541912000	1.772786000
6	-0.126591000	3.401356000	-0.532827000
1	1.368053000	1.988856000	-0.026495000
1	0.774229000	1.696859000	2.343541000
1	1.014414000	3.411805000	1.960990000
1	-0.632202000	2.754008000	2.124926000
1	-0.122501000	3.157873000	-1.598282000
1	-1.146839000	3.666533000	-0.251824000
1	0.532591000	4.257424000	-0.367443000

1_t (TE = -1348.230235)

6	-0.777284000	-1.690805000	-0.410360000
6	-2.180646000	-1.474938000	-0.406486000
1	-0.393017000	-2.688097000	-0.590347000
1	-2.874786000	-2.281105000	-0.598397000

7	-2.700859000	-0.231843000	-0.057418000
15	0.377060000	-0.501844000	-0.167458000
5	-1.893866000	0.879126000	0.182001000
7	1.552899000	-0.769229000	1.001954000
7	1.650774000	-0.261970000	-1.240714000
14	2.906488000	-0.530142000	-0.066573000
6	1.523685000	0.324176000	-2.548401000
1	0.495111000	0.213338000	-2.905759000
1	1.765158000	1.394674000	-2.552514000
1	2.174573000	-0.171766000	-3.272016000
6	3.936624000	-2.053202000	-0.304756000
1	4.492681000	-2.286851000	0.606917000
1	3.304256000	-2.908263000	-0.550086000
1	4.666684000	-1.921175000	-1.106280000
6	3.992574000	0.941024000	0.262196000
1	4.746046000	0.711311000	1.018911000
1	4.524384000	1.232061000	-0.647848000
1	3.414407000	1.800597000	0.606635000
6	1.341210000	-1.371810000	2.291956000
1	1.395568000	-0.640652000	3.105108000
1	0.351700000	-1.838780000	2.324612000
1	2.084020000	-2.150828000	2.488533000
6	-4.155746000	-0.095613000	0.084893000
6	-4.690441000	-0.950963000	1.216201000
6	-4.875017000	-0.364390000	-1.221945000
1	-4.302969000	0.959666000	0.349613000
1	-4.154018000	-0.739580000	2.143375000
1	-5.751895000	-0.748500000	1.375246000
1	-4.583120000	-2.015905000	0.996085000
1	-4.462276000	0.251939000	-2.022987000
1	-4.788691000	-1.412200000	-1.519750000
1	-5.938155000	-0.135200000	-1.120811000
7	-0.460589000	0.928724000	0.023617000
6	0.262441000	2.188051000	0.245490000
6	0.336509000	2.512521000	1.723913000
6	-0.381554000	3.311834000	-0.539360000
1	1.280288000	2.046762000	-0.138768000
1	0.825634000	1.707484000	2.277171000
1	0.888714000	3.439439000	1.897469000
1	-0.676913000	2.633813000	2.120948000
1	-0.431395000	3.068134000	-1.602842000
1	-1.403375000	3.480578000	-0.183378000
1	0.184282000	4.238035000	-0.417075000

2_s (TE = -1565.917698)

7	-2.766844000	-0.249011000	0.042602000
6	-2.087420000	-1.346420000	0.354190000
6	-0.732231000	-1.498192000	0.455712000
1	-2.669091000	-2.251884000	0.555644000
1	-0.334325000	-2.475496000	0.707207000
13	-2.130627000	1.545667000	-0.273201000
6	0.723087000	2.270244000	-0.175053000
1	1.716850000	1.935392000	0.154904000
6	0.836675000	2.666109000	-1.634807000
1	1.573504000	3.463991000	-1.761855000
1	1.143580000	1.812903000	-2.244417000
1	-0.125188000	3.027738000	-2.009884000
6	0.350469000	3.452260000	0.698560000
1	0.267756000	3.153213000	1.745977000
1	1.111955000	4.232257000	0.618956000
1	-0.608571000	3.880003000	0.394952000
6	-4.231145000	-0.373702000	-0.035452000
1	-4.581470000	0.631502000	-0.314342000
6	-4.851464000	-0.712407000	1.305530000
1	-4.551172000	0.017511000	2.060785000
1	-5.941801000	-0.709690000	1.237601000
1	-4.545294000	-1.704207000	1.651621000
6	-4.667328000	-1.326168000	-1.131120000
1	-5.754557000	-1.318713000	-1.237062000
1	-4.225721000	-1.037285000	-2.087570000
1	-4.364608000	-2.355067000	-0.914802000
15	0.464925000	-0.294006000	0.166845000
7	1.753976000	-0.370454000	1.227711000
7	1.540221000	-0.732875000	-1.044462000
14	2.905057000	-0.892626000	0.025074000
6	3.507904000	-2.637556000	0.186797000
1	4.003140000	-2.958697000	-0.733201000
1	4.227447000	-2.744902000	1.001003000
1	2.668863000	-3.310925000	0.375822000
6	4.311249000	0.286841000	-0.235471000
1	3.946626000	1.292000000	-0.456863000
1	4.936868000	0.338593000	0.659597000
1	4.949880000	-0.035677000	-1.060565000
6	1.806900000	0.222910000	2.539775000
1	0.810959000	0.559835000	2.840312000
1	2.151983000	-0.490436000	3.291920000
1	2.471220000	1.095030000	2.565293000
6	1.139357000	-1.268192000	-2.321600000
1	1.878165000	-1.031904000	-3.090220000
1	1.000597000	-2.355321000	-2.299023000

1	0.189960000	-0.821238000	-2.635826000
7	-0.231695000	1.146668000	0.008373000

2_t (TE = -1565.852723)

7	-2.603708000	-0.905023000	-0.013502000
6	-1.814038000	-1.641833000	0.774275000
6	-0.431891000	-1.620735000	0.810333000
1	-2.321144000	-2.358668000	1.425740000
1	0.071920000	-2.418413000	1.349707000
13	-1.806814000	0.253307000	-1.245277000
6	-0.066280000	2.189449000	0.161005000
1	0.949717000	2.243329000	0.575238000
6	-0.186675000	3.226365000	-0.934533000
1	-0.036023000	4.234373000	-0.541092000
1	0.544359000	3.042704000	-1.725966000
1	-1.187530000	3.181048000	-1.381751000
6	-1.064067000	2.437844000	1.275020000
1	-0.974256000	1.675861000	2.055148000
1	-0.925088000	3.422800000	1.727645000
1	-2.084381000	2.385594000	0.874088000
6	-4.046107000	-1.003054000	0.191842000
1	-4.257146000	-2.000882000	0.604244000
6	-4.780605000	-0.861968000	-1.123756000
1	-4.459683000	-1.619269000	-1.841699000
1	-5.859202000	-0.950218000	-0.978406000
1	-4.585824000	0.127464000	-1.559071000
6	-4.511190000	0.042175000	1.188947000
1	-5.580358000	-0.052061000	1.394778000
1	-3.965863000	-0.050017000	2.131505000
1	-4.323643000	1.043380000	0.784983000
15	0.603056000	-0.440579000	0.102159000
7	1.871559000	-0.031752000	1.124566000
7	1.764808000	-0.962416000	-0.997485000
14	3.109307000	-0.395053000	-0.043888000
6	4.324008000	-1.665215000	0.541332000
1	4.973391000	-1.997253000	-0.271405000
1	4.965585000	-1.251803000	1.323913000
1	3.803569000	-2.534989000	0.945690000
6	3.958832000	1.059179000	-0.824633000
1	3.215468000	1.800838000	-1.129268000
1	4.668638000	1.538340000	-0.147413000
1	4.511331000	0.748807000	-1.715696000
6	1.807863000	0.217422000	2.540583000
1	0.896802000	-0.217844000	2.963136000

1	2.659084000	-0.238842000	3.053837000
1	1.806545000	1.287482000	2.776327000
6	1.554727000	-1.003814000	-2.424188000
1	1.355582000	-0.008832000	-2.845960000
1	2.436810000	-1.415248000	-2.920801000
1	0.696703000	-1.639578000	-2.667162000
7	-0.254144000	0.843968000	-0.406007000

3_s (TE = -3248.307304)

6	-1.779931000	-1.637964000	0.340562000
6	-0.411794000	-1.674686000	0.430816000
7	-2.561704000	-0.616684000	0.035082000
1	-2.271263000	-2.595662000	0.550441000
1	0.059455000	-2.621652000	0.673963000
31	-2.091231000	1.358816000	-0.221416000
7	-0.044552000	1.009923000	0.049078000
15	0.710336000	-0.396263000	0.164214000
7	2.007479000	-0.421152000	1.229013000
7	1.816341000	-0.785195000	-1.045359000
14	3.186100000	-0.851177000	0.022329000
6	2.032519000	0.190287000	2.532686000
1	2.296372000	-0.525458000	3.315616000
1	2.746945000	1.021232000	2.575776000
1	1.046052000	0.595341000	2.776103000
6	1.474584000	-1.325979000	-2.335640000
1	1.414715000	-0.550811000	-3.106800000
1	2.216674000	-2.061429000	-2.657466000
1	0.504977000	-1.834312000	-2.296129000
6	4.512873000	0.424796000	-0.213989000
1	5.181977000	0.152248000	-1.032989000
1	4.083694000	1.404613000	-0.433736000
1	5.122841000	0.513473000	0.689165000
6	3.919004000	-2.549581000	0.152439000
1	4.408392000	-2.830449000	-0.783951000
1	4.670151000	-2.606027000	0.942964000
1	3.137813000	-3.283039000	0.362882000
6	0.824444000	2.191221000	-0.112267000
6	0.369286000	3.327538000	0.784148000
1	0.312300000	3.001573000	1.825197000
1	1.067827000	4.165651000	0.720865000
1	-0.619187000	3.690936000	0.490544000
6	0.900571000	2.624948000	-1.564482000
1	-0.089238000	2.915851000	-1.928956000
1	1.570690000	3.480940000	-1.682985000

1	1.268250000	1.809574000	-2.191883000
1	1.844974000	1.929206000	0.206764000
6	-4.007360000	-0.858537000	-0.002204000
1	-4.447608000	0.094525000	-0.332442000
6	-4.400677000	-1.912544000	-1.020441000
1	-5.487888000	-1.972573000	-1.109503000
1	-3.986926000	-1.674478000	-2.002441000
1	-4.040934000	-2.904745000	-0.733023000
6	-4.570755000	-1.160918000	1.373896000
1	-4.315432000	-0.363245000	2.075308000
1	-5.658883000	-1.254993000	1.338470000
1	-4.168574000	-2.098886000	1.768481000

3_t (TE = -3248.212392)

6	-1.907185000	-1.482008000	0.637999000
6	-0.532718000	-1.596201000	0.637941000
7	-2.621791000	-0.450312000	0.193922000
1	-2.463671000	-2.340932000	1.018548000
1	-0.102739000	-2.546538000	0.941867000
31	-1.697927000	0.945246000	-0.777647000
7	-0.031864000	1.060484000	0.265098000
15	0.655455000	-0.407437000	0.241945000
7	2.000501000	-0.480714000	1.239951000
7	1.679904000	-0.796367000	-1.024550000
14	3.116341000	-0.856482000	-0.043359000
6	2.079594000	0.007123000	2.592675000
1	2.371160000	-0.779027000	3.294270000
1	2.800565000	0.827963000	2.684280000
1	1.105709000	0.388701000	2.912625000
6	1.291026000	-1.230940000	-2.342065000
1	1.111143000	-0.386340000	-3.016061000
1	2.073248000	-1.859107000	-2.778839000
1	0.364438000	-1.813481000	-2.297685000
6	4.385216000	0.469816000	-0.315935000
1	4.977078000	0.283066000	-1.214449000
1	3.909188000	1.447937000	-0.414501000
1	5.078580000	0.511656000	0.528569000
6	3.902455000	-2.534221000	0.004926000
1	4.336898000	-2.782328000	-0.967024000
1	4.705566000	-2.581523000	0.743399000
1	3.158521000	-3.294696000	0.249974000
6	0.771119000	2.279727000	0.246107000
6	0.085517000	3.341857000	1.079463000
1	-0.027088000	3.009737000	2.113362000

1	0.649699000	4.277147000	1.068265000
1	-0.915252000	3.536054000	0.676131000
6	1.030989000	2.764878000	-1.169707000
1	0.084076000	3.050002000	-1.643715000
1	1.687214000	3.639023000	-1.173334000
1	1.490070000	1.979672000	-1.775756000
1	1.744770000	2.053226000	0.707558000
6	-4.081056000	-0.559042000	0.115803000
1	-4.413759000	0.407628000	-0.284895000
6	-4.525331000	-1.643725000	-0.848474000
1	-5.609948000	-1.623897000	-0.977538000
1	-4.056146000	-1.502216000	-1.824761000
1	-4.253214000	-2.637246000	-0.481313000
6	-4.703039000	-0.729310000	1.488265000
1	-4.375468000	0.063744000	2.162470000
1	-5.792675000	-0.697769000	1.417845000
1	-4.429591000	-1.690141000	1.932668000

I_s (TE = -599.083716)

6	0.834618000	1.166831000	-0.342662000
6	2.293404000	0.876497000	-0.004179000
6	2.379670000	-0.637482000	0.266622000
6	0.961418000	-1.104334000	0.495275000
7	0.188786000	-0.103407000	0.170585000
1	2.575265000	1.429189000	0.897391000
1	2.963702000	1.200940000	-0.804880000
6	-1.236791000	-0.235080000	0.151517000
6	-2.004977000	0.273158000	1.185630000
6	-3.381624000	0.128550000	1.153388000
6	-3.989382000	-0.520164000	0.091353000
6	-3.216539000	-1.035592000	-0.936528000
6	-1.840506000	-0.894623000	-0.906737000
1	-1.518129000	0.761619000	2.021623000
1	-3.981240000	0.518282000	1.967552000
1	-5.066839000	-0.633236000	0.069584000
1	-3.686360000	-1.556471000	-1.762477000
1	-1.215760000	-1.307445000	-1.691695000
6	3.239880000	-0.949045000	1.479209000
1	3.270124000	-2.024951000	1.663527000
1	4.263356000	-0.593547000	1.323717000
1	2.844945000	-0.464156000	2.375897000
6	2.908001000	-1.410623000	-0.939393000
1	3.937736000	-1.109290000	-1.153320000
1	2.893555000	-2.484343000	-0.741454000

1	2.309151000	-1.229420000	-1.835794000
6	0.308595000	2.389592000	0.380166000
1	-0.745406000	2.572982000	0.159751000
1	0.429789000	2.290229000	1.461391000
1	0.873658000	3.267324000	0.056795000
6	0.576289000	1.296898000	-1.833543000
1	1.075958000	2.189792000	-2.216444000
1	0.954327000	0.432622000	-2.383527000
1	-0.491661000	1.396222000	-2.042454000

I_t (TE = -599.015730)

6	-0.889817000	1.254266000	-0.064810000
6	-2.335149000	0.735410000	-0.242712000
6	-2.353019000	-0.791128000	-0.002800000
6	-0.940796000	-1.055301000	-0.366854000
7	-0.091811000	-0.002964000	-0.178704000
1	-2.657346000	0.922318000	-1.270706000
1	-3.025320000	1.262583000	0.423229000
6	1.276609000	-0.161682000	-0.091640000
6	2.183824000	0.895246000	0.055571000
6	3.540976000	0.646293000	0.136326000
6	4.043209000	-0.643696000	0.069925000
6	3.151272000	-1.694972000	-0.084267000
6	1.794607000	-1.465149000	-0.168445000
1	1.840781000	1.917976000	0.111218000
1	4.217993000	1.485302000	0.253340000
1	5.108841000	-0.826120000	0.131932000
1	3.518037000	-2.713805000	-0.144164000
1	1.103672000	-2.292689000	-0.297138000
6	-3.355000000	-1.484307000	-0.908176000
1	-3.319113000	-2.567146000	-0.768743000
1	-4.371322000	-1.150839000	-0.678981000
1	-3.146627000	-1.268236000	-1.958108000
6	-2.653303000	-1.144741000	1.454349000
1	-3.656427000	-0.805365000	1.732715000
1	-2.608365000	-2.226409000	1.598440000
1	-1.934975000	-0.688611000	2.137651000
6	-0.568218000	2.232379000	-1.182224000
1	0.411965000	2.696829000	-1.077817000
1	-0.608911000	1.725426000	-2.148897000
1	-1.314990000	3.030953000	-1.184744000
6	-0.709623000	1.896418000	1.302180000
1	-1.355445000	2.775401000	1.370829000
1	-0.988657000	1.209113000	2.102029000

1	0.315445000	2.219850000	1.480309000

II_s (TE = -1009.409541)

7	1.387059000	-0.292958000	0.000000000
6	1.245034000	-1.614172000	-0.000002000
6	0.000000000	-2.238665000	-0.000003000
6	-1.245034000	-1.614172000	-0.000003000
7	-1.387059000	-0.292958000	-0.000001000
1	0.000000000	-3.320138000	-0.000004000
13	0.000000000	1.111552000	0.000002000
6	2.702341000	0.255494000	-0.000001000
6	3.330391000	0.562599000	1.199493000
6	3.330385000	0.562610000	-1.199495000
6	4.586112000	1.145328000	1.197834000
1	2.819561000	0.341444000	2.131052000
6	4.586106000	1.145339000	-1.197837000
1	2.819550000	0.341463000	-2.131054000
6	5.218883000	1.434383000	-0.000002000
1	5.069227000	1.381386000	2.138856000
1	5.069217000	1.381405000	-2.138859000
1	6.199541000	1.895077000	-0.000002000
6	-2.702341000	0.255494000	0.000002000
6	-3.330386000	0.562604000	1.199496000
6	-3.330389000	0.562605000	-1.199491000
6	-4.586107000	1.145333000	1.197840000
1	-2.819553000	0.341452000	2.131055000
6	-4.586111000	1.145334000	-1.197831000
1	-2.819559000	0.341455000	-2.131051000
6	-5.218883000	1.434383000	0.000006000
1	-5.069219000	1.381394000	2.138863000
1	-5.069225000	1.381397000	-2.138852000
1	-6.199541000	1.895077000	0.000007000
6	2.456287000	-2.492855000	-0.000006000
1	3.078761000	-2.293351000	-0.875096000
1	3.078767000	-2.293353000	0.875078000
1	2.178287000	-3.544749000	-0.000006000
6	-2.456287000	-2.492855000	0.000000000
1	-3.078760000	-2.293355000	0.875091000
1	-3.078768000	-2.293349000	-0.875083000
1	-2.178287000	-3.544749000	-0.000005000

II_t (TE= -1009.306275)

7	1.421517000	-0.275169000	-0.000008000
6	1.291221000	-1.631984000	-0.000006000
6	0.000000000	-2.210016000	-0.000004000
6	-1.291221000	-1.631984000	-0.000003000
7	-1.421517000	-0.275169000	-0.000004000
1	0.000000000	-3.297110000	-0.000002000
13	0.000000000	1.120239000	-0.000037000
6	2.729876000	0.267692000	-0.000002000
6	3.361947000	0.568781000	1.200320000
6	3.361952000	0.568798000	-1.200317000
6	4.620254000	1.145737000	1.197769000
1	2.851546000	0.346114000	2.131604000
6	4.620259000	1.145755000	-1.197752000
1	2.851556000	0.346145000	-2.131607000
6	5.253907000	1.432896000	0.000012000
1	5.105199000	1.378013000	2.138856000
1	5.105209000	1.378045000	-2.138834000
1	6.236689000	1.889002000	0.000018000
6	-2.729876000	0.267691000	0.000002000
6	-3.361940000	0.568795000	1.200325000
6	-3.361959000	0.568784000	-1.200313000
6	-4.620247000	1.145751000	1.197773000
1	-2.851534000	0.346140000	2.131608000
6	-4.620266000	1.145740000	-1.197747000
1	-2.851568000	0.346119000	-2.131603000
6	-5.253907000	1.432896000	0.000017000
1	-5.105187000	1.378039000	2.138861000
1	-5.105221000	1.378019000	-2.138829000
1	-6.236689000	1.889002000	0.000022000
6	2.488659000	-2.520704000	-0.000003000
1	3.125512000	-2.353485000	-0.875750000
1	3.125511000	-2.353481000	0.875743000
1	2.190232000	-3.568943000	-0.000001000
6	-2.488659000	-2.520704000	0.000006000
1	-3.125506000	-2.353481000	0.875756000
1	-3.125517000	-2.353485000	-0.875737000
1	-2.190232000	-3.568943000	0.000007000

III_s (TE = -2691.803457)

7	1.429727000	0.439595000	-0.043843000
6	1.254896000	1.750016000	-0.103683000
6	-0.000001000	2.360103000	-0.138875000
6	-1.254890000	1.750010000	-0.103536000
7	-1.429711000	0.439587000	-0.043734000

1	-0.000008000	3.440031000	-0.203275000
6	2.737761000	-0.098537000	0.009156000
6	3.319189000	-0.624270000	-1.139055000
6	3.416156000	-0.198567000	1.219024000
6	4.570337000	-1.214864000	-1.081913000
1	2.775613000	-0.560675000	-2.076172000
6	4.666659000	-0.788668000	1.272283000
1	2.946017000	0.190506000	2.116544000
6	5.250107000	-1.295535000	0.121969000
1	5.014053000	-1.618684000	-1.984701000
1	5.185988000	-0.859540000	2.221170000
1	6.227383000	-1.761218000	0.166340000
6	-2.737753000	-0.098539000	0.009244000
6	-3.319571000	-0.623385000	-1.139174000
6	-3.415761000	-0.199426000	1.219253000
6	-4.570731000	-1.213953000	-1.082069000
1	-2.776281000	-0.559132000	-2.076413000
6	-4.666279000	-0.789505000	1.272477000
1	-2.945316000	0.188992000	2.116896000
6	-5.250119000	-1.295483000	0.121973000
1	-5.014758000	-1.617084000	-1.985012000
1	-5.185311000	-0.861049000	2.221475000
1	-6.227405000	-1.761150000	0.166310000
31	0.000003000	-1.096824000	-0.001400000
6	2.451237000	2.653466000	-0.150925000
1	3.026488000	2.583997000	0.774916000
1	3.125183000	2.359612000	-0.958779000
1	2.156418000	3.690686000	-0.297027000
6	-2.451253000	2.653439000	-0.150531000
1	-3.125052000	2.359953000	-0.958643000
1	-3.026656000	2.583463000	0.775180000
1	-2.156465000	3.690744000	-0.296082000

III_t (TE = -2691.716905)

7	1.435827000	0.423160000	-0.190873000
6	1.273015000	1.801817000	-0.135506000
6	0.000095000	2.369970000	-0.122425000
6	-1.272889000	1.801919000	-0.135024000
7	-1.435811000	0.423319000	-0.190779000
1	0.000136000	3.455237000	-0.151175000
6	2.641560000	-0.201635000	0.116525000
6	3.118587000	-1.256513000	-0.667192000
6	3.363516000	0.143855000	1.265648000
6	4.264276000	-1.945069000	-0.310903000

1	2.593938000	-1.509644000	-1.583491000
6	4.512729000	-0.540924000	1.605210000
1	2.984410000	0.926550000	1.911866000
6	4.974732000	-1.589828000	0.822518000
1	4.612453000	-2.757103000	-0.939133000
1	5.047179000	-0.262004000	2.506570000
1	5.877952000	-2.121831000	1.095150000
6	-2.641575000	-0.201502000	0.116532000
6	-3.118870000	-1.255898000	-0.667661000
6	-3.363255000	0.143451000	1.265985000
6	-4.264569000	-1.944516000	-0.311515000
1	-2.594427000	-1.508594000	-1.584197000
6	-4.512482000	-0.541374000	1.605406000
1	-2.983934000	0.925763000	1.912539000
6	-4.974756000	-1.589805000	0.822238000
1	-4.612964000	-2.756172000	-0.940113000
1	-5.046723000	-0.262879000	2.507021000
1	-5.877980000	-2.121855000	1.094765000
31	-0.000075000	-0.609384000	-0.971849000
6	2.473023000	2.686763000	-0.245948000
1	3.043879000	2.778632000	0.683139000
1	3.170689000	2.304517000	-0.998249000
1	2.171649000	3.692290000	-0.540323000
6	-2.472861000	2.687009000	-0.244658000
1	-3.170957000	2.305027000	-0.996692000
1	-3.043222000	2.778722000	0.684748000
1	-2.171519000	3.692574000	-0.538937000

Cartesian coordinates of the optimized geometries of the substrates considered for activation i,e., H_2, NH_3, PH_3 and SIH_3Ph.

