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Supporting Information

Probing the Potential of Metalla-*N*-heterocyclic Carbenes

Towards Activation of Enthalpically Strong Bonds

Bijoy Ghosh and Ashwini K. Phukan*

Department of Chemical Sciences, Tezpur University, Napaam 784028, Assam, India

E-Mail: *ashwini@tezu.ernet.in*

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Table S1 Calculated ΔE_{S-T} values (in kcal mol^{-1}) for the experimentally trapped MNHCs (bipy = bipyridine).

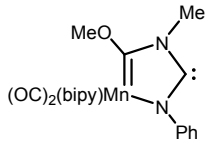
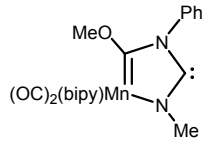
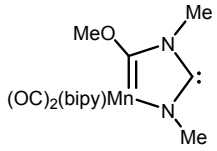
Sl. No.	Molecules	ΔE_{S-T}
1		27.2
2		24.6
3		24.2

Table S2 Calculated important geometrical parameters and natural charges at hydridic ($q_H^{\delta-}$) and positively polarized hydrogen atom ($q_H^{\delta+}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the transition states involved in the activation of hydrogen by **1**, **3** and **IV** (CAAC). Bond lengths, bond angles ($\angle$N-C_c-X, X = C, N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H^{\delta+} - H^{\delta-}$	$C_c - H^{\delta-}$	$C_c - H^{\delta+}$	C_c-X	$\angle$N-C_c-X	$q_H^{\delta-}$	$q_H^{\delta+}$	Occ_{p_π}
IVTS^{H-H}	1.076	1.950	1.214	1.325/1.502	108.0	-0.196	0.185	0.756
	(0.314)	(0.465)	(0.621)	(1.298)/(0.997)				
1TS^{H-H}	1.249	2.217	1.186	1.297/1.403	114.0	-0.423	0.206	0.815
	(0.266)	(0.312)	(0.651)	(1.497)/(1.004)				
3TS^{H-H}	1.091	2.009	1.201	1.353/1.353	124.1	-0.197	0.179	0.770
	(0.320)	(0.413)	(0.615)	(1.155)/(1.154)				

Table S3 Calculated C-X (X = C, N) bond lengths (in Å), their corresponding Wiberg bond index (WBI) values and ∠N – C – X bond angles (in degree) for the H – H splitting product obtained for **1**, **3** and **IV** (CAAC).

Molecules	C-X	WBI	∠N-C-X
IVP^{H-H}	1.518/1.448	0.979/0.981	104.8
1P^{H-H}	1.464/1.412	0.913/1.052	108.6
3P^{H-H}	1.445/1.444	0.954/0.958	114.4

Table S4 Calculated important geometrical parameters and natural charges at the nitrogen atom of the $NH_2^{\delta-}$ fragment ($q_{NH_2}{}^{\delta-}$) and hydrogen atom ($q_H{}^{\delta+}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the transition states involved in the activation of N-H bond of NH_3 by **1**, **3**, DAC (**III**) and CAAC (**IV**) via nucleophilic pathway. Bond lengths, bond angles (∠N-C_c-X, X = C, N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H_2N^{\delta-} – H^{\delta+}$	$C_c – NH_2^{\delta-}$	$C_c – H^{\delta+}$	C_c-X	∠N-C_c-X	$q_{NH_2}{}^{\delta-}$	$q_H{}^{\delta+}$	Occ_{P_π}
IIITS$_{Nu}^{N-H}$	1.513	2.332	1.149	1.354/1.354	119.9	-1.080	0.333	0.745
	(0.185)	(0.436)	(0.681)	(1.160)/(1.160)				
IVTS$_{Nu}^{N-H}$	1.542	2.428	1.156	1.314/1.496	109.5	-1.165	0.324	0.792
	(0.177)	(0.401)	(0.695)	(1.378)/(0.995)				
1TS$_{Nu}^{N-H}$	1.688	2.486	1.125	1.294/1.397	115.0	-1.210	0.320	0.810
	(0.117)	(0.296)	(0.743)	(1.494)/(1.013)				
3TS$_{Nu}^{N-H}$	1.539	2.384	1.144	1.351/1.351	124.9	-1.110	0.329	0.749
	(0.176)	(0.410)	(0.689)	(1.176)/(1.176)				

Table S5 Calculated C-X (X = C, N) bond lengths (in Å), their corresponding Wiberg bond index (WBI) values and ∠N – C – X bond angles (in degree) for the N – H splitting product obtained for **1**, **3**, DAC (**III**) and CAAC (**IV**).

Molecules	C-X	WBI	∠N-C-X
IIIP^{N-H}	1.461/1.445	0.922/0.947	110.8
IVP^{N-H}	1.450/ 1.538	0.968/0943	102.6
1P^{N-H}	1.416/ 1.508	1.046/0.840	105.6
3P^{N-H}	1.464/1.447	0.919/0.947	114.2

Table S6 Calculated important geometrical parameters and natural charges at the nitrogen atom of NH_3 (q_{NH_3}) and carbenic carbon (q_{Cc}) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the first transition state (**TS_1^{N-H}**) and the intermediate (**Int^{N-H}**) involved in the activation of N-H bond of NH_3 by **3** and DAC (**III**) via electrophilic pathway. Bond lengths, bond angles (∠N-C_c-N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H_3N - C_c$	C_c-N	∠N-C_c-N	q_{NH_3}	q_{Cc}	Occ_{P_π}
III-TS_1^{N-H}	1.822	1.407/ 1.407	113.3	-0.826	0.185	0.588
	(0.547)	(1.020)/(1.020)				
III-Int^{N-H}	1.597	1.425/1.425	113.3	-0.737	0.097	0.677
	(0.756)	(0.978)/(0.978)				
3TS_1^{N-H}	1.856	1.398/ 1.398	118.9	-0.843	0.199	0.574
	(0.515)	(1.041)/(1.042)				
3Int^{N-H}	1.570	1.417/ 1.417	119.1	-0.726	0.089	0.696
	(0.783)	(0.986)/(0.986)				

Table S7 Calculated important geometrical parameters and natural charges at the nitrogen atom of the $NH_2^{\delta-}$ fragment ($q_{NH_2}^{\delta-}$) and hydrogen atom ($q_H^{\delta+}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the second transition state (**TS_2^{N-H}**) involved in the activation of N-H bond of NH_3 by **3** and DAC (**III**) via electrophilic pathway. Bond lengths, bond angles (∠N-C_c-N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H_2N^{\delta-} - H^{\delta+}$	$C_c - NH_2^{\delta-}$	$C_c - H^{\delta+}$	C_c-N	∠N-C_c-N	$q_{NH_2}^{\delta-}$	$q_H^{\delta+}$	Occ_{P_π}
III-TS_2^{N-H}	1.515	2.295	1.168	1.350/1.350	119.8	-1.119	0.316	0.710
	(0.224)	(0.377)	(0.652)	(1.171)/(1.171)				
3TS_2^{N-H}	1.531	2.347	1.164	1.346/1.346	124.7	-1.144	0.313	0.709
	(0.218)	(0.348)	(0.657)	(1.192)/(1.192)				

Table S8 Calculated important geometrical parameters and natural charges at the phosphorus atom of the $PH_2^{\delta-}$ fragment ($q_{PH_2}^{\delta-}$) and hydrogen atom ($q_H^{\delta+}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the transition states involved in the activation of P-H bond of PH_3 by **1**, **3**, DAC (**III**) and CAAC (**IV**) via nucleophilic pathway. Bond lengths, bond angles (∠N-C_c-X, X = C, N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H_2P^{\delta-} - H^{\delta+}$	$C_c - PH_2^{\delta-}$	$C_c - H^{\delta+}$	C_c-X	∠N-C_c-X	$q_{PH_2}^{\delta-}$	$q_H^{\delta+}$	Occ_{P_π}
IIITS$_{Nu}^{P-H}$	1.708	2.931	1.338	1.354/1.356	118.4	-0.089	0.119	0.734
	(0.470)	(0.358)	(0.487)	(1.169)/(1.169)				
IVTS$_{Nu}^{P-H}$	1.733	3.030	1.376	1.310/1.507	108.5	-0.234	0.132	0.828
	(0.480)	(0.331)	(0.480)	(1.428)/(0.992)				
1TS$_{Nu}^{P-H}$	1.749	2.984	1.347	1.295/1.410	112.5	-0.232	0.135	0.801
	(0.461)	(0.282)	(0.489)	(1.519)/(0.992)				
3TS$_{Nu}^{P-H}$	1.697	2.984	1.367	1.349/1.348	123.4	-0.132	0.115	0.707
	(0.501)	(0.326)	(0.456)	(1.195)/(1.196)				

Table S9 Calculated C-X (X = C, N) bond lengths (in Å), their corresponding Wiberg bond index (WBI) values and ∠N – C – X bond angles (in degree) for the P – H splitting product obtained for **1**, **3**, DAC (**III**) and CAAC (**IV**).

Molecules	C-X	WBI	∠N-C-X
IIIP^{P-H}	1.443/1.446	0.958/0.956	111.8
IVP^{P-H}	1.450/1.536	0.972/0.966	102.9
1P^{P-H}	1.415/1.469	1.056/0.913	108.4
3P^{P-H}	1.444/1.451	0.957/0.950	115.6

Table S10 Calculated important geometrical parameters and natural charges at the phosphorus atom of PH_3 (q_{PH_3}) and carbenic carbon (q_{Cc}) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the first transition state (**TS_1^{P-H}**) and the intermediate (**Int^{P-H}**) involved in the activation of P-H bond of PH_3 by **3** and DAC (**III**) via electrophilic pathway. Bond lengths, bond angles (∠N-C_c-N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H_3P - C_c$	C_c-N	∠N-C_c-N	q_{PH_3}	q_{Cc}	Occ_{p_π}
III-TS_1^{P-H}	1.922	1.393/1.393	114.9	0.476	-0.009	0.864
	(0.930)	(1.045)/(1.045)				
III-Int^{P-H}	1.739	1.415/1.415	115.7	0.755	-0.244	1.020
	(1.156)	(0.988)/(0.988)				
3TS_1^{P-H}	2.021	1.380/1.380	119.5	0.370	0.083	0.782
	(0.798)	(1.080)/(1.080)				
3Int^{P-H}	1.685	1.419/1.413	119.2	0.891	-0.308	1.049
	(1.171)	(0.964)/(0.975)				

Table S11 Calculated important geometrical parameters and natural charges at the phosphorus atom of the $PH_2^{\delta-}$ fragment ($q_{PH_2}^{\delta-}$) and hydrogen atom ($q_H^{\delta+}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) for the second transition state (**TS_2^{P-H}**) involved in the activation of P-H bond of PH_3 by **3** and DAC (**III**) via electrophilic pathway. Bond lengths, bond angles (**∠N-C_c-N**) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H_2P^{\delta-} - H^{\delta+}$	$C_c - PH_2^{\delta-}$	$C_c - H^{\delta+}$	C_c-N	∠N-C_c-N	$q_{PH_2}^{\delta-}$	$q_H^{\delta+}$	Occ_{p_π}
III-TS_2^{P-H}	1.709	2.934	1.332	1.355/1.355	118.3	-0.141	0.120	0.738
	(0.461)	(0.335)	(0.496)	(1.170)/(1.170)				
3TS_2^{P-H}	1.701	2.994	1.359	1.348/1.348	123.4	-0.173	0.115	0.710
	(0.489)	(0.307)	(0.468)	(1.197)/(1.197)				

Table S12 Calculated important geometrical parameters and natural charges at the silicon atom of the SiH_2Ph fragment (q_{SiH_2Ph}) and hydrogen atom ($q_H^{\delta+}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the transition states involved in activation of the Si-H bond of SiH_3Ph by **1**, **3**, DAC (**III**) and CAAC (**IV**) via proton transfer pathway. Bond lengths, bond angles (∠N-C_c-X, X = C, N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$PhH_2Si^{\delta+} - H^{\delta-}$	$C_c - SiH_2Ph$	$C_c - H^{\delta+}$	C_c-X	∠N-C_c-X	q_{SiH_2Ph}	$q_H^{\delta+}$	Occ_{p_π}
$IIITS_{PT}^{Si-H}$	1.817	2.922	1.261	1.369/1.369	118.0	0.837	0.068	0.995
	(0.356)	(0.339)	(0.583)	(1.117)/(1.115)				
$IVTS_{PT}^{Si-H}$	1.861	2.983	1.281	1.325/1.506	107.7	0.706	0.095	0.825
	(0.370)	(0.365)	(0.575)	(1.323)/(0.995)				
$1TS_{PT}^{Si-H}$	1.889	3.016	1.280	1.301/1.411	113.2	0.659	0.096	0.951
	(0.383)	(0.276)	(0.551)	(1.461)/(1.272)				
$3TS_{PT}^{Si-H}$	1.819	2.998	1.274	1.359/1.361	123.2	0.793	0.062	0.895
	(0.379)	(0.323)	(0.561)	(1.148)/(1.141)				

Table S13 Calculated C-X (X = C, N) bond lengths (in Å), their corresponding Wiberg bond index (WBI) values and ∠N – C – X bond angles (in degree) for the Si – H splitting product obtained for **1**, **3**, DAC (**III**) and CAAC (**IV**).

Molecules	C-X	WBI	∠N-C-X
$IIIP^{Si-H}$	1.454/1.455	0.957/0.953	111.9
IVP^{Si-H}	1.455/1.539	0.979/0.970	102.3
$1P^{Si-H}$	1.470/1.432	0.917/1.038	108.3
$3P^{Si-H}$	1.455/1.459	0.952/0.946	115.5

Table S14 Calculated geometrical parameters and natural charges at the silicon atom of SiH_3Ph (q_{SiH_3Ph}) and carbenic carbon (q_{Cc}) of the van der Walls complexes obtained for **1**, **3** and **III-IV** (*indicated by the subscript* **V**) with SiH_3Ph. Bond lengths, bond angles (∠N-C_c-X, X = C, N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	C_c – SiH_3Ph	C_c-X	∠N-C_c-X	q_{SiH_3Ph}	q_{Cc}
$\mathbf{III_V}$	3.176	1.350/1.352	116.5	0.947	0.291
	(0.038)	(1.214)/(1.208)			
$\mathbf{IV_V}$	2.983	1.303/1.507	106.8	0.962	0.208
	(0.079)	(1.488)/(0.985)			
$\mathbf{1_V}$	3.146	1.290/1.425	109.7	0.947	0.227
	(0.046)	(1.602)/(0.963)			
$\mathbf{3_V}$	3.244	1.348/1.357	120.5	0.951	0.289
	(0.036)	(1.233)/(1.228)			

Table S15 Calculated important geometrical parameters and natural charges at the silicon atom of the $SiH_2Ph^{\delta+}$ fragment ($q_{SiH_2Ph}{}^{\delta+}$) and hydridic hydrogen atom ($q_H{}^{\delta-}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the transition states involved in activation of the Si-H bond of SiH_3Ph by **1**, **3**, DAC (**III**) and CAAC (**IV**) via hydride transfer pathway. Bond lengths, bond angles (∠N-C_c-X, X = C, N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$PhH_2Si^{\delta+}$ – $H^{\delta-}$	C_c –$SiH_2Ph^{\delta+}$	C_c – $H^{\delta-}$	C_c-X	∠N-C_c-X	$q_{SiH_2Ph}{}^{\delta+}$	$q_H{}^{\delta-}$	Occ_{p_π}
$\mathbf{IIITS_{hy}^{Si\text{-}H}}$	1.609	2.045	1.787	1.371/1.373	116.0	0.997	-0.091	0.735
	(0.514)	(0.551)	(0.322)	(1.121)/(1.113)				
$\mathbf{IVTS_{hy}^{Si\text{-}H}}$	1.619	1.956	1.909	1.319/1.518	108.6	0.978	-0.150	0.737
	(0.534)	(0.645)	(0.282)	(1.327)/(0.983)				
$\mathbf{1TS_{hy}^{Si\text{-}H}}$	1.775	1.908	1.863	1.307/1.421	111.6	1.014	-0.224	0.856
	(0.380)	(0.713)	(0.292)	(1.432)/(0.969)				
$\mathbf{3TS_{hy}^{Si\text{-}H}}$	1.577	2.093	1.781	1.372/1.368	119.7	1.000	-0.090	0.714
	(0.550)	(0.499)	(0.307)	(1.112)/(1.122)				

Table S16 Calculated important geometrical parameters and natural charges at the carbon atom of the $CH_3^{\delta-}$ fragment ($q_{CH_3}^{\delta-}$) and hydrogen atom ($q_H^{\delta+}$) and occupancies of the formally vacant p_π orbital at the carbene center (Occ_{P_π}) of the transition states involved in activation of the C-H bond of CH_4 by **1**, **3**, DAC (**III**) and CAAC (**IV**). Bond lengths, bond angles (∠N-C_c-X, X = C, N) are given in Å and in degree (°) respectively and Wiberg Bond Index (WBI) values are given within parentheses.

Molecules	$H_3C^{\delta-} - H^{\delta+}$	$C_c - CH_3^{\delta-}$	$C_c - H^{\delta+}$	C_c-X	∠N-C_c-X	$q_{H_3C}^{\delta-}$	$q_H^{\delta+}$	Occ_{P_π}
IIITS^{C-H}	1.557	2.342	1.155	1.368/1.368	119.0	-0.778	0.279	0.807
	(0.222)	(0.496)	(0.675)	(1.107)/(1.107)				
IVTS^{C-H}	1.557	2.343	1.167	1.338/1.502	108.0	-0.827	0.277	0.832
	(0.224)	(0.518)	(0.674)	(1.247)/(0.995)				
1TS^{C-H}	1.772	2.483	1.131	1.305/1.400	114.6	-0.916	0.286	0.878
	(0.143)	(0.370)	(0.736)	(1.411)/(1.002)				
3TS^{C-H}	1.536	2.366	1.166	1.364/1.364	124.3	-0.786	0.271	0.788
	(0.244)	(0.471)	(0.653)	(1.119)/(1.119)				

Table S17 Calculated C-X (X = C, N) bond lengths (in Å), their corresponding Wiberg bond index (WBI) values and ∠N – C – X bond angles (in degree) for the C – H splitting product obtained for **1**, **3**, DAC (**III**) and CAAC (**IV**).

Molecules	C-X	WBI	∠N-C-X
IIIP^{C-H}	1.453/1.452	0.946/0.946	111.4
IVP^{C-H}	1.462/1.533	0.958/0.961	103.0
1P^{C-H}	1.479/1.428	0.898/1.034	106.8
3P^{C-H}	1.456/1.455	0.942/0.943	115.2

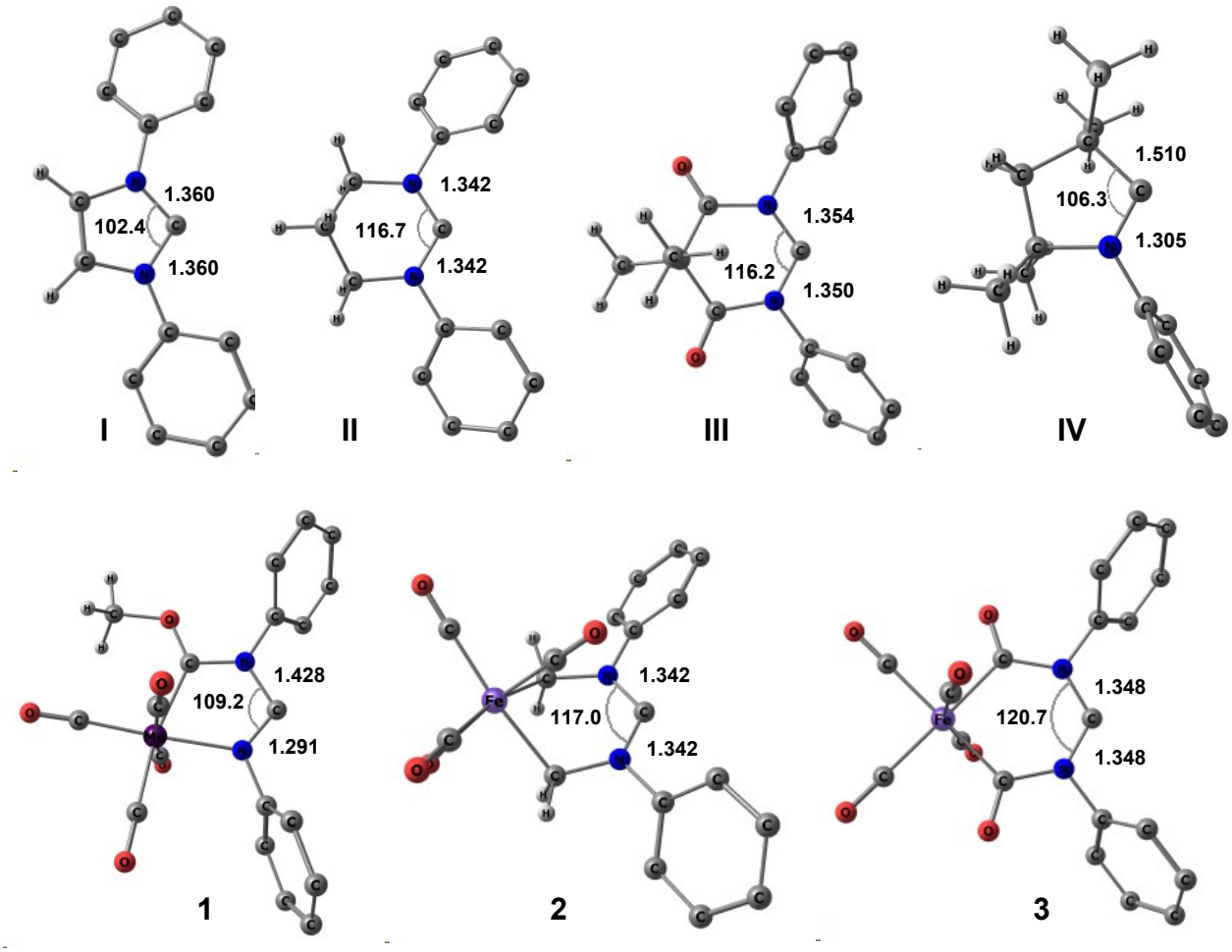
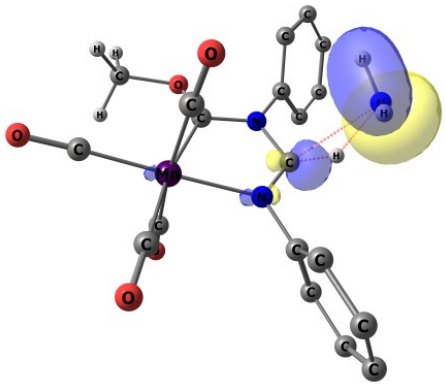
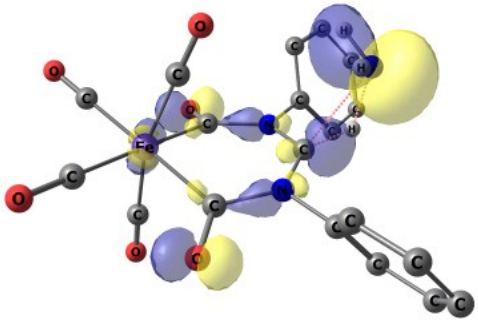


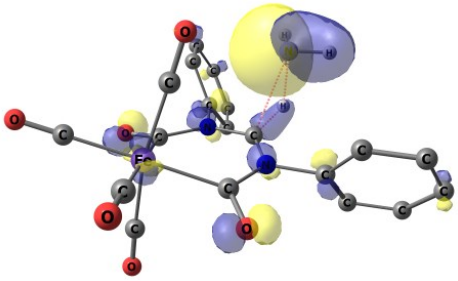
Fig. **S1** Singlet state optimized geometries of **I-IV** and **1-3**. The hydrogen atoms of the phenyl rings are omitted for clarity.



$1TS_{Nu}^{N-H}$

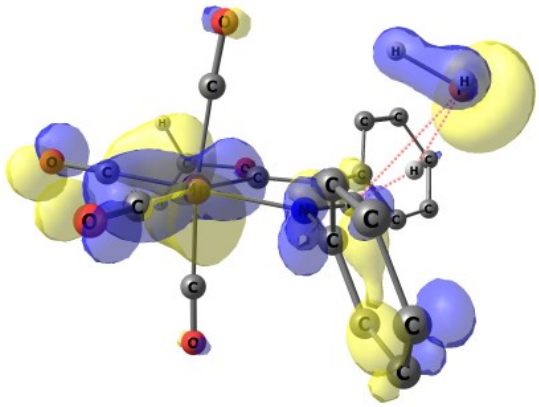


$3TS_{Nu}^{N-H}$

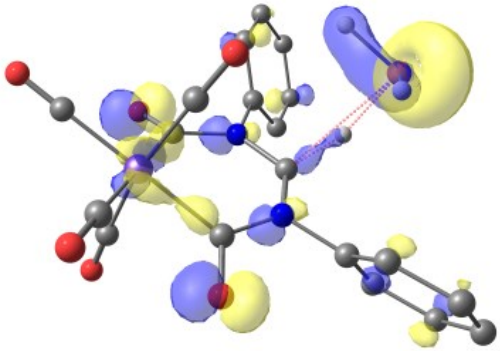


$3TS_2^{N-H}$

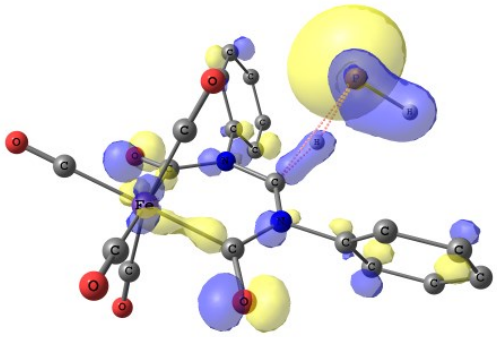
Fig. **S2** Molecular orbitals showing the orientation of the nitrogen lone pair for the TSs (**$1TS_{Nu}^{N-H}$**, **$3TS_{Nu}^{N-H}$** and **$3TS_2^{N-H}$**) involved in the activation of N-H bond of NH_3. The hydrogen atoms of the phenyl rings are omitted for clarity.



$1TS_{Nu}^{P-H}$



$3TS_{Nu}^{P-H}$



$3TS_2^{P-H}$

Fig. **S3** Molecular orbitals showing the orientation of the phosphorus lone pair for the TSs (**$1TS_{Nu}^{P-H}$**, **$3TS_{Nu}^{P-H}$** and **$3TS_2^{P-H}$**) involved in the activation of P- H bond of PH_3. The hydrogen atoms of the phenyl rings are omitted for clarity.

