Supporting Information for

Si-H Addition followed by C-H bond activation induced by a terminal thorium imido metallocene: A combined experimental and computational study

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X-ray Crystallography. Single-crystal X-ray diffraction measurements were carried out on a Bruker SMART CCD diffractometer using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). An empirical absorption correction was applied using the SADABS program.[1] All structures were solved by direct methods and refined by full-matrix least squares on F^2 using the SHELXL-97 program package.[2] The hydride atom in **2a** was located from a difference-Fourier map and refined isotropically. Hydrogen atoms were geometrically fixed using the riding model. Disordered solvents in the voids of **2a** and **6** were modeled or removed by using the SQUEEZE program.[3] Crystallographic details for **2a**, **4** and **6** are listed in Tables S1-S3.

Table S1. Crystallographic details for **2a**.

Empirical formula	C_{47} H_{73} N Si Th
Formula weight	912.19
Temperature / K	110(2)
Wavelength / Å	0.71073
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 10.4251(6) Å alpha = 90° b = 20.7650(12) Å beta = 90° c = 44.289(3) Å gamma = 90°
Volume / $Å^3$	9587.6(10)
Z, Calculated density / mg m^{-3}	8, 1.264
Absorption coefficient / mm^{-1}	3.164
F(000)	3728
Crystal size / mm	0.39 x 0.21 x 0.11 mm
Theta range for data collection / °	1.96 to 27.67
Limiting indices	0<=h<=13, 0<=k<=26, 0<=l<=57
Reflections collected / unique	11151 / 11151 [R(int) = 0.0000]
Completeness to theta = 27.67°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7223 and 0.3717
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	11151 / 210 / 528
Goodness-of-fit on F^2	1.097
Final R indices [I>2sigma(I)]	R1 = 0.0324, wR2 = 0.0636
R indices (all data)	R1 = 0.0457, wR2 = 0.0664
Largest diff. peak and hole / $e.Å^{-3}$	1.082 and -1.520
Platon squeeze solvent void volume / $Å^3$	267
Platon squeeze void count electrons / $e.Å^{-3}$	41

Table S2. Crystallographic details for **4**.

Empirical formula	C_{53} H_{75} N Si Th
Formula weight	986.27
Temperature / K	110(2)
Wavelength / Å	0.71073
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 16.578(3) Å alpha = 90° b = 16.572(3) Å beta = 97.936(3)° c = 17.515(3) Å gamma = 90°
Volume / $Å^3$	4765.9(13)
Z, Calculated density	4, 1.375 Mg/m^3
Absorption coefficient / mm^{-1}	3.188
F(000)	2016
Crystal size / mm	0.25 x 0.18 x 0.10
Theta range for data collection / °	2.20 to 27.61
Limiting indices	-17<=h<=21, -21<=k<=19, -18<=l<=22
Reflections collected / unique	26706 / 10881 [R(int) = 0.0512]
Completeness to theta = 27.61°	98.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7410 and 0.5029
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10881 / 36 / 527
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.1213
R indices (all data)	R1 = 0.0912, wR2 = 0.1463

Largest diff. peak and hole / e.Å^{-3}	8.729 and -3.181

Table S3. Crystallographic details for **6**.

Empirical formula	C_{54} H_{87} N_3 Th
Formula weight	1010.31
Temperature / K	150(2)
Wavelength / Å	0.71073
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.436(2) Å alpha = 92.787(3)° b = 15.509(3) Å beta = 92.250(3)° c = 20.314(4) Å gamma = 109.072(3)°
Volume / Å^3	3098.4(10)
Z, Calculated density	2, 1.083 Mg/m^3
Absorption coefficient / mm^{-1}	2.436
F(000)	1044
Crystal size / mm	0.45 x 0.20 x 0.11
Theta range for data collection / °	1.77 to 25.25
Limiting indices	-12<=h<=12, -18<=k<=18, 0<=l<=24
Reflections collected / unique	10908 / 10908 [R(int) = 0.0000]
Completeness to theta = 25.25°	97.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7755 and 0.4070
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10908 / 60 / 542
Goodness-of-fit on F^2	1.118

Final R indices [I>2sigma(I)]	R1 = 0.0776, wR2 = 0.2236
R indices (all data)	R1 = 0.0851, wR2 = 0.2304
Largest diff. peak and hole / e.Å^{-3}	5.744 and -7.006 e.Å^{-3}
Platon squeeze solvent void volume / Å^{3}	829
Platon squeeze void count electrons / e.Å^{-3}	201