H_2

1	0.000000000	0.000000000	0.373453000
1	0.000000000	0.000000000	-0.373453000

CH_4

6	0.000000000	0.000000000	0.000000000
1	0.628267000	0.628267000	0.628267000
1	-0.628267000	-0.628267000	0.628267000
1	-0.628267000	0.628267000	-0.628267000
1	0.628267000	-0.628267000	-0.628267000

NH_3

7	0.000000000	0.000000000	0.113823000
1	0.000000000	0.938252000	-0.265586000
1	-0.812550000	-0.469126000	-0.265586000
1	0.812550000	-0.469126000	-0.265586000

PH_3

15	0.000000000	0.000000000	0.127890000
1	0.000000000	1.192299000	-0.639451000
1	-1.032561000	-0.596150000	-0.639451000
1	1.032561000	-0.596150000	-0.639451000

SiH_3Ph

14	-2.328683000	0.000028000	0.005205000
1	-2.827228000	1.215757000	-0.672763000
1	-2.827726000	-1.206959000	-0.687882000
1	-2.852586000	-0.008841000	1.389067000
6	-0.463633000	0.000150000	-0.011629000
6	0.252994000	-1.195708000	-0.008932000
6	0.253177000	1.195817000	-0.008940000
6	1.637534000	-1.199044000	0.002972000
1	-0.279071000	-2.142852000	-0.021279000
6	1.637789000	1.198888000	0.002970000
1	-0.278704000	2.143046000	-0.021247000
6	2.331434000	-0.000114000	0.009974000
1	2.177663000	-2.138931000	0.003128000
1	2.178040000	2.138704000	0.003119000
1	3.415413000	-0.000248000	0.016496000

Cartesian coordinates of the optimized geometries of the transition states involved in activation of H_2 (**TS$^{H–H}$**), CH_4 (**TS$^{C–H}$**), NH_3 (**TS$^{N–H}$**), PH_3 (**TS$^{P–H}$**) and SiH_3Ph (**TS$^{Si–H}$**) by the proposed carbenoids **1**-**3** and the experimentally known carbenoids **I**-**III**.

1_TS$^{H–H}$

6	0.738868000	-1.509347000	-0.805332000
6	2.088894000	-1.284221000	-0.711999000
1	0.364310000	-2.379211000	-1.329140000

1	2.760729000	-1.981647000	-1.212098000
7	2.646390000	-0.279486000	-0.039610000
15	-0.405938000	-0.367529000	-0.234037000
5	1.883864000	0.884983000	0.481264000
7	-1.723574000	-0.126869000	-1.228264000
7	-1.474313000	-0.874170000	0.942967000
14	-2.897144000	-0.624972000	-0.035924000
6	-1.175389000	-1.621476000	2.142001000
1	-0.209424000	-2.125332000	2.047471000
1	-1.126265000	-0.978580000	3.024776000
1	-1.939989000	-2.384594000	2.314880000
6	-3.812952000	-2.195815000	-0.386388000
1	-4.595289000	-2.045279000	-1.133111000
1	-3.128851000	-2.965135000	-0.749148000
1	-4.295982000	-2.567170000	0.521133000
6	-4.053831000	0.728486000	0.478754000
1	-4.717750000	0.995162000	-0.347892000
1	-4.683676000	0.415304000	1.314113000
1	-3.506010000	1.624020000	0.778914000
6	-1.727142000	0.612302000	-2.465808000
1	-0.700817000	0.794810000	-2.796143000
1	-2.233255000	0.058970000	-3.260020000
1	-2.219833000	1.586097000	-2.360748000
6	4.093517000	-0.312241000	0.219454000
6	4.871241000	0.134107000	-0.999949000
6	4.560859000	-1.657591000	0.740129000
1	4.231155000	0.435143000	1.008447000
1	4.533486000	1.121229000	-1.321710000
1	5.941031000	0.184015000	-0.784423000
1	4.729057000	-0.567243000	-1.828227000
1	3.916938000	-2.001567000	1.552818000
1	4.572821000	-2.423857000	-0.040299000
1	5.580163000	-1.571859000	1.121782000
7	0.457884000	0.980451000	0.075917000
6	-0.276629000	2.248868000	0.283500000
6	0.372054000	3.370272000	-0.497650000
6	-0.402046000	2.575362000	1.757131000
1	-1.288274000	2.100407000	-0.117238000
1	0.395100000	3.140871000	-1.565514000
1	-0.181414000	4.300915000	-0.353540000
1	1.400385000	3.513170000	-0.157778000
1	-0.874647000	1.753689000	2.301485000
1	0.587130000	2.749088000	2.187214000
1	-1.003755000	3.476313000	1.900308000
1	2.113289000	0.966145000	1.868739000
1	1.800027000	0.182046000	2.241999000

2_TS^{H-H}

7	-2.782221000	-0.258291000	0.128090000
6	-2.088579000	-1.359925000	0.386953000
6	-0.729647000	-1.530318000	0.345059000
1	-2.662211000	-2.247909000	0.663270000
1	-0.328357000	-2.516688000	0.553895000
13	-1.967943000	1.294777000	-0.540352000
6	0.703239000	2.304905000	0.060838000
1	1.667681000	2.001122000	0.491455000
6	0.952013000	2.787857000	-1.355445000
1	1.648054000	3.630641000	-1.363974000
1	1.367302000	1.987950000	-1.972702000
1	0.014108000	3.119004000	-1.813664000
6	0.139176000	3.403166000	0.937867000
1	-0.003971000	3.050890000	1.961598000
1	0.812481000	4.263019000	0.956103000
1	-0.829844000	3.741931000	0.556471000
6	-4.250987000	-0.340838000	0.124996000
1	-4.594013000	0.700552000	0.073028000
6	-4.824857000	-0.946791000	1.390559000
1	-4.427571000	-0.449975000	2.277758000
1	-5.911533000	-0.840118000	1.394329000
1	-4.607070000	-2.015220000	1.470342000
6	-4.742167000	-1.051592000	-1.122238000
1	-5.833236000	-1.040372000	-1.177009000
1	-4.343517000	-0.572007000	-2.019025000
1	-4.414272000	-2.095748000	-1.125154000
15	0.489339000	-0.329339000	0.111729000
7	1.740805000	-0.432249000	1.214326000
7	1.599324000	-0.729822000	-1.072442000
14	2.944629000	-0.857483000	0.028795000
6	3.627369000	-2.576454000	0.130869000
1	4.151643000	-2.839136000	-0.791595000
1	4.340998000	-2.676762000	0.951245000
1	2.819912000	-3.295706000	0.282771000
6	4.299287000	0.397280000	-0.137291000
1	3.891918000	1.395993000	-0.307644000
1	4.905502000	0.425479000	0.772161000
1	4.966966000	0.153241000	-0.966281000
6	1.726283000	0.072852000	2.563348000
1	0.719254000	0.405364000	2.829328000
1	2.019518000	-0.693516000	3.285004000
1	2.399101000	0.930167000	2.684323000

6	1.320613000	-1.221911000	-2.401601000
1	2.041704000	-1.995960000	-2.679163000
1	0.319025000	-1.658158000	-2.448744000
1	1.367256000	-0.426262000	-3.150459000
7	-0.191960000	1.131098000	0.074278000
1	-2.205977000	1.568701000	-2.104348000
1	-1.624588000	0.497674000	-2.291079000

3_TS^{H-H}

6	1.877198000	-1.526846000	0.253855000
6	0.510408000	-1.582468000	0.178285000
7	2.663056000	-0.463642000	0.204620000
1	2.376214000	-2.492160000	0.369529000
1	0.045511000	-2.563295000	0.208764000
31	1.939991000	1.283869000	-0.175767000
7	0.073895000	1.101572000	0.371809000
15	-0.657645000	-0.306708000	0.111486000
7	-1.712961000	-0.442831000	-1.181409000
7	-1.959311000	-0.659383000	1.098466000
14	-3.071311000	-0.935153000	-0.213716000
6	-1.386333000	-0.430688000	-2.586339000
1	-0.370304000	-0.801402000	-2.750818000
1	-2.077526000	-1.072019000	-3.139506000
1	-1.439657000	0.576260000	-3.012185000
6	-1.918083000	-0.906824000	2.515711000
1	-2.500824000	-0.168404000	3.075902000
1	-2.303801000	-1.901104000	2.761018000
1	-0.887493000	-0.857666000	2.877994000
6	-4.562313000	0.165068000	-0.267533000
1	-5.097554000	0.037363000	-1.211644000
1	-5.257538000	-0.088910000	0.536508000
1	-4.291335000	1.217350000	-0.168071000
6	-3.568623000	-2.707447000	-0.437310000
1	-4.284031000	-3.016726000	0.328515000
1	-4.046660000	-2.857741000	-1.408607000
1	-2.696090000	-3.361246000	-0.380468000
6	-0.621262000	2.400107000	0.472480000
6	-1.644366000	2.457552000	1.590004000
1	-1.212118000	2.113178000	2.531647000
1	-1.980538000	3.488072000	1.725238000
1	-2.521758000	1.844079000	1.374055000
6	-1.208362000	2.847522000	-0.854071000
1	-2.032383000	2.196069000	-1.158699000
1	-1.591093000	3.868089000	-0.778271000

1	-0.451869000	2.822944000	-1.642063000
1	0.170790000	3.116147000	0.731446000
6	4.119385000	-0.635282000	0.160964000
1	4.533098000	0.357706000	0.376776000
6	4.650520000	-1.586783000	1.215453000
1	5.740889000	-1.537209000	1.241062000
1	4.271081000	-1.328408000	2.205897000
1	4.382867000	-2.625607000	1.005175000
6	4.564258000	-1.033619000	-1.234261000
1	4.200549000	-0.318412000	-1.975294000
1	5.653688000	-1.082402000	-1.301320000
1	4.162834000	-2.018111000	-1.494306000
1	2.263797000	1.962056000	-1.555801000
1	1.637246000	0.872556000	-2.101778000

I_TS^{H-H}

6	-0.845499000	1.213588000	0.349628000
6	-2.310496000	0.853903000	0.058921000
6	-2.353959000	-0.657955000	-0.216907000
6	-0.937703000	-0.975623000	-0.605161000
7	-0.153567000	-0.033166000	-0.100689000
1	-2.642415000	1.384040000	-0.838956000
1	-2.967606000	1.152557000	0.880759000
6	1.259757000	-0.183068000	-0.097428000
6	2.035724000	0.372473000	-1.104613000
6	3.409032000	0.191020000	-1.091026000
6	4.005856000	-0.542323000	-0.079552000
6	3.227538000	-1.106335000	0.919339000
6	1.856013000	-0.929877000	0.908590000
1	1.557916000	0.926184000	-1.903884000
1	4.014595000	0.620591000	-1.880381000
1	5.080611000	-0.680790000	-0.072410000
1	3.690920000	-1.687653000	1.707776000
1	1.224480000	-1.369729000	1.673970000
6	-3.394738000	-1.043907000	-1.247397000
1	-3.310758000	-2.104457000	-1.499051000
1	-4.399398000	-0.871284000	-0.851305000
1	-3.277172000	-0.468454000	-2.166962000
6	-2.620537000	-1.448790000	1.069141000
1	-3.595540000	-1.171347000	1.479162000
1	-2.623719000	-2.521828000	0.865545000
1	-1.862488000	-1.256519000	1.831959000
6	-0.403049000	2.404730000	-0.478986000
1	0.636027000	2.675949000	-0.278549000

1	-0.517275000	2.194533000	-1.546263000
1	-1.028317000	3.267906000	-0.237261000
6	-0.559298000	1.463641000	1.818387000
1	-1.066545000	2.373176000	2.147811000
1	-0.904126000	0.636422000	2.442392000
1	0.512291000	1.597677000	1.987819000
1	-0.706173000	-1.394623000	-1.720562000
1	-0.952180000	-0.739048000	-2.534398000

II_TS^{H-H}

13	0.913326000	-0.191605000	0.000000000
7	-0.340571000	-0.190379000	1.414830000
7	-0.340571000	-0.190379000	-1.414830000
6	-1.654844000	-0.115984000	1.253829000
6	-1.654844000	-0.115984000	-1.253829000
6	-2.270999000	-0.106653000	0.000000000
1	-3.352183000	-0.084630000	0.000000000
6	0.245901000	-0.068490000	2.707473000
6	0.364459000	1.182286000	3.297944000
6	0.767473000	-1.187343000	3.342242000
6	0.976561000	1.306086000	4.533508000
6	1.377096000	-1.057938000	4.578195000
6	1.480469000	0.187454000	5.176638000
1	1.066207000	2.283759000	4.992385000
1	1.777194000	-1.934633000	5.073789000
1	1.961815000	0.287160000	6.142247000
6	0.245901000	-0.068490000	-2.707473000
6	0.767473000	-1.187343000	-3.342242000
6	0.364459000	1.182286000	-3.297944000
6	1.377096000	-1.057938000	-4.578195000
6	0.976561000	1.306086000	-4.533508000
6	1.480469000	0.187454000	-5.176638000
1	1.777194000	-1.934633000	-5.073789000
1	1.066207000	2.283759000	-4.992385000
1	1.961815000	0.287160000	-6.142247000
6	-2.537104000	-0.052361000	-2.458331000
1	-3.576454000	-0.225588000	-2.187639000
1	-2.466215000	0.928398000	-2.934072000
1	-2.232076000	-0.787295000	-3.205708000
6	-2.537104000	-0.052361000	2.458331000
1	-3.576454000	-0.225588000	2.187639000
1	-2.232076000	-0.787295000	3.205708000
1	-2.466215000	0.928398000	2.934072000
1	-0.015834000	2.050880000	-2.769794000

1	0.685868000	-2.154440000	-2.857340000
1	0.685868000	-2.154440000	2.857340000
1	-0.015834000	2.050880000	2.769794000
1	1.155881000	1.765389000	0.000000000
1	2.075897000	0.894333000	0.000000000

III_TS^{H-H}

7	1.453041000	0.430215000	0.029813000
6	1.261379000	1.736129000	-0.088746000
6	0.004267000	2.343781000	-0.088696000
6	-1.257961000	1.750386000	0.016310000
7	-1.447339000	0.447832000	0.126304000
1	0.006892000	3.421903000	-0.174335000
6	2.754347000	-0.139010000	0.026352000
6	3.153764000	-0.894276000	-1.068189000
6	3.595143000	-0.018675000	1.125118000
6	4.398542000	-1.500193000	-1.073654000
1	2.475720000	-0.992716000	-1.911296000
6	4.838880000	-0.624725000	1.113333000
1	3.260365000	0.543601000	1.990310000
6	5.245354000	-1.363826000	0.013684000
1	4.706404000	-2.084399000	-1.932984000
1	5.490990000	-0.527018000	1.973500000
1	6.218005000	-1.841208000	0.009321000
6	-2.745720000	-0.126758000	0.097778000
6	-3.443286000	-0.213098000	-1.099949000
6	-3.284367000	-0.675576000	1.253532000
6	-4.688993000	-0.815493000	-1.130321000
1	-2.989287000	0.182918000	-2.002538000
6	-4.530604000	-1.276924000	1.217211000
1	-2.716425000	-0.620562000	2.176230000
6	-5.236479000	-1.345068000	0.027087000
1	-5.231027000	-0.879216000	-2.066634000
1	-4.950184000	-1.697593000	2.123529000
1	-6.210288000	-1.819377000	-0.000467000
31	-0.007680000	-0.863309000	0.057541000
6	2.449837000	2.633704000	-0.239791000
1	3.010962000	2.702832000	0.694213000
1	3.136598000	2.243380000	-0.993256000
1	2.140320000	3.636441000	-0.525915000
6	-2.446015000	2.660053000	0.006806000
1	-2.959029000	2.611566000	-0.956281000
1	-3.171248000	2.364793000	0.767020000
1	-2.145191000	3.691264000	0.179604000

1	-0.112546000	-2.049362000	-0.945960000
1	-0.171408000	-1.053592000	-1.927832000

1_TS$^{C–H}$

6	0.593797000	-1.576357000	-0.874736000
6	1.947541000	-1.355916000	-0.836478000
1	0.201001000	-2.487514000	-1.306321000
1	2.594605000	-2.108269000	-1.287602000
7	2.541739000	-0.294906000	-0.295348000
15	-0.521249000	-0.395370000	-0.332442000
5	1.828298000	0.915636000	0.187259000
7	-1.872798000	-0.181528000	-1.281624000
7	-1.546534000	-0.848077000	0.903574000
14	-3.004611000	-0.620067000	-0.023223000
6	-1.170742000	-1.493330000	2.137452000
1	-0.388467000	-2.240250000	1.967737000
1	-0.792559000	-0.778997000	2.876301000
1	-2.032486000	-2.005985000	2.569521000
6	-3.958594000	-2.184274000	-0.286060000
1	-4.789061000	-2.036990000	-0.979497000
1	-3.309969000	-2.968819000	-0.679389000
1	-4.381379000	-2.532394000	0.660167000
6	-4.119696000	0.766628000	0.495027000
1	-4.791545000	1.040320000	-0.322954000
1	-4.742626000	0.475930000	1.343671000
1	-3.546777000	1.652023000	0.778042000
6	-1.920626000	0.519827000	-2.540481000
1	-2.405605000	1.498371000	-2.445017000
1	-0.906901000	0.687873000	-2.914876000
1	-2.458392000	-0.054910000	-3.297651000
6	4.009638000	-0.300744000	-0.166449000
6	4.669080000	-0.041211000	-1.504231000
6	4.532600000	-1.558079000	0.498387000
1	4.214780000	0.552980000	0.486908000
1	4.298174000	0.892424000	-1.932626000
1	5.753235000	0.033597000	-1.393947000
1	4.461277000	-0.852183000	-2.209344000
1	3.995280000	-1.759318000	1.427958000
1	4.444416000	-2.436287000	-0.147411000
1	5.591941000	-1.437040000	0.733619000
7	0.367334000	0.950900000	-0.086021000
6	-0.374172000	2.218561000	0.119386000
6	0.183516000	3.311374000	-0.766721000
6	-0.398309000	2.620078000	1.578726000

1	-1.410507000	2.035604000	-0.194535000
1	0.146408000	3.016634000	-1.818204000
1	-0.396405000	4.228823000	-0.641834000
1	1.225209000	3.510552000	-0.506693000
1	-0.819934000	1.822990000	2.197437000
1	0.613402000	2.827922000	1.932320000
1	-1.004836000	3.519146000	1.713777000
1	2.235409000	1.204563000	1.450672000
6	2.080966000	0.290237000	2.578024000
1	3.100503000	0.167534000	2.946775000
1	1.462110000	0.835661000	3.291930000
1	1.641005000	-0.677802000	2.332691000

2_TS$^{C–H}$

7	2.677407000	-0.376054000	-0.268352000
6	1.954776000	-1.469074000	-0.441699000
6	0.586820000	-1.596846000	-0.395929000
1	2.501367000	-2.395471000	-0.637088000
1	0.159596000	-2.585935000	-0.525285000
13	1.960646000	1.315977000	0.132062000
6	-0.781121000	2.263223000	-0.209297000
1	-1.784688000	1.926225000	-0.502681000
6	-0.882365000	2.870175000	1.176046000
1	-1.586649000	3.706097000	1.181878000
1	-1.220720000	2.126381000	1.901890000
1	0.092070000	3.247490000	1.501584000
6	-0.333034000	3.280737000	-1.238740000
1	-0.282337000	2.831816000	-2.233213000
1	-1.030896000	4.120751000	-1.270946000
1	0.659372000	3.670425000	-0.993129000
6	4.143712000	-0.490326000	-0.284151000
1	4.506005000	0.496461000	0.037578000
6	4.664867000	-0.738998000	-1.685065000
1	4.319533000	0.042073000	-2.366183000
1	5.757070000	-0.752168000	-1.698683000
1	4.313635000	-1.702925000	-2.065751000
6	4.659585000	-1.511427000	0.711672000
1	5.747098000	-1.447181000	0.787259000
1	4.233166000	-1.335296000	1.701717000
1	4.414910000	-2.534061000	0.411565000
15	-0.595269000	-0.360410000	-0.195096000
7	-1.894617000	-0.487552000	-1.236332000
7	-1.665150000	-0.679430000	1.054169000
14	-3.051024000	-0.859014000	0.014788000