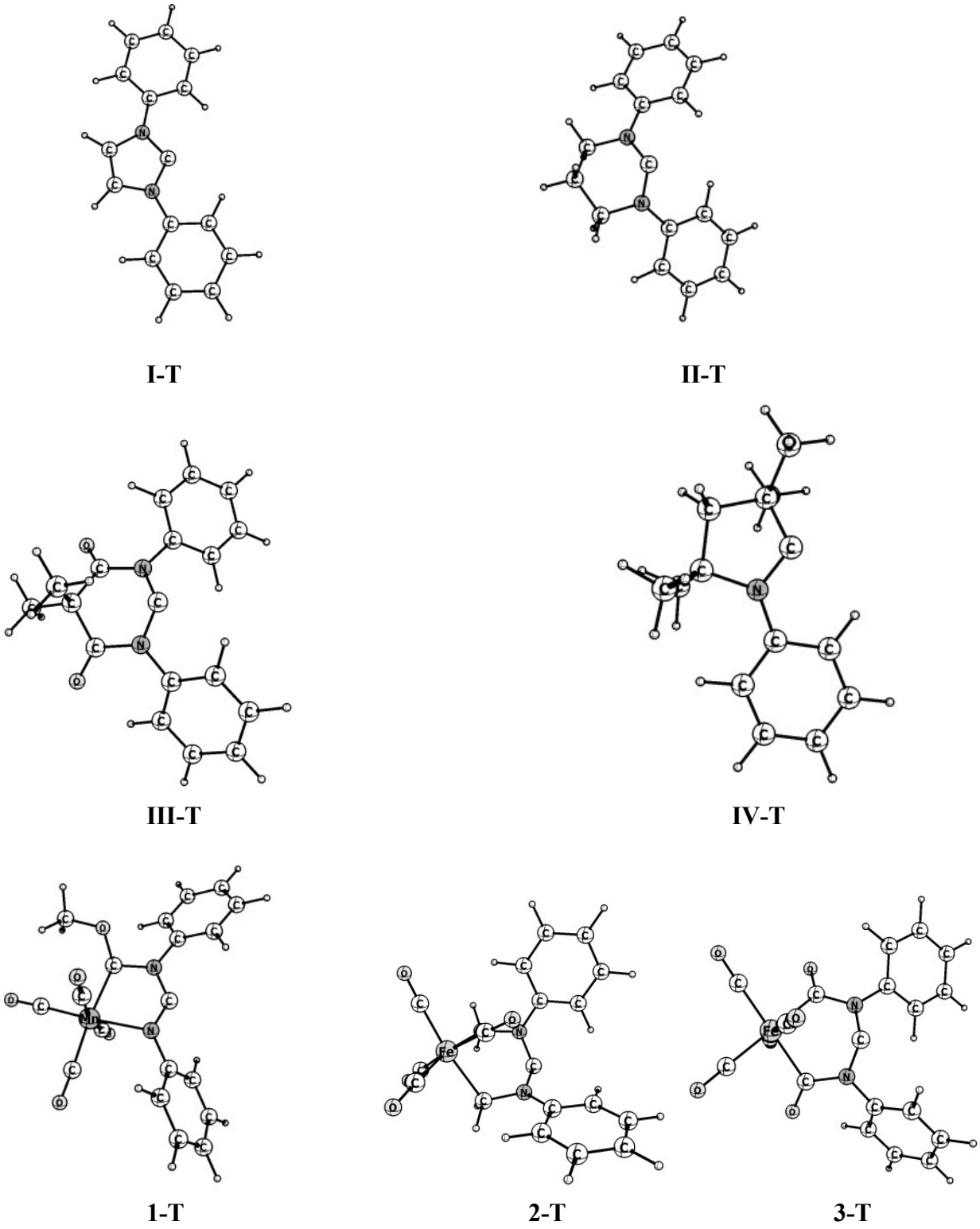
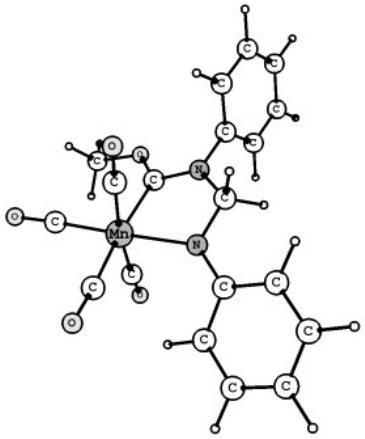
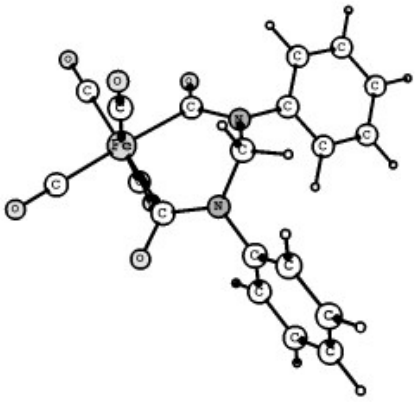


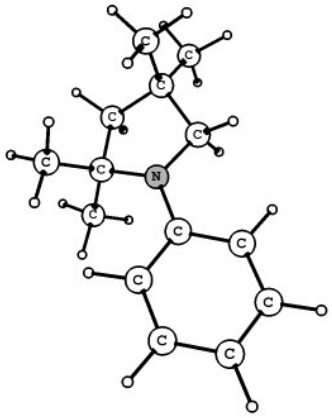
Fig. **S4** Triplet state optimized geometries of **I-IV** and **1-3**.



1P^{H-H}

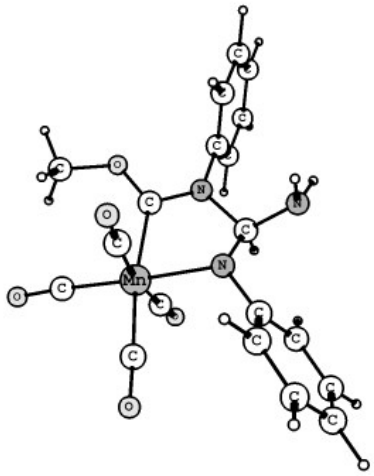


3P^{H-H}

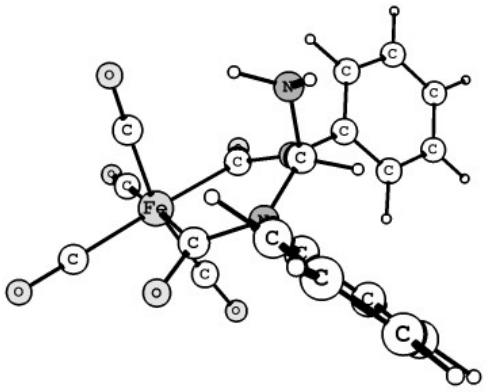


IVP^{H-H}

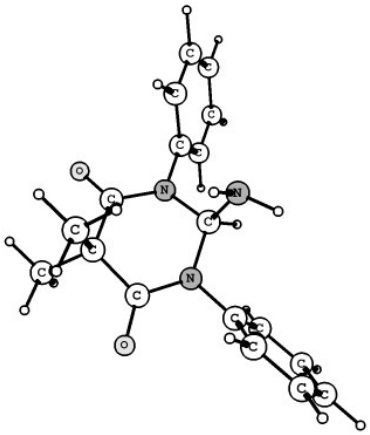
Fig. **S5** Optimized geometries of the H-H splitting product obtained for **1**, **3** and CAAC (**IV)**.



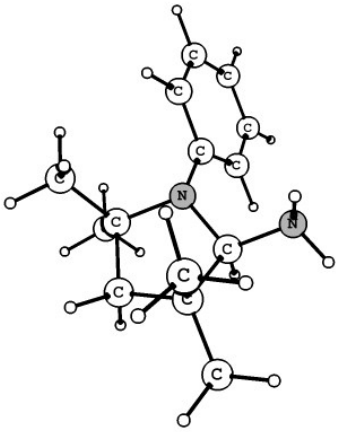
1P^{N-H}



3P^{N-H}



IIIP^{N-H}



IVP^{N-H}

Fig. **S6** Optimized geometries of the N-H bond splitting product obtained for **1**, **3** and **III-IV**.

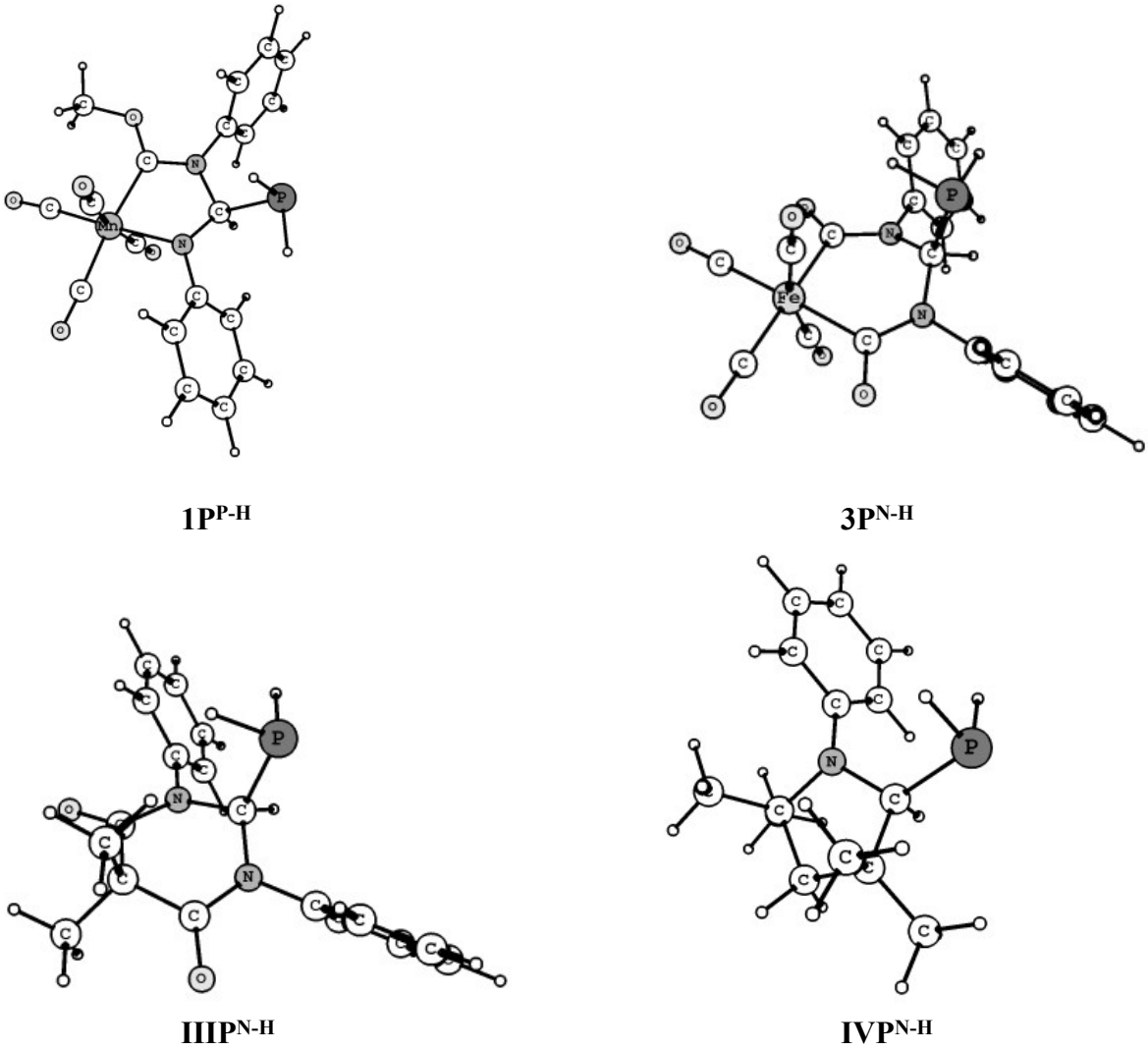
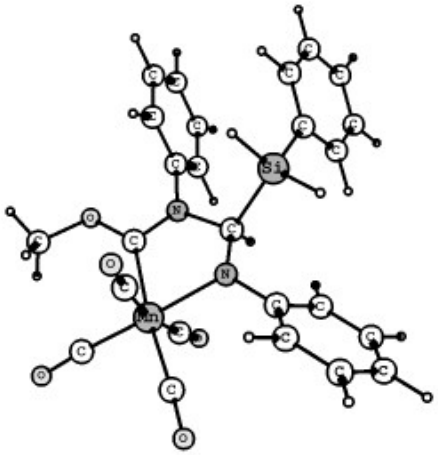
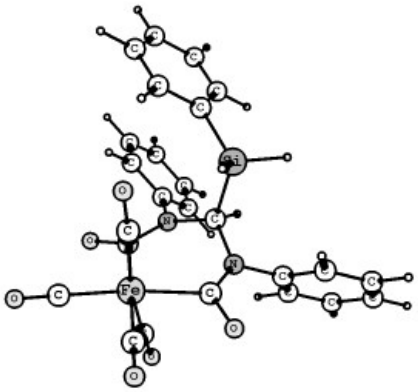


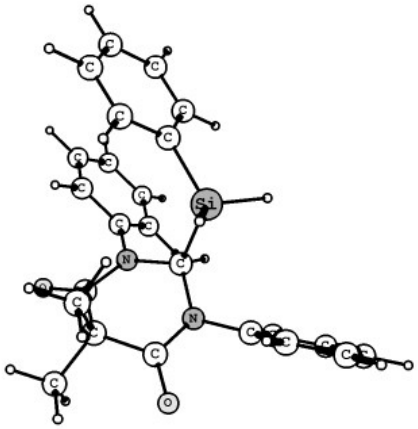
Fig. **S7** Optimized geometries of the P-H bond splitting product obtained for **1**, **3** and **III**-**IV**.



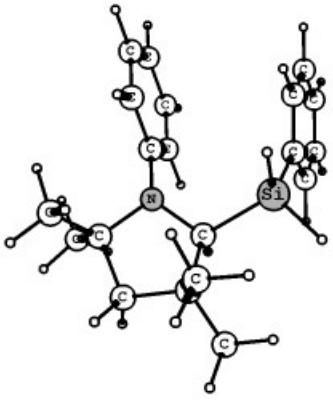
1P^{Si-H}



3P^{Si-H}



IIIP^{Si-H}



IVPSi-H

Fig. **S8** Optimized geometries of the Si-H bond splitting product obtained for **1**, **3** and **III-IV**.

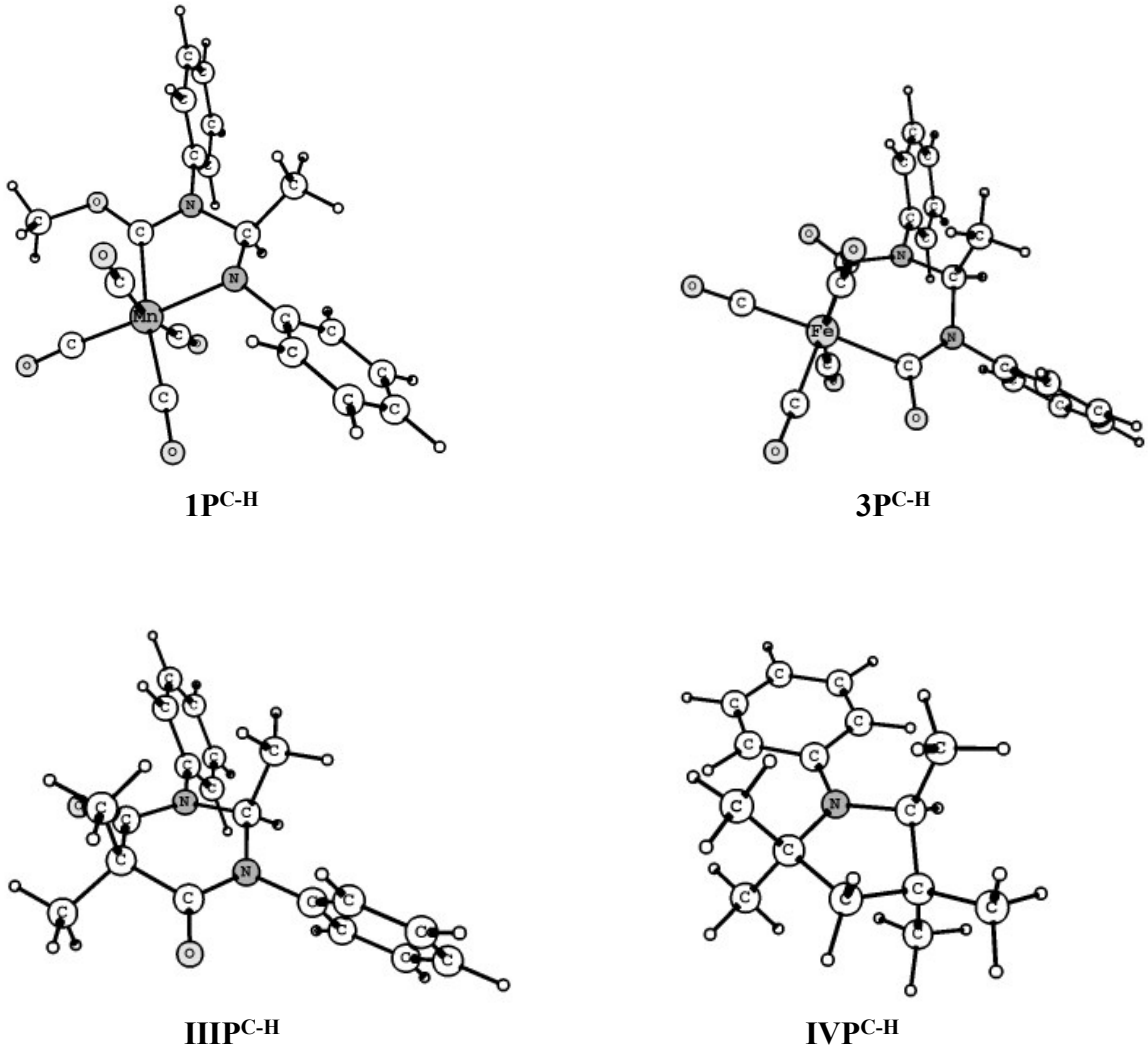
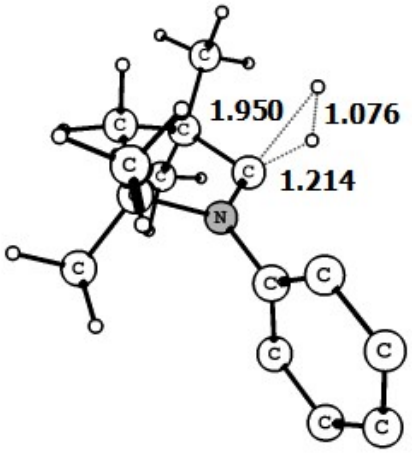
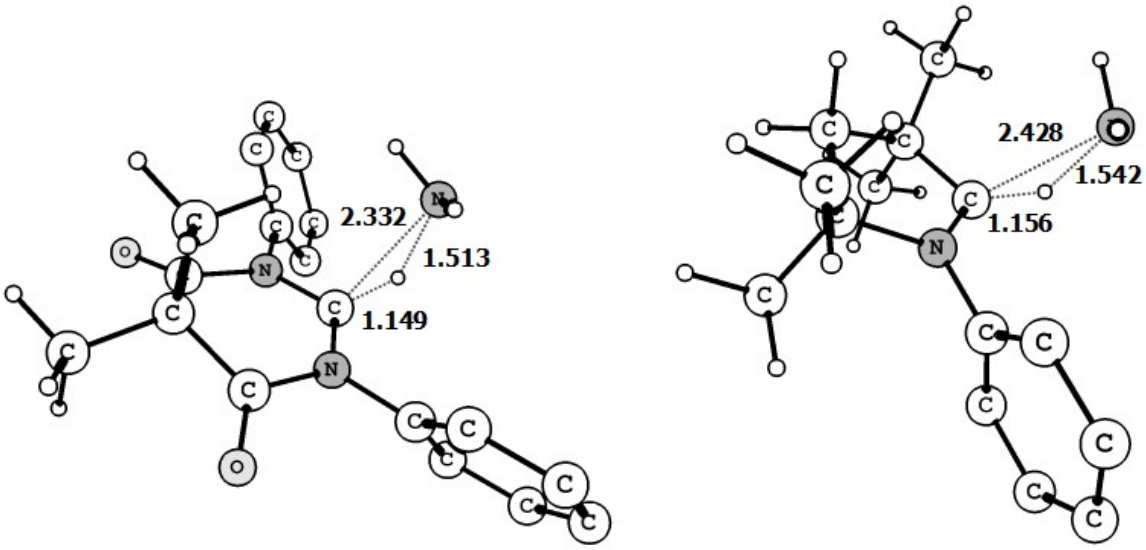


Fig. **S9** Optimized geometries of the C-H bond splitting product obtained for **1**, **3** and **III**-**IV**.



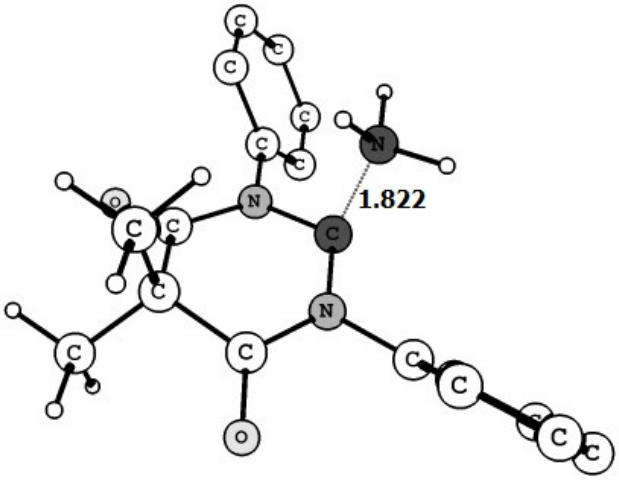
IV-TS^{H-H}

Fig. **S10** Optimized geometry of the transition state obtained for the activation of dihydrogen by CAAC (**IV**). The hydrogen atoms of the phenyl ring are omitted for clarity.

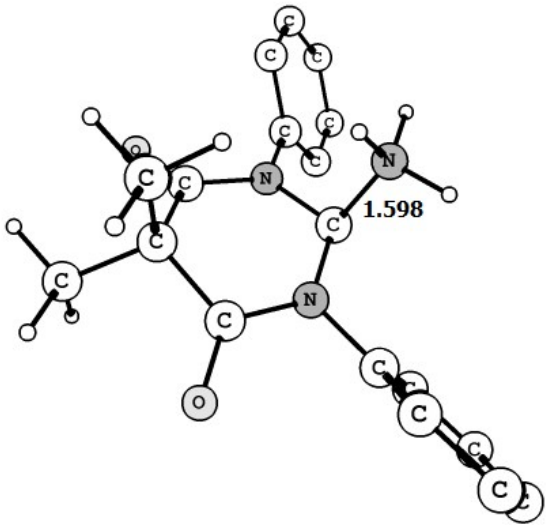


III-TS$_{Nu}^{N-H}$ **IV-TS^{N-H}**

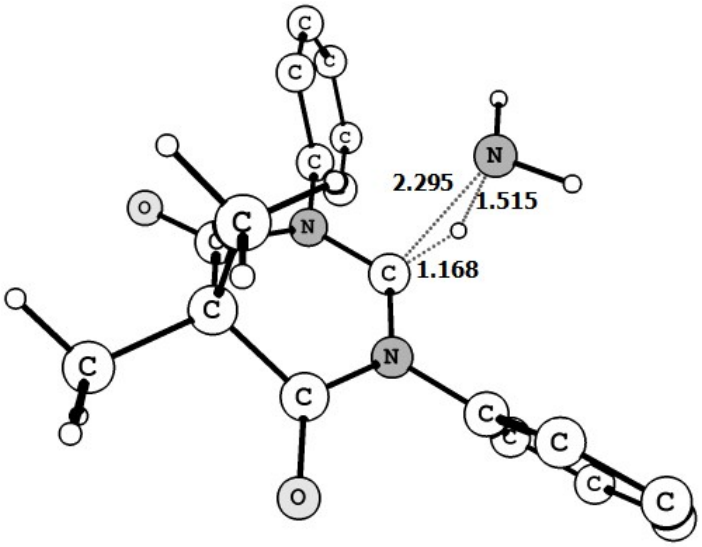
Fig. **S11** Optimized geometry of the transition states obtained for the activation of N – H bond of NH_3 by DAC (**III**) and CAAC (**IV**) via nucleophilic pathway. The hydrogen atoms of the phenyl ring are omitted for clarity.



III-TS$_1^{N-H}$

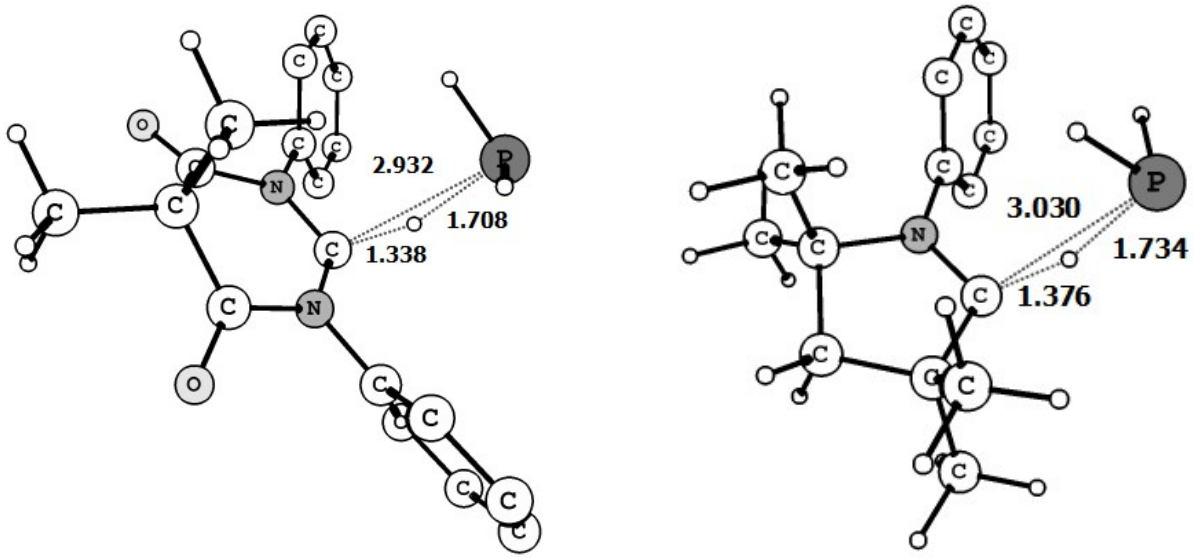


III-Int^{N-H}



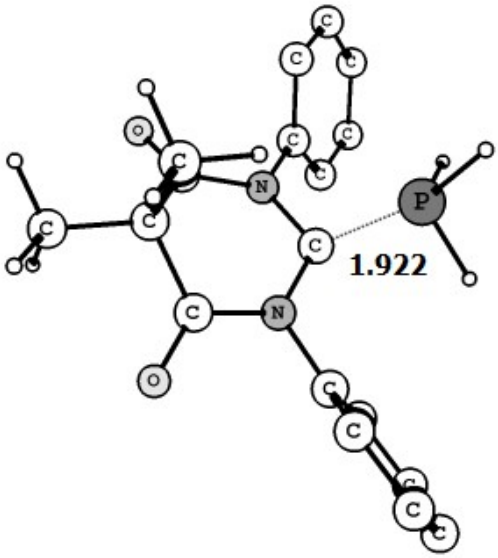
III-TS$_2^{N-H}$

Fig. **S12** Optimized geometries of the transition states and intermediate involved in the activation of N – H bond of NH_3 by DAC (**III**) via electrophilic pathway. The hydrogen atoms of the phenyl ring are omitted for clarity.

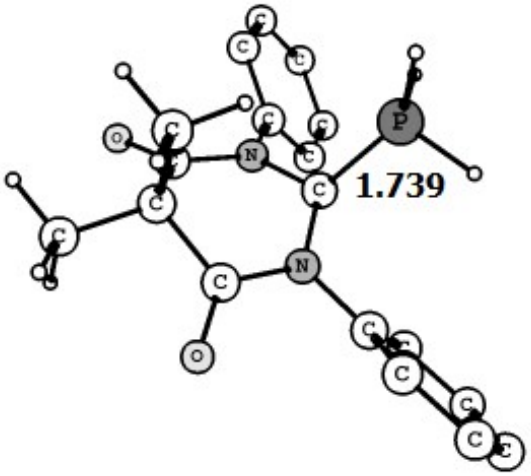


III-TS$_{Nu}^{P-H}$ **IV-TS^{P-H}**

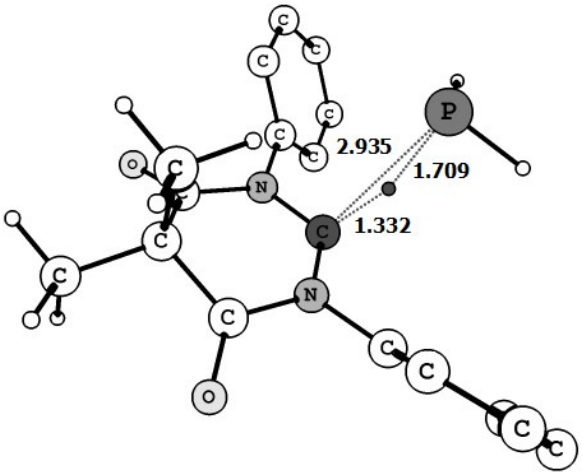
Fig. **S13** Optimized geometry of the transition states obtained for the activation of P – H bond of PH_3 by DAC (**III**) and CAAC (**IV**) via nucleophilic pathway. The hydrogen atoms of the phenyl ring are omitted for clarity.