6	-3.735418000	-2.580333000	0.010951000
1	-4.193569000	-2.810461000	0.976584000
1	-4.502873000	-2.711037000	-0.754581000
1	-2.937273000	-3.303519000	-0.169070000
6	-4.398785000	0.401188000	0.192120000
1	-3.986895000	1.404554000	0.318317000
1	-5.040135000	0.402175000	-0.693294000
1	-5.033311000	0.180762000	1.053296000
6	-1.934032000	-0.031794000	-2.602635000
1	-0.933199000	0.263696000	-2.929372000
1	-2.281640000	-0.815479000	-3.279911000
1	-2.590072000	0.838609000	-2.721818000
6	-1.305942000	-1.123794000	2.379009000
1	-0.857604000	-0.316908000	2.968026000
1	-2.194390000	-1.471745000	2.909370000
1	-0.586419000	-1.949537000	2.348268000
7	0.115374000	1.086061000	-0.213029000
1	2.501327000	2.001033000	1.464944000
6	1.963648000	0.807041000	2.481815000
1	2.920201000	0.726209000	2.999717000
1	1.256175000	1.388480000	3.075362000
1	1.568755000	-0.196670000	2.286486000

3_TS^{C-H}

7	2.491478000	-0.645734000	-0.281843000
6	1.695722000	-1.682982000	-0.444953000
6	0.321096000	-1.726206000	-0.409707000
1	2.182890000	-2.646152000	-0.621900000
1	-0.158339000	-2.692921000	-0.526385000
6	-0.880589000	2.196755000	-0.252379000
1	-1.902844000	1.913188000	-0.540997000
6	-0.939084000	2.797418000	1.138497000
1	-1.592747000	3.673316000	1.156494000
1	-1.314603000	2.068661000	1.861015000
1	0.057523000	3.112799000	1.461842000
6	-0.389291000	3.200601000	-1.275717000
1	-0.359314000	2.757462000	-2.273388000
1	-1.047491000	4.072202000	-1.301162000
1	0.619436000	3.544575000	-1.029253000
6	3.945515000	-0.843974000	-0.283339000
1	4.364520000	0.121523000	0.030679000
6	4.463320000	-1.141432000	-1.676621000
1	4.166418000	-0.353323000	-2.372131000
1	5.553294000	-1.214559000	-1.680751000

1	4.062518000	-2.090076000	-2.046275000
6	4.391296000	-1.881685000	0.729560000
1	5.480320000	-1.884811000	0.811299000
1	3.970409000	-1.664423000	1.713689000
1	4.084074000	-2.890569000	0.441051000
15	-0.804476000	-0.438946000	-0.213301000
7	-2.125537000	-0.536615000	-1.232458000
7	-1.869139000	-0.696351000	1.057654000
14	-3.275458000	-0.838272000	0.042041000
6	-4.030017000	-2.530087000	0.078549000
1	-4.485983000	-2.723927000	1.053082000
1	-4.811041000	-2.642849000	-0.676113000
1	-3.264413000	-3.288724000	-0.096879000
6	-4.569981000	0.477722000	0.214989000
1	-4.116526000	1.466447000	0.310740000
1	-5.227782000	0.484721000	-0.658248000
1	-5.195940000	0.301783000	1.092537000
6	-2.167507000	-0.102116000	-2.605236000
1	-1.156907000	0.116050000	-2.961015000
1	-2.585425000	-0.871691000	-3.258611000
1	-2.764404000	0.809763000	-2.727051000
6	-1.510095000	-1.132075000	2.385035000
1	-2.400097000	-1.466073000	2.922115000
1	-0.800307000	-1.966387000	2.358048000
1	-1.049685000	-0.325872000	2.965686000
7	-0.050564000	0.979804000	-0.276705000
1	2.464578000	1.870547000	1.320412000
6	1.825099000	0.656612000	2.472457000
1	1.363122000	-0.323782000	2.321628000
1	2.794349000	0.539015000	2.959878000
1	1.173018000	1.307680000	3.057381000
31	1.863367000	1.153787000	0.072586000

I_TS$^{C–H}$

6	-0.806999000	1.378230000	0.039928000
6	-2.189249000	0.989455000	-0.489510000
6	-2.297117000	-0.544418000	-0.392305000
6	-0.863595000	-0.974885000	-0.238852000
7	-0.066336000	0.101075000	-0.203346000
1	-2.267622000	1.296832000	-1.536965000
1	-2.982995000	1.502160000	0.060351000
6	1.334016000	-0.052078000	-0.214181000
6	1.879124000	-1.149726000	-0.880796000
6	3.242583000	-1.362779000	-0.888842000

6	4.096866000	-0.486390000	-0.238045000
6	3.562751000	0.604926000	0.422301000
6	2.195808000	0.823180000	0.441734000
1	1.210651000	-1.826435000	-1.399235000
1	3.642132000	-2.220885000	-1.417012000
1	5.167006000	-0.653956000	-0.245672000
1	4.213616000	1.297204000	0.943750000
1	1.811235000	1.671443000	0.988620000
6	-2.819371000	-1.122627000	-1.707987000
1	-2.889617000	-2.211272000	-1.652696000
1	-3.814166000	-0.722653000	-1.928255000
1	-2.156702000	-0.865520000	-2.538151000
6	-3.218157000	-0.999115000	0.730492000
1	-4.239214000	-0.668779000	0.517547000
1	-3.224191000	-2.087727000	0.810816000
1	-2.923746000	-0.594735000	1.699719000
6	-0.236949000	2.534337000	-0.757440000
1	0.703839000	2.912287000	-0.357606000
1	-0.075920000	2.240231000	-1.797170000
1	-0.955096000	3.357593000	-0.744880000
6	-0.878793000	1.707749000	1.525591000
1	-1.491522000	2.601740000	1.665827000
1	-1.337785000	0.892948000	2.087033000
1	0.100187000	1.903072000	1.963254000
1	-0.541854000	-1.932601000	0.323658000
6	-0.471487000	-2.069662000	1.926812000
1	-1.299639000	-2.692964000	2.261094000
1	0.477371000	-2.608210000	1.942022000
1	-0.400782000	-1.140325000	2.490703000

II_TS$^{C–H}$

7	1.419861000	0.404451000	-0.223665000
6	1.255637000	1.711433000	-0.071887000
6	0.000568000	2.324168000	-0.021632000
7	-1.418812000	0.404033000	-0.224468000
1	0.000413000	3.401919000	0.066130000
13	0.000983000	-0.855974000	-0.330841000
6	2.720124000	-0.174420000	-0.184402000
6	3.300017000	-0.645722000	-1.354298000
6	3.379853000	-0.337882000	1.026492000
6	4.545837000	-1.247944000	-1.315664000
1	2.762943000	-0.532272000	-2.289955000
6	4.625146000	-0.941333000	1.060333000
1	2.900502000	0.004501000	1.937974000

6	5.212142000	-1.394102000	-0.110010000
1	4.995683000	-1.608772000	-2.233131000
1	5.135604000	-1.065037000	2.008283000
1	6.185286000	-1.869643000	-0.080996000
6	-2.719157000	-0.174478000	-0.185957000
6	-3.288103000	-0.667000000	-1.352536000
6	-3.390489000	-0.316739000	1.021334000
6	-4.533982000	-1.269248000	-1.314831000
1	-2.742724000	-0.569704000	-2.285188000
6	-4.635748000	-0.920113000	1.054289000
1	-2.920244000	0.041914000	1.931264000
6	-5.211603000	-1.394225000	-0.113181000
1	-4.974984000	-1.646537000	-2.229967000
1	-5.154917000	-1.027140000	1.999540000
1	-6.184763000	-1.869761000	-0.084762000
6	-2.454146000	2.599046000	0.021178000
1	-3.203287000	2.326562000	-0.724479000
1	-2.931486000	2.499365000	0.998502000
1	-2.175109000	3.641754000	-0.115378000
6	-1.254467000	1.711369000	-0.074815000
6	2.455821000	2.597496000	0.030375000
1	2.936264000	2.485573000	1.004890000
1	3.202415000	2.332800000	-0.720695000
1	2.177449000	3.641931000	-0.093482000
1	0.002242000	-2.153792000	0.572762000
6	-0.007496000	-1.275924000	2.005741000
1	-0.918328000	-1.716980000	2.411002000
1	0.872540000	-1.756812000	2.432848000
1	0.014658000	-0.197878000	2.209529000

III_TS$^{C–H}$

7	-1.451643000	0.512694000	-0.239631000
6	-1.260361000	1.814535000	-0.110858000
6	0.000495000	2.419710000	-0.092308000
6	1.261877000	1.815624000	-0.110382000
7	1.453218000	0.514851000	-0.245037000
1	-0.000076000	3.499334000	-0.027913000
6	-2.739850000	-0.069883000	-0.126341000
6	-3.379555000	-0.138148000	1.105446000
6	-3.331866000	-0.650077000	-1.240452000
6	-4.614829000	-0.752074000	1.211835000
1	-2.889991000	0.282503000	1.977669000
6	-4.567659000	-1.264256000	-1.128619000
1	-2.812409000	-0.609653000	-2.191978000

6	-5.213782000	-1.313465000	0.095342000
1	-5.107816000	-0.800621000	2.175777000
1	-5.026169000	-1.709025000	-2.004074000
1	-6.179386000	-1.797321000	0.181729000
6	2.740594000	-0.068884000	-0.127623000
6	3.360662000	-0.164118000	1.112219000
6	3.350032000	-0.623138000	-1.245404000
6	4.595237000	-0.778607000	1.223925000
1	2.855188000	0.235399000	1.985378000
6	4.585123000	-1.237790000	-1.128268000
1	2.844569000	-0.562431000	-2.203381000
6	5.212315000	-1.313414000	0.104238000
1	5.073483000	-0.848401000	2.193969000
1	5.057981000	-1.662286000	-2.006153000
1	6.177404000	-1.797604000	0.194528000
31	0.001691000	-0.786662000	-0.431039000
6	-2.447770000	2.719272000	0.007366000
1	-3.243033000	2.416892000	-0.675865000
1	-2.863818000	2.682269000	1.016476000
1	-2.167087000	3.749485000	-0.202643000
6	2.449666000	2.718339000	0.016332000
1	2.870411000	2.663899000	1.022754000
1	3.241619000	2.425826000	-0.675136000
1	2.169187000	3.752011000	-0.175977000
1	0.009439000	-2.130472000	0.337127000
6	-0.006559000	-1.262810000	1.935160000
1	-0.945896000	-1.685761000	2.292447000
1	0.845700000	-1.813818000	2.333175000
1	0.064621000	-0.201429000	2.197329000

1_TS$^{N–H}$

6	0.571783000	-1.773266000	-0.612145000
6	1.914389000	-1.551966000	-0.576716000
1	0.181864000	-2.763506000	-0.805779000
1	2.572469000	-2.396497000	-0.782377000
7	2.505255000	-0.381047000	-0.304723000
15	-0.536679000	-0.499312000	-0.288874000
5	1.804178000	0.909442000	-0.173851000
7	-1.947246000	-0.559403000	-1.155898000
7	-1.445067000	-0.596342000	1.095261000
14	-2.976125000	-0.627929000	0.264444000
6	-0.925344000	-0.557820000	2.447043000
1	0.089556000	-0.135519000	2.457982000
1	-1.551953000	0.080241000	3.075810000

1	-0.890440000	-1.553340000	2.897604000
6	-3.950277000	-2.194139000	0.409052000
1	-4.754334000	-2.219269000	-0.330373000
1	-3.309666000	-3.063274000	0.251934000
1	-4.411384000	-2.277897000	1.395638000
6	-4.049691000	0.854003000	0.554032000
1	-4.865086000	0.895858000	-0.171960000
1	-4.502568000	0.805523000	1.547539000
1	-3.478311000	1.781791000	0.486893000
6	-2.088076000	-0.370364000	-2.577956000
1	-2.334719000	0.666351000	-2.834063000
1	-1.155042000	-0.626301000	-3.087525000
1	-2.870584000	-1.016245000	-2.981247000
6	3.962569000	-0.386963000	-0.077370000
6	4.719954000	-0.671060000	-1.356647000
6	4.351021000	-1.318507000	1.052573000
1	4.179761000	0.640705000	0.227251000
1	4.439085000	0.044134000	-2.132828000
1	5.796288000	-0.594199000	-1.188461000
1	4.517495000	-1.679963000	-1.729181000
1	3.749803000	-1.110142000	1.940642000
1	4.213768000	-2.369627000	0.781862000
1	5.404953000	-1.183171000	1.304519000
7	0.350625000	0.864506000	-0.424726000
6	-0.408476000	2.140616000	-0.494720000
6	0.092760000	2.971186000	-1.655314000
6	-0.375198000	2.900699000	0.813074000
1	-1.453101000	1.874616000	-0.704571000
1	0.003529000	2.420418000	-2.594913000
1	-0.483183000	3.895844000	-1.736887000
1	1.145338000	3.221594000	-1.505055000
1	-0.726976000	2.279807000	1.640860000
1	0.641671000	3.224945000	1.039883000
1	-1.014830000	3.784349000	0.745865000
1	2.260260000	1.602287000	0.957683000
7	2.166435000	1.238493000	2.291550000
1	3.147894000	1.170119000	2.565760000
1	1.850993000	2.115859000	2.707962000

2_TS^{N-H}

7	2.667232000	-0.403978000	-0.197464000
6	1.940523000	-1.509092000	-0.222640000
6	0.575948000	-1.628812000	-0.116247000
1	2.478745000	-2.455544000	-0.336093000

1	0.146699000	-2.625562000	-0.112524000
13	1.941534000	1.286988000	0.293871000
6	-0.749703000	2.230457000	-0.442100000
1	-1.741617000	1.876654000	-0.757896000
6	-0.922507000	2.981354000	0.864984000
1	-1.629114000	3.807093000	0.746035000
1	-1.292762000	2.316938000	1.650116000
1	0.033711000	3.402170000	1.193362000
6	-0.222469000	3.134728000	-1.537532000
1	-0.127737000	2.590692000	-2.479663000
1	-0.893719000	3.983569000	-1.690201000
1	0.765574000	3.521831000	-1.270924000
6	4.121265000	-0.527698000	-0.371077000
1	4.497855000	0.502234000	-0.310991000
6	4.486904000	-1.074901000	-1.736673000
1	4.031135000	-0.473850000	-2.526093000
1	5.570039000	-1.066566000	-1.878111000
1	4.146020000	-2.107734000	-1.856808000
6	4.768096000	-1.317031000	0.751502000
1	5.855188000	-1.316078000	0.644362000
1	4.521323000	-0.880364000	1.722080000
1	4.438345000	-2.360079000	0.753441000
15	-0.600974000	-0.369497000	-0.121124000
7	-1.862902000	-0.628333000	-1.186688000
7	-1.723119000	-0.519688000	1.115894000
14	-3.065664000	-0.844121000	0.056273000
6	-3.742791000	-2.559697000	0.238302000
1	-4.267418000	-2.665337000	1.191464000
1	-4.451670000	-2.804732000	-0.555160000
1	-2.929909000	-3.288911000	0.213381000
6	-4.420970000	0.420590000	0.021936000
1	-4.011435000	1.432863000	0.035804000
1	-5.026348000	0.308572000	-0.881446000
1	-5.089824000	0.309211000	0.877991000
6	-1.841452000	-0.362249000	-2.602144000
1	-0.816269000	-0.174011000	-2.932600000
1	-2.220281000	-1.210511000	-3.177237000
1	-2.438514000	0.520274000	-2.861606000
6	-1.390881000	-0.772424000	2.496080000
1	-1.328719000	-1.842911000	2.723931000
1	-0.419156000	-0.325556000	2.735777000
1	-2.131668000	-0.323390000	3.161494000
7	0.129957000	1.053738000	-0.280476000
1	2.862157000	1.968453000	1.569514000
7	2.024154000	1.065591000	2.249259000
1	1.537823000	1.692328000	2.881420000

1	2.366480000	0.254912000	2.765866000

3_TS^{N-H}

7	2.478294000	-0.663041000	-0.336623000
6	1.682874000	-1.715762000	-0.278610000
6	0.316206000	-1.751647000	-0.145349000
1	2.162598000	-2.697657000	-0.342583000
1	-0.162452000	-2.724166000	-0.086179000
6	-0.857530000	2.163345000	-0.524199000
1	-1.879455000	1.865754000	-0.802719000
6	-0.938065000	2.925634000	0.785289000
1	-1.581075000	3.804000000	0.685339000
1	-1.337239000	2.290704000	1.580284000
1	0.055879000	3.270269000	1.088924000
6	-0.318935000	3.032046000	-1.642837000
1	-0.288715000	2.477832000	-2.583327000
1	-0.943381000	3.918249000	-1.779597000
1	0.697902000	3.365160000	-1.413910000
6	3.924951000	-0.868415000	-0.456558000
1	4.338910000	0.128039000	-0.657365000
6	4.305998000	-1.763477000	-1.620385000
1	3.840371000	-1.419111000	-2.545683000
1	5.389433000	-1.760391000	-1.757697000
1	4.004788000	-2.801299000	-1.453057000
6	4.522138000	-1.358496000	0.850298000
1	5.607744000	-1.455965000	0.773550000
1	4.297626000	-0.661555000	1.660951000
1	4.114203000	-2.337623000	1.119665000
15	-0.808028000	-0.445032000	-0.152597000
7	-2.115123000	-0.675758000	-1.172346000
7	-1.894352000	-0.529598000	1.123241000
14	-3.279818000	-0.829235000	0.113840000
6	-4.007859000	-2.515536000	0.365175000
1	-4.499358000	-2.577956000	1.339679000
1	-4.753825000	-2.756441000	-0.394790000
1	-3.221961000	-3.273461000	0.331158000
6	-4.594883000	0.478026000	0.086612000
1	-4.152186000	1.476060000	0.060745000
1	-5.231233000	0.362762000	-0.794891000
1	-5.240075000	0.411159000	0.965147000
6	-2.142664000	-0.406363000	-2.586814000
1	-1.161932000	-0.056639000	-2.921451000
1	-2.391751000	-1.297142000	-3.169391000
1	-2.870521000	0.375950000	-2.831724000

6	-1.529019000	-0.795280000	2.493741000
1	-2.226544000	-0.309755000	3.180162000
1	-1.513056000	-1.867513000	2.722324000
1	-0.528937000	-0.395839000	2.697067000
7	-0.043455000	0.945182000	-0.392259000
1	2.675325000	1.863845000	1.376019000
7	1.830189000	0.893169000	2.241981000
1	1.304043000	1.509868000	2.852161000
1	2.253695000	0.149436000	2.791329000
31	1.848739000	1.131422000	0.154804000

I_TS$^{N–H}$

6	0.765425000	-1.316036000	-0.574292000
6	2.243561000	-0.913981000	-0.499785000
6	2.329839000	0.310663000	0.424301000
6	0.932546000	0.846912000	0.400561000
7	0.111401000	-0.090514000	-0.019594000
1	2.590481000	-0.630375000	-1.497897000
1	2.868677000	-1.742818000	-0.157340000
6	-1.300957000	0.049656000	0.101448000
6	-2.090330000	0.327914000	-1.003568000
6	-3.458171000	0.472717000	-0.846991000
6	-4.035018000	0.343181000	0.405137000
6	-3.241594000	0.076459000	1.509372000
6	-1.874766000	-0.068682000	1.358538000
1	-1.629948000	0.454827000	-1.975790000
1	-4.074470000	0.700327000	-1.708461000
1	-5.105783000	0.460002000	0.522663000
1	-3.688267000	-0.015847000	2.492148000
1	-1.231924000	-0.270441000	2.209494000
6	3.389838000	1.300460000	-0.015365000
1	3.356400000	2.204405000	0.597299000
1	4.382831000	0.854495000	0.089514000
1	3.249872000	1.590833000	-1.057561000
6	2.601524000	-0.093868000	1.878310000
1	3.570347000	-0.596419000	1.945169000
1	2.624812000	0.787056000	2.523145000
1	1.838153000	-0.772072000	2.266665000
6	0.335225000	-1.557594000	-2.008496000
1	-0.716232000	-1.844714000	-2.076540000
1	0.500571000	-0.663524000	-2.615652000
1	0.931538000	-2.370194000	-2.430480000
6	0.416639000	-2.518412000	0.283601000
1	0.903455000	-3.410123000	-0.116990000

1	0.743927000	-2.387505000	1.316916000
1	-0.661538000	-2.696597000	0.284929000
1	0.638916000	1.964054000	0.342826000
7	0.625640000	2.864139000	-0.905923000
1	1.554344000	3.017582000	-1.298064000
1	0.111985000	2.395323000	-1.654004000

II_TS^{N-H}

7	-1.387080000	0.493512000	-0.213377000
6	-1.226763000	1.796704000	-0.039932000
6	0.028100000	2.411988000	0.002294000
6	1.271663000	1.780942000	0.003863000
7	1.422533000	0.475692000	-0.184951000
1	0.032910000	3.487057000	0.119327000
13	0.014702000	-0.752375000	-0.670297000
6	-2.678199000	-0.088838000	-0.102729000
6	-3.245925000	-0.300294000	1.148033000
6	-3.341274000	-0.531274000	-1.239981000
6	-4.474485000	-0.926966000	1.258315000
1	-2.705966000	0.025501000	2.031736000
6	-4.571074000	-1.158506000	-1.124551000
1	-2.880144000	-0.380043000	-2.209446000
6	-5.141549000	-1.355977000	0.121372000
1	-4.910492000	-1.085973000	2.237815000
1	-5.084000000	-1.497896000	-2.016877000
1	-6.102114000	-1.849765000	0.208218000
6	2.709561000	-0.118721000	-0.076917000
6	3.210179000	-0.482987000	1.166495000
6	3.435656000	-0.417215000	-1.222748000
6	4.439337000	-1.111934000	1.263949000
1	2.617803000	-0.272899000	2.051186000
6	4.664896000	-1.046500000	-1.120909000
1	3.022827000	-0.151190000	-2.189974000
6	5.171423000	-1.391575000	0.121078000
1	4.824677000	-1.390064000	2.238097000
1	5.227218000	-1.272471000	-2.019373000
1	6.131990000	-1.886977000	0.198264000
6	-2.426008000	2.676182000	0.125529000
1	-3.199158000	2.424664000	-0.602913000
1	-2.870565000	2.544831000	1.114659000
1	-2.155023000	3.724143000	0.013225000
6	2.478747000	2.633474000	0.233859000
1	2.945060000	2.389856000	1.191262000
1	3.233198000	2.454799000	-0.535241000