III-TS$_1$$^{P-H}$

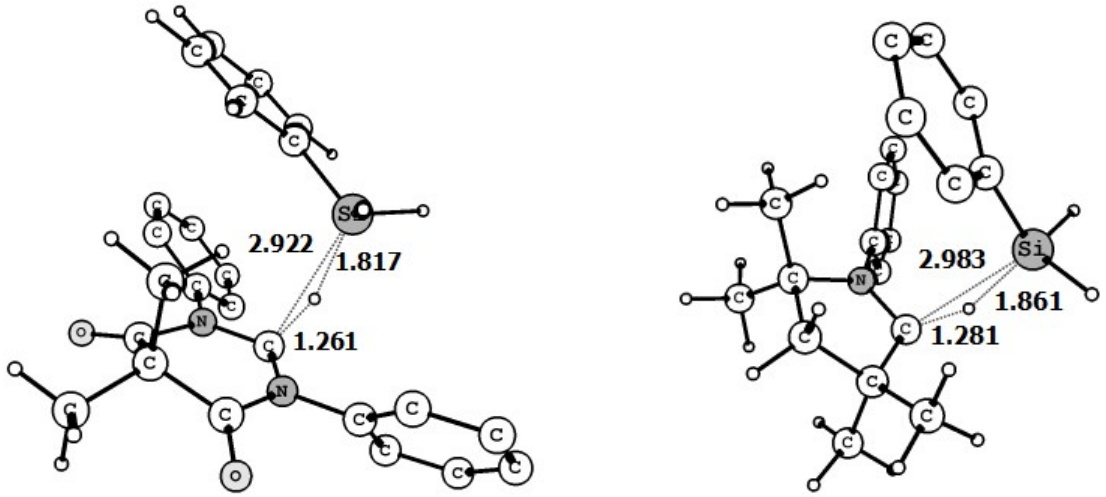


III-Int^{P-H}



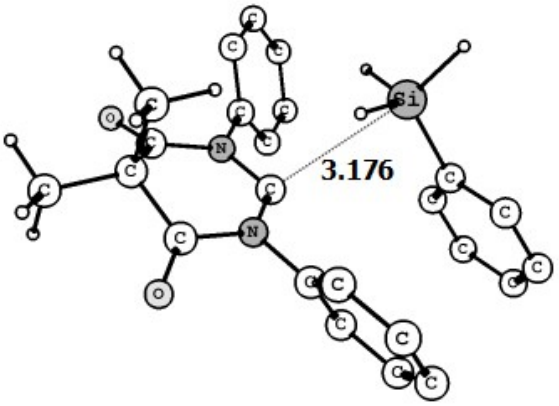
III-TS$_2$$^{P-H}$

Fig. **S14** Optimized geometries of the transition states and intermediate involved in the activation of P – H bond of PH_3 by DAC (**III**) via electrophilic pathway. The hydrogen atoms of the phenyl ring are omitted for clarity.

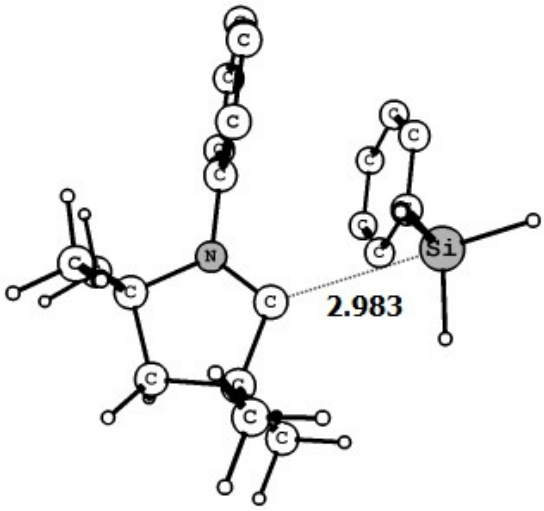


III-TS$_{PT}^{Si-H}$ **IV-TS$_{PT}^{Si-H}$**

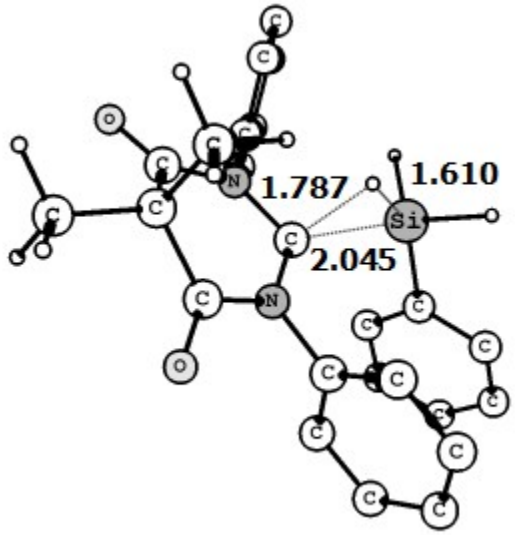
Fig. **S15** Optimized geometries of the transition states involved in the activation of Si – H bond of SiH_3Ph by DAC (**III**) and CAAC (**IV**) via proton transfer pathway. The hydrogen atoms of the phenyl ring are omitted for clarity.



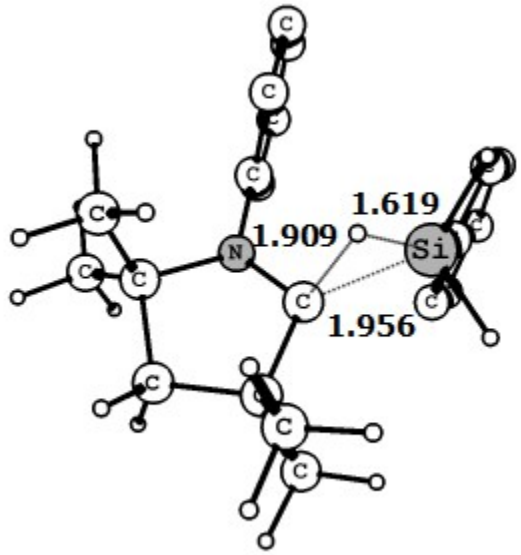
III$_V$



IV$_V$

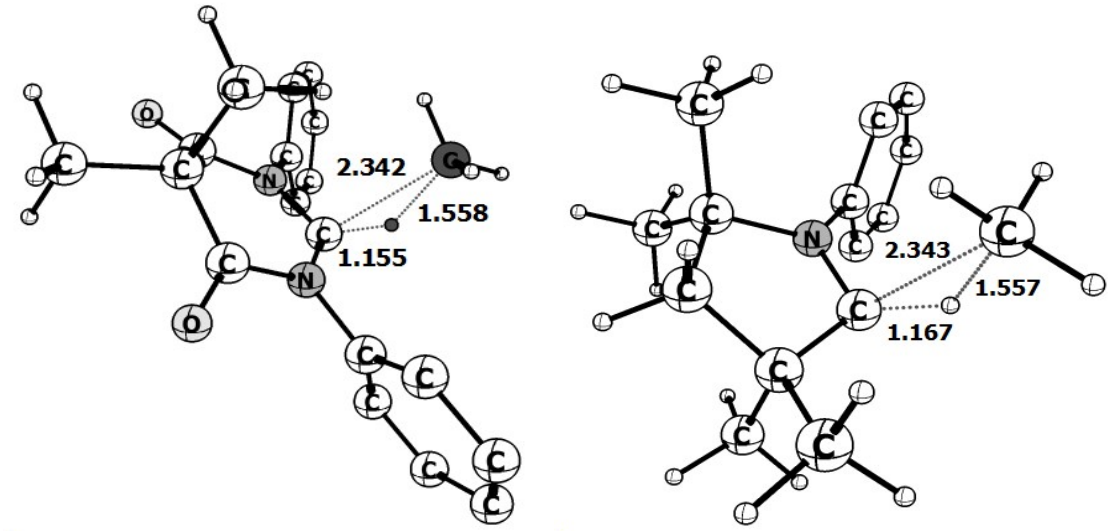


III-TS$_{hy}^{Si-H}$



IV-TS$_{hy}^{Si-H}$

Fig. **S16** Optimized geometries of the van der Waals complexes and transition states involved in the activation of Si – H bond of SiH_3Ph by DAC (**III**) and CAAC (**IV**) via hydride transfer pathway. The hydrogen atoms of the phenyl ring are omitted for clarity.



III-TS^{C-H} **IV-TS^{C-H}**

Fig. **S17** Optimized geometries of the transition states involved in the activation of C – H bond of CH_4 by DAC (**III**) and CAAC (**IV**).

Cartesian coordinates of **1-3** and **I-IV** in their optimized singlet and triplet state, along with their total energies (in hartrees) including zero point vibrational correction.

1-S (TE = -2367.842935)

6	0.450022000	-1.438352000	-0.004860000
6	1.193331000	0.841327000	-0.063858000
7	1.496006000	-0.465438000	-0.007609000
7	-0.691245000	-0.836021000	-0.038885000
25	-0.798812000	1.226640000	0.004160000
6	-0.658231000	1.088256000	1.858634000
8	-0.544608000	0.982532000	2.982702000
6	-0.820023000	3.044811000	0.070035000
8	-0.901961000	4.184226000	0.116625000
6	-2.650956000	1.205955000	0.077672000
8	-3.786053000	1.197678000	0.130860000
6	-0.778279000	1.213575000	-1.858844000
8	-0.736997000	1.197805000	-2.993291000
6	-1.868972000	-1.627496000	-0.008057000
6	-2.591798000	-1.844104000	-1.171886000
6	-2.331863000	-2.136700000	1.195789000

6	-3.773960000	-2.562202000	-1.129349000
1	-2.215721000	-1.447895000	-2.109391000
6	-3.517052000	-2.851601000	1.235110000
1	-1.749259000	-1.967339000	2.095245000
6	-4.243666000	-3.062331000	0.074747000
1	-4.331380000	-2.733049000	-2.043069000
1	-3.873469000	-3.248188000	2.178818000
1	-5.172494000	-3.619245000	0.107421000
6	2.844778000	-0.958506000	-0.002905000
6	3.280684000	-1.736713000	-1.059871000
6	3.680525000	-0.690289000	1.066997000
6	4.569610000	-2.240754000	-1.050390000
1	2.599264000	-1.952690000	-1.874146000
6	4.968359000	-1.195606000	1.071120000
1	3.315132000	-0.094401000	1.895633000
6	5.415487000	-1.968996000	0.012208000
1	4.912246000	-2.852831000	-1.876205000
1	5.622768000	-0.990538000	1.910067000
1	6.423196000	-2.367258000	0.019297000
8	2.262224000	1.585827000	-0.161379000
6	2.162806000	2.998203000	-0.274249000
1	1.550226000	3.274994000	-1.132737000
1	1.752939000	3.428578000	0.639379000
1	3.177863000	3.358654000	-0.421277000

1-**T** (TE = -2367.773420)

6	0.397945000	1.191654000	-0.173435000
6	1.200629000	-0.979787000	-0.012082000
7	1.462997000	0.411516000	-0.102754000
7	-0.812078000	0.806425000	-0.296104000
25	-0.848840000	-1.318985000	0.079143000
6	-0.637935000	-1.632744000	-1.742541000
8	-0.421979000	-1.812591000	-2.843383000
6	-0.756105000	-3.079779000	0.481830000
8	-0.730940000	-4.187699000	0.762722000
6	-2.688625000	-1.424393000	0.085959000
8	-3.822629000	-1.540195000	0.089501000
6	-0.716310000	-0.861956000	1.896583000
8	-0.577745000	-0.563721000	2.982048000
6	-1.907515000	1.682396000	-0.181796000

6	-3.003523000	1.520756000	-1.020127000
6	-1.913626000	2.699005000	0.768567000
6	-4.092062000	2.365752000	-0.907378000
1	-2.985409000	0.735573000	-1.768065000
6	-3.004276000	3.542502000	0.872659000
1	-1.057141000	2.810458000	1.425741000
6	-4.098521000	3.378967000	0.038242000
1	-4.940679000	2.233764000	-1.568265000
1	-3.001322000	4.330185000	1.617198000
1	-4.953698000	4.038201000	0.124984000
6	2.765676000	0.996112000	-0.067250000
6	3.735692000	0.469006000	0.771118000
6	3.035740000	2.108920000	-0.846352000
6	4.982040000	1.063637000	0.823315000
1	3.501828000	-0.394226000	1.383355000
6	4.282618000	2.705740000	-0.776424000
1	2.268060000	2.495682000	-1.507844000
6	5.259705000	2.182656000	0.053090000
1	5.741388000	0.654027000	1.478889000
1	4.492484000	3.578005000	-1.383907000
1	6.238266000	2.645150000	0.099623000
8	2.212254000	-1.649348000	-0.613793000
6	2.323739000	-3.015156000	-0.301413000
1	2.300937000	-3.173976000	0.782446000
1	1.519120000	-3.596363000	-0.763759000
1	3.277329000	-3.358746000	-0.699099000

2-**S** (TE = -2405.888257)

6	-1.319194000	0.685845000	-0.863716000
6	-0.003463000	-1.425011000	-0.446388000
6	1.317341000	0.679997000	-0.869666000
7	1.142583000	-0.736938000	-0.568567000
7	-1.147070000	-0.732731000	-0.567000000
6	2.343632000	-1.478636000	-0.349642000
6	3.450776000	-1.284761000	-1.165485000
6	2.415816000	-2.396289000	0.690216000
6	4.613339000	-2.003767000	-0.944775000
1	3.395404000	-0.584852000	-1.991278000
6	3.578741000	-3.112414000	0.904860000
1	1.542781000	-2.540913000	1.314830000

6	4.683786000	-2.919832000	0.090479000
1	5.466470000	-1.851147000	-1.595802000
1	3.623777000	-3.823491000	1.721844000
1	5.594329000	-3.481541000	0.262074000
6	-2.350356000	-1.471265000	-0.348700000
6	-3.456662000	-1.273504000	-1.164690000
6	-2.425479000	-2.389328000	0.690547000
6	-4.621352000	-1.989357000	-0.944890000
1	-3.398991000	-0.572896000	-1.989740000
6	-3.590551000	-3.102206000	0.904380000
1	-1.553045000	-2.536885000	1.315310000
6	-4.694725000	-2.905958000	0.089697000
1	-5.473851000	-1.833849000	-1.596063000
1	-3.637930000	-3.813672000	1.720894000
1	-5.606908000	-3.465226000	0.260556000
1	1.187866000	0.852525000	-1.940360000
1	2.341093000	0.950060000	-0.616184000
1	-2.340629000	0.957794000	-0.602720000
1	-1.196671000	0.860780000	-1.934831000
26	0.004005000	1.945046000	0.154027000
6	0.002412000	0.748056000	1.540108000
6	-1.399225000	2.877472000	0.869204000
6	0.004121000	2.908767000	-1.388156000
6	1.415009000	2.869100000	0.864644000
8	0.003761000	3.444055000	-2.385319000
8	2.312593000	3.420735000	1.281716000
8	-2.292141000	3.434620000	1.288954000
8	0.000763000	0.012884000	2.398095000

2-**T** (TE = -2405.814365)

6	-0.715811000	1.573618000	1.100568000
6	0.826098000	-0.085372000	1.796535000
6	-1.211684000	-1.155955000	1.285604000
7	0.219953000	-1.226685000	1.309794000
7	0.650260000	1.138486000	1.182191000
6	0.941383000	-2.198864000	0.608376000
6	0.310297000	-3.197750000	-0.136287000
6	2.338493000	-2.180057000	0.641807000
6	1.060097000	-4.131296000	-0.831146000
1	-0.768814000	-3.248178000	-0.198188000

6	3.072434000	-3.116807000	-0.055022000
1	2.841583000	-1.424613000	1.232744000
6	2.442503000	-4.101479000	-0.801593000
1	0.545378000	-4.890054000	-1.409713000
1	4.154848000	-3.077501000	-0.010464000
1	3.021988000	-4.834518000	-1.348951000
6	1.702359000	1.799847000	0.542191000
6	1.481445000	2.806125000	-0.399984000
6	3.021110000	1.455513000	0.850672000
6	2.550492000	3.428775000	-1.020349000
1	0.475143000	3.093601000	-0.677975000
6	4.076955000	2.084178000	0.223840000
1	3.203630000	0.707324000	1.613165000
6	3.853962000	3.075586000	-0.719849000
1	2.352744000	4.198625000	-1.757621000
1	5.090203000	1.801544000	0.485949000
1	4.685079000	3.567962000	-1.209311000
1	-1.538676000	-0.821587000	2.271134000
1	-1.648677000	-2.134717000	1.103690000
1	-0.763955000	2.609240000	0.772686000
1	-1.138206000	1.521360000	2.105688000
26	-1.938468000	0.302029000	-0.121884000
6	-0.468601000	-0.001427000	-1.179139000
6	-2.408145000	1.765172000	-1.102898000
6	-3.196550000	0.595529000	1.151088000
6	-2.885637000	-1.026149000	-0.937307000
8	-3.926227000	0.773227000	1.999180000
8	-3.455881000	-1.888219000	-1.405300000
8	-2.670722000	2.708781000	-1.675733000
8	0.433981000	-0.173660000	-1.836945000

3-**S** (TE = -2554.009118)

6	-1.446960000	0.622565000	0.256118000
7	-1.169958000	-0.763417000	0.054553000
6	0.000036000	-1.430221000	-0.000230000
7	1.170003000	-0.763325000	-0.054776000
6	1.446993000	0.622714000	-0.255816000
8	-2.561680000	0.953524000	0.552020000
6	-2.337873000	-1.621905000	0.059339000
6	-3.214782000	-1.570104000	-1.007476000

6	-4.324240000	-2.396691000	-1.018810000
6	-4.552907000	-3.266022000	0.035410000
6	-3.668232000	-3.309097000	1.100534000
6	-2.557074000	-2.483913000	1.115330000
1	-3.022176000	-0.883687000	-1.825550000
1	-5.011180000	-2.363432000	-1.856148000
1	-5.421350000	-3.914014000	0.025169000
1	-3.842236000	-3.990069000	1.925292000
1	-1.845760000	-2.512849000	1.932467000
6	2.337965000	-1.621752000	-0.059493000
6	2.557496000	-2.483443000	-1.115671000
6	3.668683000	-3.308589000	-1.100795000
6	4.553051000	-3.265785000	-0.035406000
6	4.324053000	-2.396761000	1.018998000
6	3.214566000	-1.570214000	1.007586000
1	1.846415000	-2.512170000	-1.933018000
1	3.842945000	-3.989320000	-1.925698000
1	5.421514000	-3.913748000	-0.025101000
1	5.010756000	-2.363715000	1.856538000
1	3.021689000	-0.884026000	1.825791000
8	2.561816000	0.953857000	-0.551128000
26	-0.000081000	1.991140000	0.000013000
6	0.340006000	1.689151000	1.768027000
8	0.562513000	1.424488000	2.844997000
6	-0.340047000	1.688934000	-1.767984000
8	-0.562307000	1.424314000	-2.845016000
6	-1.323508000	3.292789000	0.253878000
8	-2.114535000	4.080332000	0.405338000
6	1.323152000	3.292961000	-0.254038000
8	2.114058000	4.080595000	-0.405650000

3-**T** (TE = -2553.951406)

6	-0.839337000	1.460786000	-0.262789000
7	0.463618000	1.259986000	0.222506000
6	0.730450000	0.054667000	0.815923000
7	0.589907000	-1.178547000	0.225555000
6	-0.700903000	-1.561567000	-0.165362000
8	-1.139608000	2.461502000	-0.859954000
6	1.529515000	2.193813000	0.038922000
6	1.330511000	3.555969000	0.210945000

6	2.396250000	4.423645000	0.052578000
6	3.657063000	3.944113000	-0.263217000
6	3.851308000	2.582257000	-0.423348000
6	2.791239000	1.706581000	-0.276383000
1	0.348629000	3.930202000	0.464737000
1	2.238219000	5.487410000	0.185920000
1	4.486861000	4.630486000	-0.381869000
1	4.832930000	2.195402000	-0.670078000
1	2.937381000	0.639207000	-0.408990000
6	1.738679000	-2.024567000	0.138761000
6	2.694290000	-1.945750000	1.144443000
6	3.845371000	-2.707814000	1.064935000
6	4.043670000	-3.559558000	-0.008622000
6	3.086249000	-3.635829000	-1.006440000
6	1.934829000	-2.870766000	-0.943419000
1	2.525273000	-1.283246000	1.987088000
1	4.586072000	-2.639502000	1.852846000
1	4.942433000	-4.161498000	-0.068271000
1	3.237566000	-4.293740000	-1.854149000
1	1.195354000	-2.925307000	-1.729285000
8	-0.922359000	-2.647427000	-0.635186000
26	-2.146970000	-0.105689000	0.044569000
6	-2.098616000	-0.170084000	-1.785306000
8	-2.026143000	-0.210404000	-2.911689000
6	-1.756266000	-0.033572000	1.838506000
8	-1.600736000	0.008402000	2.959430000
6	-3.446718000	1.211142000	0.150207000
8	-4.226000000	2.025301000	0.207825000
6	-3.329693000	-1.520315000	0.242412000
8	-4.039094000	-2.389934000	0.358373000

I-S (TE = -687.771091)

6	-0.000001000	0.348905000	-0.082099000
6	0.670277000	-1.746075000	0.546092000
6	-0.670270000	-1.746074000	0.546104000
1	1.367598000	-2.518454000	0.822584000
1	-1.367588000	-2.518455000	0.822599000
7	1.060128000	-0.467966000	0.162728000
7	-1.060126000	-0.467966000	0.162736000
6	-2.408784000	-0.055393000	0.020909000

6	-3.387175000	-0.972804000	-0.331285000
6	-2.746092000	1.273034000	0.234545000
6	-4.702770000	-0.561119000	-0.459665000
1	-3.119741000	-2.004124000	-0.529026000
6	-4.060549000	1.676497000	0.094276000
1	-1.965638000	1.972690000	0.504963000
6	-5.045077000	0.762967000	-0.248533000
1	-5.461863000	-1.282488000	-0.738418000
1	-4.318986000	2.715440000	0.262572000
1	-6.074725000	1.083376000	-0.352790000
6	2.408785000	-0.055393000	0.020886000
6	3.387165000	-0.972800000	-0.331348000
6	2.746100000	1.273028000	0.234547000
6	4.702759000	-0.561117000	-0.459742000
1	3.119722000	-2.004114000	-0.529107000
6	4.060556000	1.676490000	0.094262000
1	1.965653000	1.972680000	0.504997000
6	5.045075000	0.762963000	-0.248586000
1	5.461844000	-1.282482000	-0.738527000
1	4.319001000	2.715428000	0.262577000
1	6.074722000	1.083372000	-0.352856000

I-T (TE = -687.660750)

6	0.000000000	0.188850000	0.000021000
6	-0.670986000	-1.916326000	0.000060000
6	0.670986000	-1.916326000	0.000060000
1	-1.346978000	-2.753549000	0.000080000
1	1.346978000	-2.753550000	0.000083000
7	-1.129157000	-0.600364000	0.000070000
7	1.129157000	-0.600364000	0.000060000
6	-2.423551000	-0.119589000	0.000015000
6	-2.614918000	1.265755000	0.000048000
6	-3.532595000	-0.967501000	-0.000071000
6	-3.893934000	1.785147000	0.000023000
1	-1.745521000	1.918361000	0.000064000
6	-4.802832000	-0.429051000	-0.000090000
1	-3.404325000	-2.043064000	-0.000139000
6	-4.998367000	0.946854000	-0.000036000
1	-4.029239000	2.860771000	0.000051000
1	-5.657030000	-1.096488000	-0.000163000

1	-5.999989000	1.358236000	-0.000045000
6	2.423551000	-0.119588000	0.000008000
6	2.614918000	1.265755000	0.000017000
6	3.532595000	-0.967502000	-0.000050000
6	3.893934000	1.785147000	-0.000004000
1	1.745522000	1.918361000	0.000007000
6	4.802832000	-0.429051000	-0.000067000
1	3.404325000	-2.043065000	-0.000095000
6	4.998367000	0.946854000	-0.000036000
1	4.029239000	2.860771000	0.000006000
1	5.657030000	-1.096488000	-0.000116000
1	5.999989000	1.358235000	-0.000041000

II-**S** (TE = -728.217605)

6	-1.227226000	2.102399000	0.145231000
6	-0.000005000	-0.064052000	0.042320000
6	1.227252000	2.102379000	0.145344000
6	-0.000015000	2.633590000	0.834670000
7	1.143109000	0.639395000	0.068987000
7	-1.143105000	0.639411000	0.068953000
6	2.370367000	-0.071348000	-0.028530000
6	3.495515000	0.535385000	-0.574838000
6	2.465048000	-1.382743000	0.426585000
6	4.691033000	-0.159831000	-0.666249000
1	3.444607000	1.548525000	-0.953475000
6	3.659738000	-2.068040000	0.329911000
1	1.583157000	-1.847979000	0.846359000
6	4.782471000	-1.463210000	-0.215740000
1	5.555208000	0.328366000	-1.102063000
1	3.716323000	-3.087635000	0.694128000
1	5.718415000	-2.004320000	-0.286439000
6	-2.370370000	-0.071322000	-0.028530000
6	-3.495429000	0.535300000	-0.575142000
6	-2.465137000	-1.382586000	0.426932000
6	-4.690951000	-0.159912000	-0.666525000
1	-3.444433000	1.548339000	-0.954039000
6	-3.659830000	-2.067883000	0.330283000
1	-1.583313000	-1.847721000	0.846963000
6	-4.782474000	-1.463171000	-0.215682000
1	-5.555058000	0.328185000	-1.102583000

1	-3.716492000	-3.087378000	0.694770000
1	-5.718420000	-2.004279000	-0.286361000
1	1.318395000	2.531273000	-0.860314000
1	2.129595000	2.370527000	0.697916000
1	0.000000000	3.724413000	0.820170000
1	-0.000069000	2.316467000	1.881920000
1	-2.129626000	2.370595000	0.697687000
1	-1.318240000	2.531252000	-0.860457000

II-**T** (TE = -728.132541)

6	1.384201000	2.284644000	-0.169333000
6	-0.000317000	0.462402000	-0.838467000
6	-1.075200000	2.194117000	0.374032000
6	0.034219000	2.958463000	-0.325808000
7	-1.133080000	0.832172000	-0.151435000
7	1.242506000	0.852071000	-0.423014000
6	-2.245296000	0.024554000	-0.038004000
6	-2.260599000	-1.226445000	-0.668203000
6	-3.369120000	0.418939000	0.694181000
6	-3.362533000	-2.049064000	-0.561076000
1	-1.399667000	-1.531476000	-1.254911000
6	-4.465276000	-0.419088000	0.788912000
1	-3.381219000	1.370281000	1.211001000
6	-4.477176000	-1.656471000	0.166275000
1	-3.352361000	-3.012108000	-1.059394000
1	-5.323114000	-0.096545000	1.368541000
1	-5.339942000	-2.305990000	0.246546000
6	2.259866000	-0.044805000	-0.132059000
6	2.013999000	-1.420733000	-0.184518000
6	3.544352000	0.395950000	0.195138000
6	3.019176000	-2.320293000	0.101432000
1	1.020237000	-1.768808000	-0.449164000
6	4.541716000	-0.520449000	0.478130000
1	3.768731000	1.454614000	0.229366000
6	4.292821000	-1.881668000	0.436264000
1	2.804834000	-3.382382000	0.061180000
1	5.531087000	-0.158146000	0.734212000
1	5.079686000	-2.592532000	0.656180000
1	-0.900337000	2.169022000	1.459181000
1	-2.034170000	2.692830000	0.207186000

1	0.090126000	3.970130000	0.079982000
1	-0.214471000	3.050110000	-1.386693000
1	2.123450000	2.738512000	-0.840163000
1	1.752150000	2.412461000	0.856708000

III-S (TE = -954.860199)

6	1.250636000	1.463475000	-0.337664000
7	1.138078000	0.075452000	-0.080186000
6	-0.018483000	-0.615498000	0.015055000
7	-1.158355000	0.115223000	-0.028958000
6	-1.261821000	1.522833000	-0.073827000
6	0.044751000	2.268945000	0.070437000
8	2.252826000	1.949884000	-0.775975000
6	0.217534000	2.515727000	1.585637000
1	-0.619067000	3.116046000	1.946243000
1	0.251196000	1.583451000	2.153484000
1	1.146152000	3.063912000	1.756252000
6	-0.004915000	3.593225000	-0.667519000
1	-0.110278000	3.444815000	-1.743280000
1	-0.852483000	4.179301000	-0.315739000
1	0.914607000	4.149111000	-0.489674000
6	2.357642000	-0.690616000	-0.073110000
6	3.354698000	-0.362224000	0.828080000
6	4.518219000	-1.108873000	0.858788000
6	4.680749000	-2.178307000	-0.007327000
6	3.675944000	-2.500168000	-0.904186000
6	2.510435000	-1.754370000	-0.941039000
1	3.214211000	0.474133000	1.504975000
1	5.299288000	-0.856895000	1.566063000
1	5.592570000	-2.763041000	0.018867000
1	3.798638000	-3.336479000	-1.581999000
1	1.708391000	-1.997278000	-1.627513000
6	-2.390312000	-0.634842000	0.017763000
6	-2.643067000	-1.439341000	1.112569000
6	-3.810291000	-2.181125000	1.159205000
6	-4.718455000	-2.112848000	0.115812000
6	-4.455512000	-1.304078000	-0.977573000
6	-3.288891000	-0.562005000	-1.030631000
1	-1.913979000	-1.488763000	1.912913000
1	-4.009492000	-2.815231000	2.014860000

1	-5.632514000	-2.693532000	0.153271000
1	-5.161040000	-1.251822000	-1.798170000
1	-3.073830000	0.071585000	-1.882424000
8	-2.318274000	2.083428000	-0.139894000

III-T (TE = -954.790481)