1	2.216480000	3.689358000	0.237611000
1	0.508726000	-2.788044000	0.803061000
1	-0.888212000	-2.179675000	1.465935000
1	-0.532862000	-2.379360000	-0.675737000
7	-0.242478000	-2.117202000	0.677030000

III_TS$^{N–H}$

7	1.454318000	0.569119000	0.180057000
6	1.271441000	1.870162000	0.027436000
6	0.018561000	2.487236000	0.050318000
6	-1.241276000	1.879935000	0.061122000
7	-1.427920000	0.579015000	0.199152000
1	0.021737000	3.565825000	-0.030875000
6	2.732103000	-0.021052000	0.021988000
6	3.229191000	-0.287079000	-1.248357000
6	3.455127000	-0.422996000	1.138193000
6	4.451210000	-0.919004000	-1.398065000
1	2.636981000	-0.002260000	-2.111791000
6	4.676933000	-1.055747000	0.983527000
1	3.045787000	-0.232740000	2.124760000
6	5.180279000	-1.301486000	-0.283266000
1	4.832652000	-1.121036000	-2.392346000
1	5.236776000	-1.361811000	1.859644000
1	6.135180000	-1.799505000	-0.402241000
6	-2.708192000	-0.004067000	0.043912000
6	-3.280917000	-0.122505000	-1.217703000
6	-3.362155000	-0.544759000	1.144105000
6	-4.503909000	-0.750247000	-1.371144000
1	-2.746940000	0.273346000	-2.075656000
6	-4.585591000	-1.173713000	0.985160000
1	-2.898945000	-0.465476000	2.121547000
6	-5.161744000	-1.275378000	-0.269837000
1	-4.942559000	-0.836612000	-2.358583000
1	-5.090215000	-1.588712000	1.849900000
1	-6.117804000	-1.770356000	-0.391821000
31	0.011135000	-0.734859000	0.616627000
6	2.464224000	2.750099000	-0.186773000
1	3.248501000	2.527719000	0.539629000
1	2.894700000	2.579793000	-1.176187000
1	2.192429000	3.800860000	-0.109376000
6	-2.428818000	2.779497000	-0.098019000
1	-2.836085000	2.709510000	-1.109030000
1	-3.230210000	2.496365000	0.586725000
1	-2.153005000	3.816818000	0.081925000

1	0.609002000	-2.613100000	-1.169300000
1	-0.413232000	-2.330683000	0.542115000
7	-0.191501000	-2.025470000	-0.958848000
1	-0.853016000	-2.059327000	-1.732602000

1_TS^{P-H}

6	0.389754000	-1.903774000	-0.335964000
6	1.737231000	-1.735043000	-0.452203000
1	-0.039604000	-2.896660000	-0.315512000
1	2.350433000	-2.631562000	-0.551897000
7	2.376785000	-0.558782000	-0.464244000
15	-0.669559000	-0.555925000	-0.256307000
5	1.736589000	0.772891000	-0.623269000
7	-2.102464000	-0.708703000	-1.085913000
7	-1.562938000	-0.412118000	1.140059000
14	-3.107517000	-0.538405000	0.337992000
6	-1.072973000	-0.522482000	2.494311000
1	-0.136883000	-1.088022000	2.520683000
1	-0.873675000	0.455836000	2.940881000
1	-1.799638000	-1.046666000	3.119766000
6	-4.069639000	-2.033977000	0.848268000
1	-4.956281000	-2.171438000	0.226055000
1	-3.452064000	-2.931080000	0.778096000
1	-4.409345000	-1.931918000	1.882295000
6	-4.169465000	0.979093000	0.309558000
1	-4.885447000	0.925170000	-0.515072000
1	-4.743103000	1.078200000	1.233313000
1	-3.568012000	1.881380000	0.180964000
6	-2.282777000	-0.558769000	-2.509675000
1	-2.828816000	0.359681000	-2.753430000
1	-1.311223000	-0.507428000	-3.008861000
1	-2.827627000	-1.403964000	-2.935524000
6	3.851913000	-0.582944000	-0.421217000
6	4.426370000	-0.972788000	-1.765766000
6	4.387508000	-1.446823000	0.703472000
1	4.115706000	0.461710000	-0.225699000
1	4.056276000	-0.299796000	-2.541886000
1	5.517263000	-0.920687000	-1.750291000
1	4.146191000	-1.996861000	-2.032696000
1	3.891270000	-1.215770000	1.649583000
1	4.261538000	-2.515025000	0.503774000
1	5.457305000	-1.267578000	0.827341000
7	0.254686000	0.728898000	-0.672049000
6	-0.480068000	2.002411000	-0.911888000

6	-0.051006000	2.631873000	-2.218293000
6	-0.330202000	2.951088000	0.257049000
1	-1.543100000	1.744152000	-1.003132000
1	-0.198612000	1.942258000	-3.052862000
1	-0.635931000	3.535499000	-2.405734000
1	1.008421000	2.890900000	-2.175959000
1	-0.662726000	2.483697000	1.188472000
1	0.716008000	3.244156000	0.368690000
1	-0.927780000	3.851310000	0.093454000
1	2.274318000	1.538529000	0.831815000
15	2.312669000	1.360812000	2.376533000
1	3.732567000	1.323011000	2.405890000
1	2.257167000	2.762210000	2.600724000

2_TS^{P-H}

7	2.540974000	-0.536383000	-0.465118000
6	1.796170000	-1.631923000	-0.413966000
6	0.433639000	-1.721306000	-0.297843000
1	2.324095000	-2.587603000	-0.462141000
1	-0.014109000	-2.707382000	-0.233246000
13	1.878943000	1.220626000	-0.468479000
6	-0.863620000	2.152245000	-0.669201000
1	-1.893183000	1.804987000	-0.830160000
6	-0.835486000	2.949836000	0.619921000
1	-1.515438000	3.803545000	0.562462000
1	-1.130956000	2.328814000	1.469000000
1	0.171331000	3.333850000	0.813454000
6	-0.488363000	3.002381000	-1.866084000
1	-0.523944000	2.417191000	-2.787591000
1	-1.175398000	3.846071000	-1.962966000
1	0.524689000	3.402857000	-1.759114000
6	4.004206000	-0.684378000	-0.517450000
1	4.396570000	0.332126000	-0.367910000
6	4.462870000	-1.160162000	-1.881398000
1	4.105841000	-0.486233000	-2.663677000
1	5.553063000	-1.203849000	-1.933776000
1	4.076839000	-2.161912000	-2.092886000
6	4.547322000	-1.550669000	0.602856000
1	5.637040000	-1.487581000	0.630000000
1	4.159030000	-1.226082000	1.570961000
1	4.287490000	-2.603890000	0.466551000
15	-0.716017000	-0.438762000	-0.237777000

7	-2.086895000	-0.706797000	-1.151857000
7	-1.693011000	-0.503821000	1.117438000
14	-3.157570000	-0.809104000	0.221881000
6	-3.874453000	-2.478053000	0.581406000
1	-4.292421000	-2.508374000	1.590886000
1	-4.679053000	-2.728592000	-0.112859000
1	-3.100608000	-3.245193000	0.507994000
6	-4.460713000	0.509033000	0.242353000
1	-4.017551000	1.505352000	0.185043000
1	-5.138399000	0.387239000	-0.606985000
1	-5.063958000	0.454586000	1.150882000
6	-2.226410000	-0.458345000	-2.564670000
1	-1.262954000	-0.168147000	-2.992886000
1	-2.570843000	-1.345910000	-3.100701000
1	-2.932979000	0.356231000	-2.762647000
6	-1.267412000	-0.751588000	2.475988000
1	-1.288708000	0.157665000	3.083939000
1	-1.912687000	-1.496066000	2.950669000
1	-0.241718000	-1.130590000	2.496798000
7	0.012242000	0.961739000	-0.579273000
1	2.469667000	2.044479000	0.825165000
1	1.994524000	2.390451000	2.974443000
1	3.505605000	1.044437000	2.550885000
15	2.085962000	1.063513000	2.471410000

3_TS^{P-H}

7	2.227239000	-1.031767000	-0.303246000
6	1.354334000	-2.004253000	-0.097074000
6	-0.009383000	-1.926216000	0.013328000
1	1.766774000	-3.012350000	0.007465000
1	-0.557106000	-2.840244000	0.218748000
6	-0.927000000	1.960530000	-0.925741000
1	-1.976435000	1.683477000	-1.102066000
6	-0.892089000	2.928728000	0.240331000
1	-1.505824000	3.807944000	0.027372000
1	-1.266075000	2.456668000	1.151613000
1	0.130167000	3.266935000	0.432606000
6	-0.414483000	2.600854000	-2.199712000
1	-0.454029000	1.896721000	-3.033598000
1	-1.012880000	3.478285000	-2.455348000
1	0.623308000	2.927901000	-2.080307000
6	3.657086000	-1.371401000	-0.332484000
1	4.177282000	-0.415701000	-0.476114000
6	4.004776000	-2.263376000	-1.508793000

1	3.680238000	-1.811192000	-2.448113000
1	5.083422000	-2.427668000	-1.559420000
1	3.526072000	-3.242957000	-1.420673000
6	4.129448000	-1.953347000	0.986529000
1	5.215156000	-2.070837000	0.985450000
1	3.854534000	-1.295403000	1.813605000
1	3.691440000	-2.938997000	1.169082000
15	-1.025419000	-0.541750000	-0.116136000
7	-2.440214000	-0.825355000	-0.952736000
7	-1.967815000	-0.282511000	1.241178000
14	-3.476852000	-0.607807000	0.436614000
6	-4.334114000	-2.134866000	1.039522000
1	-4.743464000	-1.977894000	2.040521000
1	-5.162904000	-2.416306000	0.386583000
1	-3.630413000	-2.968829000	1.084523000
6	-4.651997000	0.816847000	0.280284000
1	-4.121507000	1.737282000	0.027447000
1	-5.391027000	0.620515000	-0.500945000
1	-5.198795000	0.981731000	1.211138000
6	-2.592048000	-0.841435000	-2.385559000
1	-1.612878000	-0.775815000	-2.867975000
1	-3.068356000	-1.761300000	-2.733285000
1	-3.189718000	0.007299000	-2.738187000
6	-1.457126000	-0.239188000	2.590200000
1	-0.446003000	0.182148000	2.597250000
1	-2.079608000	0.402016000	3.217448000
1	-1.407454000	-1.231275000	3.051881000
7	-0.173894000	0.721501000	-0.639994000
1	3.270475000	1.709129000	0.087962000
1	2.509742000	3.107931000	1.469161000
1	3.465090000	2.177175000	3.098565000
31	1.787855000	0.868254000	-0.445599000
15	2.916189000	1.796863000	1.810616000

I_TS^{P-H}

6	-2.206100000	-1.420259000	-0.026441000
6	-2.331756000	0.002130000	0.551876000
6	-0.798828000	-1.535668000	-0.612291000
7	-0.121139000	-0.412184000	0.124626000
6	1.296396000	-0.270690000	0.186129000
6	2.041052000	0.018969000	-0.947140000
6	3.412036000	0.180405000	-0.840120000
6	4.036575000	0.058901000	0.389675000
6	3.286597000	-0.219786000	1.520861000

6	1.916998000	-0.383860000	1.420209000
1	1.546819000	0.157890000	-1.900094000
1	3.992063000	0.418814000	-1.723574000
1	5.109259000	0.189632000	0.468223000
1	3.769520000	-0.309695000	2.486590000
1	1.308674000	-0.596553000	2.292353000
6	-0.134225000	-2.852549000	-0.273725000
1	-0.093872000	-3.000858000	0.808280000
1	-0.706657000	-3.673384000	-0.711383000
1	0.883154000	-2.903540000	-0.668334000
6	-0.776322000	-1.296325000	-2.113111000
1	-1.421505000	-2.028030000	-2.604641000
1	-1.139325000	-0.297433000	-2.365254000
1	0.226760000	-1.414948000	-2.525648000
6	-0.903360000	0.453256000	0.721077000
15	-0.289230000	3.169413000	-0.465041000
1	-0.576038000	1.772322000	0.521479000
1	-0.433828000	2.427044000	-1.672816000
1	-2.319627000	-2.152796000	0.778696000
1	-2.973899000	-1.635692000	-0.773671000
6	-3.102169000	0.940434000	-0.372735000
1	-3.113732000	1.957285000	0.024701000
1	-2.671971000	0.977653000	-1.375578000
1	-4.136302000	0.595357000	-0.459628000
6	-3.008437000	-0.011751000	1.916900000
1	-3.080615000	0.998981000	2.324098000
1	-4.018359000	-0.424144000	1.832469000
1	-2.447935000	-0.625131000	2.626934000
1	1.113105000	2.932082000	-0.406952000

II_TS^{P-H}

7	1.331156000	0.666591000	0.157702000
6	1.155605000	1.938575000	-0.177370000
6	-0.105069000	2.510601000	-0.357963000
6	-1.338940000	1.874415000	-0.253381000
7	-1.468562000	0.604465000	0.120372000
1	-0.123923000	3.558249000	-0.625223000
13	-0.046518000	-0.616238000	0.559595000
6	2.648125000	0.127725000	0.225988000
6	3.341936000	-0.172014000	-0.940069000
6	3.206830000	-0.181697000	1.457748000
6	4.593662000	-0.755991000	-0.871530000
1	2.879174000	0.043828000	-1.897760000
6	4.458896000	-0.772212000	1.521898000

1	2.649279000	0.042733000	2.360691000
6	5.154098000	-1.059161000	0.359904000
1	5.129013000	-0.987226000	-1.784917000
1	4.890030000	-1.010570000	2.487070000
1	6.131242000	-1.524437000	0.412050000
6	-2.763965000	0.011222000	0.172379000
6	-3.317514000	-0.556786000	-0.966987000
6	-3.439912000	-0.073822000	1.381675000
6	-4.551229000	-1.180565000	-0.900911000
1	-2.763921000	-0.509861000	-1.899113000
6	-4.673967000	-0.698553000	1.443578000
1	-2.985208000	0.352993000	2.269659000
6	-5.233682000	-1.249716000	0.302861000
1	-4.977739000	-1.621953000	-1.794088000
1	-5.197409000	-0.759814000	2.390521000
1	-6.197211000	-1.742621000	0.353839000
6	2.343473000	2.828047000	-0.366915000
1	3.065690000	2.692195000	0.440219000
1	2.863899000	2.589833000	-1.297030000
1	2.041438000	3.872660000	-0.404867000
6	-2.561144000	2.675339000	-0.568547000
1	-3.079077000	2.260691000	-1.436276000
1	-3.270506000	2.643887000	0.261283000
1	-2.306421000	3.711859000	-0.778646000
1	-0.419273000	-3.368975000	-0.457402000
1	0.842648000	-3.311537000	-2.166946000
1	1.011403000	-2.261788000	0.529970000
15	0.525348000	-2.476593000	-0.997229000

III_TS^{P-H}

7	1.514061000	0.674898000	0.029302000
6	1.363404000	1.949087000	-0.307770000
6	0.127664000	2.588208000	-0.391928000
6	-1.145374000	2.040882000	-0.214569000
7	-1.360839000	0.773099000	0.098288000
1	0.156907000	3.638725000	-0.647400000
6	2.805081000	0.084663000	0.087562000
6	3.264512000	-0.672336000	-0.982387000
6	3.574704000	0.184995000	1.239360000
6	4.496112000	-1.300627000	-0.908670000
1	2.642158000	-0.763427000	-1.866363000
6	4.805831000	-0.443393000	1.307645000
1	3.193985000	0.757905000	2.078712000
6	5.271075000	-1.184604000	0.233347000

1	4.848873000	-1.888445000	-1.748016000
1	5.401928000	-0.359212000	2.208889000
1	6.233066000	-1.679785000	0.290577000
6	-2.678274000	0.250064000	0.171470000
6	-3.399968000	-0.005849000	-0.988838000
6	-3.211965000	-0.103604000	1.403235000
6	-4.650187000	-0.590929000	-0.913039000
1	-2.956795000	0.238515000	-1.948743000
6	-4.462575000	-0.694916000	1.473896000
1	-2.633455000	0.085352000	2.301364000
6	-5.184683000	-0.938291000	0.318303000
1	-5.205238000	-0.790008000	-1.822319000
1	-4.871925000	-0.968995000	2.439136000
1	-6.160734000	-1.405170000	0.374961000
31	0.038807000	-0.605755000	0.448105000
6	2.580383000	2.761683000	-0.623645000
1	3.237403000	2.831662000	0.245831000
1	3.162313000	2.286887000	-1.416748000
1	2.309806000	3.767116000	-0.938545000
6	-2.312157000	2.963675000	-0.388073000
1	-2.834275000	2.757971000	-1.324914000
1	-3.039630000	2.827189000	0.414147000
1	-1.986094000	4.001638000	-0.402633000
1	0.473625000	-3.285112000	-0.468684000
1	-0.866403000	-2.182952000	0.706699000
1	-0.931531000	-3.559411000	-2.024562000
15	-0.660737000	-2.600019000	-0.955411000

1_TS$^{Si–H}$

6	-1.100235000	1.146381000	-1.751803000
6	0.168303000	1.642258000	-1.604203000
1	-1.640578000	1.296510000	-2.677238000
1	0.586866000	2.220618000	-2.427932000
7	0.938488000	1.478325000	-0.526595000
15	-1.922769000	0.386928000	-0.455126000
5	0.455507000	0.990133000	0.792669000
7	-3.529784000	0.788849000	-0.278425000
7	-2.412923000	-1.189198000	-0.693008000
14	-4.112353000	-0.845228000	-0.493489000
6	-1.637288000	-2.263571000	-1.264681000
1	-0.890240000	-1.874969000	-1.963116000
1	-1.108818000	-2.844394000	-0.501802000
1	-2.287637000	-2.946121000	-1.817055000
6	-5.101808000	-1.171663000	-2.023035000

1	-6.123285000	-0.798730000	-1.924393000
1	-4.639224000	-0.695014000	-2.889048000
1	-5.164870000	-2.245855000	-2.215453000
6	-4.939593000	-1.541285000	1.011213000
1	-5.857675000	-0.989780000	1.231124000
1	-5.215771000	-2.587168000	0.861785000
1	-4.287201000	-1.480746000	1.884773000
6	-4.041543000	2.014768000	0.283410000
1	-4.478974000	1.855861000	1.275860000
1	-3.234780000	2.745227000	0.390335000
1	-4.804682000	2.460405000	-0.358276000
6	2.344798000	1.920776000	-0.594897000
6	2.448255000	3.414256000	-0.372339000
6	3.043827000	1.490024000	-1.868834000
1	2.817238000	1.414123000	0.253501000
1	1.986928000	3.686968000	0.579065000
1	3.493477000	3.731220000	-0.357343000
1	1.943373000	3.961801000	-1.174773000
1	2.845982000	0.439695000	-2.096359000
1	2.747615000	2.092502000	-2.732536000
1	4.123164000	1.604804000	-1.745372000
7	-0.992755000	0.672109000	0.859405000
6	-1.593972000	0.369181000	2.183389000
6	-1.409657000	1.533691000	3.131146000
6	-1.050373000	-0.924459000	2.751026000
1	-2.671935000	0.238763000	2.021647000
1	-1.852591000	2.444643000	2.721734000
1	-1.884678000	1.315847000	4.090450000
1	-0.345074000	1.716708000	3.290763000
1	-1.207568000	-1.755118000	2.057298000
1	0.021279000	-0.832355000	2.942102000
1	-1.549191000	-1.165134000	3.693015000
1	1.313840000	-0.256124000	1.052591000
1	1.542707000	-2.822489000	1.110964000
1	1.433630000	-1.927952000	-1.111719000
14	1.871495000	-1.629002000	0.282555000
6	3.722480000	-1.362518000	0.230179000
6	4.493320000	-1.630294000	-0.902366000
6	4.359091000	-0.762863000	1.320768000
6	5.842028000	-1.319327000	-0.945723000
1	4.025781000	-2.087712000	-1.770150000
6	5.707593000	-0.451009000	1.284396000
1	3.782382000	-0.517400000	2.209332000
6	6.453239000	-0.728138000	0.149032000
1	6.419942000	-1.538564000	-1.836960000
1	6.178391000	0.016305000	2.142331000

1	7.508674000	-0.482323000	0.117125000

2_TS$^{Si–H}$

7	1.772560000	-1.912166000	-0.437705000
6	1.019131000	-1.708689000	-1.508884000
6	-0.228811000	-1.142971000	-1.574587000
1	1.434234000	-2.034227000	-2.465613000
1	-0.699179000	-1.052783000	-2.548207000
13	1.211114000	-1.602963000	1.326858000
6	-1.137320000	-0.195289000	2.316032000
1	-1.964568000	0.444631000	1.980500000
6	-1.728342000	-1.351827000	3.097498000
1	-2.281054000	-0.988693000	3.967362000
1	-2.410026000	-1.932830000	2.472069000
1	-0.937264000	-2.019951000	3.452854000
6	-0.225117000	0.662693000	3.168465000
1	0.175560000	1.500685000	2.592142000
1	-0.769282000	1.061787000	4.027105000
1	0.616893000	0.076762000	3.552307000
6	3.063343000	-2.602352000	-0.604109000
1	3.551287000	-2.538893000	0.378378000
6	3.974646000	-1.923304000	-1.607137000
1	4.130426000	-0.873757000	-1.349760000
1	4.949147000	-2.415713000	-1.616279000
1	3.575572000	-1.976556000	-2.623654000
6	2.859365000	-4.070641000	-0.924212000
1	3.814736000	-4.599063000	-0.952301000
1	2.225871000	-4.543628000	-0.169968000
1	2.379506000	-4.194279000	-1.899584000
15	-1.210659000	-0.557349000	-0.283659000
7	-1.934572000	0.917170000	-0.549811000
7	-2.740735000	-1.235185000	-0.307844000
14	-3.550521000	0.267937000	-0.666024000
6	-4.318303000	0.288397000	-2.351479000
1	-5.187561000	-0.373689000	-2.382833000
1	-4.656251000	1.287583000	-2.633087000
1	-3.599586000	-0.056486000	-3.098164000
6	-4.712833000	0.918460000	0.621727000
1	-4.309326000	0.776575000	1.626283000
1	-4.886499000	1.987253000	0.471055000
1	-5.682883000	0.420020000	0.567770000
6	-1.352489000	2.215916000	-0.306548000
1	-0.279926000	2.125490000	-0.113668000
1	-1.469373000	2.875565000	-1.168913000