6	1.317914000	1.623336000	-0.192466000
7	1.211670000	0.286499000	0.189957000
6	-0.002166000	-0.118840000	0.667061000
7	-1.194731000	0.358306000	0.183152000
6	-1.230386000	1.716278000	-0.134167000
6	0.081504000	2.451927000	0.160403000
8	2.289986000	2.074230000	-0.743137000
6	0.123124000	2.748825000	1.670525000
1	-0.735970000	3.366568000	1.939198000
1	0.102914000	1.842459000	2.278201000
1	1.033612000	3.304277000	1.903997000
6	0.111599000	3.757084000	-0.609726000
1	0.078852000	3.586865000	-1.686284000
1	-0.746555000	4.368489000	-0.333902000
1	1.027709000	4.299280000	-0.378331000
6	2.239314000	-0.685086000	0.009391000
6	3.575410000	-0.364932000	0.200328000
6	4.535265000	-1.349087000	0.046675000
6	4.174064000	-2.645371000	-0.282242000
6	2.837015000	-2.959335000	-0.459925000
6	1.868933000	-1.982872000	-0.316713000
1	3.857949000	0.645172000	0.460784000
1	5.579017000	-1.097408000	0.192858000
1	4.933092000	-3.409665000	-0.397571000
1	2.542479000	-3.969742000	-0.717317000
1	0.818750000	-2.218233000	-0.462889000
6	-2.287772000	-0.551310000	0.093095000
6	-2.203055000	-1.730687000	0.827361000
6	-3.209630000	-2.673770000	0.747413000
6	-4.313518000	-2.448080000	-0.056950000
6	-4.395050000	-1.271798000	-0.781773000
6	-3.392061000	-0.319718000	-0.717238000
1	-1.346945000	-1.898278000	1.474006000
1	-3.130763000	-3.586494000	1.325969000

1	-5.105922000	-3.184216000	-0.117130000
1	-5.251624000	-1.086659000	-1.419326000
1	-3.461505000	0.591374000	-1.290348000
8	-2.202072000	2.269919000	-0.583112000

IV-S (TE = -599.083898)

6	-0.834585000	1.167201000	0.341199000
6	-2.293293000	0.876531000	0.002692000
6	-2.379777000	-0.637795000	-0.265835000
6	-0.961484000	-1.104996000	-0.493753000
7	-0.188744000	-0.103925000	-0.170043000
1	-2.574729000	1.427875000	-0.899825000
1	-2.963780000	1.202257000	0.802694000
6	1.236861000	-0.235451000	-0.150921000
6	2.004567000	0.269970000	-1.186767000
6	3.381242000	0.125557000	-1.154641000
6	3.989454000	-0.520136000	-0.091000000
6	3.217058000	-1.032677000	0.938670000
6	1.840981000	-0.891886000	0.909035000
1	1.517347000	0.756237000	-2.023832000
1	3.980518000	0.513092000	-1.970098000
1	5.066926000	-0.633039000	-0.069312000
1	3.687244000	-1.551120000	1.765941000
1	1.216659000	-1.302416000	1.695532000
6	-3.240019000	-0.950948000	-1.478000000
1	-3.270742000	-2.027135000	-1.660692000
1	-4.263354000	-0.594879000	-1.322982000
1	-2.844966000	-0.467494000	-2.375411000
6	-2.908332000	-1.409082000	0.941289000
1	-3.937926000	-1.107012000	1.154801000
1	-2.894467000	-2.483104000	0.744868000
1	-2.309401000	-1.226873000	1.837423000
6	-0.308045000	2.388649000	-0.383421000
1	0.745924000	2.572122000	-0.162935000
1	-0.428939000	2.287613000	-1.464517000
1	-0.873016000	3.266981000	-0.061554000
6	-0.576639000	1.299441000	1.831927000
1	-1.076535000	2.192862000	2.213271000
1	-0.954721000	0.435964000	2.383126000
1	0.491234000	1.399276000	2.040949000

IV-T (TE = -599.015824)

6	-0.889815000	1.254200000	-0.065375000
6	-2.334901000	0.735235000	-0.244249000
6	-2.353149000	-0.791062000	-0.002604000
6	-0.940599000	-1.055786000	-0.364985000
7	-0.091672000	-0.003278000	-0.177627000
1	-2.655979000	0.920864000	-1.272819000
1	-3.025738000	1.263219000	0.420341000
6	1.276693000	-0.161782000	-0.091089000
6	2.183872000	0.895215000	0.056380000
6	3.541055000	0.646346000	0.136863000
6	4.043456000	-0.643607000	0.070004000
6	3.151588000	-1.694932000	-0.084411000
6	1.794864000	-1.465213000	-0.168374000
1	1.840759000	1.917889000	0.112507000
1	4.218002000	1.485388000	0.254064000
1	5.109118000	-0.825918000	0.131881000
1	3.518419000	-2.713723000	-0.144697000
1	1.104084000	-2.292831000	-0.297395000
6	-3.354403000	-1.484997000	-0.908256000
1	-3.318862000	-2.567704000	-0.767687000
1	-4.370828000	-1.151048000	-0.680239000
1	-3.145075000	-1.269946000	-1.958207000
6	-2.655033000	-1.143197000	1.454566000
1	-3.658256000	-0.803020000	1.731537000
1	-2.610864000	-2.224784000	1.599565000
1	-1.937139000	-0.686889000	2.138196000
6	-0.567096000	2.231511000	-1.183137000
1	0.412728000	2.696507000	-1.077798000
1	-0.606415000	1.723817000	-2.149480000
1	-1.314215000	3.029736000	-1.187122000
6	-0.710726000	1.897116000	1.301388000
1	-1.355545000	2.776960000	1.368432000
1	-0.991840000	1.210761000	2.101310000
1	0.314511000	2.219375000	1.480675000

Cartesian coordinates of H_2, NH_3, PH_3, SiH_3Ph and CH_4, along with their total energies (in hartrees) including zero point vibrational correction.

H_2 (TE = -1.160836)

1	0.000000000	0.000000000	0.373457000
1	0.000000000	0.000000000	-0.373457000

NH_3 (TE = -56.509166)

7	0.000000000	0.000000000	0.114416000
1	0.000000000	0.938276000	-0.266971000
1	-0.812571000	-0.469138000	-0.266971000
1	0.812571000	-0.469138000	-0.266971000

PH_3 (TE = -343.109705)

15	0.000000000	0.000000000	0.127733000
1	0.000000000	1.192412000	-0.638667000
1	-1.032659000	-0.596206000	-0.638667000
1	1.032659000	-0.596206000	-0.638667000

SiH_3Ph (TE = -522.717016)

14	-2.328705000	0.000028000	0.005195000
1	-2.827744000	-1.206911000	-0.687965000
1	-2.827241000	1.215800000	-0.672689000
1	-2.852591000	-0.008933000	1.389066000
6	-0.463638000	0.000151000	-0.011617000
6	0.252990000	-1.195725000	-0.008920000
6	0.253174000	1.195836000	-0.008928000
6	1.637548000	-1.199060000	0.002968000
1	-0.279062000	-2.142875000	-0.021232000
6	1.637806000	1.198902000	0.002967000
1	-0.278692000	2.143071000	-0.021199000
6	2.331460000	-0.000115000	0.009960000
1	2.177675000	-2.138948000	0.003127000
1	2.178055000	2.138719000	0.003118000
1	3.415438000	-0.000250000	0.016471000

CH_4 (TE = -40.448443)

6	0.000000000	0.000000000	0.000000000
1	0.628315000	0.628315000	0.628315000
1	-0.628315000	-0.628315000	0.628315000

1	-0.628315000	0.628315000	-0.628315000
1	0.628315000	-0.628315000	-0.628315000

Cartesian coordinates of the transition states involved in the activation of hydrogen by **1**, **3** and **IV**, along with their total energies (in hartrees) including zero point vibrational correction.

1TS^{H-H} (TE = -2368.963393)

6	-0.443476000	-1.315068000	0.061975000
6	-1.172795000	0.923036000	0.075863000
7	-1.488406000	-0.378794000	0.050991000
7	0.734576000	-0.788354000	0.189847000
25	0.828093000	1.274196000	-0.056718000
6	0.667260000	0.873412000	-1.884795000
8	0.541715000	0.577332000	-2.969545000
6	0.818726000	3.067139000	-0.362667000
8	0.875044000	4.188863000	-0.571087000
6	2.678727000	1.291157000	-0.169922000
8	3.810940000	1.331060000	-0.250110000
6	0.852634000	1.501360000	1.793115000
8	0.844711000	1.632085000	2.920470000
6	1.863985000	-1.641975000	0.145322000
6	2.823081000	-1.568920000	1.147557000
6	2.032900000	-2.529822000	-0.909336000
6	3.942116000	-2.379266000	1.095445000
1	2.681383000	-0.877653000	1.971874000
6	3.159786000	-3.332534000	-0.958547000
1	1.270213000	-2.586072000	-1.681432000
6	4.116431000	-3.261255000	0.040227000
1	4.682403000	-2.322260000	1.884948000
1	3.288578000	-4.020767000	-1.785992000
1	4.995925000	-3.892786000	-0.000795000
6	-2.830350000	-0.891789000	0.077257000
6	-3.246891000	-1.617815000	1.176428000
6	-3.663917000	-0.693868000	-1.009141000
6	-4.527189000	-2.146552000	1.193181000
1	-2.566128000	-1.767928000	2.006599000
6	-4.942535000	-1.217995000	-0.982643000
1	-3.295870000	-0.148247000	-1.870373000
6	-5.374110000	-1.943413000	0.117404000
1	-4.861474000	-2.718446000	2.050338000

1	-5.599851000	-1.073641000	-1.831473000
1	-6.374726000	-2.359013000	0.131243000
8	-2.233890000	1.669482000	0.210810000
6	-2.126217000	3.083960000	0.286277000
1	-1.432267000	3.378684000	1.073955000
1	-1.809894000	3.494391000	-0.672408000
1	-3.122486000	3.447186000	0.524962000
1	-0.731437000	-2.261845000	-0.591117000
1	-1.027047000	-2.365786000	-1.800555000

3TS$^{H\text{-}H}$ (TE = -2555.137412)

6	1.463559000	0.671713000	0.341698000
7	1.195216000	-0.701533000	0.155455000
6	-0.000409000	-1.309121000	-0.025595000
7	-1.195719000	-0.700856000	0.155311000
6	-1.463247000	0.672536000	0.341643000
8	2.570673000	1.008020000	0.670274000
6	2.320048000	-1.596216000	0.054686000
6	2.493665000	-2.595326000	0.993618000
6	3.554873000	-3.473887000	0.860943000
6	4.428508000	-3.351011000	-0.207421000
6	4.240531000	-2.351831000	-1.148499000
6	3.181431000	-1.471201000	-1.021212000
1	1.794674000	-2.677045000	1.818350000
1	3.700538000	-4.256217000	1.596187000
1	5.258510000	-4.040153000	-0.308917000
1	4.917106000	-2.261456000	-1.989709000
1	3.012700000	-0.686857000	-1.751425000
6	-2.320994000	-1.594982000	0.054605000
6	-2.494914000	-2.594096000	0.993480000
6	-3.556536000	-3.472172000	0.860915000
6	-4.430286000	-3.348823000	-0.207298000
6	-4.242014000	-2.349648000	-1.148324000
6	-3.182500000	-1.469500000	-1.021144000
1	-1.795812000	-2.676208000	1.818079000
1	-3.702427000	-4.254497000	1.596120000
1	-5.260605000	-4.037593000	-0.308722000
1	-4.918679000	-2.258912000	-1.989423000
1	-3.013539000	-0.685187000	-1.751332000
8	-2.570137000	1.009487000	0.670318000

26	0.000548000	2.019817000	0.013827000
6	0.000561000	1.439325000	-1.725320000
8	0.000614000	1.071499000	-2.793588000
6	0.000512000	2.137746000	1.841574000
8	0.000484000	2.165085000	2.970604000
6	1.363378000	3.268266000	-0.251630000
8	2.193332000	4.014032000	-0.410188000
6	-1.361596000	3.268979000	-0.251902000
8	-2.191145000	4.015146000	-0.410689000
1	-0.000555000	-1.875726000	-1.952728000
1	-0.000622000	-2.139327000	-0.894094000

IVTS$^{H\text{-}H}$ (TE = -600.210632)

6	-0.845676000	1.214313000	0.348005000
6	-2.310395000	0.854412000	0.056643000
6	-2.353989000	-0.657975000	-0.216142000
6	-0.937440000	-0.976954000	-0.601787000
7	-0.153599000	-0.033100000	-0.100821000
1	-2.641267000	1.382850000	-0.842618000
1	-2.968235000	1.154854000	0.877207000
6	1.259831000	-0.183050000	-0.097220000
6	2.035766000	0.370825000	-1.105311000
6	3.409068000	0.189270000	-1.091267000
6	4.005742000	-0.542415000	-0.078486000
6	3.227335000	-1.104714000	0.921322000
6	1.855803000	-0.928245000	0.910146000
1	1.558118000	0.923302000	-1.905510000
1	4.014723000	0.617490000	-1.881275000
1	5.080488000	-0.680909000	-0.071011000
1	3.690621000	-1.684675000	1.710803000
1	1.224203000	-1.366688000	1.676284000
6	-3.393337000	-1.045614000	-1.247496000
1	-3.309720000	-2.106781000	-1.496618000
1	-4.398470000	-0.871312000	-0.853354000
1	-3.273825000	-0.472330000	-2.168154000
6	-2.622579000	-1.446347000	1.071044000
1	-3.598176000	-1.167878000	1.478915000
1	-2.625712000	-2.519778000	0.869536000
1	-1.865720000	-1.252726000	1.834700000
6	-0.402304000	2.404416000	-0.481519000

1	0.636747000	2.675481000	-0.280786000
1	-0.516040000	2.193266000	-1.548644000
1	-1.027418000	3.267973000	-0.240818000
6	-0.560219000	1.465585000	1.816682000
1	-1.067634000	2.375456000	2.144874000
1	-0.905432000	0.639012000	2.441308000
1	0.511273000	1.599781000	1.986548000
1	-0.703789000	-1.401803000	-1.714481000
1	-0.945183000	-0.753933000	-2.538839000

Cartesian coordinates of the transition states and the intermediates involved in the activation of N – H bond of NH_3 by **1**, **3** and **III-IV**, along with their total energies (in hartrees) including zero point vibrational correction.

1TS$_{Nu}^{N-H}$ (TE = -2424.312253)

6	-0.413034000	-1.176214000	0.080321000
6	-1.099190000	1.057157000	0.173674000
7	-1.446512000	-0.236718000	0.118290000
7	0.780866000	-0.677323000	0.084565000
25	0.909693000	1.373223000	-0.009537000
6	0.629650000	1.220543000	-1.855847000
8	0.421484000	1.090979000	-2.961589000
6	0.960799000	3.191944000	-0.088091000
8	1.061555000	4.327860000	-0.151225000
6	2.754864000	1.342898000	-0.184520000
8	3.886213000	1.345791000	-0.281992000
6	1.021425000	1.351835000	1.857041000
8	1.061988000	1.300695000	2.988701000
6	1.858965000	-1.593383000	0.121994000
6	2.108329000	-2.320931000	1.277456000
6	2.674429000	-1.761855000	-0.988904000
6	3.168996000	-3.209132000	1.321584000
1	1.461636000	-2.176805000	2.136769000
6	3.731846000	-2.652233000	-0.940715000
1	2.464801000	-1.200650000	-1.893801000
6	3.983559000	-3.375795000	0.214083000
1	3.359645000	-3.773338000	2.227042000
1	4.359325000	-2.786565000	-1.813862000
1	4.813678000	-4.071110000	0.249134000
6	-2.800324000	-0.720169000	0.142729000

6	-3.208896000	-1.518853000	1.193036000
6	-3.655687000	-0.418516000	-0.901878000
6	-4.499462000	-2.021341000	1.199335000
1	-2.513991000	-1.749242000	1.992467000
6	-4.943162000	-0.919630000	-0.886923000
1	-3.300418000	0.190440000	-1.725783000
6	-5.365722000	-1.720416000	0.163174000
1	-4.825465000	-2.652921000	2.016748000
1	-5.616145000	-0.695538000	-1.705627000
1	-6.373633000	-2.117804000	0.167815000
8	-2.141411000	1.824845000	0.339838000
6	-1.994007000	3.231170000	0.470269000
1	-1.313987000	3.472882000	1.287700000
1	-1.638694000	3.667922000	-0.463008000
1	-2.985164000	3.616025000	0.695906000
1	-0.712369000	-2.206968000	-0.256778000
7	-1.032570000	-2.588383000	-1.869519000
1	-0.147085000	-2.420629000	-2.353977000
1	-1.685835000	-1.953130000	-2.332456000

3TS$_{Nu}^{N-H}$ (TE =-2610.484624)

6	1.457988000	0.766329000	0.357949000
7	1.198030000	-0.609554000	0.170365000
6	0.000585000	-1.210788000	-0.000610000
7	-1.197427000	-0.610713000	0.170460000
6	-1.458611000	0.764904000	0.358329000
8	2.561521000	1.106813000	0.694097000
6	2.324188000	-1.511796000	0.155423000
6	2.407501000	-2.510911000	1.105894000
6	3.465952000	-3.402116000	1.064528000
6	4.430458000	-3.287124000	0.078318000
6	4.336957000	-2.281874000	-0.871361000
6	3.281032000	-1.390634000	-0.836117000
1	1.639459000	-2.588098000	1.867616000
1	3.535519000	-4.188650000	1.806225000
1	5.257509000	-3.986284000	0.045856000
1	5.086244000	-2.196363000	-1.649008000
1	3.189037000	-0.604366000	-1.577881000
6	-2.322724000	-1.514022000	0.155484000
6	-2.404649000	-2.513760000	1.105425000

6	-3.462241000	-3.405980000	1.064024000
6	-4.427298000	-3.291377000	0.078310000
6	-4.335183000	-2.285516000	-0.870856000
6	-3.280111000	-1.393266000	-0.835587000
1	-1.636201000	-2.590629000	1.866767000
1	-3.530706000	-4.192997000	1.805310000
1	-5.253686000	-3.991320000	0.045824000
1	-5.084886000	-2.200307000	-1.648135000
1	-3.189191000	-0.606540000	-1.576997000
8	-2.562330000	1.104313000	0.694953000
26	-0.001014000	2.112583000	0.018757000
6	-0.000919000	1.523423000	-1.712810000
8	-0.000861000	1.140132000	-2.775952000
6	-0.000861000	2.250829000	1.848312000
8	-0.000745000	2.289073000	2.976421000
6	1.362802000	3.361096000	-0.253452000
8	2.193260000	4.104664000	-0.417052000
6	-1.366130000	3.359728000	-0.253165000
8	-2.197373000	4.102453000	-0.416609000
1	0.001040000	-2.200988000	-0.573798000
7	0.000950000	-2.327448000	-2.107427000
1	0.807688000	-1.844042000	-2.504302000
1	-0.806520000	-1.845034000	-2.504029000

IIITS$_{Nu}^{N-H}$ (TE = -1011.335086)

6	1.263064000	1.608772000	-0.410036000
7	1.172399000	0.224575000	-0.212226000
6	0.000036000	-0.430496000	-0.035777000
7	-1.172374000	0.224499000	-0.212197000
6	-1.263149000	1.608684000	-0.410027000
6	-0.000071000	2.373141000	-0.074539000
8	2.284259000	2.134001000	-0.756015000
6	-0.000057000	2.531266000	1.460995000
1	-0.887100000	3.090386000	1.765436000
1	0.000070000	1.566910000	1.976643000
1	0.886861000	3.090603000	1.765393000
6	-0.000123000	3.732075000	-0.742968000
1	-0.000163000	3.640880000	-1.829932000
1	-0.888143000	4.288816000	-0.446914000
1	0.887898000	4.288850000	-0.446982000

6	2.369700000	-0.565089000	-0.164717000
6	3.342746000	-0.263818000	0.772193000
6	4.477109000	-1.050032000	0.846215000
6	4.631068000	-2.131171000	-0.007378000
6	3.648903000	-2.427217000	-0.937077000
6	2.512879000	-1.640961000	-1.020216000
1	3.202440000	0.579427000	1.440207000
1	5.241066000	-0.822098000	1.579495000
1	5.519971000	-2.747300000	0.055713000
1	3.766760000	-3.272592000	-1.604016000
1	1.733291000	-1.857100000	-1.741862000
6	-2.369632000	-0.565212000	-0.164706000
6	-3.342792000	-0.263776000	0.772027000
6	-4.477165000	-1.049970000	0.846048000
6	-4.631013000	-2.131255000	-0.007386000
6	-3.648722000	-2.427476000	-0.936895000
6	-2.512682000	-1.641241000	-1.020025000
1	-3.202538000	0.579630000	1.439858000
1	-5.241226000	-0.821901000	1.579178000
1	-5.519933000	-2.747363000	0.055683000
1	-3.766499000	-3.272966000	-1.603704000
1	-1.733001000	-1.857505000	-1.741536000
8	-2.284394000	2.133808000	-0.756013000
1	0.000055000	-1.393759000	0.590834000
7	0.000055000	-1.359632000	2.103541000
1	0.810331000	-0.849430000	2.457264000
1	-0.810216000	-0.849415000	2.457253000

$IVTS_{Nu}^{N-H}$ (TE = -655.559058)

6	-0.766491000	1.319131000	-0.570683000
6	-2.244444000	0.916049000	-0.498115000
6	-2.330552000	-0.312146000	0.421317000
6	-0.932541000	-0.846016000	0.398681000
7	-0.111945000	0.092015000	-0.019646000
1	-2.591066000	0.636411000	-1.497426000
1	-2.869932000	1.743240000	-0.152481000
6	1.300526000	-0.048255000	0.101010000
6	2.089736000	-0.323000000	-1.004989000
6	3.457583000	-0.468269000	-0.848833000
6	4.034400000	-0.342655000	0.403736000

6	3.241013000	-0.079387000	1.508838000
6	1.874155000	0.066186000	1.358510000
1	1.629328000	-0.446743000	-1.977611000
1	4.073911000	-0.693058000	-1.711017000
1	5.105168000	-0.459792000	0.520885000
1	3.687707000	0.009891000	2.491876000
1	1.231307000	0.265423000	2.210060000
6	-3.387172000	-1.302759000	-0.024806000
1	-3.354257000	-2.208324000	0.585465000
1	-4.381299000	-0.858818000	0.077727000
1	-3.242905000	-1.589995000	-1.067313000
6	-2.606257000	0.086409000	1.876195000
1	-3.576647000	0.585930000	1.942725000
1	-2.628332000	-0.796794000	2.517946000
1	-1.845609000	0.765532000	2.268316000
6	-0.335623000	1.565422000	-2.003810000
1	0.715636000	1.853556000	-2.070395000
1	-0.500018000	0.673123000	-2.613842000
1	-0.932338000	2.378923000	-2.423441000
6	-0.418546000	2.518509000	0.291660000
1	-0.905778000	3.411332000	-0.105890000
1	-0.746094000	2.383617000	1.324388000
1	0.659524000	2.697287000	0.293937000
1	-0.637408000	-1.962459000	0.342914000
7	-0.617569000	-2.871499000	-0.902983000
1	-1.543768000	-3.020352000	-1.302925000
1	-0.095252000	-2.406852000	-1.647739000

$3TS_1^{N-H}$ (TE = -2610.501350)

6	-1.476501000	0.762323000	-0.136100000
7	-1.225358000	-0.593711000	0.015304000
6	-0.038420000	-1.298943000	0.236209000
7	1.181708000	-0.661920000	-0.009501000
6	1.496620000	0.672025000	-0.218829000
8	-2.590935000	1.161648000	-0.380466000
6	-2.370414000	-1.467132000	-0.053424000
6	-2.458367000	-2.396653000	-1.075668000
6	-3.534717000	-3.262247000	-1.127725000
6	-4.522501000	-3.206887000	-0.155309000
6	-4.430506000	-2.277667000	0.866349000

6	-3.355635000	-1.404210000	0.917122000
1	-1.665175000	-2.439070000	-1.813246000
1	-3.603006000	-3.987009000	-1.930663000
1	-5.363780000	-3.888703000	-0.195588000
1	-5.199643000	-2.227806000	1.628273000
1	-3.282867000	-0.660902000	1.704602000
6	2.281201000	-1.591778000	-0.066999000
6	2.308645000	-2.565449000	-1.050458000
6	3.345777000	-3.478973000	-1.083639000
6	4.352981000	-3.427403000	-0.131144000
6	4.320028000	-2.454731000	0.853185000
6	3.284906000	-1.534073000	0.885052000
1	1.500494000	-2.603617000	-1.771722000
1	3.368186000	-4.238226000	-1.856718000
1	5.163113000	-4.146598000	-0.157339000
1	5.103911000	-2.408346000	1.600132000
1	3.256127000	-0.757505000	1.643152000
8	2.614166000	1.000362000	-0.543263000
26	0.055346000	2.098556000	-0.072036000
6	0.106712000	1.763020000	1.694887000
8	0.143506000	1.500136000	2.802129000
6	-0.006430000	1.827638000	-1.880641000
8	-0.044815000	1.604747000	-2.989224000
6	-1.254113000	3.423946000	0.002249000
8	-2.042748000	4.228918000	0.054346000
6	1.444975000	3.341204000	-0.084283000
8	2.283092000	4.096348000	-0.084439000
7	-0.027293000	-1.534568000	2.076810000
1	-0.862302000	-2.081058000	2.259187000
1	0.777240000	-2.129085000	2.245686000
1	0.001715000	-0.744483000	2.721199000

3Int$^{N\text{-}H}$ (TE = -2610.501534)

6	-1.501889000	0.715870000	-0.165162000
7	-1.222148000	-0.605338000	0.102662000
6	0.000058000	-1.226670000	0.462315000
7	1.222255000	-0.605231000	0.102940000
6	1.501916000	0.716007000	-0.164865000
8	-2.597635000	1.067523000	-0.543389000
6	-2.315461000	-1.533807000	-0.009742000

6	-2.285301000	-2.525821000	-0.976952000
6	-3.322169000	-3.435136000	-1.062168000
6	-4.389493000	-3.364833000	-0.177236000
6	-4.415940000	-2.375716000	0.789712000
6	-3.380544000	-1.457575000	0.872707000
1	-1.433683000	-2.577283000	-1.645397000
1	-3.298982000	-4.205911000	-1.823857000
1	-5.199154000	-4.081883000	-0.244405000
1	-5.246884000	-2.312989000	1.482725000
1	-3.399869000	-0.665432000	1.614402000
6	2.315665000	-1.533649000	-0.009606000
6	2.285436000	-2.525616000	-0.976850000
6	3.322357000	-3.434863000	-1.062194000
6	4.389760000	-3.364534000	-0.177354000
6	4.416244000	-2.375460000	0.789630000
6	3.380813000	-1.457374000	0.872755000
1	1.433744000	-2.577123000	-1.645195000
1	3.299165000	-4.205605000	-1.823917000
1	5.199426000	-4.081569000	-0.244638000
1	5.247244000	-2.312722000	1.482578000
1	3.400126000	-0.665256000	1.614463000
8	2.597683000	1.067741000	-0.542970000
26	-0.000043000	2.108480000	-0.078236000
6	-0.000377000	1.824039000	1.687139000
8	-0.000796000	1.582108000	2.803118000
6	0.000160000	1.771274000	-1.879266000
8	0.000155000	1.510896000	-2.980411000
6	-1.354021000	3.383789000	-0.085235000
8	-2.174778000	4.158572000	-0.077708000
6	1.353891000	3.383839000	-0.084745000
8	2.174613000	4.158654000	-0.076891000
7	-0.000125000	-1.386289000	2.023959000
1	-0.818917000	-1.941219000	2.267412000
1	0.818715000	-1.941078000	2.267547000
1	-0.000258000	-0.540922000	2.614199000

$3TS_2^{N-H}$ (TE = -2610.483132)

6	1.457708000	0.760359000	0.374268000
7	1.194222000	-0.625133000	0.247095000
6	0.003113000	-1.236490000	0.109264000

7	-1.190911000	-0.630887000	0.247083000
6	-1.460964000	0.753371000	0.375056000
8	2.570997000	1.106455000	0.668762000
6	2.329793000	-1.513443000	0.187224000
6	2.514653000	-2.457756000	1.177923000
6	3.584886000	-3.332876000	1.091003000
6	4.458269000	-3.255326000	0.019759000
6	4.260780000	-2.305733000	-0.971132000
6	3.193483000	-1.431254000	-0.890315000
1	1.817504000	-2.503479000	2.007162000
1	3.736123000	-4.075860000	1.864886000
1	5.294984000	-3.940550000	-0.046902000
1	4.937686000	-2.250848000	-1.815177000
1	3.010162000	-0.695113000	-1.665463000
6	-2.322370000	-1.524402000	0.187230000
6	-2.502521000	-2.470053000	1.177515000
6	-3.568869000	-3.349901000	1.090651000
6	-4.443116000	-3.275703000	0.019881000
6	-4.250379000	-2.324713000	-0.970597000
6	-3.186973000	-1.445508000	-0.889839000
1	-1.804788000	-2.513075000	2.006405000
1	-3.716427000	-4.093933000	1.864237000
1	-5.276808000	-3.964608000	-0.046724000
1	-4.927972000	-2.272372000	-1.814255000
1	-3.007566000	-0.707901000	-1.664521000
8	-2.575719000	1.093957000	0.670358000
26	-0.004939000	2.093807000	0.021482000
6	-0.004691000	1.510207000	-1.727088000
8	-0.005202000	1.181493000	-2.805295000
6	-0.004711000	2.258853000	1.843991000
8	-0.004523000	2.313867000	2.972136000
6	1.354647000	3.342421000	-0.269364000
8	2.180416000	4.089682000	-0.440673000
6	-1.370481000	3.336120000	-0.268218000
8	-2.199806000	4.079612000	-0.438768000
1	0.005521000	-2.181969000	-0.570339000
7	0.005946000	-2.041586000	-2.095251000
1	0.812284000	-2.652634000	-2.242396000
1	-0.799947000	-2.652987000	-2.243361000

III-TS$_1^{N-H}$ (TE = -1011.354162)

6	1.273178000	1.530090000	-0.356529000
7	1.176179000	0.176635000	-0.108480000
6	0.000000000	-0.569055000	0.096192000
7	-1.176179000	0.176635000	-0.108481000
6	-1.273179000	1.530091000	-0.356529000
6	0.000000000	2.332986000	-0.157548000
8	2.306624000	2.057399000	-0.698106000
6	0.000000000	2.817455000	1.300897000
1	-0.887884000	3.425842000	1.484534000
1	-0.000003000	1.991780000	2.015758000
1	0.887886000	3.425838000	1.484536000
6	0.000000000	3.540547000	-1.080279000
1	0.000001000	3.236698000	-2.128271000
1	-0.889184000	4.142945000	-0.900518000
1	0.889183000	4.142946000	-0.900516000
6	2.382212000	-0.594565000	-0.104238000
6	3.376761000	-0.303054000	0.815605000
6	4.528307000	-1.070796000	0.853609000
6	4.685389000	-2.129745000	-0.024856000
6	3.686002000	-2.419263000	-0.941125000
6	2.533381000	-1.655398000	-0.980935000
1	3.246068000	0.535388000	1.492232000
1	5.305219000	-0.839300000	1.572756000
1	5.586808000	-2.730444000	0.004030000
1	3.805617000	-3.245802000	-1.631814000
1	1.734237000	-1.875812000	-1.678152000
6	-2.382212000	-0.594565000	-0.104237000
6	-3.376759000	-0.303057000	0.815608000
6	-4.528305000	-1.070799000	0.853612000
6	-4.685389000	-2.129744000	-0.024856000
6	-3.686004000	-2.419259000	-0.941129000
6	-2.533383000	-1.655395000	-0.980939000
1	-3.246064000	0.535383000	1.492238000
1	-5.305215000	-0.839304000	1.572762000
1	-5.586808000	-2.730443000	0.004030000
1	-3.805622000	-3.245796000	-1.631820000
1	-1.734240000	-1.875807000	-1.678158000
8	-2.306624000	2.057399000	-0.698105000
7	0.000000000	-0.814901000	1.901730000

1	-0.822489000	-1.377889000	2.093329000
1	0.822483000	-1.377899000	2.093326000
1	0.000006000	-0.004146000	2.522089000

III-Int^{N-H} (TE = -1011.353288)

6	1.277573000	1.522147000	-0.342784000
7	1.190466000	0.190939000	-0.016737000
6	0.000016000	-0.528496000	0.294522000
7	-1.190377000	0.190960000	-0.016474000
6	-1.277653000	1.522100000	-0.342701000
6	-0.000073000	2.334888000	-0.177563000
8	2.301326000	2.034543000	-0.741114000
6	-0.000081000	2.923220000	1.240514000
1	-0.887594000	3.543985000	1.380323000
1	-0.000328000	2.158205000	2.020758000
1	0.887610000	3.543684000	1.380479000
6	-0.000179000	3.482590000	-1.175866000
1	0.000224000	3.112305000	-2.202178000
1	-0.890035000	4.094319000	-1.035488000
1	0.889181000	4.094927000	-1.035049000
6	2.380548000	-0.600885000	-0.057066000
6	3.454578000	-0.275109000	0.756649000
6	4.594251000	-1.061943000	0.746036000
6	4.662438000	-2.174890000	-0.074464000
6	3.584639000	-2.499366000	-0.884874000
6	2.443861000	-1.718138000	-0.875165000
1	3.395795000	0.606879000	1.385381000
1	5.432214000	-0.801675000	1.382091000
1	5.554369000	-2.790233000	-0.083592000
1	3.634026000	-3.367676000	-1.531656000
1	1.584995000	-1.965451000	-1.487487000
6	-2.380483000	-0.600869000	-0.056921000
6	-3.453813000	-0.276021000	0.758062000
6	-4.593563000	-1.062735000	0.747376000
6	-4.662452000	-2.174613000	-0.074525000
6	-3.585353000	-2.498125000	-0.886247000
6	-2.444494000	-1.717001000	-0.876447000
1	-3.394383000	0.605222000	1.387808000
1	-5.431019000	-0.803254000	1.384416000
1	-5.554434000	-2.789883000	-0.083745000

1	-3.635363000	-3.365594000	-1.534107000
1	-1.586134000	-1.963601000	-1.489779000
8	-2.301463000	2.034306000	-0.741120000
7	0.000263000	-0.651629000	1.887352000
1	-0.821849000	-1.190819000	2.151742000
1	0.822430000	-1.190873000	2.151475000
1	0.000376000	0.226329000	2.426268000

III-TS$_2^{N-H}$ (TE = -1011.334036)

6	1.263106000	1.604780000	-0.422572000
7	1.168226000	0.214491000	-0.254285000
6	-0.000019000	-0.440796000	-0.083861000
7	-1.168243000	0.214556000	-0.254234000
6	-1.263093000	1.604857000	-0.422387000
6	0.000058000	2.364707000	-0.084495000
8	2.290166000	2.130721000	-0.747386000
6	0.000191000	2.500900000	1.456815000
1	-0.886591000	3.060949000	1.761681000
1	0.000235000	1.526521000	1.956741000
1	0.887014000	3.060969000	1.761524000
6	0.000053000	3.730445000	-0.738944000
1	0.000049000	3.652668000	-1.827229000
1	-0.887646000	4.283844000	-0.435754000
1	0.887755000	4.283847000	-0.435768000
6	2.365231000	-0.572730000	-0.180281000
6	3.295142000	-0.302181000	0.808341000
6	4.427171000	-1.089775000	0.904578000
6	4.621200000	-2.141439000	0.022170000
6	3.680705000	-2.408008000	-0.958264000
6	2.547370000	-1.619940000	-1.063620000
1	3.117323000	0.512965000	1.501478000
1	5.158155000	-0.886069000	1.677617000
1	5.508932000	-2.757412000	0.102378000
1	3.830116000	-3.229893000	-1.648012000
1	1.799609000	-1.810604000	-1.825101000
6	-2.365260000	-0.572655000	-0.180258000
6	-3.295071000	-0.302294000	0.808508000
6	-4.427108000	-1.089886000	0.904685000
6	-4.621243000	-2.141360000	0.022076000
6	-3.680847000	-2.407742000	-0.958505000

6	-2.547506000	-1.619677000	-1.063800000
1	-3.117178000	0.512707000	1.501794000
1	-5.158016000	-0.886326000	1.677835000
1	-5.508981000	-2.757331000	0.102238000
1	-3.830341000	-3.229479000	-1.648412000
1	-1.799818000	-1.810198000	-1.825388000
8	-2.290188000	2.130872000	-0.746972000
1	-0.000072000	-1.326689000	0.677546000
7	-0.000074000	-0.969043000	2.149463000
1	-0.808250000	-1.548215000	2.385950000
1	0.808042000	-1.548265000	2.386021000

Cartesian coordinates of the transition states and the intermediates involved in the activation of P – H bond of PH_3 by **1**, **3** and **III-IV**, along with their total energies (in hartrees) including zero point vibrational correction.

$1TS_{Nu}^{P-H}$ (TE = -2710.942139)

6	0.456641000	-1.031339000	-0.368886000
6	0.958783000	1.270691000	-0.161651000
7	1.403465000	0.009656000	-0.275715000
7	-0.757310000	-0.613142000	-0.202376000
25	-1.061570000	1.408702000	0.070903000
6	-0.746665000	1.148299000	1.893246000
8	-0.517791000	0.962736000	2.988010000
6	-1.263073000	3.205734000	0.281688000
8	-1.459339000	4.321670000	0.427837000
6	-2.894271000	1.209962000	0.260629000
8	-4.020725000	1.112896000	0.369727000
6	-1.204748000	1.514056000	-1.791397000
8	-1.265825000	1.548994000	-2.923001000
6	-1.780061000	-1.587551000	-0.301456000
6	-2.026819000	-2.217906000	-1.512922000
6	-2.542059000	-1.911618000	0.813142000
6	-3.035195000	-3.161743000	-1.609395000
1	-1.419578000	-1.953452000	-2.372109000
6	-3.544285000	-2.859541000	0.713256000
1	-2.330482000	-1.427348000	1.761168000
6	-3.796473000	-3.483830000	-0.498261000
1	-3.226625000	-3.647576000	-2.559148000
1	-4.128831000	-3.115580000	1.589025000

1	-4.585236000	-4.222684000	-0.574819000
6	2.789113000	-0.359593000	-0.362784000
6	3.231210000	-1.044093000	-1.479232000
6	3.641394000	-0.097683000	0.696298000
6	4.547203000	-1.470960000	-1.536549000
1	2.537154000	-1.250932000	-2.285397000
6	4.954878000	-0.523179000	0.630537000
1	3.264451000	0.415150000	1.574209000
6	5.408480000	-1.210362000	-0.484645000
1	4.897885000	-2.013306000	-2.406280000
1	5.623195000	-0.331001000	1.461093000
1	6.436097000	-1.550742000	-0.528941000
8	1.934763000	2.132577000	-0.247664000
6	1.682524000	3.529418000	-0.193533000
1	0.989737000	3.825780000	-0.981531000
1	1.291218000	3.811244000	0.783940000
1	2.642947000	4.012968000	-0.352668000
1	0.920986000	-2.113686000	0.284263000
15	1.422317000	-2.853241000	1.788233000
1	1.315661000	-1.592812000	2.447029000
1	0.064689000	-3.184119000	2.062945000

3TS$_{Nu}^{P-H}$ (TE = -2897.112485)

6	-1.495899000	1.065677000	-0.750809000
7	-1.219336000	-0.321326000	-0.595116000
6	-0.026485000	-0.949394000	-0.560454000
7	1.154148000	-0.307382000	-0.677861000
6	1.405478000	1.082904000	-0.841827000
8	-2.604465000	1.402456000	-1.067770000
6	-2.352059000	-1.214666000	-0.527497000
6	-2.462955000	-2.253396000	-1.431824000
6	-3.520231000	-3.141030000	-1.323277000
6	-4.457368000	-2.985652000	-0.316259000
6	-4.336847000	-1.941671000	0.587514000
6	-3.282214000	-1.054119000	0.485096000
1	-1.714125000	-2.363525000	-2.207865000
1	-3.610234000	-3.956939000	-2.030380000
1	-5.282873000	-3.682326000	-0.232031000
1	-5.062893000	-1.823078000	1.382706000
1	-3.170074000	-0.240977000	1.194213000

6	2.296810000	-1.190523000	-0.692366000
6	2.349697000	-2.226477000	-1.605133000
6	3.416042000	-3.109061000	-1.573016000
6	4.420219000	-2.951270000	-0.633270000
6	4.358217000	-1.909661000	0.279120000
6	3.295042000	-1.026666000	0.252582000
1	1.548712000	-2.339097000	-2.326806000
1	3.460523000	-3.923047000	-2.286595000
1	5.252722000	-3.644252000	-0.607879000
1	5.137327000	-1.789183000	1.022116000
1	3.228326000	-0.214896000	0.968843000
8	2.489081000	1.434180000	-1.223076000
26	-0.041213000	2.410235000	-0.401610000
6	0.013874000	1.746295000	1.302124000
8	0.045163000	1.309975000	2.344002000
6	-0.097877000	2.626743000	-2.223091000
8	-0.132444000	2.714617000	-3.347719000
6	-1.404559000	3.634354000	-0.035864000
8	-2.237732000	4.360455000	0.183353000
6	1.325946000	3.652174000	-0.119924000
8	2.160736000	4.389903000	0.048371000
1	0.016033000	-1.944434000	0.376210000
15	0.092589000	-2.532408000	1.966732000
1	1.099370000	-1.599883000	2.339528000
1	-0.961290000	-1.685904000	2.408813000

IIITS$_{Nu}^{P-H}$ (TE = -1297.963184)

6	1.259424000	1.748594000	-0.375246000
7	1.164523000	0.345176000	-0.343572000
6	-0.000004000	-0.349036000	-0.322428000
7	-1.164538000	0.345164000	-0.343573000
6	-1.259441000	1.748585000	-0.375247000
6	-0.000011000	2.466801000	0.054587000
8	2.275464000	2.310760000	-0.671873000
6	-0.000011000	2.432013000	1.597860000
1	-0.886919000	2.949472000	1.969452000
1	-0.000070000	1.412662000	1.992373000
1	0.886956000	2.949370000	1.969454000
6	-0.000019000	3.899259000	-0.436985000
1	-0.000069000	3.945878000	-1.526702000

1	-0.887777000	4.414648000	-0.073021000
1	0.887785000	4.414628000	-0.073102000
6	2.368096000	-0.436378000	-0.367732000
6	3.358143000	-0.185344000	0.567975000
6	4.493764000	-0.972642000	0.582648000
6	4.635166000	-2.008022000	-0.327984000
6	3.637196000	-2.255806000	-1.254840000
6	2.499058000	-1.467957000	-1.278718000
1	3.231040000	0.619051000	1.284155000
1	5.268672000	-0.781681000	1.315056000
1	5.525596000	-2.625040000	-0.312286000
1	3.744108000	-3.064562000	-1.967645000
1	1.705880000	-1.647554000	-1.995015000
6	-2.368108000	-0.436395000	-0.367720000
6	-3.358177000	-0.185335000	0.567957000
6	-4.493797000	-0.972635000	0.582629000
6	-4.635176000	-2.008046000	-0.327969000
6	-3.637180000	-2.255864000	-1.254788000
6	-2.499046000	-1.468011000	-1.278669000
1	-3.231085000	0.619062000	1.284136000
1	-5.268720000	-0.781652000	1.315015000
1	-5.525605000	-2.625066000	-0.312271000
1	-3.744070000	-3.064649000	-1.967563000
1	-1.705849000	-1.647632000	-1.994939000
8	-2.275479000	2.310749000	-0.671878000
1	0.000043000	-1.348450000	0.567870000
15	0.000089000	-1.832294000	2.206304000
1	1.031299000	-0.910360000	2.539314000
1	-1.031588000	-0.910852000	2.539217000

IVTS$_{Nu}^{P-H}$ (TE = -942.183304)

6	-2.216621000	-1.411565000	-0.016008000
6	-2.334662000	0.018148000	0.545034000
6	-0.808902000	-1.542429000	-0.597678000
7	-0.126050000	-0.413448000	0.126420000
6	1.292182000	-0.277059000	0.186134000
6	2.037614000	-0.004446000	-0.950852000
6	3.408960000	0.155068000	-0.845822000
6	4.033069000	0.048640000	0.385616000
6	3.282316000	-0.213317000	1.520281000

6	1.912317000	-0.375609000	1.421659000
1	1.543997000	0.123282000	-1.905701000
1	3.989606000	0.380387000	-1.732294000
1	5.106019000	0.178074000	0.462594000
1	3.764919000	-0.291499000	2.487183000
1	1.303486000	-0.575239000	2.296515000
6	-0.152135000	-2.858244000	-0.239967000
1	-0.114910000	-2.992158000	0.844018000
1	-0.728069000	-3.681753000	-0.667890000
1	0.865756000	-2.919938000	-0.631703000
6	-0.781762000	-1.324043000	-2.101609000
1	-1.431299000	-2.058015000	-2.583910000
1	-1.136929000	-0.326352000	-2.369036000
1	0.221145000	-1.456088000	-2.510361000
6	-0.903923000	0.460216000	0.715848000
15	-0.256397000	3.171757000	-0.471605000
1	-0.564500000	1.777647000	0.511607000
1	-0.395725000	2.430292000	-1.680537000
1	-2.335981000	-2.133521000	0.797790000
1	-2.984399000	-1.631381000	-0.761969000
6	-3.089367000	0.952452000	-0.396771000
1	-3.096565000	1.973512000	-0.010165000
1	-2.649427000	0.975800000	-1.395859000
1	-4.125266000	0.614338000	-0.489588000
6	-3.021321000	0.026553000	1.904862000
1	-3.087130000	1.042643000	2.299657000
1	-4.034418000	-0.377368000	1.817780000
1	-2.471892000	-0.583637000	2.626179000
1	1.143307000	2.922556000	-0.399533000

$3TS_1^{P\text{-}H}$ (TE = -2897.116724)

6	0.845738000	1.448854000	-0.389957000
7	-0.515740000	1.192683000	-0.183520000
6	-1.150975000	0.000213000	0.099080000
7	-0.516145000	-1.192348000	-0.184103000
6	0.845229000	-1.448977000	-0.390590000
8	1.195619000	2.531511000	-0.791196000
6	-1.410352000	2.318129000	-0.254582000
6	-2.439232000	2.309450000	-1.179435000
6	-3.349389000	3.350984000	-1.201672000

6	-3.230037000	4.397422000	-0.300410000
6	-2.194456000	4.403294000	0.619690000
6	-1.281208000	3.363408000	0.644264000
1	-2.525116000	1.473757000	-1.864807000
1	-4.155204000	3.345951000	-1.926067000
1	-3.945454000	5.211082000	-0.316303000
1	-2.099204000	5.218584000	1.326932000
1	-0.468790000	3.352935000	1.362648000
6	-1.411121000	-2.317497000	-0.255025000
6	-2.439963000	-2.308685000	-1.179911000
6	-3.350519000	-3.349879000	-1.201849000
6	-3.231603000	-4.396079000	-0.300247000
6	-2.196069000	-4.402067000	0.619906000
6	-1.282425000	-3.362521000	0.644178000
1	-2.525503000	-1.473168000	-1.865542000
1	-4.156317000	-3.344766000	-1.926263000
1	-3.947338000	-5.209463000	-0.315909000
1	-2.101182000	-5.217156000	1.327428000
1	-0.470080000	-3.352044000	1.362653000
8	1.194743000	-2.531651000	-0.792091000
26	2.200663000	-0.000374000	-0.011715000
6	1.617795000	-0.000933000	1.718470000
8	1.276769000	-0.001388000	2.797919000
6	2.343062000	0.000053000	-1.839607000
8	2.387851000	0.000308000	-2.968121000
6	3.434587000	1.367475000	0.265492000
8	4.170112000	2.206705000	0.429879000
6	3.434281000	-1.368678000	0.264638000
8	4.169667000	-2.208139000	0.428464000
15	-2.120337000	-0.000104000	1.872418000
1	-2.958365000	1.089216000	1.591954000
1	-2.959618000	-1.088282000	1.591275000
1	-2.354953000	-0.000276000	3.310243000

3Int^{P-H} (TE = -2897.124152)

6	0.999508000	-1.579954000	0.034685000
7	-0.253620000	-1.299831000	-0.504160000
6	-0.480345000	0.000709000	-1.008275000
7	-0.470345000	1.101972000	-0.113795000
6	0.721659000	1.351322000	0.559399000

8	1.245056000	-2.652308000	0.526868000
6	-1.376533000	-2.061366000	-0.037837000
6	-1.702464000	-2.055131000	1.311407000
6	-2.848201000	-2.695656000	1.746546000
6	-3.671961000	-3.344706000	0.839478000
6	-3.337467000	-3.364152000	-0.504099000
6	-2.185861000	-2.729802000	-0.941419000
1	-1.059724000	-1.530208000	2.011252000
1	-3.103931000	-2.681291000	2.799438000
1	-4.571898000	-3.841257000	1.182128000
1	-3.969683000	-3.882696000	-1.215272000
1	-1.903266000	-2.759248000	-1.989281000
6	-1.656552000	1.852762000	0.138127000
6	-2.887553000	1.205150000	0.207046000
6	-4.047670000	1.931790000	0.407042000
6	-3.999211000	3.309265000	0.541674000
6	-2.775813000	3.954192000	0.467104000
6	-1.610209000	3.237770000	0.262810000
1	-2.933953000	0.125029000	0.112247000
1	-4.996099000	1.410330000	0.465145000
1	-4.908623000	3.876263000	0.700414000
1	-2.724019000	5.032631000	0.563137000
1	-0.659115000	3.748109000	0.202384000
8	0.823797000	2.215756000	1.396002000
26	2.280019000	0.040109000	0.122377000
6	1.990521000	0.330120000	-1.667104000
8	2.037054000	0.539573000	-2.787330000
6	2.122768000	-0.296518000	1.915369000
8	1.976791000	-0.507674000	3.016530000
6	3.623620000	-1.177992000	-0.184367000
8	4.429498000	-1.948919000	-0.372205000
6	3.364871000	1.517587000	0.298531000
8	4.014425000	2.436748000	0.409032000
15	-1.136244000	0.201771000	-2.547123000
1	-2.531025000	0.107836000	-2.805950000
1	-0.854244000	1.477819000	-3.057489000
1	-0.625097000	-0.745451000	-3.445309000

$3TS_2^{P\text{-}H}$ (TE =-2897.112256)

6	0.951288000	1.458841000	-0.416692000
7	-0.443729000	1.186938000	-0.400522000
6	-1.083589000	0.000477000	-0.394262000
7	-0.445243000	-1.186828000	-0.399693000
6	0.949370000	-1.460792000	-0.414334000
8	1.319090000	2.568182000	-0.693773000
6	-1.340172000	2.319202000	-0.396068000
6	-2.266673000	2.465563000	-1.409777000
6	-3.180648000	3.503737000	-1.349810000
6	-3.162213000	4.384738000	-0.281416000
6	-2.228261000	4.229245000	0.730679000
6	-1.314354000	3.192902000	0.676729000
1	-2.274043000	1.755855000	-2.228929000
1	-3.911045000	3.622690000	-2.141101000
1	-3.881077000	5.194045000	-0.234438000
1	-2.218672000	4.910524000	1.572856000
1	-0.589941000	3.046566000	1.471102000
6	-1.343315000	-2.317828000	-0.395398000
6	-2.267953000	-2.464113000	-1.410809000
6	-3.183486000	-3.500942000	-1.351477000
6	-3.168441000	-4.380671000	-0.281976000
6	-2.236355000	-4.225247000	0.731845000
6	-1.320882000	-3.190239000	0.678508000
1	-2.272633000	-1.755403000	-2.230847000
1	-3.912420000	-3.619868000	-2.144117000
1	-3.888500000	-5.188943000	-0.235486000
1	-2.229426000	-4.905517000	1.574864000
1	-0.597893000	-3.043889000	1.474175000
8	1.315779000	-2.571207000	-0.688922000
26	2.250150000	-0.001425000	0.063217000
6	1.443625000	0.000186000	1.706219000
8	0.902965000	0.001146000	2.698329000
6	2.588744000	-0.003099000	-1.738880000
8	2.749715000	-0.004083000	-2.856348000
6	3.461591000	1.360653000	0.477261000
8	4.183348000	2.189587000	0.724495000
6	3.459988000	-1.364251000	0.479514000
8	4.180861000	-2.193532000	0.728152000
1	-2.117424000	0.001513000	0.487612000

15	-2.849164000	0.002777000	2.023147000
1	-3.706476000	1.037557000	1.554668000
1	-3.707734000	-1.031424000	1.555700000

III-TS$_1^{P-H}$ (TE = -1297.968613)

6	1.258781000	1.690672000	-0.388894000
7	1.175106000	0.320314000	-0.203307000
6	-0.000057000	-0.374944000	0.075362000
7	-1.175092000	0.320431000	-0.203705000
6	-1.258791000	1.690876000	-0.388533000
6	0.000115000	2.455053000	-0.024480000
8	2.264047000	2.231722000	-0.777815000
6	0.000389000	2.604429000	1.506937000
1	-0.885643000	3.162195000	1.817789000
1	-0.000724000	1.639239000	2.021610000
1	0.887757000	3.160117000	1.817729000
6	0.000140000	3.821298000	-0.678208000
1	0.000302000	3.742124000	-1.766011000
1	-0.888708000	4.374527000	-0.377253000
1	0.888852000	4.374627000	-0.377022000
6	2.369745000	-0.462826000	-0.256200000
6	3.406632000	-0.189125000	0.620898000
6	4.534327000	-0.991075000	0.618509000
6	4.621644000	-2.064201000	-0.253141000
6	3.580009000	-2.333123000	-1.127379000
6	2.451715000	-1.532546000	-1.130991000
1	3.322036000	0.651677000	1.300965000
1	5.345579000	-0.779566000	1.304789000
1	5.504386000	-2.692567000	-0.252518000
1	3.648108000	-3.168925000	-1.813559000
1	1.621371000	-1.732470000	-1.798770000
6	-2.369785000	-0.462618000	-0.256496000
6	-3.406511000	-0.189124000	0.620851000
6	-4.534139000	-0.991169000	0.618576000
6	-4.621544000	-2.064185000	-0.253201000
6	-3.580074000	-2.332894000	-1.127701000
6	-2.451858000	-1.532212000	-1.131432000
1	-3.321873000	0.651580000	1.301028000
1	-5.345270000	-0.779822000	1.305049000
1	-5.504231000	-2.692628000	-0.252476000

1	-3.648244000	-3.168606000	-1.813983000
1	-1.621634000	-1.731962000	-1.799416000
8	-2.264225000	2.232151000	-0.776714000
15	-0.000276000	-1.327578000	1.745076000
1	1.103142000	-2.158010000	1.513879000
1	-0.000548000	-1.429707000	3.196758000
1	-1.103618000	-2.158090000	1.513713000

III-Int^{P-H} (TE = -1297.962408)

6	1.268616000	1.658193000	-0.409311000
7	1.198681000	0.332319000	-0.048585000
6	-0.000016000	-0.238132000	0.441852000
7	-1.198561000	0.332314000	-0.048909000
6	-1.268412000	1.658145000	-0.409767000
6	0.000031000	2.460380000	-0.122632000
8	2.245955000	2.152847000	-0.923120000
6	-0.000330000	2.843167000	1.364988000
1	-0.885810000	3.443322000	1.585221000
1	-0.000596000	1.976624000	2.028324000
1	0.885117000	3.443182000	1.585730000
6	0.000172000	3.725932000	-0.958442000
1	0.000519000	3.499064000	-2.024949000
1	-0.888872000	4.315097000	-0.736377000
1	0.888970000	4.315271000	-0.735849000
6	2.331284000	-0.522214000	-0.190666000
6	3.547994000	-0.173835000	0.376761000
6	4.629033000	-1.032207000	0.268049000
6	4.499556000	-2.239150000	-0.397629000
6	3.280361000	-2.586457000	-0.959173000
6	2.198514000	-1.731944000	-0.856499000
1	3.643925000	0.772954000	0.893757000
1	5.578024000	-0.754790000	0.711641000
1	5.347018000	-2.909222000	-0.479857000
1	3.172548000	-3.526729000	-1.487140000
1	1.239194000	-1.992298000	-1.287946000
6	-2.331238000	-0.522125000	-0.190891000
6	-3.547679000	-0.173888000	0.377191000
6	-4.628798000	-1.032179000	0.268659000
6	-4.499631000	-2.238901000	-0.397489000
6	-3.280700000	-2.586062000	-0.959695000

6	-2.198781000	-1.731612000	-0.857205000
1	-3.643324000	0.772734000	0.894565000
1	-5.577596000	-0.754896000	0.712750000
1	-5.347148000	-2.908922000	-0.479568000
1	-3.173164000	-3.526156000	-1.488033000
1	-1.239663000	-1.991817000	-1.289199000
8	-2.245584000	2.152704000	-0.923994000
15	-0.000152000	-0.857704000	2.066858000
1	-1.128404000	-1.678107000	2.169951000
1	1.128113000	-1.678080000	2.170132000
1	-0.000216000	-0.271177000	3.384723000

III-TS_2^{P-H} (TE = -1297.969203)

6	1.261744000	1.794759000	-0.356988000
7	1.163482000	0.392617000	-0.405634000
6	-0.000015000	-0.302004000	-0.425882000
7	-1.163517000	0.392611000	-0.405502000
6	-1.261760000	1.794751000	-0.356857000
6	0.000014000	2.491333000	0.100673000
8	2.284621000	2.367566000	-0.605459000
6	0.000146000	2.376135000	1.641480000
1	-0.887078000	2.873467000	2.038871000
1	0.000517000	1.337407000	1.983985000
1	0.887105000	2.874054000	2.038727000
6	-0.000035000	3.946774000	-0.317603000
1	-0.000521000	4.048874000	-1.403607000
1	-0.887501000	4.443265000	0.072480000
1	0.887873000	4.443088000	0.071694000
6	2.361905000	-0.396576000	-0.397922000
6	3.279929000	-0.212228000	0.622510000
6	4.392925000	-1.029110000	0.689233000
6	4.581403000	-2.026079000	-0.255100000
6	3.656060000	-2.203772000	-1.269831000
6	2.541129000	-1.386600000	-1.345357000
1	3.110908000	0.559959000	1.365308000
1	5.110725000	-0.893226000	1.489000000
1	5.452340000	-2.667952000	-0.197880000
1	3.801600000	-2.981932000	-2.009341000
1	1.800568000	-1.515455000	-2.125904000
6	-2.361943000	-0.396584000	-0.397799000

6	-3.279953000	-0.212322000	0.622660000
6	-4.392973000	-1.029184000	0.689299000
6	-4.581491000	-2.026041000	-0.255144000
6	-3.656165000	-2.203644000	-1.269905000
6	-2.541212000	-1.386496000	-1.345347000
1	-3.110927000	0.559799000	1.365522000
1	-5.110765000	-0.893363000	1.489083000
1	-5.452448000	-2.667891000	-0.197988000
1	-3.801738000	-2.981710000	-2.009507000
1	-1.800671000	-1.515274000	-2.125926000
8	-2.284642000	2.367576000	-0.605274000
1	0.000022000	-1.297255000	0.460115000
15	0.000091000	-1.814089000	2.089269000
1	-1.035364000	-2.725795000	1.743664000
1	1.036171000	-2.725128000	1.743770000

Cartesian coordinates of the transition states and the intermediates involved in the activation of Si –H bond of SiH_3Ph by **1**, **3** and **III-IV**, along with their total energies (in hartrees) including zero point vibrational correction.