1	-1.806851000	2.703914000	0.564166000
6	-3.008422000	-2.636810000	-0.518849000
1	-3.043582000	-2.904038000	-1.581346000
1	-2.227758000	-3.245269000	-0.051002000
1	-3.958468000	-2.920019000	-0.061363000
7	-0.415714000	-0.675267000	1.114880000
1	2.385998000	-0.987313000	2.238955000
14	3.119992000	0.720779000	1.368059000
1	3.497247000	1.391667000	2.646039000
1	4.381028000	0.183279000	0.779095000
6	2.502804000	2.081230000	0.231992000
6	2.064375000	3.312019000	0.732520000
6	2.364517000	1.864299000	-1.144860000
6	1.545790000	4.288960000	-0.101969000
1	2.150988000	3.515694000	1.796751000
6	1.851831000	2.837669000	-1.982531000
1	2.667611000	0.910000000	-1.569227000
6	1.443217000	4.059286000	-1.465216000
1	1.228289000	5.239810000	0.312950000
1	1.768172000	2.643870000	-3.046590000
1	1.044614000	4.825204000	-2.120718000

3_TS$^{Si–H}$

6	-0.991044000	1.440194000	-1.712301000
6	0.302743000	0.980127000	-1.695613000
7	-1.821316000	1.615323000	-0.700114000
1	-1.377912000	1.698898000	-2.701271000
1	0.824822000	0.908613000	-2.644527000
31	-1.287301000	1.436255000	1.152402000
7	0.432597000	0.534177000	1.006299000
15	1.282550000	0.504035000	-0.360033000
7	2.158158000	-0.895132000	-0.580715000
7	2.742378000	1.327550000	-0.340054000
14	3.705754000	-0.092742000	-0.646318000
6	1.695050000	-2.239692000	-0.335067000
1	1.769259000	-2.865694000	-1.227032000
1	2.267315000	-2.716283000	0.469370000
1	0.644581000	-2.230315000	-0.031165000
6	2.880528000	2.745685000	-0.562349000
1	3.794398000	3.120396000	-0.097039000
1	2.903995000	3.005986000	-1.627045000
1	2.040951000	3.283140000	-0.109510000
6	4.873608000	-0.615880000	0.693807000
1	5.786919000	-0.017530000	0.678227000

1	4.414035000	-0.515352000	1.679144000
1	5.165932000	-1.660444000	0.557482000
6	4.539725000	-0.057585000	-2.300233000
1	5.340649000	0.686296000	-2.309114000
1	4.984630000	-1.022290000	-2.551945000
1	3.821468000	0.205401000	-3.079982000
6	1.127098000	0.137029000	2.244950000
6	0.246366000	-0.775700000	3.072110000
1	-0.063526000	-1.649024000	2.492110000
1	0.780143000	-1.120256000	3.960427000
1	-0.654675000	-0.252721000	3.408178000
6	1.592256000	1.347851000	3.030240000
1	0.737290000	1.958094000	3.337936000
1	2.131572000	1.043121000	3.930482000
1	2.254332000	1.970394000	2.423730000
1	2.016413000	-0.441746000	1.959048000
6	-3.139245000	2.218899000	-0.942118000
1	-3.672324000	2.142299000	0.014485000
6	-3.010562000	3.691006000	-1.285094000
1	-3.993758000	4.160160000	-1.362908000
1	-2.437890000	4.215325000	-0.516298000
1	-2.498312000	3.824829000	-2.242483000
6	-3.953683000	1.463003000	-1.973231000
1	-4.061623000	0.413087000	-1.693719000
1	-4.952867000	1.896901000	-2.048272000
1	-3.502680000	1.513579000	-2.967819000
1	-2.430222000	0.955663000	2.119670000
14	-3.034889000	-0.970566000	1.216087000
1	-3.436644000	-1.634608000	2.493253000
1	-4.307039000	-0.585972000	0.531777000
6	-2.251333000	-2.325253000	0.175023000
6	-1.722546000	-3.482205000	0.755821000
6	-2.094084000	-2.174672000	-1.207615000
6	-1.097667000	-4.455398000	-0.007646000
1	-1.823095000	-3.634028000	1.827581000
6	-1.474119000	-3.143813000	-1.975376000
1	-2.469450000	-1.277399000	-1.693911000
6	-0.976443000	-4.293611000	-1.378773000
1	-0.711241000	-5.350009000	0.469257000
1	-1.377248000	-3.002969000	-3.046639000
1	-0.494841000	-5.057000000	-1.979332000

I_TS^{Si-H}

6	0.893191000	1.286275000	-0.870332000

7	1.113693000	0.493542000	0.169054000
6	1.842573000	-0.713170000	-0.005970000
6	3.150177000	-0.636343000	-0.467964000
6	3.881570000	-1.790140000	-0.675908000
6	3.308592000	-3.028569000	-0.428887000
6	2.002657000	-3.105725000	0.022551000
6	1.264892000	-1.952080000	0.235216000
1	4.903040000	-1.723807000	-1.031516000
1	3.880382000	-3.934027000	-0.594196000
1	1.545979000	-4.071740000	0.203486000
1	3.574384000	0.344156000	-0.659071000
1	0.234920000	-2.012528000	0.565239000
14	-1.289496000	-0.086937000	-2.369205000
1	-2.129167000	0.811254000	-3.212252000
1	-0.977202000	-1.300501000	-3.176424000
1	0.303331000	0.730486000	-1.862304000
6	-2.350053000	-0.669485000	-0.934070000
6	-3.201040000	0.200947000	-0.247357000
6	-2.251199000	-1.978002000	-0.455059000
6	-3.912201000	-0.209943000	0.866886000
1	-3.320224000	1.223245000	-0.598408000
6	-2.957209000	-2.396463000	0.661199000
1	-1.612858000	-2.687693000	-0.975557000
6	-3.788547000	-1.511441000	1.329294000
1	-4.569433000	0.486497000	1.375996000
1	-2.864536000	-3.420167000	1.007487000
1	-4.343791000	-1.836077000	2.201675000
6	0.381542000	2.601722000	-0.344147000
6	-0.057786000	2.280038000	1.094028000
6	0.690937000	1.011457000	1.510725000
1	0.128146000	3.103648000	1.789040000
1	-1.133954000	2.077466000	1.103063000
6	-0.729327000	3.218983000	-1.171215000
1	-0.967415000	4.218201000	-0.795687000
1	-0.428181000	3.314249000	-2.217541000
1	-1.642359000	2.621023000	-1.134616000
6	1.583407000	3.553667000	-0.370538000
1	1.872867000	3.771297000	-1.400714000
1	1.322038000	4.494232000	0.123059000
1	2.455196000	3.133636000	0.135237000
6	-0.226802000	0.050641000	2.242836000
1	-1.076008000	-0.234700000	1.617842000
1	0.297785000	-0.850456000	2.567205000
1	-0.615708000	0.546119000	3.136370000
6	1.926100000	1.277102000	2.355403000
1	1.630631000	1.678815000	3.327105000

1	2.479810000	0.350915000	2.529846000
1	2.600569000	1.991950000	1.880975000

II_TS$^{Si–H}$

13	-0.811047000	0.462922000	1.098538000
7	-2.401140000	0.758411000	0.122097000
7	0.242927000	1.767168000	0.227987000
6	-2.565056000	1.726154000	-0.769906000
6	-0.226418000	2.629174000	-0.666451000
6	-1.557091000	2.638424000	-1.093080000
1	-1.829214000	3.423596000	-1.785526000
6	-3.374986000	-0.263836000	0.297816000
6	-4.046429000	-0.371792000	1.507699000
6	-3.584458000	-1.210976000	-0.697323000
6	-4.945211000	-1.406346000	1.709443000
6	-4.483714000	-2.242153000	-0.490565000
6	-5.165752000	-2.340926000	0.711852000
1	-5.473115000	-1.481792000	2.652676000
1	-4.644024000	-2.977696000	-1.269817000
1	-5.865378000	-3.152334000	0.873285000
6	1.637080000	1.661401000	0.496120000
6	2.506811000	1.196903000	-0.482032000
6	2.111984000	1.925104000	1.773783000
6	3.847660000	1.028475000	-0.190733000
6	3.455536000	1.749835000	2.061856000
6	4.324777000	1.304190000	1.080624000
1	4.517419000	0.651652000	-0.954501000
1	3.821619000	1.960904000	3.059637000
1	5.373802000	1.157242000	1.308962000
6	0.683669000	3.661158000	-1.251095000
1	0.106835000	4.504021000	-1.627859000
1	1.406310000	4.016734000	-0.515697000
1	1.252459000	3.247715000	-2.086795000
6	-3.879651000	1.878363000	-1.464249000
1	-3.984731000	2.884799000	-1.865149000
1	-3.958293000	1.176918000	-2.297943000
1	-4.711163000	1.668450000	-0.789982000
1	1.420196000	2.272340000	2.534108000
1	2.116974000	0.943621000	-1.462901000
1	-3.027722000	-1.136606000	-1.626340000
1	-3.861744000	0.366173000	2.281256000
14	0.011009000	-1.789481000	-0.745614000
6	1.853728000	-2.102870000	-0.562464000
6	2.430258000	-2.262746000	0.700751000

6	2.710341000	-2.114860000	-1.665780000
6	3.793861000	-2.446429000	0.853896000
1	1.800637000	-2.240692000	1.586769000
6	4.075603000	-2.297429000	-1.519190000
1	2.296738000	-1.988000000	-2.662711000
6	4.622467000	-2.467808000	-0.257004000
1	4.213800000	-2.568947000	1.846391000
1	4.716235000	-2.312897000	-2.394691000
1	5.690394000	-2.613255000	-0.139064000
1	-0.712520000	-3.048240000	-0.406578000
1	-0.217328000	-1.579187000	-2.215565000
1	-0.301244000	-1.044865000	1.161233000

III_TS$^{Si–H}$

7	2.365806000	0.698721000	0.027774000
7	-0.356892000	1.721110000	-0.115741000
6	2.460626000	1.627529000	0.964260000
6	0.105475000	2.527069000	0.826793000
6	1.427839000	2.514754000	1.283478000
1	1.672330000	3.269083000	2.019496000
6	3.356244000	-0.298540000	-0.161515000
6	4.047513000	-0.354548000	-1.364238000
6	3.573407000	-1.273540000	0.805112000
6	4.972393000	-1.361036000	-1.585359000
6	4.499423000	-2.276310000	0.579254000
6	5.202087000	-2.321410000	-0.614489000
1	5.514765000	-1.394335000	-2.522891000
1	4.664359000	-3.033068000	1.337027000
1	5.923112000	-3.110703000	-0.790535000
6	-1.737956000	1.610895000	-0.419185000
6	-2.642837000	1.172240000	0.540015000
6	-2.172429000	1.842011000	-1.718111000
6	-3.973688000	0.999584000	0.208895000
6	-3.505776000	1.662308000	-2.045805000
6	-4.409419000	1.244830000	-1.083319000
1	-4.668452000	0.642768000	0.960008000
1	-3.837665000	1.849239000	-3.060308000
1	-5.450880000	1.095203000	-1.342214000
6	-0.808630000	3.536079000	1.449998000
1	-0.232954000	4.383195000	1.819748000
1	-1.557698000	3.890820000	0.741986000
1	-1.342201000	3.104465000	2.299567000
6	3.739177000	1.769413000	1.728869000
1	3.818003000	2.768382000	2.153927000

1	3.776226000	1.053278000	2.552837000
1	4.606132000	1.577406000	1.095592000
1	-1.455284000	2.168141000	-2.464300000
1	-2.288477000	0.938498000	1.538706000
1	3.001039000	-1.244621000	1.726816000
1	3.855331000	0.402790000	-2.117031000
14	-0.084814000	-1.740485000	0.726285000
6	-1.929081000	-2.094512000	0.603971000
6	-2.532791000	-2.290915000	-0.640225000
6	-2.756642000	-2.107108000	1.728771000
6	-3.894855000	-2.508834000	-0.756882000
1	-1.925310000	-2.268101000	-1.541971000
6	-4.120959000	-2.321974000	1.619713000
1	-2.321619000	-1.952074000	2.712426000
6	-4.694823000	-2.526525000	0.374930000
1	-4.336571000	-2.658359000	-1.736110000
1	-4.739604000	-2.334384000	2.510906000
1	-5.762189000	-2.695074000	0.286401000
1	0.639843000	-3.028783000	0.515023000
1	0.160731000	-1.378888000	2.163792000
1	0.284695000	-1.004920000	-1.373962000
31	0.771018000	0.443846000	-1.064089000

Cartesian coordinates of the optimized geometries of the products obtained on activation of H_2 (**P$^{H–H}$**), CH_4 (**P$^{C–H}$**), NH_3 (**P$^{N–H}$**), PH_3 (**P$^{P–H}$**) and SiH_3Ph (**P$^{Si–H}$**) by the proposed carbenoids **1-3** and the experimentally known carbenoids **I-III**.

1_P$^{H–H}$

6	0.686183000	-1.713289000	0.333423000
6	2.046939000	-1.541132000	0.178949000
1	0.277716000	-2.708606000	0.451253000
1	2.659614000	-2.441849000	0.140347000
7	2.661338000	-0.382227000	0.081771000
15	-0.415791000	-0.428524000	0.056413000
5	1.865425000	0.914269000	0.424629000
7	-1.633500000	-0.712435000	-1.054184000
7	-1.623340000	-0.282936000	1.214090000
14	-2.927827000	-0.535187000	0.097640000
6	-1.435152000	-0.277619000	2.643114000
1	-0.514860000	-0.806638000	2.907450000
1	-1.360552000	0.737396000	3.045571000
1	-2.267209000	-0.781714000	3.142564000
6	-3.926190000	-2.055570000	0.460243000

1	-4.644085000	-2.268163000	-0.334797000
1	-3.273098000	-2.921962000	0.578589000
1	-4.494936000	-1.928286000	1.385322000
6	-4.039315000	0.910133000	-0.252149000
1	-4.574878000	0.762609000	-1.194073000
1	-4.789853000	1.037919000	0.530884000
1	-3.463813000	1.835027000	-0.329175000
6	-1.485797000	-0.687377000	-2.486167000
1	-1.945570000	-1.562439000	-2.952509000
1	-1.932117000	0.210635000	-2.930978000
1	-0.425481000	-0.691855000	-2.751954000
6	4.117762000	-0.296269000	-0.013898000
6	4.761204000	-1.449748000	-0.755104000
6	4.721554000	-0.129965000	1.369539000
1	4.309986000	0.619386000	-0.583960000
1	4.274472000	-1.631953000	-1.715497000
1	5.810948000	-1.216772000	-0.943286000
1	4.741287000	-2.377344000	-0.176155000
1	4.289940000	0.730744000	1.881821000
1	4.518312000	-1.020547000	1.973206000
1	5.804461000	0.004514000	1.310986000
7	0.481301000	0.849840000	-0.323236000
6	-0.172079000	2.084380000	-0.764825000
6	0.577359000	2.699921000	-1.929446000
6	-0.346988000	3.068266000	0.377858000
1	-1.174687000	1.814238000	-1.128832000
1	0.657307000	1.990640000	-2.755924000
1	0.059446000	3.593263000	-2.286948000
1	1.586849000	2.986313000	-1.629508000
1	-0.904898000	2.612045000	1.199903000
1	0.623975000	3.384423000	0.765338000
1	-0.888605000	3.956949000	0.043236000
1	1.690852000	0.941070000	1.640463000
1	2.493709000	1.879517000	0.054427000

2_P^{H-H}

7	2.753636000	-0.333293000	-0.048575000
6	2.038439000	-1.437641000	-0.165057000
6	0.672193000	-1.555819000	-0.250768000
1	2.588731000	-2.382237000	-0.205825000
1	0.248774000	-2.548086000	-0.368618000
13	2.058071000	1.414500000	-0.221597000
6	-0.684905000	2.266605000	0.339456000
1	-1.713297000	1.994132000	0.059840000

6	-0.669405000	2.595343000	1.819357000
1	-1.327148000	3.440569000	2.037863000
1	-1.001458000	1.738337000	2.408890000
1	0.343622000	2.857251000	2.136319000
6	-0.296691000	3.466786000	-0.500562000
1	-0.309901000	3.227587000	-1.565708000
1	-0.987585000	4.293382000	-0.320962000
1	0.707738000	3.819762000	-0.244306000
6	4.217040000	-0.444599000	0.010959000
1	4.583934000	0.588644000	0.083077000
6	4.796416000	-1.042593000	-1.257447000
1	4.447869000	-0.491945000	-2.133680000
1	5.887852000	-1.005956000	-1.236602000
1	4.503964000	-2.090015000	-1.374076000
6	4.680119000	-1.174562000	1.256490000
1	5.770044000	-1.164248000	1.327354000
1	4.270433000	-0.704021000	2.152395000
1	4.359567000	-2.220327000	1.244077000
15	-0.511554000	-0.312442000	-0.094579000
7	-1.735771000	-0.356272000	-1.234904000
7	-1.670151000	-0.696941000	1.053373000
14	-2.967896000	-0.844337000	-0.106333000
6	-3.580303000	-2.587729000	-0.250214000
1	-4.129590000	-2.875513000	0.650152000
1	-4.253849000	-2.714300000	-1.099974000
1	-2.739723000	-3.275044000	-0.370530000
6	-4.375500000	0.352814000	0.033437000
1	-4.017573000	1.373944000	0.177005000
1	-4.984851000	0.328520000	-0.873800000
1	-5.028186000	0.096901000	0.870811000
6	-1.692920000	0.289788000	-2.523366000
1	-0.689837000	0.684932000	-2.712001000
1	-1.931342000	-0.402808000	-3.333951000
1	-2.392683000	1.132138000	-2.574984000
6	-1.386385000	-1.317243000	2.325955000
1	-2.130176000	-1.026522000	3.071009000
1	-1.370224000	-2.411953000	2.264187000
1	-0.409621000	-0.993741000	2.695493000
7	0.200592000	1.117667000	0.055714000
1	2.664423000	2.344862000	0.930566000
1	2.362292000	1.919570000	-1.714595000

3_P^{H-H}

6	1.746757000	-1.648017000	-0.237318000

6	0.382523000	-1.645405000	-0.417765000
7	2.540143000	-0.628947000	0.028876000
1	2.221429000	-2.629356000	-0.334012000
1	-0.097677000	-2.588700000	-0.658994000
31	1.949429000	1.218527000	-0.239300000
7	0.027563000	1.003750000	0.149387000
15	-0.741046000	-0.371488000	-0.121458000
7	-1.989277000	-0.287970000	-1.235320000
7	-1.895306000	-0.799070000	1.020716000
14	-3.215476000	-0.818335000	-0.121219000
6	-1.944166000	0.448246000	-2.474060000
1	-2.194692000	-0.180200000	-3.332158000
1	-2.633615000	1.300546000	-2.460789000
1	-0.936623000	0.843455000	-2.637908000
6	-1.605856000	-1.535366000	2.228007000
1	-2.353794000	-1.325337000	2.995437000
1	-1.577337000	-2.619391000	2.062850000
1	-0.633158000	-1.237742000	2.629420000
6	-4.580747000	0.410517000	0.127503000
1	-5.218805000	0.128765000	0.967768000
1	-4.185683000	1.410457000	0.316032000
1	-5.214628000	0.455679000	-0.762066000
6	-3.889518000	-2.526624000	-0.376586000
1	-4.425976000	-2.862273000	0.515013000
1	-4.586804000	-2.570600000	-1.215418000
1	-3.074632000	-3.228913000	-0.567233000
6	-0.767682000	2.170622000	0.558853000
6	-0.416887000	3.382959000	-0.280614000
1	-0.538601000	3.173063000	-1.345557000
1	-1.055460000	4.229305000	-0.017827000
1	0.620541000	3.688630000	-0.112030000
6	-0.584748000	2.442679000	2.038794000
1	0.467232000	2.646190000	2.257001000
1	-1.173992000	3.307093000	2.355571000
1	-0.894027000	1.577166000	2.628719000
1	-1.831420000	1.949262000	0.384456000
6	3.982355000	-0.860272000	0.154551000
1	4.399942000	0.098751000	0.486786000
6	4.322243000	-1.890836000	1.214269000
1	5.403177000	-1.937956000	1.363291000
1	3.853010000	-1.638378000	2.166876000
1	3.990349000	-2.891876000	0.925431000
6	4.609537000	-1.198730000	-1.186374000
1	4.364593000	-0.436656000	-1.929358000
1	5.696877000	-1.265533000	-1.103583000
1	4.242613000	-2.161029000	-1.555803000

1	2.125791000	1.575615000	-1.779744000
1	2.636690000	2.131654000	0.853883000

I_P^{H-H}

6	0.836577000	1.216716000	-0.224198000
6	2.259154000	0.707244000	-0.518746000
6	2.369445000	-0.697062000	0.066468000
6	0.950329000	-1.191846000	-0.151062000
7	0.112048000	-0.039614000	0.109202000
1	3.022065000	1.389500000	-0.132449000
1	2.400915000	0.643556000	-1.603275000
6	-1.262885000	-0.188794000	0.078014000
6	-2.146567000	0.869987000	0.339954000
6	-3.514129000	0.681880000	0.333709000
6	-4.068167000	-0.561668000	0.074803000
6	-3.212237000	-1.616517000	-0.183541000
6	-1.840061000	-1.440209000	-0.189004000
1	-1.765338000	1.854407000	0.567137000
1	-4.157730000	1.529159000	0.544276000
1	-5.141885000	-0.702943000	0.075933000
1	-3.612702000	-2.602175000	-0.394740000
1	-1.211371000	-2.291711000	-0.411202000
6	2.709205000	-0.690217000	1.551030000
1	2.832493000	-1.714179000	1.914944000
1	3.645299000	-0.154594000	1.732775000
1	1.925354000	-0.222295000	2.148435000
6	3.386362000	-1.541670000	-0.676053000
1	4.394879000	-1.141375000	-0.539186000
1	3.386032000	-2.570790000	-0.305159000
1	3.175020000	-1.566954000	-1.748363000
6	0.868425000	2.207650000	0.934990000
1	-0.121124000	2.566664000	1.214929000
1	1.326927000	1.767769000	1.821371000
1	1.463293000	3.078364000	0.646243000
6	0.277423000	1.883579000	-1.474538000
1	0.959034000	2.673641000	-1.800210000
1	0.189912000	1.154042000	-2.284668000
1	-0.703120000	2.333140000	-1.315868000
1	0.830728000	-1.559651000	-1.186708000
1	0.699732000	-2.020715000	0.520414000