$1TS_{PT}^{Si-H}$ (TE = -2890.539993)

6	-0.232027000	0.685533000	0.927476000
6	-0.203819000	-1.622031000	0.459082000
7	0.466340000	-0.540271000	0.892071000
7	-1.408990000	0.620853000	0.374990000
25	-2.030130000	-1.199823000	-0.357942000
6	-1.117699000	-0.804349000	-1.936397000
8	-0.530099000	-0.543289000	-2.870612000
6	-2.520366000	-2.843977000	-0.965867000
8	-2.885412000	-3.842501000	-1.384970000
6	-3.629172000	-0.524815000	-1.000765000
8	-4.623051000	-0.138736000	-1.393722000
6	-2.767358000	-1.487018000	1.339327000
8	-3.183460000	-1.638030000	2.383068000
6	-2.163171000	1.815659000	0.412891000
6	-2.514500000	2.380472000	1.633067000
6	-2.546840000	2.441269000	-0.767040000
6	-3.250777000	3.551534000	1.670851000
1	-2.205381000	1.881503000	2.545350000
6	-3.279088000	3.614375000	-0.724208000

1	-2.252091000	2.010267000	-1.718259000
6	-3.636362000	4.171027000	0.493245000
1	-3.527180000	3.981079000	2.626863000
1	-3.566360000	4.099734000	-1.649509000
1	-4.213144000	5.087702000	0.523698000
6	1.785290000	-0.561382000	1.463751000
6	2.006487000	0.108848000	2.654825000
6	2.830085000	-1.188845000	0.804328000
6	3.283429000	0.149016000	3.188948000
1	1.177069000	0.603000000	3.146654000
6	4.097969000	-1.156942000	1.352117000
1	2.657108000	-1.678217000	-0.145585000
6	4.328876000	-0.488112000	2.543577000
1	3.457251000	0.678772000	4.117903000
1	4.914949000	-1.637943000	0.828136000
1	5.327217000	-0.456321000	2.963542000
8	0.441560000	-2.728489000	0.715991000
6	-0.110863000	-3.992922000	0.385071000
1	-1.085063000	-4.124567000	0.857323000
1	-0.193715000	-4.105588000	-0.695846000
1	0.583524000	-4.733551000	0.773839000
1	0.545263000	1.659536000	0.633531000
14	1.518216000	2.454427000	-0.776956000
1	0.633609000	2.438530000	-1.981892000
1	1.904102000	3.874692000	-0.532887000
6	3.081051000	1.539006000	-1.263837000
6	3.057591000	0.505486000	-2.203778000
6	4.294621000	1.799358000	-0.622800000
6	4.196046000	-0.226484000	-2.500256000
1	2.131297000	0.277936000	-2.725519000
6	5.435831000	1.074347000	-0.916528000
1	4.346402000	2.589539000	0.122460000
6	5.391399000	0.056844000	-1.858255000
1	4.153377000	-1.016134000	-3.243017000
1	6.366815000	1.301936000	-0.408141000
1	6.285623000	-0.509400000	-2.093156000

$3TS_{PT}^{Si\text{-}H}$ (TE = -3076.715539)

6	-2.454877000	0.600630000	0.027493000
7	-1.288009000	1.266725000	0.447532000

6	-0.101203000	0.759052000	0.880566000
7	0.120338000	-0.570766000	1.053745000
6	-0.777365000	-1.643482000	0.867900000
8	-3.471064000	1.230148000	-0.119776000
6	-1.275726000	2.706902000	0.387683000
6	-0.995103000	3.437797000	1.526946000
6	-0.886840000	4.815351000	1.443498000
6	-1.053707000	5.453386000	0.225211000
6	-1.333100000	4.713455000	-0.912425000
6	-1.443943000	3.336663000	-0.834248000
1	-0.852893000	2.917389000	2.467045000
1	-0.669958000	5.392040000	2.334714000
1	-0.963586000	6.531229000	0.161290000
1	-1.456539000	5.208300000	-1.868154000
1	-1.652031000	2.744502000	-1.718804000
6	1.432787000	-0.877527000	1.565703000
6	1.910104000	-0.222073000	2.685158000
6	3.197990000	-0.476858000	3.127370000
6	3.998574000	-1.382552000	2.452770000
6	3.513524000	-2.030939000	1.327640000
6	2.232057000	-1.776764000	0.878800000
1	1.269741000	0.487815000	3.195747000
1	3.573797000	0.033878000	4.006016000
1	5.006952000	-1.578463000	2.798062000
1	4.142870000	-2.724855000	0.783644000
1	1.852682000	-2.262086000	-0.013828000
8	-0.549969000	-2.701058000	1.396705000
26	-2.396670000	-1.388468000	-0.308874000
6	-1.192698000	-1.024339000	-1.628137000
8	-0.411002000	-0.784505000	-2.410642000
6	-3.292807000	-1.446769000	1.289305000
8	-3.810204000	-1.453708000	2.293178000
6	-3.909173000	-1.141614000	-1.374705000
8	-4.819897000	-0.981112000	-2.019175000
6	-2.362355000	-3.235064000	-0.570552000
8	-2.331277000	-4.351684000	-0.722220000
1	0.874771000	1.342012000	0.305501000
14	1.802941000	1.791147000	-1.192419000
1	2.230955000	3.189202000	-0.922763000
1	0.996742000	1.756159000	-2.439672000

6	3.302479000	0.705849000	-1.410570000
6	4.411134000	0.850686000	-0.574293000
6	3.323735000	-0.325260000	-2.351677000
6	5.504197000	0.009675000	-0.682780000
1	4.417286000	1.635848000	0.177719000
6	4.413014000	-1.173389000	-2.459495000
1	2.476984000	-0.460741000	-3.018753000
6	5.508191000	-1.005801000	-1.626643000
1	6.355865000	0.142473000	-0.024600000
1	4.412259000	-1.963505000	-3.202291000
1	6.364012000	-1.665540000	-1.712873000

III-TS$_{PT}^{Si-H}$ (TE = -1477.567281)

6	-0.014996000	-2.320913000	0.391377000
7	0.150391000	-1.006384000	0.841713000
6	-0.838677000	-0.059772000	0.803442000
7	-2.047366000	-0.412138000	0.264315000
6	-2.349718000	-1.650700000	-0.300514000
6	-1.139281000	-2.508317000	-0.607538000
8	0.702385000	-3.218347000	0.745392000
6	-0.601860000	-2.013031000	-1.963545000
1	-1.354257000	-2.184854000	-2.736030000
1	-0.364241000	-0.946858000	-1.947749000
1	0.303700000	-2.566099000	-2.224593000
6	-1.527929000	-3.969327000	-0.704791000
1	-1.893743000	-4.348079000	0.250357000
1	-2.316004000	-4.092200000	-1.446441000
1	-0.663372000	-4.563864000	-0.997354000
6	1.372541000	-0.616559000	1.482170000
6	2.588495000	-1.010100000	0.943046000
6	3.763970000	-0.578474000	1.525280000
6	3.734185000	0.252062000	2.634848000
6	2.517783000	0.647736000	3.162568000
6	1.333973000	0.211586000	2.591252000
1	2.612842000	-1.639866000	0.062242000
1	4.711569000	-0.881446000	1.096116000
1	4.659540000	0.591730000	3.084781000
1	2.484662000	1.295382000	4.030670000
1	0.373594000	0.511175000	2.993384000
6	-3.048027000	0.612389000	0.299774000

6	-3.649440000	1.015834000	-0.881430000
6	-4.565981000	2.051168000	-0.859245000
6	-4.873976000	2.682404000	0.335314000
6	-4.263625000	2.276748000	1.510576000
6	-3.347349000	1.239573000	1.495828000
1	-3.392623000	0.518660000	-1.810513000
1	-5.036345000	2.370618000	-1.781338000
1	-5.590939000	3.494655000	0.349296000
1	-4.503706000	2.767437000	2.446212000
1	-2.854841000	0.909655000	2.403053000
8	-3.477435000	-1.984739000	-0.550832000
1	-0.436556000	1.050916000	0.362852000
14	0.120446000	1.891441000	-1.148337000
1	-0.109056000	3.335081000	-0.901415000
1	-0.669413000	1.437679000	-2.320759000
6	1.923803000	1.546401000	-1.435086000
6	2.348504000	0.578583000	-2.347625000
6	2.894257000	2.201093000	-0.673018000
6	3.692436000	0.279423000	-2.497557000
1	1.619014000	0.059834000	-2.963355000
6	4.236855000	1.908650000	-0.823710000
1	2.591927000	2.952506000	0.051867000
6	4.639448000	0.945043000	-1.736285000
1	4.002678000	-0.470615000	-3.216369000
1	4.974257000	2.429351000	-0.223044000
1	5.691955000	0.714383000	-1.854604000

IV-TS$_{PT}^{Si-H}$ (TE = -1121.786438)

6	-0.893809000	-1.285666000	-0.870623000
7	-1.114335000	-0.493295000	0.168858000
6	-1.842314000	0.714023000	-0.006039000
6	-3.150237000	0.638255000	-0.467283000
6	-3.880691000	1.792717000	-0.675000000
6	-3.306412000	3.030660000	-0.428499000
6	-2.000135000	3.106720000	0.022208000
6	-1.263333000	1.952412000	0.234655000
1	-4.902425000	1.727277000	-1.030009000
1	-3.877478000	3.936611000	-0.593600000
1	-1.542478000	4.072335000	0.202790000
1	-3.575536000	-0.341878000	-0.657866000

1	-0.233162000	2.011933000	0.564225000
14	1.289646000	0.087860000	-2.369064000
1	2.129180000	-0.810117000	-3.212609000
1	0.978926000	1.302194000	-3.175897000
1	-0.303536000	-0.729358000	-1.862317000
6	2.350686000	0.668984000	-0.933620000
6	3.201020000	-0.202495000	-0.247400000
6	2.252939000	1.977344000	-0.453916000
6	3.912637000	0.207258000	0.866987000
1	3.319302000	-1.224746000	-0.598888000
6	2.959399000	2.394677000	0.662498000
1	1.615123000	2.687861000	-0.973934000
6	3.790105000	1.508640000	1.330058000
1	4.569298000	-0.490001000	1.375715000
1	2.867531000	3.418265000	1.009336000
1	4.345686000	1.832381000	2.202558000
6	-0.382996000	-2.601576000	-0.344867000
6	0.055791000	-2.280777000	1.093668000
6	-0.692442000	-1.011980000	1.510568000
1	-0.130931000	-3.104610000	1.788179000
1	1.132072000	-2.078817000	1.103319000
6	0.728046000	-3.218856000	-1.171695000
1	0.965945000	-4.218086000	-0.796102000
1	0.427183000	-3.314086000	-2.218109000
1	1.641119000	-2.620974000	-1.134742000
6	-1.585256000	-3.552989000	-0.372310000
1	-1.874527000	-3.769791000	-1.402719000
1	-1.324333000	-4.493996000	0.120656000
1	-2.456988000	-3.132999000	0.133595000
6	0.225485000	-0.051745000	2.243186000
1	1.074987000	0.233372000	1.618461000
1	-0.298816000	0.849502000	2.567610000
1	0.613896000	-0.547645000	3.136691000
6	-1.928072000	-1.277235000	2.354641000
1	-1.633130000	-1.679322000	3.326340000
1	-2.481404000	-0.350832000	2.529125000
1	-2.602665000	-1.991675000	1.879778000

$\mathbf{1}_V$ (TE = -2890.576541)

6	-0.181246000	0.569063000	0.146417000
6	2.210273000	0.710878000	0.188832000
7	1.021372000	1.333302000	0.176987000
7	0.102855000	-0.684719000	0.037930000
25	2.072561000	-1.308588000	0.027207000
6	2.048632000	-1.030649000	-1.815348000
8	2.005726000	-0.809628000	-2.927978000
6	3.827179000	-1.791007000	0.034352000
8	4.908873000	-2.161176000	0.030207000
6	1.600590000	-3.094218000	-0.124890000
8	1.324740000	-4.193716000	-0.204259000
6	1.939568000	-1.369301000	1.886706000
8	1.835390000	-1.374524000	3.016664000
6	-0.975035000	-1.609276000	0.010099000
6	-1.647800000	-1.929515000	1.179545000
6	-1.323359000	-2.233981000	-1.179217000
6	-2.662173000	-2.871512000	1.158327000
1	-1.370539000	-1.422606000	2.097908000
6	-2.338243000	-3.174341000	-1.196010000
1	-0.794974000	-1.973320000	-2.090727000
6	-3.006852000	-3.499807000	-0.026717000
1	-3.190598000	-3.110586000	2.074111000
1	-2.609417000	-3.654236000	-2.129317000
1	-3.800434000	-4.237571000	-0.040714000
6	0.868664000	2.760325000	0.207763000
6	0.201540000	3.342937000	1.269808000
6	1.311432000	3.527193000	-0.855347000
6	-0.023020000	4.708647000	1.267314000
1	-0.156349000	2.715541000	2.077839000
6	1.088476000	4.892734000	-0.850921000
1	1.809017000	3.047202000	-1.690897000
6	0.420236000	5.484698000	0.208586000
1	-0.551224000	5.167514000	2.094613000
1	1.426196000	5.494586000	-1.686143000
1	0.238465000	6.552810000	0.205745000
8	3.199530000	1.555708000	0.301823000
6	4.544691000	1.102793000	0.360554000
1	4.687939000	0.431588000	1.207563000
1	4.823896000	0.606958000	-0.569219000

1	5.154442000	1.992752000	0.494710000
14	-2.319715000	1.694378000	-1.867664000
1	-1.339702000	0.723598000	-2.407563000
1	-1.641866000	2.899480000	-1.347679000
1	-3.153439000	2.110588000	-3.028512000
6	-3.471194000	0.962390000	-0.595198000
6	-4.316981000	-0.088986000	-0.939239000
6	-3.533897000	1.458488000	0.704855000
6	-5.189304000	-0.638386000	-0.013937000
1	-4.290440000	-0.495029000	-1.947698000
6	-4.413189000	0.923840000	1.630660000
1	-2.871165000	2.267281000	0.998220000
6	-5.240474000	-0.129397000	1.272909000
1	-5.828055000	-1.467747000	-0.297226000
1	-4.450383000	1.324781000	2.637654000
1	-5.924126000	-0.555223000	1.998953000

1TS$_{hy}^{Si-H}$ (TE = -2890.553257)

6	0.389480000	0.254895000	0.524809000
6	-1.424006000	1.546815000	-0.270527000
7	-0.160201000	1.514495000	0.161139000
7	-0.413735000	-0.728100000	0.213435000
25	-2.363793000	-0.250287000	-0.243556000
6	-2.629307000	0.025398000	1.593186000
8	-2.769208000	0.207963000	2.701963000
6	-4.077864000	0.236532000	-0.617587000
8	-5.171396000	0.482421000	-0.839194000
6	-2.901516000	-2.023809000	-0.132198000
8	-3.232059000	-3.108365000	-0.069868000
6	-1.935983000	-0.412497000	-2.051866000
8	-1.654945000	-0.483804000	-3.148543000
6	-0.020333000	-2.075461000	0.400775000
6	0.355226000	-2.837585000	-0.697398000
6	-0.082991000	-2.661846000	1.657939000
6	0.671091000	-4.175025000	-0.538695000
1	0.410934000	-2.364077000	-1.672064000
6	0.235555000	-4.000440000	1.812897000
1	-0.376986000	-2.057658000	2.510243000
6	0.609890000	-4.760422000	0.716307000
1	0.973483000	-4.760941000	-1.398848000

1	0.190195000	-4.451760000	2.797012000
1	0.855516000	-5.808362000	0.840052000
6	0.656404000	2.692613000	0.254806000
6	1.598413000	2.937723000	-0.725890000
6	0.507350000	3.538368000	1.338528000
6	2.426415000	4.040717000	-0.606435000
1	1.691561000	2.251877000	-1.561003000
6	1.339493000	4.637040000	1.452847000
1	-0.237933000	3.310368000	2.092161000
6	2.300993000	4.884314000	0.484889000
1	3.175765000	4.235862000	-1.364250000
1	1.243056000	5.298877000	2.304904000
1	2.955926000	5.742002000	0.582002000
8	-1.766201000	2.753886000	-0.636895000
6	-3.058996000	3.014584000	-1.162503000
1	-3.266801000	2.371795000	-2.018617000
1	-3.819463000	2.881033000	-0.393328000
1	-3.046996000	4.053176000	-1.483119000
14	2.018778000	0.148388000	1.512064000
1	2.612491000	1.460638000	1.864011000
1	2.082646000	-0.951451000	2.505737000
6	3.314709000	-0.499357000	0.253221000
6	3.517800000	-1.866176000	0.068342000
6	4.079962000	0.369458000	-0.523969000
6	4.419735000	-2.349363000	-0.866143000
1	2.953228000	-2.575832000	0.670158000
6	4.990479000	-0.099305000	-1.458684000
1	3.970709000	1.443647000	-0.385615000
6	5.156974000	-1.463669000	-1.636324000
1	4.551946000	-3.419345000	-0.990938000
1	5.576805000	0.599012000	-2.046897000
1	5.866561000	-1.835742000	-2.367129000
1	0.535304000	0.671679000	2.334857000

3_V (TE = -3076.743925)

6	1.355465000	-1.629246000	0.432803000
7	0.077939000	-0.997330000	0.306076000
6	-0.249883000	0.308170000	0.262143000
7	0.707536000	1.256257000	0.319156000
6	2.126534000	1.136471000	0.459040000

8	1.403602000	-2.781536000	0.761713000
6	-1.053572000	-1.900758000	0.299397000
6	-1.961713000	-1.881605000	1.339364000
6	-3.042764000	-2.745322000	1.315091000
6	-3.211740000	-3.618989000	0.254101000
6	-2.299330000	-3.627146000	-0.788452000
6	-1.215745000	-2.767267000	-0.766111000
1	-1.823739000	-1.177877000	2.152331000
1	-3.763354000	-2.725119000	2.124061000
1	-4.063804000	-4.288514000	0.234453000
1	-2.432486000	-4.303248000	-1.624656000
1	-0.492325000	-2.761007000	-1.575231000
6	0.199325000	2.610670000	0.308416000
6	-0.662622000	3.033254000	1.300605000
6	-1.203559000	4.306534000	1.237284000
6	-0.872718000	5.151853000	0.190933000
6	0.004824000	4.723934000	-0.792439000
6	0.542170000	3.450962000	-0.734892000
1	-0.922888000	2.351147000	2.102077000
1	-1.887645000	4.638339000	2.009473000
1	-1.299915000	6.146296000	0.141277000
1	0.262714000	5.379880000	-1.615250000
1	1.214834000	3.096174000	-1.509127000
8	2.757106000	2.093903000	0.811929000
26	3.013863000	-0.595346000	-0.034838000
6	2.247837000	-0.362372000	-1.678339000
8	1.725850000	-0.201290000	-2.668205000
6	3.338952000	-0.706657000	1.768048000
8	3.496333000	-0.762897000	2.884210000
6	3.806946000	-2.232923000	-0.458203000
8	4.268019000	-3.229752000	-0.710520000
6	4.543480000	0.402295000	-0.427114000
8	5.455621000	1.022226000	-0.658939000
14	-2.428121000	0.833046000	-2.084025000
1	-1.383155000	-0.202879000	-2.250104000
1	-1.819106000	2.142046000	-1.771307000
1	-3.115278000	0.939332000	-3.397311000
6	-3.720946000	0.383151000	-0.815237000
6	-4.652819000	-0.615210000	-1.090563000
6	-3.814261000	1.050744000	0.404260000

6	-5.642378000	-0.943228000	-0.178690000
1	-4.605259000	-1.150535000	-2.035819000
6	-4.804231000	0.731580000	1.318120000
1	-3.096120000	1.830044000	0.641173000
6	-5.719912000	-0.267769000	1.027886000
1	-6.353953000	-1.728389000	-0.409602000
1	-4.863956000	1.265074000	2.260432000
1	-6.495906000	-0.518917000	1.742426000

$3TS_{hy}^{Si\text{-}H}$ (TE = -3076.721379)

6	-2.018378000	1.208586000	-0.036318000
7	-0.612429000	1.318228000	0.053604000
6	0.309081000	0.312456000	0.202234000
7	0.032829000	-0.938379000	-0.278965000
6	-1.224466000	-1.517724000	-0.564644000
8	-2.671770000	2.208800000	-0.179270000
6	-0.073089000	2.648598000	-0.106510000
6	-0.309215000	3.631423000	0.838085000
6	0.236395000	4.888866000	0.661454000
6	1.009722000	5.163887000	-0.456313000
6	1.229607000	4.180270000	-1.404808000
6	0.680309000	2.920237000	-1.233049000
1	-0.906789000	3.400486000	1.711957000
1	0.061802000	5.658355000	1.403786000
1	1.438584000	6.150035000	-0.588724000
1	1.826369000	4.392337000	-2.283974000
1	0.838739000	2.136268000	-1.967021000
6	1.157136000	-1.834666000	-0.381033000
6	1.332116000	-2.809617000	0.585266000
6	2.415777000	-3.666494000	0.496991000
6	3.306556000	-3.547837000	-0.556712000
6	3.117702000	-2.573125000	-1.523809000
6	2.038811000	-1.712798000	-1.437952000
1	0.615345000	-2.892993000	1.396773000
1	2.563229000	-4.428492000	1.252787000
1	4.156652000	-4.216473000	-0.623508000
1	3.818208000	-2.478277000	-2.344699000
1	1.879332000	-0.933641000	-2.175681000
8	-1.254424000	-2.588626000	-1.112635000
14	1.697852000	0.506917000	1.755558000

1	2.106614000	-0.102687000	3.075351000
1	0.244750000	-0.079140000	1.938254000
1	1.502671000	1.947479000	2.006311000
6	3.318458000	0.230758000	0.833048000
6	3.660698000	0.991818000	-0.283736000
6	4.253151000	-0.680052000	1.312379000
6	4.887889000	0.843153000	-0.904441000
1	2.953591000	1.720600000	-0.670940000
6	5.478029000	-0.851543000	0.684356000
1	4.015169000	-1.274683000	2.190521000
6	5.797951000	-0.088144000	-0.424539000
1	5.140046000	1.455111000	-1.763693000
1	6.184857000	-1.581267000	1.064223000
1	6.757722000	-0.212873000	-0.913360000
26	-2.915905000	-0.593248000	0.003173000
6	-2.390348000	-0.827716000	1.743642000
8	-2.123139000	-1.016490000	2.826054000
6	-4.481818000	0.309082000	0.481880000
8	-5.419685000	0.864504000	0.767890000
6	-3.742369000	-2.266486000	-0.066889000
8	-4.230764000	-3.280953000	-0.116469000
6	-3.071805000	-0.273514000	-1.796476000
8	-3.125328000	-0.070440000	-2.905811000

III$_V$ (TE = -1477.596093)

6	-2.932352000	-0.954780000	-0.338808000
7	-1.921988000	0.034756000	-0.323426000
6	-0.587736000	-0.186994000	-0.341946000
7	-0.191381000	-1.477955000	-0.333343000
6	-1.038268000	-2.610610000	-0.346854000
6	-2.459423000	-2.326440000	0.074472000
8	-4.073592000	-0.696898000	-0.591286000
6	-2.430457000	-2.301822000	1.620115000
1	-2.101385000	-3.275821000	1.987698000
1	-1.756735000	-1.534769000	2.010091000
1	-3.437486000	-2.107764000	1.994692000
6	-3.404202000	-3.404592000	-0.414091000
1	-3.439916000	-3.437069000	-1.503800000
1	-3.072552000	-4.377585000	-0.054287000
1	-4.410273000	-3.209937000	-0.045134000

6	-2.335473000	1.413149000	-0.343669000
6	-3.172265000	1.884065000	0.652231000
6	-3.501840000	3.226600000	0.686372000
6	-2.993903000	4.091940000	-0.269409000
6	-2.161359000	3.609753000	-1.265785000
6	-1.833192000	2.265456000	-1.307788000
1	-3.547435000	1.201059000	1.407055000
1	-4.149410000	3.600325000	1.470330000
1	-3.247870000	5.144697000	-0.237053000
1	-1.764381000	4.282604000	-2.016582000
1	-1.169448000	1.871938000	-2.068774000
6	1.229040000	-1.714590000	-0.365758000
6	1.811079000	-2.457046000	0.646199000
6	3.178339000	-2.667424000	0.636121000
6	3.954683000	-2.134126000	-0.379801000
6	3.363202000	-1.385011000	-1.383027000
6	1.996053000	-1.172776000	-1.378773000
1	1.191121000	-2.864737000	1.438136000
1	3.638505000	-3.246607000	1.427692000
1	5.026309000	-2.295651000	-0.384804000
1	3.969293000	-0.956128000	-2.171984000
1	1.517637000	-0.577133000	-2.147367000
8	-0.632915000	-3.707220000	-0.602950000
14	0.796029000	1.331485000	2.080505000
1	0.417458000	-0.097607000	2.202397000
1	-0.380181000	2.143473000	1.705237000
1	1.245510000	1.750454000	3.432165000
6	2.204970000	1.606338000	0.890758000
6	3.476262000	1.121803000	1.190193000
6	2.034701000	2.323477000	-0.291660000
6	4.545222000	1.343241000	0.338331000
1	3.636597000	0.557407000	2.105744000
6	3.100721000	2.552669000	-1.145096000
1	1.049406000	2.701233000	-0.549523000
6	4.358686000	2.063050000	-0.830142000
1	5.525694000	0.951366000	0.585571000
1	2.951361000	3.116810000	-2.059074000
1	5.194469000	2.242016000	-1.497333000

III-TS$_{hy}^{Si-H}$ (TE = -1477.574031)

6	-2.714418000	-1.094185000	-0.461013000
7	-1.844932000	-0.038371000	-0.153823000
6	-0.509375000	-0.181735000	0.121945000
7	0.042623000	-1.400733000	-0.187610000
6	-0.681918000	-2.567813000	-0.453931000
6	-2.166798000	-2.475519000	-0.196711000
8	-3.831272000	-0.892135000	-0.850515000
6	-2.350581000	-2.722985000	1.315034000
1	-1.979762000	-3.719277000	1.562679000
1	-1.816182000	-1.990733000	1.928078000
1	-3.413089000	-2.671226000	1.560514000
6	-2.921754000	-3.519544000	-0.993684000
1	-2.807967000	-3.360930000	-2.066869000
1	-2.543098000	-4.511696000	-0.752113000
1	-3.982740000	-3.471176000	-0.752458000
6	-2.419457000	1.277348000	-0.100175000
6	-3.288591000	1.583226000	0.931085000
6	-3.794424000	2.865443000	1.032730000
6	-3.431763000	3.829077000	0.104322000
6	-2.576724000	3.506544000	-0.936381000
6	-2.072901000	2.221760000	-1.045289000
1	-3.544276000	0.817284000	1.656594000
1	-4.466712000	3.117007000	1.843943000
1	-3.822818000	4.835846000	0.189908000
1	-2.302588000	4.256135000	-1.668751000
1	-1.405914000	1.947448000	-1.854804000
6	1.471417000	-1.541636000	-0.086712000
6	2.005951000	-2.052169000	1.082621000
6	3.380416000	-2.163937000	1.207079000
6	4.201473000	-1.776871000	0.161293000
6	3.653471000	-1.287152000	-1.013982000
6	2.281927000	-1.171302000	-1.142660000
1	1.341894000	-2.356662000	1.885739000
1	3.808839000	-2.554667000	2.121953000
1	5.277303000	-1.859081000	0.260952000
1	4.297616000	-0.984319000	-1.830588000
1	1.833700000	-0.778437000	-2.047899000
8	-0.135117000	-3.579127000	-0.798633000
14	0.429034000	0.997310000	1.504333000

1	1.138241000	0.862186000	2.827157000
1	-0.491400000	-0.260210000	1.907476000
1	-0.546618000	2.097120000	1.630694000
6	1.906193000	1.590787000	0.484684000
6	1.760431000	2.072173000	-0.814557000
6	3.176714000	1.613572000	1.048205000
6	2.841321000	2.557179000	-1.528254000
1	0.779026000	2.059515000	-1.282378000
6	4.271136000	2.083631000	0.336735000
1	3.314490000	1.245936000	2.061854000
6	4.104295000	2.557265000	-0.952783000
1	2.703992000	2.935909000	-2.535242000
1	5.256466000	2.077952000	0.789896000
1	4.956140000	2.928607000	-1.511386000

IV$_V$ (TE = -1121.816877)

6	-1.205092000	-0.760859000	0.223195000
7	-1.184033000	0.506508000	-0.080102000
6	-0.050262000	1.326008000	0.227976000
6	0.823857000	1.725698000	-0.768460000
6	1.923495000	2.501203000	-0.443870000
6	2.150404000	2.875367000	0.869916000
6	1.278392000	2.464740000	1.865541000
6	0.177215000	1.690390000	1.545522000
1	0.656991000	1.403999000	-1.789705000
1	2.615891000	2.799289000	-1.222456000
1	3.014799000	3.478945000	1.120531000
1	1.457855000	2.744399000	2.896926000
1	-0.508272000	1.343533000	2.311717000
14	0.905926000	-2.245355000	1.719529000
1	-0.087194000	-3.258362000	1.312939000
1	0.346052000	-1.211708000	2.613887000
1	1.904549000	-2.969078000	2.566377000
6	1.915980000	-1.584218000	0.289728000
6	3.044122000	-0.811112000	0.551789000
6	1.616274000	-1.872130000	-1.040243000
6	3.839480000	-0.327670000	-0.475016000
1	3.305922000	-0.572455000	1.580196000
6	2.413486000	-1.404826000	-2.071358000
1	0.736996000	-2.466839000	-1.270911000

6	3.526814000	-0.627086000	-1.790041000
1	4.705058000	0.284961000	-0.247113000
1	2.166492000	-1.646660000	-3.099448000
1	4.149868000	-0.256090000	-2.596284000
6	-2.589811000	-1.262477000	-0.096651000
6	-2.456231000	1.133118000	-0.609549000
6	-3.287561000	-0.121732000	-0.861269000
1	-4.327265000	0.017873000	-0.553122000
1	-3.294390000	-0.346193000	-1.932268000
6	-3.258005000	-1.558693000	1.244642000
1	-4.277591000	-1.920728000	1.083434000
1	-2.699587000	-2.322633000	1.790299000
1	-3.310023000	-0.668979000	1.877996000
6	-2.516465000	-2.537075000	-0.920343000
1	-1.980757000	-2.365882000	-1.858498000
1	-1.995279000	-3.324505000	-0.371053000
1	-3.521807000	-2.892715000	-1.165622000
6	-3.045460000	2.042193000	0.454344000
1	-2.368279000	2.867422000	0.687457000
1	-3.983429000	2.470268000	0.093391000
1	-3.252571000	1.497168000	1.377855000
6	-2.200554000	1.917661000	-1.879316000
1	-3.154288000	2.263115000	-2.285651000
1	-1.577784000	2.796319000	-1.697710000
1	-1.717158000	1.293932000	-2.635073000

IV-TS$_{hy}^{Si\text{-}H}$ (TE = -1121.807217)

6	1.143705000	-0.725604000	-0.272516000
7	1.122169000	0.520120000	0.162436000
6	-0.025050000	1.360692000	0.017072000
6	-0.878363000	1.544159000	1.093425000
6	-2.009702000	2.324738000	0.945960000
6	-2.288557000	2.919390000	-0.274924000
6	-1.434609000	2.733664000	-1.348065000
6	-0.297597000	1.954718000	-1.205553000
1	-0.660426000	1.046625000	2.031898000
1	-2.685727000	2.454497000	1.782536000
1	-3.180863000	3.522908000	-0.391302000
1	-1.655330000	3.189537000	-2.305711000
1	0.366260000	1.785290000	-2.045960000

14	-0.117952000	-1.422156000	-1.594970000
1	0.306747000	-2.842250000	-1.697899000
1	1.219823000	-0.722353000	-2.180118000
1	-0.840150000	-1.037956000	-2.870551000
6	-1.693331000	-1.386735000	-0.503440000
6	-2.895288000	-0.894175000	-0.998575000
6	-1.678978000	-1.844116000	0.813290000
6	-4.038026000	-0.843216000	-0.212565000
1	-2.932362000	-0.529094000	-2.022960000
6	-2.815113000	-1.817280000	1.603651000
1	-0.751750000	-2.229310000	1.234646000
6	-4.000280000	-1.308402000	1.090927000
1	-4.960346000	-0.440225000	-0.617663000
1	-2.781437000	-2.191014000	2.621758000
1	-4.891172000	-1.275565000	1.708357000
6	2.470836000	-1.352775000	0.116671000
6	2.462404000	1.084525000	0.524635000
6	3.232859000	-0.200857000	0.809725000
1	4.265949000	-0.129081000	0.462064000
1	3.264819000	-0.372893000	1.889403000
6	3.267856000	-1.947996000	-1.034640000
1	4.177481000	-2.406474000	-0.635973000
1	2.699568000	-2.717915000	-1.557753000
1	3.557233000	-1.187878000	-1.762129000
6	2.160845000	-2.458441000	1.126357000
1	1.558145000	-2.075629000	1.955336000
1	1.618464000	-3.281990000	0.656633000
1	3.093602000	-2.850151000	1.541174000
6	3.025714000	1.840112000	-0.665662000
1	2.427854000	2.725568000	-0.893073000
1	4.043186000	2.169478000	-0.444019000
1	3.057859000	1.206352000	-1.556129000
6	2.362591000	1.986121000	1.734019000
1	3.364248000	2.304283000	2.031290000
1	1.775116000	2.882411000	1.522427000
1	1.907873000	1.461040000	2.577482000

Cartesian coordinates of the transition states involved in the activation of C – H bond of CH_4 by **1**, **3** and **III**-**IV**, along with their total energies (in hartrees) including zero point vibrational correction.

1TS^{C-H} (TE = -2408.234110)

6	0.426759000	-1.191730000	-0.056252000
6	1.102344000	1.050776000	-0.136466000
7	1.451787000	-0.238435000	-0.091240000
7	-0.778820000	-0.692034000	-0.019364000
25	-0.920534000	1.366044000	-0.025734000
6	-0.732008000	1.357372000	1.833215000
8	-0.598848000	1.336443000	2.958860000
6	-0.985473000	3.182617000	-0.079253000
8	-1.100440000	4.319791000	-0.099516000
6	-2.767169000	1.341042000	0.072129000
8	-3.902670000	1.354985000	0.120129000
6	-0.953045000	1.202401000	-1.892087000
8	-0.942446000	1.054276000	-3.015956000
6	-1.840757000	-1.617319000	-0.074765000
6	-1.988321000	-2.454837000	-1.175073000
6	-2.749653000	-1.703975000	0.973364000
6	-3.033746000	-3.359920000	-1.227514000
1	-1.274143000	-2.377070000	-1.988383000
6	-3.793342000	-2.610009000	0.917121000
1	-2.616563000	-1.066500000	1.841703000
6	-3.941112000	-3.439107000	-0.183483000
1	-3.143216000	-4.003862000	-2.092634000
1	-4.491868000	-2.674089000	1.743292000
1	-4.760720000	-4.146462000	-0.226176000
6	2.804872000	-0.719201000	-0.123518000
6	3.204020000	-1.512346000	-1.182329000
6	3.670956000	-0.425955000	0.914934000
6	4.492828000	-2.020197000	-1.202461000
1	2.501022000	-1.731477000	-1.977920000
6	4.956820000	-0.930961000	0.885852000
1	3.325026000	0.178019000	1.745829000
6	5.368692000	-1.728254000	-0.171722000
1	4.811160000	-2.644969000	-2.028284000
1	5.637710000	-0.712015000	1.699534000
1	6.376072000	-2.126973000	-0.187793000

8	2.147856000	1.825357000	-0.297870000
6	1.996075000	3.231522000	-0.387068000
1	1.367825000	3.500072000	-1.237256000
1	1.576724000	3.635392000	0.534988000
1	2.995616000	3.632870000	-0.535036000
1	0.738358000	-2.185408000	0.385147000
6	0.994922000	-2.205197000	2.138386000
1	1.932785000	-2.723857000	2.342403000
1	0.974865000	-1.207733000	2.583257000
1	0.122342000	-2.790902000	2.431689000

3TS^{C-H} (TE = -2594.411983)

6	1.466094000	0.822009000	0.239651000
7	1.216552000	-0.535668000	0.004009000
6	0.024009000	-1.148069000	-0.249554000
7	-1.195407000	-0.578687000	-0.025713000
6	-1.495043000	0.766034000	0.225884000
8	2.571126000	1.174841000	0.569045000
6	2.335551000	-1.443796000	0.019410000
6	2.339845000	-2.491271000	0.923480000
6	3.389156000	-3.392770000	0.922838000
6	4.428955000	-3.246004000	0.019211000
6	4.416676000	-2.196489000	-0.884916000
6	3.369174000	-1.292411000	-0.888256000
1	1.514114000	-2.592851000	1.619072000
1	3.395059000	-4.211547000	1.632496000
1	5.250406000	-3.952640000	0.018134000
1	5.225684000	-2.081802000	-1.596413000
1	3.349138000	-0.467553000	-1.591182000
6	-2.284088000	-1.522723000	-0.045005000
6	-2.273669000	-2.583747000	0.842877000
6	-3.294748000	-3.516549000	0.807594000
6	-4.320903000	-3.387333000	-0.114042000
6	-4.323094000	-2.324159000	-1.002233000
6	-3.303815000	-1.389108000	-0.971148000
1	-1.458756000	-2.671502000	1.552910000
1	-3.289408000	-4.346129000	1.504590000
1	-5.120227000	-4.118352000	-0.141899000
1	-5.120973000	-2.223175000	-1.728236000
1	-3.294329000	-0.553867000	-1.662202000

8	-2.614531000	1.074913000	0.550504000
26	-0.040148000	2.165288000	0.088386000
6	-0.039216000	1.853507000	-1.708985000
8	-0.045160000	1.673003000	-2.825954000
6	-0.040614000	1.990378000	1.910561000
8	-0.040739000	1.832140000	3.029665000
6	1.293110000	3.469723000	0.015872000
8	2.098883000	4.256828000	-0.028600000
6	-1.419530000	3.420426000	0.016813000
8	-2.252970000	4.178367000	-0.025003000
1	0.049564000	-1.953418000	-1.092508000
6	0.065597000	-1.566417000	-2.578411000
1	0.948728000	-0.988461000	-2.839142000
1	0.127381000	-2.595104000	-2.931463000
1	-0.864309000	-1.085302000	-2.871315000

III-TS^{C-H} (TE = -995.263169)

6	1.268242000	1.581953000	-0.406827000
7	1.178668000	0.213669000	-0.167719000
6	-0.000009000	-0.450245000	0.036618000
7	-1.178668000	0.213707000	-0.167717000
6	-1.268242000	1.582014000	-0.406667000
6	0.000037000	2.364768000	-0.122670000
8	2.288699000	2.101285000	-0.776923000
6	0.000156000	2.658980000	1.389979000
1	-0.886759000	3.243275000	1.643845000
1	0.000317000	1.747502000	1.989912000
1	0.887006000	3.243457000	1.643658000
6	0.000010000	3.667578000	-0.898659000
1	-0.000171000	3.490391000	-1.975067000
1	-0.888097000	4.245883000	-0.647895000
1	0.888277000	4.245754000	-0.648165000
6	2.367350000	-0.584767000	-0.147587000
6	3.399511000	-0.253987000	0.714503000
6	4.528412000	-1.050715000	0.761936000
6	4.622173000	-2.174986000	-0.042923000
6	3.583099000	-2.502276000	-0.897947000
6	2.452212000	-1.706403000	-0.953110000
1	3.311194000	0.625121000	1.343139000
1	5.336926000	-0.794997000	1.436146000

1	5.507489000	-2.798273000	-0.002032000
1	3.653566000	-3.379265000	-1.530209000
1	1.628900000	-1.946883000	-1.616162000
6	-2.367359000	-0.584717000	-0.147602000
6	-3.399410000	-0.254101000	0.714681000
6	-4.528316000	-1.050825000	0.762081000
6	-4.622187000	-2.174924000	-0.043004000
6	-3.583220000	-2.502050000	-0.898223000
6	-2.452329000	-1.706182000	-0.953352000
1	-3.311005000	0.624879000	1.343483000
1	-5.336749000	-0.795237000	1.436438000
1	-5.507506000	-2.798207000	-0.002140000
1	-3.653776000	-3.378904000	-1.530661000
1	-1.629098000	-1.946529000	-1.616554000
8	-2.288741000	2.101416000	-0.776550000
1	-0.000042000	-1.293009000	0.827115000
6	-0.000095000	-0.902546000	2.335006000
1	0.910132000	-0.375803000	2.612936000
1	-0.910123000	-0.375388000	2.612805000
1	-0.000357000	-1.936410000	2.677851000

IV-TS$^{C\text{-}H}$ (TE = -639.483317)

6	0.741029000	-1.340687000	0.358587000
6	2.223897000	-0.951173000	0.269685000
6	2.288618000	0.393616000	-0.471989000
6	0.918398000	0.967750000	-0.248024000
7	0.084732000	-0.042790000	0.026447000
1	2.813896000	-1.731847000	-0.219089000
1	2.626605000	-0.822447000	1.279008000
6	-1.318669000	0.118871000	-0.080047000
6	-1.869080000	0.381740000	-1.328956000
6	-3.233059000	0.555872000	-1.468194000
6	-4.061222000	0.466377000	-0.359573000
6	-3.515504000	0.213010000	0.886962000
6	-2.147966000	0.043658000	1.031563000
1	-1.203595000	0.447370000	-2.183780000
1	-3.653270000	0.757939000	-2.446578000
1	-5.130989000	0.600973000	-0.467566000
1	-4.156167000	0.158707000	1.759417000
1	-1.717057000	-0.120630000	2.011656000

6	2.414919000	0.183751000	-1.986307000
1	2.462237000	1.146792000	-2.499557000
1	3.328793000	-0.373747000	-2.212099000
1	1.568184000	-0.369305000	-2.397870000
6	3.440432000	1.267536000	-0.018932000
1	4.390844000	0.828269000	-0.335037000
1	3.366494000	2.261754000	-0.468002000
1	3.463519000	1.385604000	1.064504000
6	0.333223000	-2.399256000	-0.652607000
1	-0.747259000	-2.563272000	-0.626241000
1	0.609273000	-2.116559000	-1.670110000
1	0.821666000	-3.347656000	-0.417554000
6	0.392759000	-1.821515000	1.757885000
1	1.024193000	-2.677045000	2.012531000
1	0.569928000	-1.035844000	2.496345000
1	-0.647456000	-2.146049000	1.829432000
1	0.753927000	2.011298000	0.247682000
6	1.022726000	2.144385000	1.775970000
1	-0.012457000	2.297918000	2.083685000
1	1.473449000	1.311114000	2.312520000
1	1.619107000	3.052573000	1.865441000

Cartesian coordinates of the optimized geometries of the dihydrogen splitting product obtained for **1**, **3** and **IV**, along with their total energies (in hartrees) including zero point vibrational correction.

1P^{H-H} (TE = -2369.054765)

6	0.413371000	-1.306021000	0.401956000
6	1.131145000	0.871853000	-0.271526000
7	1.462754000	-0.380221000	-0.028801000
7	-0.839716000	-0.769935000	0.032646000
25	-0.831742000	1.302374000	0.110060000
6	-0.359121000	1.174464000	1.909170000
8	-0.037319000	1.077346000	2.993731000
6	-0.743186000	3.113515000	0.147457000
8	-0.753787000	4.257262000	0.193107000
6	-2.616630000	1.441530000	0.574472000
8	-3.695470000	1.585353000	0.903824000
6	-1.141926000	1.244411000	-1.736323000
8	-1.281724000	1.173331000	-2.859456000

6	-1.883648000	-1.650769000	-0.019011000
6	-3.097118000	-1.312388000	-0.649590000
6	-1.807689000	-2.953477000	0.517846000
6	-4.144889000	-2.203332000	-0.737246000
1	-3.203236000	-0.334203000	-1.102953000
6	-2.865095000	-3.840358000	0.416836000
1	-0.917025000	-3.272059000	1.046138000
6	-4.047021000	-3.482982000	-0.207254000
1	-5.054959000	-1.893644000	-1.240299000
1	-2.759504000	-4.829759000	0.850111000
1	-4.872871000	-4.179867000	-0.278933000
6	2.805149000	-0.879472000	-0.034577000
6	3.286161000	-1.551436000	-1.144066000
6	3.588878000	-0.713233000	1.094145000
6	4.574304000	-2.056846000	-1.123736000
1	2.647665000	-1.672400000	-2.012021000
6	4.875933000	-1.222093000	1.108628000
1	3.180106000	-0.185331000	1.950105000
6	5.367931000	-1.892038000	0.000344000
1	4.959568000	-2.582429000	-1.989186000
1	5.495550000	-1.095833000	1.988297000
1	6.375531000	-2.290207000	0.013194000
8	2.169060000	1.576915000	-0.662831000
6	2.024435000	2.942266000	-1.016804000
1	1.204715000	3.081029000	-1.722608000
1	1.864418000	3.555754000	-0.130102000
1	2.960375000	3.230493000	-1.489549000
1	0.620888000	-2.272031000	-0.083623000
1	0.559079000	-1.470978000	1.491677000

3P^{H-H} (TE = -2555.250956)

6	0.848098000	-1.465453000	-0.009484000
7	-0.420664000	-1.273455000	0.482975000
6	-0.747271000	-0.072394000	1.214716000
7	-0.606418000	1.147624000	0.453180000
6	0.624669000	1.539318000	-0.012278000
8	1.178585000	-2.502095000	-0.536759000
6	-1.468994000	-2.203794000	0.208449000
6	-1.331680000	-3.547604000	0.520827000
6	-2.368198000	-4.423756000	0.249793000

6	-3.544129000	-3.966617000	-0.321683000
6	-3.680007000	-2.623129000	-0.629382000
6	-2.643250000	-1.743816000	-0.373276000
1	-0.413532000	-3.899648000	0.971822000
1	-2.256260000	-5.473374000	0.495210000
1	-4.353502000	-4.656779000	-0.528012000
1	-4.593491000	-2.255823000	-1.082014000
1	-2.739657000	-0.693483000	-0.632323000
6	-1.756507000	1.967112000	0.246774000
6	-2.503365000	2.406703000	1.328729000
6	-3.647321000	3.158501000	1.119179000
6	-4.037773000	3.486156000	-0.167659000
6	-3.283482000	3.054046000	-1.247425000
6	-2.147561000	2.292609000	-1.044116000
1	-2.182310000	2.164418000	2.336227000
1	-4.228961000	3.497518000	1.968267000
1	-4.929809000	4.079115000	-0.330532000
1	-3.585684000	3.305339000	-2.257220000
1	-1.555609000	1.941899000	-1.882250000
8	0.799208000	2.631159000	-0.501889000
26	2.146806000	0.143951000	-0.032915000
6	1.632599000	0.118315000	-1.791867000
8	1.258904000	0.108426000	-2.858894000
6	2.208021000	0.143789000	1.781377000
8	2.280868000	0.144559000	2.913742000
6	3.494630000	-1.123352000	-0.197789000
8	4.308687000	-1.898210000	-0.298326000
6	3.293197000	1.597540000	-0.190197000
8	3.985498000	2.483534000	-0.283709000
1	-1.783551000	-0.151057000	1.534981000
1	-0.149085000	-0.024042000	2.127102000

IVP$^{H\text{-}H}$ (TE = -600.325466)

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

Cartesian coordinates of the optimized geometries of the N-H bond splitting product obtained for **1**, **3** and **III**-**IV**, along with their total energies (in hartrees) including zero point vibrational correction.

1P^{N-H} (TE = -2424.386095)

6	-0.438975000	-1.349226000	0.073300000
6	-1.146685000	0.969883000	-0.091203000
7	-1.508755000	-0.295411000	-0.069974000
7	0.757429000	-0.741855000	-0.378744000
25	0.854845000	1.287380000	0.105434000
6	0.908827000	1.553978000	-1.743584000

8	0.906239000	1.659123000	-2.873376000
6	0.857397000	3.054525000	0.514709000
8	0.925795000	4.162677000	0.795660000
6	2.696561000	1.311457000	0.278110000
8	3.823567000	1.375358000	0.415119000
6	0.668915000	0.770756000	1.885398000
8	0.537311000	0.409657000	2.954454000
6	1.909323000	-1.519906000	-0.248063000
6	2.111087000	-2.457095000	0.772296000
6	2.946893000	-1.351657000	-1.172349000
6	3.295221000	-3.167071000	0.868121000
1	1.331415000	-2.635867000	1.504169000
6	4.129637000	-2.056326000	-1.069460000
1	2.801810000	-0.649237000	-1.987411000
6	4.318007000	-2.971975000	-0.044803000
1	3.418797000	-3.882881000	1.674025000
1	4.910446000	-1.896352000	-1.805167000
1	5.243047000	-3.530317000	0.034350000
6	-2.871210000	-0.725695000	-0.033873000
6	-3.439512000	-1.062153000	1.183177000
6	-3.597644000	-0.837293000	-1.207364000
6	-4.747428000	-1.516306000	1.224201000
1	-2.853031000	-0.962371000	2.090745000
6	-4.905457000	-1.285501000	-1.160163000
1	-3.128128000	-0.568913000	-2.147364000
6	-5.480026000	-1.626914000	0.054392000
1	-5.195518000	-1.780550000	2.174568000
1	-5.477936000	-1.372320000	-2.075923000
1	-6.503524000	-1.980773000	0.088175000
8	-2.186470000	1.769335000	-0.210242000
6	-2.019046000	3.174110000	-0.293576000
1	-1.730478000	3.586890000	0.673133000
1	-1.280202000	3.439814000	-1.050435000
1	-2.988788000	3.574759000	-0.579916000
1	-0.475642000	-1.622500000	1.149671000
7	-0.728073000	-2.533234000	-0.658979000
1	-1.565926000	-3.012167000	-0.357731000
1	-0.748513000	-2.352976000	-1.655359000

3P^{N-H} (TE = -2610.576532)

6	1.488146000	0.738890000	0.104944000
7	1.229779000	-0.597018000	-0.054754000
6	0.021029000	-1.200879000	-0.619917000
7	-1.214021000	-0.625875000	-0.132852000
6	-1.513632000	0.703463000	-0.002212000
8	2.610596000	1.127074000	0.347688000
6	2.330500000	-1.514101000	0.025000000
6	2.357305000	-2.440988000	1.053985000
6	3.388249000	-3.361962000	1.125480000
6	4.394077000	-3.350778000	0.173161000
6	4.366680000	-2.419367000	-0.852435000
6	3.334116000	-1.501408000	-0.930207000
1	1.564096000	-2.429224000	1.795427000
1	3.408800000	-4.086003000	1.931312000
1	5.203392000	-4.068884000	0.231453000
1	5.153912000	-2.407331000	-1.596897000
1	3.303382000	-0.762552000	-1.723238000
6	-2.291116000	-1.572212000	-0.035763000
6	-2.388731000	-2.347198000	1.107076000
6	-3.403505000	-3.282667000	1.218516000
6	-4.318943000	-3.433223000	0.190268000
6	-4.217940000	-2.651234000	-0.949692000
6	-3.201403000	-1.720130000	-1.066964000
1	-1.664879000	-2.204862000	1.904327000
1	-3.482601000	-3.889591000	2.112694000
1	-5.116095000	-4.162121000	0.277806000
1	-4.934748000	-2.768988000	-1.753769000
1	-3.103123000	-1.102864000	-1.951968000
8	-2.657290000	1.061156000	0.177243000
26	-0.030415000	2.099258000	0.103193000
6	0.050652000	2.024889000	-1.699326000
8	0.107383000	1.941233000	-2.831128000
6	-0.098006000	1.593095000	1.856816000
8	-0.139419000	1.201629000	2.918206000
6	1.293443000	3.401752000	0.296305000
8	2.081372000	4.200575000	0.410221000
6	-1.398695000	3.368361000	0.175621000
8	-2.213958000	4.146533000	0.214263000
1	0.030727000	-2.226352000	-0.241251000

7	0.002028000	-1.313640000	-2.053776000
1	0.102411000	-0.419104000	-2.516672000
1	0.738189000	-1.928497000	-2.378461000

IIIP^{N-H} (TE = -1011.428065)

6	1.280865000	1.522222000	-0.304606000
7	1.197704000	0.178881000	-0.064188000
6	-0.000081000	-0.529935000	0.325557000
7	-1.194111000	0.180343000	-0.125750000
6	-1.277269000	1.528488000	-0.339244000
6	0.001120000	2.328892000	-0.158796000
8	2.330378000	2.056794000	-0.582347000
6	-0.019159000	2.884606000	1.273585000
1	-0.906166000	3.505488000	1.410951000
1	-0.035159000	2.093956000	2.028306000
1	0.869938000	3.495136000	1.440616000
6	0.017361000	3.487840000	-1.143656000
1	0.035122000	3.131119000	-2.175057000
1	-0.874670000	4.097353000	-1.008104000
1	0.903934000	4.098051000	-0.978744000
6	2.400595000	-0.596884000	-0.054108000
6	3.301150000	-0.462679000	0.988452000
6	4.455689000	-1.222559000	0.998158000
6	4.705160000	-2.120664000	-0.028155000
6	3.800660000	-2.253619000	-1.067577000
6	2.646944000	-1.487231000	-1.083796000
1	3.084952000	0.241294000	1.784396000
1	5.162961000	-1.117274000	1.812211000
1	5.609618000	-2.717415000	-0.017737000
1	3.995966000	-2.950028000	-1.874373000
1	1.936111000	-1.569206000	-1.899337000
6	-2.395866000	-0.592012000	-0.099239000
6	-3.326062000	-0.390496000	0.908649000
6	-4.472490000	-1.162482000	0.950507000
6	-4.686354000	-2.140723000	-0.007960000
6	-3.754053000	-2.342176000	-1.011592000
6	-2.608583000	-1.565419000	-1.060673000
1	-3.145102000	0.382485000	1.648200000
1	-5.202002000	-1.000798000	1.735104000
1	-5.584567000	-2.745735000	0.026509000

1	-3.921587000	-3.101516000	-1.766044000
1	-1.877767000	-1.702934000	-1.850383000
8	-2.322315000	2.070209000	-0.621892000
1	0.002119000	-1.489173000	-0.205021000
7	0.031434000	-0.847259000	1.724976000
1	-0.110090000	-0.025491000	2.301514000
1	-0.671078000	-1.536107000	1.962604000

IVP^{N-H} (TE = -655.652774)

6	-0.664109000	1.346511000	-0.321000000
6	-2.138854000	0.987363000	-0.594809000
6	-2.390305000	-0.383481000	0.023085000
6	-0.999681000	-1.017466000	-0.151367000
7	-0.108113000	0.069275000	0.206275000
1	-2.303716000	0.929854000	-1.676012000
1	-2.821904000	1.749236000	-0.207938000
6	1.284645000	-0.140472000	0.131711000
6	1.859129000	-1.014506000	-0.789052000
6	3.231484000	-1.177656000	-0.847859000
6	4.063110000	-0.468101000	0.003171000
6	3.502021000	0.394977000	0.929579000
6	2.128520000	0.546575000	1.001851000
1	1.224772000	-1.576000000	-1.464320000
1	3.655613000	-1.865293000	-1.571200000
1	5.137833000	-0.597351000	-0.046369000
1	4.136685000	0.942021000	1.617786000
1	1.690188000	1.186429000	1.758525000
6	-3.455362000	-1.160719000	-0.723710000
1	-3.575461000	-2.166279000	-0.308055000
1	-4.424826000	-0.660167000	-0.650363000
1	-3.206539000	-1.258236000	-1.784243000
6	-2.779897000	-0.271500000	1.489175000
1	-3.688493000	0.328524000	1.587546000
1	-2.990078000	-1.253853000	1.921187000
1	-1.996354000	0.199970000	2.085786000
6	0.016129000	1.763170000	-1.618454000
1	1.057977000	2.049450000	-1.455509000
1	-0.003581000	0.949777000	-2.349321000
1	-0.507127000	2.619601000	-2.051836000
6	-0.547914000	2.475409000	0.690084000

1	-1.060909000	3.363402000	0.310630000
1	-1.000620000	2.199947000	1.645036000
1	0.493755000	2.749559000	0.866399000
1	-0.913172000	-1.299511000	-1.221912000
7	-0.677640000	-2.194008000	0.610449000
1	-0.797677000	-2.022150000	1.602035000
1	-1.259592000	-2.976434000	0.340639000

Cartesian coordinates of the optimized geometries for the P – H bond splitting product obtained for **1**, **3** and **III-IV,** along with their total energies (in hartrees) including zero point vibrational correction.