II_P^{H-H}

7	1.408310000	-0.335684000	-0.000002000
6	1.251472000	-1.651368000	-0.000004000
6	0.000000000	-2.271841000	-0.000004000
6	-1.251472000	-1.651368000	-0.000002000
7	-1.408310000	-0.335684000	0.000001000
1	0.000000000	-3.353079000	-0.000006000
13	0.000000000	0.950229000	0.000002000
6	2.710638000	0.239635000	-0.000002000
6	3.330937000	0.557053000	1.201122000
6	3.330934000	0.557059000	-1.201126000
6	4.576692000	1.160511000	1.198642000
1	2.821730000	0.327880000	2.131417000
6	4.576689000	1.160518000	-1.198646000
1	2.821724000	0.327891000	-2.131421000
6	5.203309000	1.460120000	-0.000002000
1	5.057393000	1.403145000	2.139166000
1	5.057387000	1.403156000	-2.139170000
1	6.176672000	1.936148000	-0.000002000
6	-2.710637000	0.239635000	0.000003000
6	-3.330934000	0.557054000	1.201128000
6	-3.330937000	0.557058000	-1.201120000
6	-4.576690000	1.160512000	1.198650000
1	-2.821725000	0.327882000	2.131422000
6	-4.576692000	1.160516000	-1.198638000
1	-2.821729000	0.327889000	-2.131416000
6	-5.203309000	1.460120000	0.000007000
1	-5.057388000	1.403147000	2.139175000
1	-5.057392000	1.403154000	-2.139161000
1	-6.176672000	1.936148000	0.000009000
6	2.461142000	-2.529520000	-0.000007000
1	3.082805000	-2.328789000	-0.875525000
1	3.082807000	-2.328791000	0.875510000
1	2.183377000	-3.580985000	-0.000008000
6	-2.461142000	-2.529520000	-0.000002000
1	-3.082805000	-2.328792000	0.875517000
1	-3.082808000	-2.328788000	-0.875517000
1	-2.183377000	-3.580985000	-0.000004000
1	-0.000001000	1.781661000	-1.358041000
1	0.000001000	1.781656000	1.358047000

III_P$^{H–H}$

6	1.746757000	-1.648017000	-0.237318000
6	0.382523000	-1.645405000	-0.417765000
7	2.540143000	-0.628947000	0.028876000

1	2.221429000	-2.629356000	-0.334012000
1	-0.097677000	-2.588700000	-0.658994000
31	1.949429000	1.218527000	-0.239300000
7	0.027563000	1.003750000	0.149387000
15	-0.741046000	-0.371488000	-0.121458000
7	-1.989277000	-0.287970000	-1.235320000
7	-1.895306000	-0.799070000	1.020716000
14	-3.215476000	-0.818335000	-0.121219000
6	-1.944166000	0.448246000	-2.474060000
1	-2.194692000	-0.180200000	-3.332158000
1	-2.633615000	1.300546000	-2.460789000
1	-0.936623000	0.843455000	-2.637908000
6	-1.605856000	-1.535366000	2.228007000
1	-2.353794000	-1.325337000	2.995437000
1	-1.577337000	-2.619391000	2.062850000
1	-0.633158000	-1.237742000	2.629420000
6	-4.580747000	0.410517000	0.127503000
1	-5.218805000	0.128765000	0.967768000
1	-4.185683000	1.410457000	0.316032000
1	-5.214628000	0.455679000	-0.762066000
6	-3.889518000	-2.526624000	-0.376586000
1	-4.425976000	-2.862273000	0.515013000
1	-4.586804000	-2.570600000	-1.215418000
1	-3.074632000	-3.228913000	-0.567233000
6	-0.767682000	2.170622000	0.558853000
6	-0.416887000	3.382959000	-0.280614000
1	-0.538601000	3.173063000	-1.345557000
1	-1.055460000	4.229305000	-0.017827000
1	0.620541000	3.688630000	-0.112030000
6	-0.584748000	2.442679000	2.038794000
1	0.467232000	2.646190000	2.257001000
1	-1.173992000	3.307093000	2.355571000
1	-0.894027000	1.577166000	2.628719000
1	-1.831420000	1.949262000	0.384456000
6	3.982355000	-0.860272000	0.154551000
1	4.399942000	0.098751000	0.486786000
6	4.322243000	-1.890836000	1.214269000
1	5.403177000	-1.937956000	1.363291000
1	3.853010000	-1.638378000	2.166876000
1	3.990349000	-2.891876000	0.925431000
6	4.609537000	-1.198730000	-1.186374000
1	4.364593000	-0.436656000	-1.929358000
1	5.696877000	-1.265533000	-1.103583000
1	4.242613000	-2.161029000	-1.555803000
1	2.125791000	1.575615000	-1.779744000
1	2.636690000	2.131654000	0.853883000

1_P$^{C–H}$

6	0.545718000	-1.800481000	0.160252000
6	1.914551000	-1.625580000	0.233182000
1	0.111731000	-2.764029000	0.395105000
1	2.502912000	-2.464376000	0.606610000
7	2.566299000	-0.540332000	-0.118326000
15	-0.515433000	-0.460784000	0.023007000
5	1.828446000	0.628858000	-0.872559000
7	-1.827659000	-0.697656000	-0.993905000
7	-1.622404000	-0.273360000	1.261329000
14	-3.024372000	-0.477990000	0.247501000
6	-1.319023000	0.173645000	2.595204000
1	-0.262170000	-0.002447000	2.818308000
1	-1.511688000	1.244815000	2.731355000
1	-1.904893000	-0.373574000	3.337206000
6	-4.052240000	-1.984468000	0.575301000
1	-4.713765000	-2.185535000	-0.271609000
1	-3.415146000	-2.857485000	0.727157000
1	-4.682952000	-1.855648000	1.457587000
6	-4.093205000	1.032284000	0.108710000
1	-4.899839000	0.881738000	-0.612174000
1	-4.555569000	1.265760000	1.071432000
1	-3.506998000	1.897455000	-0.208344000
6	-1.782992000	-1.165034000	-2.355518000
1	-2.735833000	-1.623188000	-2.630037000
1	-1.580168000	-0.355349000	-3.064164000
1	-1.002572000	-1.922085000	-2.482641000
6	3.989009000	-0.371958000	0.167428000
6	4.790543000	-1.656439000	0.148321000
6	4.155597000	0.361948000	1.485949000
1	4.368480000	0.270666000	-0.636116000
1	4.616089000	-2.224027000	-0.768226000
1	5.854101000	-1.417492000	0.204494000
1	4.562860000	-2.299907000	1.002804000
1	3.587855000	1.294657000	1.479184000
1	3.780472000	-0.260856000	2.304854000
1	5.205294000	0.592788000	1.683719000
7	0.422343000	0.829719000	-0.181643000
6	-0.152708000	2.167925000	-0.011346000
6	-0.329956000	2.882414000	-1.337360000
6	0.660312000	2.993735000	0.968151000
1	-1.152473000	2.041929000	0.427735000
1	-0.946968000	2.288345000	-2.017173000

1	-0.813415000	3.851650000	-1.189915000
1	0.636435000	3.053888000	-1.817326000
1	0.765792000	2.469252000	1.920949000
1	1.660422000	3.188597000	0.577022000
1	0.171831000	3.953718000	1.152849000
1	2.473795000	1.644800000	-0.703881000
6	1.737030000	0.238452000	-2.439244000
1	1.219879000	-0.714419000	-2.608357000
1	1.212873000	0.998179000	-3.028719000
1	2.738240000	0.134267000	-2.873391000

2_P^{C-H}

7	2.618779000	-0.538198000	0.055256000
6	1.865319000	-1.554337000	-0.323705000
6	0.504484000	-1.566693000	-0.524891000
1	2.370439000	-2.505835000	-0.515139000
1	0.046330000	-2.486434000	-0.874173000
13	2.002932000	1.255846000	0.039814000
6	-0.701943000	2.096862000	0.851134000
1	-1.751344000	1.904781000	0.582949000
6	-0.604975000	2.135659000	2.363398000
1	-1.225842000	2.935905000	2.774381000
1	-0.934008000	1.187579000	2.794016000
1	0.429710000	2.310521000	2.669889000
6	-0.319837000	3.426990000	0.233420000
1	-0.403410000	3.395220000	-0.854968000
1	-0.970599000	4.220411000	0.607595000
1	0.709281000	3.698256000	0.489780000
6	4.061852000	-0.752603000	0.217667000
1	4.475628000	0.235888000	0.459594000
6	4.727170000	-1.221081000	-1.063679000
1	4.480657000	-0.553295000	-1.892082000
1	5.812864000	-1.240675000	-0.946049000
1	4.409348000	-2.231502000	-1.335508000
6	4.364686000	-1.669106000	1.387016000
1	5.442121000	-1.751166000	1.547575000
1	3.905968000	-1.289013000	2.301833000
1	3.978030000	-2.676460000	1.205810000
15	-0.633832000	-0.335887000	-0.122332000
7	-1.855182000	-0.118213000	-1.245588000
7	-1.810800000	-0.890437000	0.936813000
14	-3.106645000	-0.772738000	-0.227774000
6	-3.774000000	-2.437178000	-0.697336000
1	-4.340326000	-2.870058000	0.131557000

1	-4.443509000	-2.379597000	-1.557724000
1	-2.955149000	-3.117704000	-0.941987000
6	-4.477475000	0.422213000	0.129149000
1	-4.089340000	1.392485000	0.444232000
1	-5.089120000	0.572738000	-0.764367000
1	-5.135865000	0.043942000	0.913985000
6	-1.790714000	0.766071000	-2.382839000
1	-0.802774000	1.233927000	-2.438836000
1	-1.959486000	0.237112000	-3.324004000
1	-2.530148000	1.571324000	-2.305167000
6	-1.549852000	-1.760500000	2.059232000
1	-2.261545000	-1.574691000	2.866602000
1	-1.605239000	-2.821782000	1.788657000
1	-0.548469000	-1.574559000	2.456951000
7	0.131564000	1.005312000	0.309052000
1	2.639872000	2.036276000	1.285513000
6	2.403267000	1.968160000	-1.757186000
1	1.993799000	1.297099000	-2.522477000
1	1.993578000	2.965208000	-1.944684000
1	3.482544000	2.028755000	-1.934539000

3_P$^{C–H}$

7	2.413753000	-0.791276000	0.101931000
6	1.602358000	-1.725722000	-0.351057000
6	0.250697000	-1.634925000	-0.599938000
1	2.045409000	-2.703019000	-0.568689000
1	-0.250721000	-2.510065000	-1.001365000
6	-0.809859000	2.033614000	0.900097000
1	-1.876426000	1.876572000	0.678090000
6	-0.648005000	2.065864000	2.407168000
1	-1.220459000	2.886834000	2.846647000
1	-0.991871000	1.128327000	2.849226000
1	0.404491000	2.201626000	2.670351000
6	-0.409596000	3.351197000	0.266860000
1	-0.537940000	3.320209000	-0.817423000
1	-1.015655000	4.168398000	0.664544000
1	0.638682000	3.584108000	0.479208000
6	3.833285000	-1.107868000	0.280700000
1	4.280989000	-0.197728000	0.700458000
6	4.520406000	-1.390641000	-1.044015000
1	4.354078000	-0.571729000	-1.747440000
1	5.596916000	-1.514934000	-0.905390000
1	4.135904000	-2.308551000	-1.498086000
6	4.055017000	-2.225540000	1.281943000

1	5.121692000	-2.362099000	1.473668000
1	3.559348000	-2.001811000	2.228278000
1	3.664441000	-3.177077000	0.910244000
15	-0.840042000	-0.381098000	-0.140354000
7	-2.074333000	-0.113841000	-1.241468000
7	-2.019010000	-0.930344000	0.925378000
14	-3.324820000	-0.760598000	-0.218835000
6	-4.036796000	-2.399754000	-0.713773000
1	-4.598639000	-2.838653000	0.115071000
1	-4.718466000	-2.310166000	-1.561779000
1	-3.236189000	-3.091718000	-0.985594000
6	-4.663619000	0.457650000	0.180940000
1	-4.246542000	1.412458000	0.506403000
1	-5.285754000	0.638650000	-0.699565000
1	-5.317879000	0.081335000	0.970155000
6	-2.004938000	0.792070000	-2.360585000
1	-0.992675000	1.198272000	-2.451591000
1	-2.247019000	0.296782000	-3.304163000
1	-2.688085000	1.640175000	-2.234339000
6	-1.756485000	-1.838274000	2.016319000
1	-2.483158000	-1.697602000	2.819365000
1	-1.786385000	-2.889657000	1.704929000
1	-0.764508000	-1.648288000	2.436088000
7	-0.040608000	0.922668000	0.322090000
1	2.569888000	1.845869000	1.268543000
6	2.232836000	1.703493000	-1.839442000
1	1.801610000	0.965687000	-2.522889000
1	1.773830000	2.672579000	-2.047640000
1	3.299760000	1.783058000	-2.060084000
31	1.909969000	1.109341000	0.030547000

I_P$^{C–H}$

6	-0.759445000	1.353573000	0.189044000
6	-2.231227000	0.909554000	0.240427000
6	-2.297851000	-0.501671000	-0.332422000
6	-0.954784000	-1.076770000	0.134070000
7	-0.049198000	0.064681000	0.016488000
1	-2.880143000	1.608142000	-0.295769000
1	-2.574674000	0.892815000	1.279885000
6	1.316824000	-0.113749000	-0.044058000
6	1.868890000	-1.402381000	-0.174265000
6	3.232474000	-1.601716000	-0.267299000
6	4.119874000	-0.540442000	-0.228182000
6	3.597347000	0.733429000	-0.090415000

6	2.235616000	0.949058000	0.002373000
1	1.225526000	-2.270610000	-0.206349000
1	3.602591000	-2.616200000	-0.369929000
1	5.188293000	-0.701860000	-0.298246000
1	4.260677000	1.590818000	-0.050672000
1	1.893419000	1.965875000	0.112063000
6	-2.335525000	-0.503752000	-1.857441000
1	-2.480517000	-1.522464000	-2.228017000
1	-3.162752000	0.108405000	-2.227956000
1	-1.408646000	-0.126706000	-2.292214000
6	-3.512423000	-1.257629000	0.173504000
1	-4.423833000	-0.804269000	-0.226355000
1	-3.492204000	-2.300619000	-0.156730000
1	-3.587898000	-1.246345000	1.262256000
6	-0.548296000	2.306662000	-0.985598000
1	0.495365000	2.581378000	-1.129839000
1	-0.909877000	1.873645000	-1.918630000
1	-1.110998000	3.226041000	-0.803908000
6	-0.410230000	2.053413000	1.500908000
1	-1.125858000	2.860771000	1.678831000
1	-0.473670000	1.352810000	2.336658000
1	0.586692000	2.492752000	1.505980000
1	-0.652606000	-1.857938000	-0.574552000
6	-0.952711000	-1.661556000	1.537198000
1	0.067105000	-1.889999000	1.851506000
1	-1.370120000	-0.959859000	2.263547000
1	-1.532690000	-2.585471000	1.585962000

II_P^{C-H}

7	-1.408146000	0.475263000	0.116872000
6	-1.251480000	1.782603000	-0.028762000
6	0.000000000	2.402338000	-0.066656000
6	1.251480000	1.782603000	-0.028762000
7	1.408146000	0.475263000	0.116872000
1	0.000000000	3.478873000	-0.168350000
13	0.000000000	-0.791283000	0.387463000
6	-2.705117000	-0.108497000	0.089964000
6	-3.329999000	-0.458546000	1.279468000
6	-3.314478000	-0.410125000	-1.121601000
6	-4.566907000	-1.081364000	1.255405000
1	-2.832836000	-0.238717000	2.218238000
6	-4.550242000	-1.031621000	-1.140749000
1	-2.800993000	-0.159032000	-2.044229000
6	-5.180825000	-1.366064000	0.047396000

1	-5.050632000	-1.348774000	2.187640000
1	-5.020110000	-1.263146000	-2.089570000
1	-6.146712000	-1.856753000	0.030482000
6	2.705117000	-0.108497000	0.089964000
6	3.329998000	-0.458548000	1.279468000
6	3.314479000	-0.410124000	-1.121601000
6	4.566906000	-1.081365000	1.255405000
1	2.832835000	-0.238719000	2.218238000
6	4.550243000	-1.031620000	-1.140749000
1	2.800994000	-0.159030000	-2.044228000
6	5.180825000	-1.366064000	0.047396000
1	5.050631000	-1.348776000	2.187640000
1	5.020111000	-1.263144000	-2.089570000
1	6.146712000	-1.856753000	0.030481000
6	-2.459199000	2.654297000	-0.161565000
1	-2.990596000	2.438152000	-1.091137000
1	-3.163590000	2.465817000	0.651578000
1	-2.184705000	3.706763000	-0.157652000
6	2.459199000	2.654297000	-0.161565000
1	3.163591000	2.465817000	0.651578000
1	2.990596000	2.438153000	-1.091136000
1	2.184705000	3.706763000	-0.157651000
1	0.000000000	-1.291725000	1.903622000
6	0.000000000	-2.153738000	-1.020254000
1	0.000001000	-1.700257000	-2.017195000
1	0.879803000	-2.801148000	-0.957603000
1	-0.879804000	-2.801147000	-0.957605000

III_P^{C-H}

7	-1.442926000	0.573195000	-0.175343000
6	-1.258164000	1.878147000	-0.090003000
6	0.000000000	2.488847000	-0.122084000
6	1.258165000	1.878147000	-0.090009000
7	1.442927000	0.573196000	-0.175350000
1	0.000000000	3.570052000	-0.090073000
6	-2.721634000	-0.011983000	-0.010127000
6	-3.302175000	-0.109517000	1.249343000
6	-3.361973000	-0.583152000	-1.103261000
6	-4.520405000	-0.745677000	1.406599000
1	-2.778161000	0.307188000	2.103418000
6	-4.580676000	-1.220370000	-0.940628000
1	-2.891706000	-0.519151000	-2.078884000
6	-5.165153000	-1.300444000	0.312224000
1	-4.964889000	-0.817010000	2.392608000

1	-5.075114000	-1.658242000	-1.800014000
1	-6.117212000	-1.802086000	0.438130000
6	2.721635000	-0.011982000	-0.010133000
6	3.302189000	-0.109487000	1.249334000
6	3.361959000	-0.583182000	-1.103258000
6	4.520419000	-0.745648000	1.406592000
1	2.778187000	0.307241000	2.103404000
6	4.580661000	-1.220402000	-0.940623000
1	2.891683000	-0.519204000	-2.078879000
6	5.165153000	-1.300446000	0.312224000
1	4.964914000	-0.816958000	2.392598000
1	5.075088000	-1.658297000	-1.800003000
1	6.117211000	-1.802089000	0.438133000
31	-0.000001000	-0.742711000	-0.539790000
6	-2.447480000	2.777808000	0.052741000
1	-3.245631000	2.483643000	-0.631453000
1	-2.858805000	2.719034000	1.062828000
1	-2.174036000	3.813203000	-0.140089000
6	2.447479000	2.777811000	0.052730000
1	2.858788000	2.719064000	1.062825000
1	3.245642000	2.483629000	-0.631444000
1	2.174038000	3.813201000	-0.140130000
1	-0.000007000	-1.091818000	-2.082490000
6	0.000002000	-2.100115000	0.891427000
1	-0.000034000	-1.605949000	1.866312000
1	-0.883774000	-2.738166000	0.831484000
1	0.883817000	-2.738117000	0.831524000

1_P^{N-H}

6	-0.558391000	-1.795558000	-0.332660000
6	-1.926129000	-1.634817000	-0.214700000
1	-0.135054000	-2.790529000	-0.382377000
1	-2.523271000	-2.539558000	-0.096002000
7	-2.564676000	-0.487262000	-0.258244000
15	0.516336000	-0.477607000	-0.107767000
5	-1.815106000	0.839591000	-0.701481000
7	1.615578000	-0.656894000	1.136911000
7	1.832740000	-0.400095000	-1.141203000
14	3.023337000	-0.548461000	0.115975000
6	1.797681000	0.019637000	-2.520979000
1	0.889380000	0.599112000	-2.720279000
1	2.652739000	0.663178000	-2.748429000
1	1.819612000	-0.828054000	-3.212568000
6	4.052278000	-2.089747000	0.127222000

1	4.543265000	-2.214434000	1.095990000
1	3.429405000	-2.967015000	-0.055939000
1	4.835145000	-2.054003000	-0.633297000
6	4.093210000	0.957183000	0.292774000
1	4.679399000	0.931573000	1.213831000
1	4.799671000	1.013134000	-0.539914000
1	3.492168000	1.869019000	0.288107000
6	1.290186000	-0.890556000	2.518179000
1	1.335283000	0.027367000	3.114578000
1	0.275363000	-1.292309000	2.603306000
1	1.970881000	-1.619698000	2.965556000
6	-3.988981000	-0.385382000	0.046205000
6	-4.166549000	0.018986000	1.498895000
6	-4.795986000	-1.624619000	-0.278282000
1	-4.361128000	0.430252000	-0.586437000
1	-3.600701000	0.926966000	1.716578000
1	-5.218257000	0.196729000	1.737006000
1	-3.796054000	-0.778427000	2.151502000
1	-4.622659000	-1.961244000	-1.302653000
1	-4.573137000	-2.452760000	0.400464000
1	-5.858535000	-1.400184000	-0.168596000
7	-0.416737000	0.825596000	0.019979000
6	0.166863000	2.067716000	0.542309000
6	-0.658354000	2.610130000	1.694202000
6	0.371974000	3.104818000	-0.544049000
1	1.154317000	1.814382000	0.953527000
1	-0.795222000	1.845061000	2.462613000
1	-0.159376000	3.470914000	2.146137000
1	-1.645383000	2.928415000	1.353694000
1	1.016051000	2.716535000	-1.336879000
1	-0.580802000	3.382251000	-0.999378000
1	0.834767000	4.004295000	-0.129004000
1	-2.463567000	1.778317000	-0.290233000
7	-1.681450000	0.931363000	-2.208823000
1	-1.426759000	0.057081000	-2.657043000
1	-2.528767000	1.252518000	-2.658627000