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1P^{P-H} (TE = -2710.984482)

6	0.451552000	-1.211534000	-0.057482000
6	1.066153000	1.111524000	0.063798000
7	1.463838000	-0.150093000	0.021385000
7	-0.802833000	-0.660035000	0.296984000
25	-0.942221000	1.395086000	-0.069852000
6	-0.962096000	1.552986000	1.794754000
8	-0.936439000	1.574195000	2.928564000
6	-0.983604000	3.176441000	-0.404917000
8	-1.085236000	4.292317000	-0.641256000
6	-2.785574000	1.430012000	-0.208680000
8	-3.913777000	1.519602000	-0.322110000
6	-0.773411000	0.898697000	-1.858264000
8	-0.636242000	0.502454000	-2.913721000
6	-1.909575000	-1.477415000	0.097905000
6	-1.987374000	-2.468550000	-0.890947000
6	-3.021894000	-1.335725000	0.940204000
6	-3.120631000	-3.252365000	-1.035456000
1	-1.155373000	-2.629713000	-1.567658000
6	-4.150386000	-2.113236000	0.787328000
1	-2.972444000	-0.602519000	1.739008000
6	-4.213852000	-3.081888000	-0.205595000
1	-3.144964000	-4.005694000	-1.815677000
1	-4.987475000	-1.972781000	1.462518000
1	-5.097419000	-3.697748000	-0.321177000
6	2.844994000	-0.529188000	-0.086937000
6	3.330544000	-0.942275000	-1.314804000
6	3.663319000	-0.505935000	1.029453000

6	4.648768000	-1.352383000	-1.422125000
1	2.673341000	-0.941427000	-2.178109000
6	4.980043000	-0.911793000	0.914566000
1	3.257646000	-0.176436000	1.979640000
6	5.472033000	-1.338546000	-0.309103000
1	5.033169000	-1.681001000	-2.380164000
1	5.624037000	-0.899780000	1.785596000
1	6.502814000	-1.660994000	-0.394702000
8	2.094700000	1.926612000	0.136096000
6	1.912476000	3.328232000	0.237398000
1	1.569293000	3.742589000	-0.710439000
1	1.209710000	3.576082000	1.033636000
1	2.890223000	3.740079000	0.476561000
1	0.520529000	-1.616229000	-1.088090000
15	1.030205000	-2.643602000	1.076960000
1	0.855594000	-1.878836000	2.263265000
1	-0.256224000	-3.231607000	1.151955000

3P$^{P\text{-}H}$ (TE = -2897.176864)

6	-0.874926000	-1.435556000	-0.179497000
7	0.469440000	-1.255785000	0.015291000
6	1.110725000	-0.080536000	0.574065000
7	0.649652000	1.187365000	0.057473000
6	-0.668249000	1.572765000	-0.022314000
8	-1.314000000	-2.525953000	-0.474204000
6	1.337020000	-2.392228000	-0.120084000
6	2.229799000	-2.429660000	-1.178602000
6	3.096634000	-3.500416000	-1.310435000
6	3.063514000	-4.534445000	-0.389059000
6	2.163414000	-4.496644000	0.663474000
6	1.299852000	-3.424269000	0.802382000
1	2.230751000	-1.617267000	-1.898847000
1	3.794165000	-3.530365000	-2.139042000
1	3.739837000	-5.374560000	-0.493584000
1	2.134336000	-5.306048000	1.383164000
1	0.590454000	-3.380097000	1.620682000
6	1.674573000	2.178832000	-0.099587000
6	2.552582000	2.054280000	-1.164525000
6	3.571879000	2.974929000	-1.331344000
6	3.706289000	4.025935000	-0.439043000

6	2.821161000	4.152668000	0.619273000
6	1.805135000	3.229116000	0.794129000
1	2.420948000	1.234171000	-1.863954000
1	4.256187000	2.876316000	-2.165590000
1	4.500608000	4.751030000	-0.570919000
1	2.922006000	4.976412000	1.315983000
1	1.104542000	3.321413000	1.615481000
8	-0.959012000	2.737663000	-0.183792000
26	-2.143311000	0.161513000	-0.162751000
6	-2.178953000	-0.019866000	1.643191000
8	-2.226303000	-0.165830000	2.766761000
6	-1.600833000	0.240433000	-1.905001000
8	-1.189160000	0.277161000	-2.958885000
6	-3.510411000	-1.077290000	-0.439419000
8	-4.348229000	-1.812032000	-0.612580000
6	-3.330008000	1.601822000	-0.214565000
8	-4.060216000	2.460848000	-0.241786000
1	2.156745000	-0.158784000	0.268886000
15	1.245033000	-0.179113000	2.476508000
1	2.285962000	0.780730000	2.557931000
1	0.240581000	0.779265000	2.761994000

IIIP^{P-H} (TE = -1298.028077)

6	1.274542000	1.594934000	-0.370912000
7	1.192083000	0.246713000	-0.139165000
6	0.002352000	-0.402866000	0.357068000
7	-1.201294000	0.248041000	-0.110744000
6	-1.285951000	1.578345000	-0.418376000
6	-0.015340000	2.396657000	-0.245807000
8	2.318200000	2.131804000	-0.665215000
6	-0.063450000	3.017576000	1.157932000
1	-0.930200000	3.677120000	1.228600000
1	-0.143158000	2.268088000	1.947694000
1	0.840604000	3.605056000	1.328699000
6	0.003489000	3.514422000	-1.279075000
1	0.052192000	3.116457000	-2.294233000
1	-0.902897000	4.110742000	-1.188550000
1	0.874102000	4.148291000	-1.118681000
6	2.368901000	-0.560779000	-0.203446000
6	3.439693000	-0.315821000	0.641261000

6	4.558714000	-1.126269000	0.580283000
6	4.606960000	-2.183503000	-0.314309000
6	3.534279000	-2.426668000	-1.155446000
6	2.416123000	-1.612622000	-1.104107000
1	3.389829000	0.514015000	1.336337000
1	5.397426000	-0.932361000	1.238197000
1	5.484463000	-2.817599000	-0.357633000
1	3.570261000	-3.246991000	-1.862292000
1	1.577055000	-1.782848000	-1.771502000
6	-2.373761000	-0.567141000	-0.170856000
6	-3.408413000	-0.368186000	0.727809000
6	-4.531470000	-1.172979000	0.666993000
6	-4.616630000	-2.178059000	-0.283157000
6	-3.579041000	-2.375083000	-1.179039000
6	-2.457260000	-1.566258000	-1.126698000
1	-3.324216000	0.422057000	1.465467000
1	-5.343040000	-1.016506000	1.367418000
1	-5.496619000	-2.808748000	-0.326823000
1	-3.646285000	-3.154818000	-1.928270000
1	-1.645079000	-1.696401000	-1.835227000
8	-2.322366000	2.086941000	-0.781161000
1	-0.006976000	-1.418335000	-0.051405000
15	-0.046795000	-0.700818000	2.241744000
1	1.063397000	-1.583248000	2.238670000
1	0.746469000	0.420847000	2.597043000

IVP^{P-H} (TE = -942.258789)

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

Cartesian coordinates of the optimized geometries for the Si – H bond splitting product obtained for **1**, **3** and **III-IV**, along with their total energies (in hartrees) including zero point vibrational correction.

1P^{Si-H} (TE = -2890.606666)

6	0.291036000	0.388584000	0.039629000
6	-0.696978000	-1.808270000	0.005393000
7	0.403982000	-1.076658000	0.016424000
7	-1.044180000	0.743517000	-0.336985000
25	-2.439408000	-0.755737000	0.104934000
6	-2.573729000	-0.943578000	-1.752373000
8	-2.582776000	-1.022118000	-2.883879000
6	-3.582182000	-2.104212000	0.509236000
8	-4.358804000	-2.897956000	0.789106000

6	-3.902132000	0.367636000	0.212622000
8	-4.844366000	0.997470000	0.312700000
6	-1.985846000	-0.401605000	1.876988000
8	-1.629258000	-0.136141000	2.921962000
6	-1.373661000	2.080466000	-0.161398000
6	-0.739285000	2.934929000	0.753277000
6	-2.376847000	2.649223000	-0.963010000
6	-1.101277000	4.269381000	0.862297000
1	0.041801000	2.558706000	1.404166000
6	-2.736228000	3.973279000	-0.844675000
1	-2.855882000	2.023536000	-1.709358000
6	-2.101725000	4.802856000	0.072914000
1	-0.587867000	4.896275000	1.583735000
1	-3.512316000	4.371617000	-1.489256000
1	-2.379484000	5.846161000	0.159825000
6	1.724692000	-1.630618000	0.124426000
6	2.432523000	-1.447017000	1.300704000
6	2.289968000	-2.313077000	-0.940259000
6	3.723318000	-1.935305000	1.404756000
1	1.971490000	-0.917697000	2.127657000
6	3.575254000	-2.810912000	-0.824666000
1	1.718193000	-2.445185000	-1.851464000
6	4.294562000	-2.617154000	0.343727000
1	4.283527000	-1.780819000	2.318989000
1	4.020249000	-3.345148000	-1.655634000
1	5.305850000	-2.997244000	0.426352000
8	-0.413527000	-3.092948000	-0.019580000
6	-1.438034000	-4.068531000	-0.082963000
1	-1.953981000	-4.150548000	0.873683000
1	-2.150587000	-3.839497000	-0.876183000
1	-0.941427000	-5.010627000	-0.304204000
1	0.585246000	0.687753000	1.066361000
14	1.486675000	1.145472000	-1.272839000
1	1.468403000	0.226015000	-2.433484000
1	0.941764000	2.459439000	-1.659825000
6	3.223220000	1.331219000	-0.616656000
6	3.444084000	2.125167000	0.509955000
6	4.310542000	0.659637000	-1.169396000
6	4.703973000	2.235918000	1.071478000
1	2.615037000	2.670191000	0.956628000

6	5.575576000	0.770806000	-0.615575000
1	4.165381000	0.029554000	-2.042246000
6	5.772790000	1.555431000	0.508298000
1	4.855568000	2.856395000	1.947492000
1	6.409225000	0.237819000	-1.059264000
1	6.761119000	1.640133000	0.945530000

3P^{Si-H} (TE = -3076.796167)

6	-2.253708000	0.237905000	-0.450026000
7	-1.282737000	1.169738000	-0.172857000
6	0.144145000	0.889477000	-0.110748000
7	0.535873000	-0.188779000	0.791207000
6	-0.112643000	-1.387246000	0.933159000
8	-3.366275000	0.583873000	-0.783764000
6	-1.637306000	2.559506000	-0.169190000
6	-1.585817000	3.250449000	1.031529000
6	-1.897040000	4.598234000	1.066361000
6	-2.271023000	5.251518000	-0.096721000
6	-2.331938000	4.555229000	-1.292914000
6	-2.013507000	3.208860000	-1.333083000
1	-1.310282000	2.716016000	1.936075000
1	-1.857635000	5.136509000	2.005927000
1	-2.520084000	6.305724000	-0.070094000
1	-2.628297000	5.063579000	-2.202765000
1	-2.060373000	2.652344000	-2.262400000
6	1.766392000	0.022661000	1.500745000
6	1.893905000	1.125803000	2.331650000
6	3.090807000	1.371339000	2.982253000
6	4.159060000	0.505422000	2.819843000
6	4.022193000	-0.607606000	2.006108000
6	2.833218000	-0.848192000	1.343402000
1	1.049999000	1.793808000	2.472293000
1	3.182699000	2.237724000	3.626523000
1	5.095737000	0.695441000	3.330295000
1	4.853944000	-1.289051000	1.870294000
1	2.730909000	-1.706084000	0.691291000
8	0.331599000	-2.256504000	1.653401000
26	-1.932999000	-1.720472000	0.057295000
6	-1.007629000	-2.074407000	-1.460972000
8	-0.418133000	-2.370180000	-2.384271000

6	-2.504614000	-1.035374000	1.653267000
8	-2.807483000	-0.562125000	2.635748000
6	-3.610245000	-2.039025000	-0.692278000
8	-4.619300000	-2.244036000	-1.152997000
6	-1.775028000	-3.474574000	0.669433000
8	-1.702461000	-4.538596000	1.036913000
1	0.581866000	1.790867000	0.326992000
14	0.917773000	0.905353000	-1.877000000
1	0.080604000	0.128452000	-2.810608000
1	0.892461000	2.332859000	-2.264210000
6	2.667774000	0.286976000	-1.835524000
6	2.998893000	-1.007224000	-2.232373000
6	3.678206000	1.106491000	-1.331229000
6	4.300086000	-1.471185000	-2.124817000
1	2.231665000	-1.662743000	-2.633928000
6	4.977863000	0.647290000	-1.221569000
1	3.443304000	2.118929000	-1.010817000
6	5.289085000	-0.644266000	-1.618233000
1	4.543237000	-2.479707000	-2.438971000
1	5.749818000	1.294502000	-0.821396000
1	6.307272000	-1.006397000	-1.533316000

IIIP^{Si-H} (TE = -1477.648329)

6	-2.302752000	1.566253000	0.234020000
7	-1.967231000	0.301473000	-0.159610000
6	-0.595625000	-0.174764000	-0.261909000
7	0.318298000	0.885889000	-0.654872000
6	0.087959000	2.212556000	-0.405047000
6	-1.150868000	2.546272000	0.414641000
8	-3.450987000	1.897705000	0.431693000
6	-1.630998000	3.943310000	0.052898000
1	-0.829879000	4.661858000	0.217946000
1	-1.931275000	4.001416000	-0.994680000
1	-2.489180000	4.205964000	0.669343000
6	-0.736777000	2.529034000	1.893064000
1	-0.366121000	1.554076000	2.215506000
1	0.051889000	3.266432000	2.056015000
1	-1.595085000	2.788794000	2.515889000
6	-2.971824000	-0.710594000	-0.249871000
6	-3.164291000	-1.369098000	-1.454130000

6	-4.096457000	-2.387970000	-1.541478000
6	-4.841184000	-2.743412000	-0.429129000
6	-4.652754000	-2.076937000	0.770748000
6	-3.717043000	-1.062449000	0.864630000
1	-2.586389000	-1.071995000	-2.323408000
1	-4.246726000	-2.899961000	-2.484438000
1	-5.572829000	-3.539576000	-0.498275000
1	-5.236087000	-2.350092000	1.641920000
1	-3.563335000	-0.532380000	1.797423000
6	1.505436000	0.489332000	-1.344231000
6	1.418324000	-0.308018000	-2.475424000
6	2.570336000	-0.726380000	-3.120228000
6	3.811369000	-0.337367000	-2.647483000
6	3.894726000	0.474840000	-1.527323000
6	2.748852000	0.884778000	-0.874077000
1	0.447149000	-0.595196000	-2.864439000
1	2.492895000	-1.349743000	-4.003102000
1	4.712820000	-0.663284000	-3.152565000
1	4.862214000	0.781574000	-1.147434000
1	2.810489000	1.505622000	0.010755000
8	0.842763000	3.082071000	-0.780519000
14	-0.090649000	-1.210980000	1.299120000
1	-0.720240000	-0.604824000	2.492237000
1	-0.635559000	-2.565866000	1.064156000
1	-0.591713000	-0.903233000	-1.078675000
6	1.752236000	-1.278849000	1.506011000
6	2.518941000	-2.161771000	0.745723000
6	2.407021000	-0.421471000	2.388559000
6	3.897186000	-2.182940000	0.857515000
1	2.030964000	-2.837868000	0.048093000
6	3.787217000	-0.440265000	2.504943000
1	1.831639000	0.270153000	2.998003000
6	4.532262000	-1.321002000	1.738326000
1	4.479423000	-2.870274000	0.254617000
1	4.282192000	0.231204000	3.197015000
1	5.612389000	-1.337358000	1.827908000

IVP$^{\text{Si-H}}$ (TE = -1121.878842)

6	2.548258000	1.001570000	0.473064000
6	3.346756000	-0.297358000	0.675283000

6	2.566157000	-1.432704000	0.003681000
6	1.125687000	-0.913114000	0.154486000
7	1.277242000	0.506792000	-0.124038000
1	3.430715000	-0.510315000	1.746180000
1	4.365564000	-0.216024000	0.283977000
6	0.137878000	1.344816000	-0.078559000
6	-0.788113000	1.288040000	0.961771000
6	-1.898857000	2.111718000	0.965622000
6	-2.100999000	3.016366000	-0.064407000
6	-1.186459000	3.085186000	-1.102317000
6	-0.080768000	2.251120000	-1.112025000
1	-0.641975000	0.581383000	1.771443000
1	-2.614394000	2.043149000	1.777263000
1	-2.973205000	3.659644000	-0.061729000
1	-1.341908000	3.780970000	-1.919011000
1	0.623522000	2.270977000	-1.936725000
6	2.785462000	-2.750386000	0.721621000
1	2.214427000	-3.560642000	0.260419000
1	3.842293000	-3.030700000	0.687911000
1	2.490040000	-2.681199000	1.772387000
6	2.975619000	-1.574011000	-1.457352000
1	4.048442000	-1.773996000	-1.528978000
1	2.457996000	-2.408225000	-1.941096000
1	2.759487000	-0.666586000	-2.024652000
6	2.330813000	1.693056000	1.812511000
1	1.771285000	2.625001000	1.699773000
1	1.786130000	1.046586000	2.506252000
1	3.296214000	1.931524000	2.266806000
6	3.239002000	1.962775000	-0.478820000
1	4.192526000	2.292964000	-0.057658000
1	3.433162000	1.488400000	-1.443305000
1	2.626274000	2.851524000	-0.649636000
1	0.823537000	-1.112987000	1.206448000
14	-0.157857000	-1.734508000	-0.979376000
1	-0.029716000	-1.200155000	-2.354025000
1	0.110712000	-3.193920000	-0.971607000
6	-1.905535000	-1.448872000	-0.392337000
6	-2.796696000	-0.665550000	-1.121286000
6	-2.334542000	-1.973263000	0.826815000
6	-4.070872000	-0.403114000	-0.645328000

1	-2.484633000	-0.239062000	-2.070494000
6	-3.604591000	-1.711510000	1.310433000
1	-1.660950000	-2.593938000	1.413822000
6	-4.474644000	-0.922283000	0.573408000
1	-4.747955000	0.215479000	-1.223639000
1	-3.919783000	-2.124623000	2.262032000
1	-5.469841000	-0.714546000	0.949816000

Cartesian coordinates of the optimized geometries for the C – H bond splitting product obtained for **1**, **3** and **III-IV**, along with their total energies (in hartrees) including zero point vibrational correction.

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1P^{C-H} (TE = -2408.325357)

6	-0.442926000	-1.344360000	-0.001685000
6	-1.141184000	0.958996000	-0.100625000
7	-1.496677000	-0.312692000	-0.110898000
7	0.782560000	-0.727661000	-0.398186000
25	0.854588000	1.299038000	0.102507000
6	0.917140000	1.580116000	-1.745569000
8	0.924411000	1.689526000	-2.874699000
6	0.830121000	3.060020000	0.535918000
8	0.886235000	4.164245000	0.834911000
6	2.692839000	1.364860000	0.286674000
8	3.816766000	1.463032000	0.431264000
6	0.667017000	0.735188000	1.867892000
8	0.532224000	0.329487000	2.920369000
6	1.924372000	-1.503941000	-0.241149000
6	2.071000000	-2.505840000	0.730236000
6	3.015917000	-1.292340000	-1.097218000
6	3.244140000	-3.234497000	0.841440000
1	1.260529000	-2.716291000	1.419476000
6	4.184324000	-2.014235000	-0.976336000
1	2.919311000	-0.543713000	-1.877448000
6	4.313396000	-2.996331000	-0.003080000
1	3.320013000	-3.997588000	1.609032000
1	5.002823000	-1.818043000	-1.660579000
1	5.228644000	-3.568636000	0.087481000
6	-2.865488000	-0.734573000	-0.043925000
6	-3.388630000	-1.115855000	1.179312000
6	-3.639046000	-0.780079000	-1.190379000

6	-4.699480000	-1.556685000	1.252963000
1	-2.764696000	-1.063999000	2.065719000
6	-4.949428000	-1.215693000	-1.110105000
1	-3.204522000	-0.475101000	-2.135825000
6	-5.479173000	-1.606827000	0.109743000
1	-5.112755000	-1.858131000	2.208017000
1	-5.559165000	-1.253659000	-2.004876000
1	-6.504744000	-1.951293000	0.168676000
8	-2.191607000	1.746685000	-0.184129000
6	-2.046539000	3.155091000	-0.233978000
1	-1.760702000	3.548604000	0.741497000
1	-1.314668000	3.449430000	-0.986942000
1	-3.023597000	3.547214000	-0.507002000
1	-0.469695000	-1.669172000	1.060834000
6	-0.795256000	-2.532588000	-0.877198000
1	-0.927228000	-2.198201000	-1.908828000
1	0.023563000	-3.250555000	-0.853166000
1	-1.701931000	-3.040690000	-0.544467000

3P^{C-H} (TE = -2594.518228)

6	-1.524248000	0.565179000	0.365345000
7	-1.223993000	-0.768944000	0.286339000
6	0.044121000	-1.394725000	0.631516000
7	1.227546000	-0.728174000	0.106198000
6	1.486919000	0.616798000	0.137139000
8	-2.674167000	0.944990000	0.305369000
6	-2.295075000	-1.697584000	0.065085000
6	-2.336148000	-2.385395000	-1.137135000
6	-3.341384000	-3.306935000	-1.371644000
6	-4.310463000	-3.532927000	-0.407816000
6	-4.271652000	-2.836885000	0.789539000
6	-3.263342000	-1.919700000	1.030005000
1	-1.575390000	-2.183317000	-1.885636000
1	-3.372529000	-3.843336000	-2.312589000
1	-5.100937000	-4.250871000	-0.591767000
1	-5.031556000	-3.008849000	1.542633000
1	-3.225905000	-1.363238000	1.959519000
6	2.296938000	-1.621588000	-0.236049000
6	2.206529000	-2.348521000	-1.412094000
6	3.210441000	-3.238394000	-1.752658000

6	4.308582000	-3.393132000	-0.922684000
6	4.400023000	-2.658291000	0.248389000
6	3.394257000	-1.773516000	0.595492000
1	1.345058000	-2.203359000	-2.057487000
1	3.138205000	-3.805711000	-2.673022000
1	5.097234000	-4.086107000	-1.190929000
1	5.260150000	-2.774774000	0.897041000
1	3.456469000	-1.188454000	1.505939000
8	2.601210000	1.036790000	-0.091711000
26	-0.036808000	1.964390000	0.323768000
6	0.103387000	1.778503000	2.121402000
8	0.191279000	1.667261000	3.247166000
6	-0.167296000	1.598517000	-1.459206000
8	-0.246076000	1.284171000	-2.544436000
6	-1.401665000	3.234990000	0.394493000
8	-2.212285000	4.018211000	0.436656000
6	1.279326000	3.280815000	0.190154000
8	2.060173000	4.091077000	0.112192000
1	0.022436000	-2.361227000	0.120667000
6	0.157221000	-1.673533000	2.118094000
1	0.187865000	-0.752115000	2.698181000
1	-0.697264000	-2.264582000	2.452359000
1	1.065705000	-2.242277000	2.323854000

IIIP^{C-H} (TE = -995.369871)

6	1.281705000	1.525976000	-0.316526000
7	1.200270000	0.183691000	-0.072765000
6	0.000022000	-0.509343000	0.362809000
7	-1.200247000	0.183668000	-0.072770000
6	-1.281665000	1.525898000	-0.316718000
6	-0.000014000	2.333058000	-0.180175000
8	2.328347000	2.061594000	-0.607448000
6	-0.000127000	2.960211000	1.221855000
1	-0.888029000	3.583735000	1.340305000
1	0.000016000	2.208770000	2.014245000
1	0.887588000	3.584005000	1.340289000
6	0.000026000	3.445284000	-1.219744000
1	-0.000003000	3.041339000	-2.233891000
1	-0.889404000	4.061150000	-1.097138000
1	0.889496000	4.061088000	-1.097141000

6	2.397505000	-0.597089000	-0.070971000
6	3.372209000	-0.369874000	0.887853000
6	4.518077000	-1.143228000	0.899401000
6	4.688138000	-2.148447000	-0.039747000
6	3.711681000	-2.374946000	-0.994706000
6	2.566591000	-1.596360000	-1.014311000
1	3.223954000	0.420687000	1.615470000
1	5.281535000	-0.962054000	1.646549000
1	5.586003000	-2.754883000	-0.028259000
1	3.844096000	-3.154908000	-1.735049000
1	1.802801000	-1.753327000	-1.768484000
6	-2.397485000	-0.597097000	-0.070944000
6	-3.372022000	-0.370001000	0.888060000
6	-4.517932000	-1.143313000	0.899660000
6	-4.688169000	-2.148351000	-0.039638000
6	-3.711867000	-2.374724000	-0.994798000
6	-2.566747000	-1.596195000	-1.014442000
1	-3.223625000	0.420450000	1.615774000
1	-5.281257000	-0.962223000	1.646962000
1	-5.586047000	-2.754769000	-0.028141000
1	-3.844460000	-3.154548000	-1.735256000
1	-1.803051000	-1.753047000	-1.768733000
8	-2.328286000	2.061463000	-0.607850000
1	0.000022000	-1.478754000	-0.149818000
6	0.000023000	-0.769756000	1.857524000
1	0.883627000	-1.343551000	2.140397000
1	-0.000167000	0.168466000	2.416068000
1	-0.883435000	-1.343813000	2.140315000

IVP^{C-H} (TE = -639.594566)

6	-0.759442000	1.353558000	0.189102000
6	-2.231198000	0.909383000	0.240675000
6	-2.297817000	-0.501704000	-0.332439000
6	-0.954765000	-1.076909000	0.133924000
7	-0.049174000	0.064675000	0.016371000
1	-2.880233000	1.607993000	-0.295308000
1	-2.574377000	0.892496000	1.280205000
6	1.316716000	-0.113694000	-0.044323000
6	1.868825000	-1.402436000	-0.174185000
6	3.232418000	-1.601828000	-0.266965000

6	4.119881000	-0.540492000	-0.227948000
6	3.597326000	0.733444000	-0.090595000
6	2.235540000	0.949131000	0.001964000
1	1.225345000	-2.270589000	-0.206383000
1	3.602564000	-2.616346000	-0.369248000
1	5.188312000	-0.702020000	-0.297705000
1	4.260582000	1.590907000	-0.051030000
1	1.893337000	1.965961000	0.111478000
6	-2.335572000	-0.503429000	-1.857462000
1	-2.480662000	-1.522086000	-2.228173000
1	-3.162708000	0.108890000	-2.227862000
1	-1.408657000	-0.126356000	-2.292183000
6	-3.512184000	-1.257985000	0.173453000
1	-4.423694000	-0.804877000	-0.226487000
1	-3.491623000	-2.300982000	-0.156709000
1	-3.587660000	-1.246599000	1.262204000
6	-0.548583000	2.306862000	-0.985432000
1	0.494615000	2.584268000	-1.128068000
1	-0.907702000	1.872823000	-1.918954000
1	-1.113742000	3.224901000	-0.804686000
6	-0.409983000	2.053403000	1.500839000
1	-1.125606000	2.860740000	1.678785000
1	-0.473256000	1.352844000	2.336664000
1	0.586936000	2.492784000	1.505448000
1	-0.652627000	-1.858111000	-0.574667000
6	-0.952700000	-1.661400000	1.537207000
1	0.067032000	-1.890535000	1.851331000
1	-1.369473000	-0.959307000	2.263547000
1	-1.533262000	-2.584936000	1.586321000