2_P^{N-H}

7	2.612459000	-0.551925000	0.046988000
6	1.851375000	-1.585283000	-0.266258000
6	0.487139000	-1.614051000	-0.431601000
1	2.356595000	-2.542798000	-0.424076000
1	0.024609000	-2.551866000	-0.721914000
13	2.020264000	1.242840000	0.060819000

6	-0.697345000	2.117030000	0.757978000
1	-1.737543000	1.931531000	0.451695000
6	-0.663768000	2.204750000	2.271293000
1	-1.286806000	3.029003000	2.628349000
1	-1.027807000	1.277885000	2.719554000
1	0.360099000	2.372653000	2.615288000
6	-0.274457000	3.424258000	0.117082000
1	-0.284897000	3.352273000	-0.972080000
1	-0.949378000	4.227347000	0.421893000
1	0.735574000	3.707579000	0.428948000
6	4.059761000	-0.767432000	0.188121000
1	4.476343000	0.217793000	0.433900000
6	4.702371000	-1.216430000	-1.110526000
1	4.472733000	-0.510447000	-1.911095000
1	5.787782000	-1.274106000	-1.001722000
1	4.348731000	-2.207021000	-1.410765000
6	4.382314000	-1.698641000	1.340788000
1	5.462228000	-1.767550000	1.489851000
1	3.928116000	-1.337814000	2.265740000
1	4.010138000	-2.709742000	1.151164000
15	-0.639327000	-0.352944000	-0.099536000
7	-1.838336000	-0.158052000	-1.253031000
7	-1.844661000	-0.854234000	0.954105000
14	-3.117566000	-0.756760000	-0.236473000
6	-3.805142000	-2.426272000	-0.657089000
1	-4.385595000	-2.821666000	0.180800000
1	-4.465685000	-2.389191000	-1.525471000
1	-2.994318000	-3.126913000	-0.869519000
6	-4.474768000	0.471743000	0.053853000
1	-4.076681000	1.442050000	0.356217000
1	-5.058358000	0.611924000	-0.859948000
1	-5.162136000	0.125554000	0.828564000
6	-1.739593000	0.683046000	-2.419683000
1	-0.747199000	1.142457000	-2.467712000
1	-1.890113000	0.121317000	-3.345021000
1	-2.474401000	1.495779000	-2.389576000
6	-1.621034000	-1.679411000	2.117386000
1	-2.341555000	-1.443910000	2.903858000
1	-1.695201000	-2.750078000	1.892154000
1	-0.622535000	-1.497162000	2.523802000
7	0.140086000	0.993236000	0.288106000
1	2.595466000	2.050355000	1.312893000
7	2.544038000	1.950914000	-1.517863000
1	2.648298000	2.939011000	-1.687048000
1	2.429678000	1.478225000	-2.401901000

3_P^{N-H}

7	2.428753000	-0.771801000	0.112186000
6	1.619934000	-1.732541000	-0.291581000
6	0.264364000	-1.663894000	-0.521885000
1	2.070424000	-2.712081000	-0.481172000
1	-0.233225000	-2.556533000	-0.888153000
6	-0.794588000	2.027141000	0.918535000
1	-1.861962000	1.859943000	0.709547000
6	-0.617260000	2.085844000	2.422927000
1	-1.185450000	2.913867000	2.854622000
1	-0.952101000	1.155645000	2.887176000
1	0.438357000	2.229561000	2.670529000
6	-0.405536000	3.335636000	0.260390000
1	-0.505518000	3.279220000	-0.824820000
1	-1.033711000	4.148265000	0.632801000
1	0.634559000	3.591296000	0.484187000
6	3.855435000	-1.064693000	0.274842000
1	4.295582000	-0.141036000	0.672007000
6	4.525730000	-1.358991000	-1.055995000
1	4.343240000	-0.548644000	-1.765247000
1	5.604966000	-1.475105000	-0.931799000
1	4.139803000	-2.284578000	-1.493282000
6	4.111308000	-2.162112000	1.290279000
1	5.182922000	-2.272925000	1.470512000
1	3.622935000	-1.934312000	2.239418000
1	3.737621000	-3.127964000	0.938885000
15	-0.831269000	-0.398624000	-0.102153000
7	-2.037623000	-0.128032000	-1.231598000
7	-2.034959000	-0.929854000	0.941163000
14	-3.315822000	-0.754553000	-0.232241000
6	-4.033536000	-2.391396000	-0.726675000
1	-4.616130000	-2.817464000	0.094506000
1	-4.697296000	-2.302413000	-1.588838000
1	-3.234830000	-3.093632000	-0.976801000
6	-4.650482000	0.479035000	0.131687000
1	-4.231195000	1.431993000	0.459588000
1	-5.251225000	0.660319000	-0.763501000
1	-5.325677000	0.114293000	0.908606000
6	-1.931905000	0.771334000	-2.355005000
1	-0.926382000	1.202477000	-2.398737000
1	-2.118855000	0.263423000	-3.304453000
1	-2.639759000	1.603499000	-2.267428000
6	-1.808764000	-1.824435000	2.050975000
1	-2.544764000	-1.655464000	2.839939000

1	-1.856414000	-2.879946000	1.756306000
1	-0.819872000	-1.648165000	2.483177000
7	-0.026421000	0.901733000	0.362785000
1	2.650585000	1.983822000	1.034900000
7	1.984282000	1.664335000	-1.835068000
1	2.883620000	2.050400000	-2.096822000
1	1.805900000	0.897836000	-2.476454000
31	1.887354000	1.111202000	-0.030089000

I_P$^{N–H}$

6	0.664072000	1.346440000	0.321355000
6	2.139030000	0.987671000	0.594396000
6	2.390408000	-0.383356000	-0.023183000
6	0.999895000	-1.017524000	0.152007000
7	0.108166000	0.069042000	-0.205576000
1	2.304574000	0.930614000	1.675525000
1	2.821678000	1.749563000	0.206831000
6	-1.284622000	-0.140673000	-0.131543000
6	-1.859591000	-1.014926000	0.788649000
6	-3.231982000	-1.177800000	0.846859000
6	-4.063122000	-0.467800000	-0.004214000
6	-3.501546000	0.395504000	-0.930087000
6	-2.128028000	0.546844000	-1.001784000
1	-1.225555000	-1.576973000	1.463742000
1	-3.656524000	-1.865695000	1.569706000
1	-5.137886000	-0.596858000	0.044886000
1	-4.135877000	0.942865000	-1.618347000
1	-1.689171000	1.186874000	-1.758004000
6	3.455913000	-1.160200000	0.723395000
1	3.576139000	-2.165823000	0.307910000
1	4.425258000	-0.659476000	0.649636000
1	3.207501000	-1.257584000	1.784035000
6	2.779358000	-0.271732000	-1.489446000
1	3.687845000	0.328362000	-1.588419000
1	2.989465000	-1.254183000	-1.921277000
1	1.995468000	0.199456000	-2.085817000
6	-0.015530000	1.763096000	1.619130000
1	-1.057570000	2.048951000	1.456824000
1	0.004925000	0.949869000	2.350151000
1	0.507658000	2.619814000	2.052062000
6	0.547071000	2.475128000	-0.689876000
1	1.059700000	3.363429000	-0.310659000
1	0.999673000	2.199753000	-1.644898000
1	-0.494789000	2.748695000	-0.866022000

1	0.913864000	-1.299347000	1.222658000
7	0.677519000	-2.194282000	-0.609269000
1	0.796595000	-2.022809000	-1.601031000
1	1.259279000	-2.976854000	-0.339523000

II_P^{N-H}

7	-1.403882000	0.423193000	0.013324000
6	-1.250154000	1.736828000	-0.078090000
6	0.000021000	2.355645000	-0.136624000
6	1.250221000	1.736819000	-0.077915000
7	1.403855000	0.423241000	0.013624000
1	0.000011000	3.434387000	-0.210880000
13	-0.000025000	-0.873179000	0.002427000
6	-2.709937000	-0.138059000	0.103876000
6	-3.243175000	-0.442380000	1.348964000
6	-3.426447000	-0.447163000	-1.044473000
6	-4.495228000	-1.025907000	1.444201000
1	-2.661235000	-0.219433000	2.237009000
6	-4.677964000	-1.029003000	-0.945322000
1	-2.984838000	-0.232565000	-2.011804000
6	-5.216785000	-1.316861000	0.298484000
1	-4.905977000	-1.258650000	2.419771000
1	-5.232453000	-1.266098000	-1.845889000
1	-6.194991000	-1.776795000	0.373949000
6	2.709872000	-0.138110000	0.104070000
6	3.242312000	-0.444215000	1.349058000
6	3.427166000	-0.445404000	-1.044295000
6	4.494374000	-1.027758000	1.444250000
1	2.659697000	-0.222661000	2.237008000
6	4.678670000	-1.027211000	-0.945177000
1	2.986014000	-0.229508000	-2.011538000
6	5.216704000	-1.316871000	0.298574000
1	4.904523000	-1.261938000	2.419728000
1	5.233821000	-1.262922000	-1.845700000
1	6.194938000	-1.776760000	0.373970000
6	-2.458865000	2.616865000	-0.109551000
1	-3.082286000	2.388264000	-0.976799000
1	-3.080626000	2.449053000	0.772753000
1	-2.178063000	3.666954000	-0.147791000
6	2.458974000	2.616796000	-0.109080000
1	3.080318000	2.448890000	0.773524000
1	3.082779000	2.388212000	-0.976034000
1	2.178228000	3.666897000	-0.147370000
1	-0.000020000	-1.738550000	1.335071000

7	0.000777000	-1.854368000	-1.493722000
1	0.000522000	-2.860897000	-1.497959000
1	-0.003822000	-1.513085000	-2.440842000

III_P^{N-H}

7	-1.448922000	0.549276000	-0.144182000
6	-1.259508000	1.849202000	-0.004666000
6	-0.000017000	2.456388000	0.020869000
6	1.259449000	1.849203000	-0.004821000
7	1.448875000	0.549238000	-0.144267000
1	-0.000008000	3.534157000	0.110235000
6	-2.741654000	-0.029027000	-0.074462000
6	-3.335122000	-0.278464000	1.157550000
6	-3.382798000	-0.430596000	-1.239664000
6	-4.570406000	-0.899274000	1.218405000
1	-2.806678000	0.008762000	2.060782000
6	-4.618740000	-1.051189000	-1.172953000
1	-2.898211000	-0.250125000	-2.193394000
6	-5.216941000	-1.283963000	0.054428000
1	-5.027958000	-1.089645000	2.182382000
1	-5.115166000	-1.357447000	-2.086450000
1	-6.182800000	-1.772439000	0.104944000
6	2.741622000	-0.029032000	-0.074574000
6	3.335763000	-0.277237000	1.157369000
6	3.382144000	-0.431823000	-1.239701000
6	4.571058000	-0.898020000	1.218204000
1	2.807859000	0.010935000	2.060617000
6	4.618102000	-1.052389000	-1.173014000
1	2.897079000	-0.252294000	-2.193363000
6	5.216962000	-1.283923000	0.054278000
1	5.029116000	-1.087414000	2.182133000
1	5.114030000	-1.359585000	-2.086466000
1	6.182836000	-1.772370000	0.104777000
31	-0.000032000	-0.768182000	-0.325943000
6	-2.453425000	2.741905000	0.132417000
1	-3.188499000	2.530080000	-0.646872000
1	-2.952154000	2.572003000	1.089279000
1	-2.166783000	3.789718000	0.076507000
6	2.453354000	2.741981000	0.131938000
1	2.951764000	2.572890000	1.089108000
1	3.188686000	2.529547000	-0.646939000
1	2.166717000	3.789748000	0.075112000
1	-0.000331000	-1.408430000	-1.767258000
7	0.000076000	-1.756403000	1.276843000

1	-0.806736000	-2.367299000	1.349590000
1	0.808945000	-2.364387000	1.351146000

1_P^{P-H}

6	-0.437630000	-1.826259000	0.036959000
6	-1.796671000	-1.675502000	0.220671000
1	0.003735000	-2.814427000	0.062076000
1	-2.372840000	-2.569217000	0.458333000
7	-2.463192000	-0.546039000	0.103989000
15	0.623810000	-0.479236000	0.053312000
5	-1.771642000	0.733681000	-0.421979000
7	1.813361000	-0.500340000	1.220304000
7	1.849647000	-0.506873000	-1.082243000
14	3.138920000	-0.517603000	0.085879000
6	1.691992000	-0.644675000	-2.509305000
1	1.099909000	0.175596000	-2.930057000
1	2.669028000	-0.632941000	-2.995089000
1	1.194477000	-1.583484000	-2.773397000
6	4.164970000	-2.059448000	0.108719000
1	4.813665000	-2.087811000	0.987342000
1	3.527250000	-2.944985000	0.120510000
1	4.808607000	-2.109744000	-0.772914000
6	4.212956000	0.993099000	0.099093000
1	4.809084000	1.041550000	1.013585000
1	4.909168000	0.980739000	-0.742942000
1	3.610518000	1.901183000	0.030275000
6	1.603667000	-0.393340000	2.640204000
1	1.715655000	0.635155000	3.002661000
1	0.594320000	-0.728641000	2.897997000
1	2.306883000	-1.024617000	3.187858000
6	-3.889968000	-0.467003000	0.423368000
6	-4.068771000	-0.140908000	1.893580000
6	-4.679757000	-1.692236000	0.014274000
1	-4.262921000	0.377006000	-0.167256000
1	-3.504055000	0.756340000	2.157523000
1	-5.120611000	0.025166000	2.138164000
1	-3.701119000	-0.968989000	2.508109000
1	-4.479850000	-1.956864000	-1.026850000
1	-4.459878000	-2.559961000	0.642115000
1	-5.746743000	-1.486735000	0.117359000
7	-0.326204000	0.822493000	0.141464000
6	0.255065000	2.113461000	0.536687000
6	-0.489842000	2.704474000	1.718878000
6	0.333673000	3.082699000	-0.625884000

1	1.282752000	1.914342000	0.870064000
1	-0.526574000	1.992944000	2.547447000
1	0.008959000	3.613093000	2.064251000
1	-1.515289000	2.962692000	1.448016000
1	0.912903000	2.658280000	-1.449798000
1	-0.662426000	3.320343000	-1.006540000
1	0.810037000	4.014924000	-0.311885000
1	-2.405256000	1.704446000	-0.080282000
15	-1.829254000	0.753960000	-2.443631000
1	-1.595833000	-0.628473000	-2.697392000
1	-3.241950000	0.629404000	-2.564962000

2_P^{P-H}

7	-2.517641000	-0.693275000	0.277399000
6	-1.735804000	-1.719619000	-0.019419000
6	-0.375968000	-1.714646000	-0.210782000
1	-2.220198000	-2.692070000	-0.141496000
1	0.102388000	-2.645412000	-0.498188000
13	-1.902596000	1.083371000	0.207495000
6	0.767145000	2.039797000	0.972116000
1	1.817778000	1.720480000	1.018415000
6	0.668543000	3.148274000	-0.057216000
1	1.329087000	3.978808000	0.202609000
1	0.941773000	2.782959000	-1.050336000
1	-0.351856000	3.542910000	-0.109495000
6	0.377919000	2.521824000	2.355361000
1	0.475579000	1.719220000	3.089177000
1	1.016697000	3.352893000	2.663689000
1	-0.659450000	2.864850000	2.368841000
6	-3.955794000	-0.926511000	0.465557000
1	-4.400878000	0.073161000	0.560640000
6	-4.228234000	-1.672804000	1.756675000
1	-3.790759000	-1.143717000	2.605655000
1	-5.302050000	-1.776308000	1.928343000
1	-3.796241000	-2.677579000	1.723011000
6	-4.604671000	-1.597311000	-0.731065000
1	-5.690225000	-1.611467000	-0.613914000
1	-4.364151000	-1.063393000	-1.653223000
1	-4.276679000	-2.634218000	-0.842816000
15	0.739342000	-0.426386000	0.065453000
7	2.043154000	-0.848404000	1.017839000
7	1.821748000	-0.223671000	-1.195209000
14	3.209409000	-0.740897000	-0.274348000
6	3.912934000	-2.347845000	-0.871659000

1	4.410536000	-2.211457000	-1.835424000
1	4.650907000	-2.752989000	-0.176408000
1	3.117924000	-3.085670000	-1.000704000
6	4.542716000	0.512444000	0.016029000
1	4.121757000	1.484008000	0.281282000
1	5.196936000	0.188893000	0.829938000
1	5.165941000	0.639224000	-0.871733000
6	2.063037000	-0.924810000	2.456260000
1	1.044530000	-0.871541000	2.850242000
1	2.499014000	-1.864812000	2.802621000
1	2.632850000	-0.099955000	2.900185000
6	1.468872000	-0.237585000	-2.597099000
1	2.226836000	0.284132000	-3.184372000
1	1.367929000	-1.255378000	-2.991829000
1	0.516596000	0.277034000	-2.758123000
7	-0.054473000	0.876019000	0.578029000
1	-2.637086000	1.986402000	1.292677000
15	-2.202726000	1.684214000	-2.084924000
1	-3.619556000	1.558668000	-2.023221000
1	-2.226808000	3.091703000	-1.885492000

3_P^{P-H}

7	2.345585000	-0.878270000	-0.304993000
6	1.509925000	-1.864886000	-0.041538000
6	0.150973000	-1.802653000	0.159523000
1	1.943509000	-2.865925000	0.040582000
1	-0.363453000	-2.723608000	0.416049000
6	-0.880880000	2.025708000	-0.902269000
1	-1.942907000	1.748477000	-0.972014000
6	-0.751088000	3.082674000	0.177091000
1	-1.378346000	3.948787000	-0.046974000
1	-1.044341000	2.681970000	1.150791000
1	0.283359000	3.434960000	0.251858000
6	-0.460189000	2.556554000	-2.258317000
1	-0.585295000	1.794186000	-3.029974000
1	-1.058678000	3.428796000	-2.531975000
1	0.591008000	2.855248000	-2.247805000
6	3.770254000	-1.170981000	-0.491366000
1	4.256948000	-0.191487000	-0.586667000
6	4.017912000	-1.933011000	-1.778884000
1	3.599630000	-1.394743000	-2.631535000
1	5.088019000	-2.073174000	-1.948058000
1	3.553850000	-2.923063000	-1.741751000
6	4.385080000	-1.867299000	0.709460000

1	5.468413000	-1.941445000	0.593030000
1	4.173733000	-1.314982000	1.628028000
1	3.999151000	-2.883330000	0.828087000
15	-0.925997000	-0.476114000	-0.077531000
7	-2.241781000	-0.829712000	-1.046939000
7	-2.009484000	-0.300432000	1.190872000
14	-3.406360000	-0.739457000	0.245698000
6	-4.160907000	-2.344040000	0.786099000
1	-4.646581000	-2.226592000	1.758550000
1	-4.917096000	-2.698119000	0.082652000
1	-3.390377000	-3.112346000	0.881826000
6	-4.702186000	0.562361000	-0.001922000
1	-4.250804000	1.529462000	-0.231447000
1	-5.362995000	0.288110000	-0.828582000
1	-5.324314000	0.676461000	0.888331000
6	-2.262972000	-0.822620000	-2.487034000
1	-1.244203000	-0.750952000	-2.877380000
1	-2.703868000	-1.738423000	-2.888084000
1	-2.828381000	0.029864000	-2.882294000
6	-1.666520000	-0.405070000	2.590874000
1	-2.427142000	0.081093000	3.204827000
1	-1.572529000	-1.446329000	2.921786000
1	-0.713478000	0.093810000	2.791533000
7	-0.111185000	0.819726000	-0.557813000
31	1.804158000	0.986487000	-0.130251000
1	2.552777000	1.879801000	-1.194564000
15	2.044221000	1.399524000	2.197891000
1	3.444578000	1.147642000	2.172444000
1	2.208209000	2.806412000	2.083123000

I_P^{P-H}

6	-0.557400000	1.592034000	-0.159762000
6	-2.045014000	1.344537000	-0.465260000
6	-2.360381000	-0.100365000	-0.077206000
6	-0.997883000	-0.757876000	-0.346414000
7	-0.059683000	0.221281000	0.166497000
1	-2.222335000	1.470990000	-1.538438000
1	-2.692595000	2.057471000	0.053533000
6	1.327562000	-0.018109000	0.071131000
6	1.903355000	-0.647349000	-1.031229000
6	3.270061000	-0.855796000	-1.093904000
6	4.092224000	-0.428191000	-0.064487000
6	3.530755000	0.195548000	1.037609000
6	2.162142000	0.386961000	1.109940000

1	1.274414000	-0.972856000	-1.852914000
1	3.696462000	-1.349948000	-1.959667000
1	5.162450000	-0.589499000	-0.116356000
1	4.160625000	0.518458000	1.858774000
1	1.714890000	0.834882000	1.989849000
6	-3.461932000	-0.682246000	-0.941221000
1	-3.659104000	-1.727137000	-0.686595000
1	-4.391340000	-0.123818000	-0.798243000
1	-3.200491000	-0.633904000	-2.002003000
6	-2.761229000	-0.193913000	1.389563000
1	-3.642774000	0.426009000	1.573971000
1	-3.020510000	-1.219817000	1.667876000
1	-1.961613000	0.145255000	2.050687000
6	0.135279000	2.170653000	-1.386045000
1	1.192456000	2.372404000	-1.196674000
1	0.063759000	1.487047000	-2.236750000
1	-0.343033000	3.111484000	-1.670997000
6	-0.370189000	2.537007000	1.014713000
1	-0.814550000	3.508928000	0.783588000
1	-0.847375000	2.145974000	1.915825000
1	0.688286000	2.701250000	1.227150000
1	-0.920734000	-0.897976000	-1.444401000
15	-0.869569000	-2.479459000	0.356363000
1	0.431669000	-2.772253000	-0.120702000
1	-0.411331000	-2.107400000	1.646985000

II_P^{P-H}

7	-1.408419000	0.651145000	0.180775000
6	-1.251444000	1.937594000	-0.099756000
6	0.000000000	2.551983000	-0.186018000
6	1.251444000	1.937595000	-0.099756000
7	1.408419000	0.651146000	0.180775000
1	0.000000000	3.614090000	-0.388945000
13	0.000000000	-0.556483000	0.598274000
6	-2.695870000	0.044824000	0.159088000
6	-3.321005000	-0.284333000	1.354357000
6	-3.284644000	-0.311601000	-1.048091000
6	-4.538574000	-0.944459000	1.339611000
1	-2.839973000	-0.020303000	2.290081000
6	-4.501170000	-0.970034000	-1.056993000
1	-2.768498000	-0.080909000	-1.974546000
6	-5.131986000	-1.285780000	0.136130000
1	-5.022951000	-1.196295000	2.275736000
1	-4.954032000	-1.247274000	-2.001665000

1	-6.082034000	-1.806521000	0.126865000
6	2.695870000	0.044824000	0.159088000
6	3.321005000	-0.284333000	1.354357000
6	3.284644000	-0.311602000	-1.048091000
6	4.538574000	-0.944459000	1.339611000
1	2.839973000	-0.020303000	2.290081000
6	4.501170000	-0.970034000	-1.056993000
1	2.768498000	-0.080909000	-1.974546000
6	5.131986000	-1.285780000	0.136130000
1	5.022951000	-1.196295000	2.275736000
1	4.954032000	-1.247274000	-2.001665000
1	6.082034000	-1.806521000	0.126866000
6	-2.458127000	2.786750000	-0.338567000
1	-2.936289000	2.519701000	-1.283645000
1	-3.203322000	2.632430000	0.444527000
1	-2.191461000	3.840625000	-0.376430000
6	2.458127000	2.786751000	-0.338567000
1	3.203322000	2.632431000	0.444527000
1	2.936289000	2.519702000	-1.283645000
1	2.191461000	3.840626000	-0.376429000
1	0.000000000	-0.942925000	2.140425000
15	0.000000000	-2.319279000	-0.979593000
1	1.038557000	-3.017044000	-0.300541000
1	-1.038557000	-3.017044000	-0.300540000

III_P^{P-H}

7	-1.445294000	0.723007000	-0.191116000
6	-1.258564000	2.011206000	0.037373000
6	-0.000011000	2.620045000	0.074112000
6	1.258547000	2.011221000	0.037339000
7	1.445291000	0.723025000	-0.191164000
1	-0.000015000	3.691450000	0.222650000
6	-2.719354000	0.112207000	-0.081139000
6	-3.296305000	-0.107892000	1.164413000
6	-3.346762000	-0.372574000	-1.222292000
6	-4.498830000	-0.784813000	1.262417000
1	-2.780136000	0.239997000	2.053298000
6	-4.549561000	-1.050360000	-1.118422000
1	-2.877720000	-0.213164000	-2.187455000
6	-5.129865000	-1.256254000	0.122137000
1	-4.939987000	-0.955045000	2.237600000
1	-5.034000000	-1.422306000	-2.013694000
1	-6.068521000	-1.791414000	0.201916000
6	2.719351000	0.112231000	-0.081171000

6	3.296340000	-0.107768000	1.164381000
6	3.346716000	-0.372663000	-1.222301000
6	4.498858000	-0.784698000	1.262407000
1	2.780198000	0.240195000	2.053254000
6	4.549507000	-1.050458000	-1.118410000
1	2.877646000	-0.213332000	-2.187463000
6	5.129849000	-1.256250000	0.122149000
1	4.940041000	-0.954853000	2.237592000
1	5.033911000	-1.422492000	-2.013664000
1	6.068498000	-1.791419000	0.201945000
31	-0.000003000	-0.547259000	-0.633093000
6	-2.448257000	2.889173000	0.273770000
1	-3.255084000	2.653369000	-0.422435000
1	-2.843956000	2.740419000	1.280893000
1	-2.179748000	3.938492000	0.169721000
6	2.448227000	2.889214000	0.273711000
1	2.843839000	2.740600000	1.280889000
1	3.255112000	2.653322000	-0.422396000
1	2.179722000	3.938519000	0.169503000
1	-0.000055000	-0.859490000	-2.181567000
15	0.000042000	-2.230796000	1.012510000
1	-1.036635000	-2.958896000	0.365284000
1	1.037048000	-2.958609000	0.365485000

1_P$^{Si–H}$

6	-0.036342000	0.722477000	-1.715248000
6	1.018135000	1.604003000	-1.620776000
1	-0.470850000	0.499548000	-2.681942000
1	1.359737000	2.084379000	-2.537605000
7	1.657562000	1.910125000	-0.509111000
15	-0.978898000	0.360460000	-0.324992000
5	1.432657000	1.120009000	0.811890000
7	-2.465991000	1.143148000	-0.329630000
7	-1.814837000	-1.079247000	-0.312245000
14	-3.387185000	-0.333476000	-0.439270000
6	-1.331962000	-2.356280000	0.159659000
1	-0.338998000	-2.244965000	0.602358000
1	-1.996352000	-2.760659000	0.930236000
1	-1.249357000	-3.090235000	-0.645570000
6	-4.246680000	-0.498795000	-2.072775000
1	-5.072779000	0.213398000	-2.146192000
1	-3.545644000	-0.291550000	-2.884976000
1	-4.659612000	-1.498613000	-2.219448000
6	-4.511380000	-0.755798000	0.971100000

1	-5.408768000	-0.133821000	0.961629000
1	-4.835760000	-1.797158000	0.897633000
1	-4.009066000	-0.621522000	1.930863000
6	-2.651719000	2.491457000	-0.809881000
1	-3.488642000	2.972377000	-0.299031000
1	-1.757649000	3.090263000	-0.607273000
1	-2.837119000	2.531957000	-1.890072000
6	2.618541000	3.014126000	-0.472247000
6	1.889583000	4.302270000	-0.137399000
6	3.454800000	3.151243000	-1.726925000
1	3.299324000	2.773872000	0.351864000
1	1.301548000	4.182241000	0.775900000
1	2.586934000	5.131389000	0.003890000
1	1.206048000	4.564497000	-0.951939000
1	3.908448000	2.196987000	-2.004484000
1	2.875127000	3.521971000	-2.576684000
1	4.255420000	3.871431000	-1.549604000
7	-0.062828000	0.686835000	0.955216000
6	-0.701399000	0.664361000	2.280008000
6	-0.978379000	2.070245000	2.776329000
6	0.117200000	-0.139237000	3.270481000
1	-1.668238000	0.152807000	2.168711000
1	-1.633247000	2.599175000	2.080160000
1	-1.462226000	2.047816000	3.755822000
1	-0.046611000	2.632942000	2.868680000
1	0.289511000	-1.155208000	2.905450000
1	1.088744000	0.327323000	3.447656000
1	-0.406038000	-0.204105000	4.227070000
1	1.722602000	1.847862000	1.739663000
14	2.834701000	-0.393082000	0.864999000
1	3.304301000	-0.722180000	2.245368000
1	4.061329000	0.040352000	0.121506000
6	2.365921000	-2.071698000	0.132837000
6	2.220551000	-3.206810000	0.929034000
6	2.101420000	-2.205249000	-1.231621000
6	1.822761000	-4.422910000	0.391833000
1	2.425769000	-3.140353000	1.994391000
6	1.710668000	-3.414805000	-1.778300000
1	2.191774000	-1.335745000	-1.878711000
6	1.567268000	-4.529676000	-0.964713000
1	1.717741000	-5.290776000	1.034043000
1	1.515516000	-3.491323000	-2.842637000
1	1.260775000	-5.479070000	-1.389498000

2_P^{Si-H}

7	-1.718680000	1.957137000	-0.420711000
6	-0.939889000	1.815097000	-1.481905000
6	0.272701000	1.179881000	-1.560009000
1	-1.301003000	2.246615000	-2.419551000
1	0.774103000	1.143183000	-2.521525000
13	-1.410639000	1.186510000	1.273493000
6	1.074086000	0.042773000	2.302803000
1	1.902996000	-0.601390000	1.976934000
6	1.657388000	1.200304000	3.090142000
1	2.189155000	0.838006000	3.973728000
1	2.357419000	1.771593000	2.477115000
1	0.862388000	1.873835000	3.421355000
6	0.162903000	-0.809892000	3.162021000
1	-0.255431000	-1.644422000	2.593243000
1	0.717121000	-1.215822000	4.011004000
1	-0.667125000	-0.221983000	3.568350000
6	-2.961626000	2.730594000	-0.553764000
1	-3.474844000	2.626449000	0.412971000
6	-3.892927000	2.173443000	-1.613374000
1	-4.112004000	1.119834000	-1.424635000
1	-4.837341000	2.721514000	-1.613640000
1	-3.464713000	2.260961000	-2.615627000
6	-2.672821000	4.205088000	-0.757547000
1	-3.597376000	4.786593000	-0.759987000
1	-2.028597000	4.581717000	0.039811000
1	-2.168127000	4.376155000	-1.713063000
15	1.206778000	0.516583000	-0.268705000
7	1.962715000	-0.931207000	-0.607410000
7	2.729941000	1.212353000	-0.198843000
14	3.569957000	-0.254575000	-0.627603000
6	4.395872000	-0.146221000	-2.282607000
1	5.258122000	0.524196000	-2.236840000
1	4.754218000	-1.119557000	-2.623380000
1	3.698907000	0.245164000	-3.027109000
6	4.700205000	-0.978188000	0.650240000
1	4.255443000	-0.925681000	1.646019000
1	4.909632000	-2.027031000	0.423957000
1	5.657062000	-0.452488000	0.673609000
6	1.400669000	-2.248913000	-0.425361000
1	0.348188000	-2.176606000	-0.136991000
1	1.444916000	-2.839150000	-1.343372000
1	1.924455000	-2.800566000	0.363972000
6	2.989374000	2.623443000	-0.351143000
1	3.906775000	2.904530000	0.170422000

1	3.084159000	2.923084000	-1.401533000
1	2.174153000	3.207339000	0.086463000
7	0.360615000	0.526257000	1.099118000
1	-1.514789000	2.297652000	2.419318000
14	-3.048503000	-0.669265000	1.381305000
1	-3.257320000	-1.365082000	2.685745000
1	-4.419571000	-0.272358000	0.931312000
6	-2.494610000	-2.028544000	0.185427000
6	-2.224563000	-3.331692000	0.602035000
6	-2.283801000	-1.728512000	-1.162724000
6	-1.776961000	-4.297841000	-0.287391000
1	-2.374248000	-3.599951000	1.644454000
6	-1.844469000	-2.687713000	-2.058832000
1	-2.459562000	-0.715857000	-1.520386000
6	-1.590901000	-3.979346000	-1.622291000
1	-1.578925000	-5.305250000	0.062668000
1	-1.692183000	-2.425602000	-3.100307000
1	-1.245699000	-4.733583000	-2.320557000

3_P$^{Si–H}$

6	0.895628000	-1.625503000	-1.662745000
6	-0.361943000	-1.071651000	-1.664313000
7	1.738896000	-1.751700000	-0.657819000
1	1.233452000	-2.001534000	-2.633496000
1	-0.902542000	-1.043663000	-2.605008000
31	1.451675000	-1.042403000	1.147984000
7	-0.431770000	-0.461155000	1.012170000
15	-1.300518000	-0.501359000	-0.335113000
7	-2.162693000	0.901969000	-0.628104000
7	-2.778315000	-1.297998000	-0.269168000
14	-3.721510000	0.125907000	-0.607126000
6	-1.684235000	2.247605000	-0.420220000
1	-1.816000000	2.865470000	-1.311639000
1	-2.202820000	2.734865000	0.414160000
1	-0.615542000	2.239981000	-0.187420000
6	-2.973175000	-2.717890000	-0.421847000
1	-3.104302000	-3.222373000	0.540667000
1	-3.856798000	-2.923864000	-1.032091000
1	-2.112589000	-3.172036000	-0.923732000
6	-4.842783000	0.744789000	0.734337000
1	-5.769590000	0.168357000	0.770357000
1	-4.362281000	0.682488000	1.712903000
1	-5.114554000	1.788123000	0.552839000
6	-4.616312000	0.017873000	-2.226713000

1	-5.424320000	-0.716504000	-2.172318000
1	-5.062942000	0.974588000	-2.505003000
1	-3.929209000	-0.287272000	-3.018815000
6	-1.130878000	-0.050543000	2.242522000
6	-0.248859000	0.836772000	3.097067000
1	0.113872000	1.699353000	2.531775000
1	-0.805242000	1.202473000	3.962816000
1	0.618126000	0.285866000	3.476244000
6	-1.621417000	-1.255674000	3.022423000
1	-0.778934000	-1.891354000	3.308432000
1	-2.140431000	-0.945518000	3.933178000
1	-2.309752000	-1.852206000	2.420296000
1	-2.006672000	0.550213000	1.956524000
6	3.018400000	-2.435805000	-0.873962000
1	3.567345000	-2.333606000	0.072351000
6	2.816688000	-3.918005000	-1.124702000
1	3.775761000	-4.437418000	-1.184925000
1	2.230245000	-4.365060000	-0.319211000
1	2.285828000	-4.086353000	-2.066339000
6	3.861925000	-1.780598000	-1.951713000
1	4.023401000	-0.722709000	-1.730851000
1	4.837786000	-2.266333000	-2.017831000
1	3.391569000	-1.857032000	-2.935831000
1	1.572791000	-2.241078000	2.184856000
14	2.931420000	0.877683000	1.235938000
1	3.129439000	1.515163000	2.566928000
1	4.294085000	0.533885000	0.733653000
6	2.256489000	2.226218000	0.104712000
6	1.952261000	3.505058000	0.569012000
6	2.002199000	1.948501000	-1.240328000
6	1.427938000	4.472937000	-0.275119000
1	2.133691000	3.752346000	1.611465000
6	1.485421000	2.910634000	-2.090464000
1	2.203279000	0.953013000	-1.630298000
6	1.198554000	4.178964000	-1.608853000
1	1.202844000	5.461760000	0.109353000
1	1.297815000	2.668003000	-3.130754000
1	0.792085000	4.934680000	-2.271576000

I_P$^{Si–H}$

6	2.547285000	1.003234000	0.473246000
6	3.347082000	-0.294944000	0.675227000
6	2.567463000	-1.430983000	0.003636000
6	1.126526000	-0.912772000	0.154556000

7	1.276754000	0.507284000	-0.123835000
1	3.431458000	-0.507902000	1.746093000
1	4.365746000	-0.212579000	0.283744000
6	0.136578000	1.344213000	-0.078353000
6	-0.789149000	1.286792000	0.962156000
6	-1.900900000	2.109075000	0.965825000
6	-2.104313000	3.012979000	-0.064570000
6	-1.189998000	3.082515000	-1.102612000
6	-0.083309000	2.249806000	-1.112157000
1	-0.642152000	0.580529000	1.772013000
1	-2.616352000	2.039768000	1.777475000
1	-2.977356000	3.655116000	-0.062074000
1	-1.346463000	3.777709000	-1.919613000
1	0.620729000	2.269952000	-1.937059000
6	2.788030000	-2.748552000	0.721397000
1	2.217543000	-3.559223000	0.260254000
1	3.845074000	-3.028039000	0.687432000
1	2.492795000	-2.679733000	1.772241000
6	2.976855000	-1.571733000	-1.457459000
1	4.049873000	-1.770603000	-1.529299000
1	2.460011000	-2.406427000	-1.941193000
1	2.759630000	-0.664489000	-2.024623000
6	2.329184000	1.694327000	1.812788000
1	1.768592000	2.625642000	1.700199000
1	1.785234000	1.047196000	2.506486000
1	3.294328000	1.933810000	2.267104000
6	3.236996000	1.965264000	-0.478557000
1	4.190190000	2.296447000	-0.057421000
1	3.431598000	1.491180000	-1.443092000
1	2.623315000	2.853370000	-0.649253000
1	0.824556000	-1.113018000	1.206519000
14	-0.156380000	-1.735015000	-0.979477000
1	-0.028240000	-1.200759000	-2.354132000
1	0.112938000	-3.194287000	-0.971420000
6	-1.904129000	-1.449782000	-0.392559000
6	-2.795222000	-0.666374000	-1.121458000
6	-2.333114000	-1.974079000	0.826620000
6	-4.069229000	-0.403596000	-0.645323000
1	-2.483096000	-0.239833000	-2.070616000
6	-3.603015000	-1.712024000	1.310392000
1	-1.659564000	-2.594863000	1.413565000
6	-4.472941000	-0.922588000	0.573483000
1	-4.746198000	0.215217000	-1.223527000
1	-3.918187000	-2.125054000	2.262035000
1	-5.468029000	-0.714575000	0.950027000

II_P$^{Si–H}$

13	-0.672201000	0.179090000	0.744689000
7	-2.403452000	0.676095000	0.125936000
7	0.202999000	1.736556000	0.088917000
6	-2.723491000	1.857494000	-0.384750000
6	-0.406080000	2.802768000	-0.408383000
6	-1.790004000	2.875121000	-0.591382000
1	-2.174155000	3.806608000	-0.983869000
6	-3.348701000	-0.384020000	0.195819000
6	-3.822817000	-0.799813000	1.433009000
6	-3.710725000	-1.082845000	-0.950157000
6	-4.670085000	-1.892325000	1.518695000
6	-4.558202000	-2.171883000	-0.858968000
6	-5.041453000	-2.578332000	0.375046000
1	-5.037835000	-2.210218000	2.487211000
1	-4.833045000	-2.714119000	-1.756069000
1	-5.699373000	-3.436225000	0.444966000
6	1.622700000	1.686183000	0.202896000
6	2.391088000	1.231995000	-0.861064000
6	2.231202000	1.993598000	1.412175000
6	3.761371000	1.106326000	-0.721193000
6	3.604215000	1.868732000	1.546397000
6	4.370530000	1.426964000	0.480990000
1	4.353527000	0.736932000	-1.550145000
1	4.074939000	2.110770000	2.492114000
1	5.442712000	1.315171000	0.591519000
6	0.412200000	3.988774000	-0.804048000
1	-0.219540000	4.809303000	-1.136404000
1	1.027896000	4.328514000	0.031790000
1	1.100309000	3.727348000	-1.611208000
6	-4.143231000	2.132996000	-0.764007000
1	-4.296652000	3.194737000	-0.945136000
1	-4.413559000	1.590637000	-1.672684000
1	-4.827678000	1.798522000	0.018033000
1	1.615017000	2.322884000	2.242273000
1	1.898546000	0.962972000	-1.790737000
1	-3.303548000	-0.773227000	-1.907349000
1	-3.516114000	-0.260287000	2.322753000
1	-0.586734000	0.127264000	2.336490000
14	0.060547000	-1.842264000	-0.461973000
1	-0.198881000	-1.778549000	-1.933213000
1	-0.640472000	-3.080346000	-0.007792000
6	1.919762000	-2.134394000	-0.305513000
6	2.568886000	-1.926330000	0.912049000

6	2.701795000	-2.504415000	-1.399086000
6	3.938042000	-2.088000000	1.037312000
1	1.993230000	-1.618888000	1.782504000
6	4.073960000	-2.663683000	-1.283568000
1	2.228555000	-2.668593000	-2.363126000
6	4.695611000	-2.456817000	-0.063009000
1	4.418033000	-1.913991000	1.994284000
1	4.660557000	-2.951907000	-2.149298000
1	5.768957000	-2.578898000	0.030202000

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7	-1.937141000	0.944028000	0.137257000
6	-1.863358000	1.848138000	1.099178000
6	-0.714783000	2.602714000	1.359360000
6	0.587461000	2.395598000	0.889917000
7	0.888864000	1.552146000	-0.084979000
1	-0.821130000	3.371974000	2.113488000
6	-3.034787000	0.064523000	0.000814000
6	-3.333536000	-0.877957000	0.979192000
6	-3.760128000	0.064904000	-1.185534000
6	-4.350974000	-1.793371000	0.778557000
1	-2.746891000	-0.900240000	1.891800000
6	-4.775746000	-0.854251000	-1.382832000
1	-3.517954000	0.796156000	-1.950063000
6	-5.075675000	-1.785588000	-0.402450000
1	-4.569862000	-2.526795000	1.545849000
1	-5.334881000	-0.842862000	-2.311116000
1	-5.866810000	-2.508505000	-0.560795000
6	2.210339000	1.158137000	-0.378548000
6	3.068089000	0.668801000	0.602829000
6	2.630473000	1.146339000	-1.705851000
6	4.326685000	0.208612000	0.265245000
1	2.723238000	0.606963000	1.628775000
6	3.887565000	0.673703000	-2.040439000
1	1.963953000	1.522974000	-2.475925000
6	4.743850000	0.208403000	-1.056417000
1	4.976753000	-0.178961000	1.041404000
1	4.198931000	0.673156000	-3.078479000
1	5.726851000	-0.163730000	-1.318907000
31	-0.522504000	0.760255000	-1.250254000
6	-3.053593000	2.109790000	1.970918000
1	-3.986742000	2.005272000	1.416213000
1	-3.090185000	1.403849000	2.803567000
1	-2.996808000	3.111702000	2.393374000

6	1.656409000	3.210672000	1.555610000
1	2.006127000	2.729744000	2.471513000
1	2.519711000	3.360755000	0.908727000
1	1.248078000	4.180683000	1.838234000
1	-0.848604000	1.787387000	-2.411388000
14	-0.014930000	-1.586668000	-1.485380000
1	-1.250681000	-2.415232000	-1.538298000
1	0.791159000	-1.933853000	-2.684210000
6	0.993752000	-2.093008000	0.017958000
6	2.228081000	-2.727067000	-0.103819000
6	0.549855000	-1.773800000	1.302492000
6	2.988402000	-3.039204000	1.012189000
1	2.608705000	-2.972757000	-1.091145000
6	1.301198000	-2.086191000	2.422034000
1	-0.401888000	-1.261105000	1.429607000
6	2.525829000	-2.721191000	2.277939000
1	3.948395000	-3.529427000	0.892285000
1	0.934101000	-1.831780000	3.410385000
1	3.118570000	-2.965353000	3.152303000