Computational Methods. All calculations were carried out with the Gaussian 09 program (G09),[4] employing the B3PW91 method, plus polarizable continuum model (PCM) and D3[5] (denoted as B3PW91-PCM+D3), with standard 6-31G(d) basis set for C, H, O, N and Si elements and Stuttgart RLC ECP from EMSL basis set exchange (https://bse.pnl.gov/bse/portal) for Th element,[6] to fully optimize the geometries of reactants, complexes, transition state, intermediates, and product structures, and to mimic experimental toluene-solvent conditions (dielectricity constant ε = 2.379). All stationary points were subsequently characterized by vibrational analyses, from which their respective zero-point (vibrational) energy (ZPE) were extracted and used in the relative energy determinations; in addition to ensure that the reactant, complex, intermediate, product and transition state structures resided at minima and 1st order saddle points, respectively, on their potential energy hyper surfaces. Cartesian coordinates, frequencies and energitcs for all of stationary points along the reaction path are listed in Tables S4-7. To properly describe the reaction profile dispersion effects (D3) had to be considered for these sterically encumbered thorium complexes. The implications of the dispersion correction on the overall energy profile can be seen in Figures S3 and S4.

In imido complex **1**, the thorium-nitrogen interaction is described by the three highest molecular orbitals (MOs) (Figure S1). The HOMO-13 describes the σ-interaction between N and Th atoms, whereas the HOMO and HOMO-3 describe the π interactions, labeled as π_1 and π_2 bond, respectively. 5f orbitals are involved in forming the Th=N bond, and the Wiberg bond order is 0.92. This means that the π-bonding between the Th and N atoms is weak and that the Th=N bond is strongly polarized. Consistent with this picture a natural bond orbital (NBO) analysis gives a charge of +2.15 on Th, -0.39 on 1,2,4-$(Me_3C)_3C_5H_2$, so that the total positive charge on [1,2,4-$(Me_3C)_3C_5H_2]_2$Th fragment is +1.37, whereas the charges on the imido moiety are -1.41 on N, and +0.04 on the *p*-tolyl group, resulting in a total negative charge on the nitrene fragment of -1.37. In addition, the NBO analysis reveals that the σ-bond is formed by a nitrogen sp-hybrid (55% s and 45% p character) donating to a vacant Th orbital. Furthermore, one Th=N π bond (π_1) is polarized towards the nitrogen atom and consists of a pure 2p nitrogen-based orbital (89%) and a thorium hybrid orbital (11%) of 39% 5f and 55% 6d and 6% 7p character, whereas the other

donor-acceptor π-interaction (*i.e.* the Th=N π_2 bond) between the nitrogen 2p orbital and the thorium orbitals is only small, since the thorium contribution is less than 5%. From all these observations we conclude that the π-interaction results mainly from Coulombic attraction between the oppositely charged atoms over a short distance augmented by a small orbital contribution and that the covalent contributions to the bonding are small. This clearly supports the picture of a very polarized double bond and it should be better described as Th^{+}-N^{-}. In addition, it also establishes the involvement of the thorium 5f orbitals in the formation of a weak π-bond.

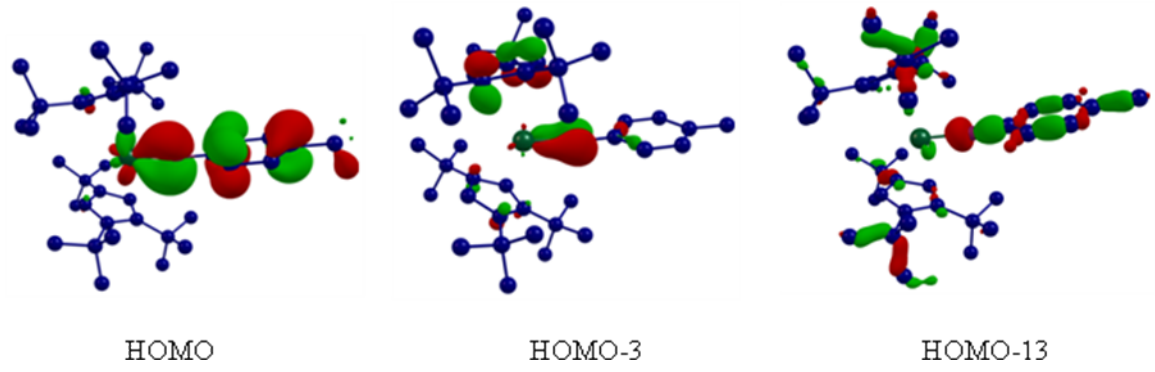


Figure S1. Plots of HOMOs for complex **1** (the hydrogen atoms have been omitted for clarity).

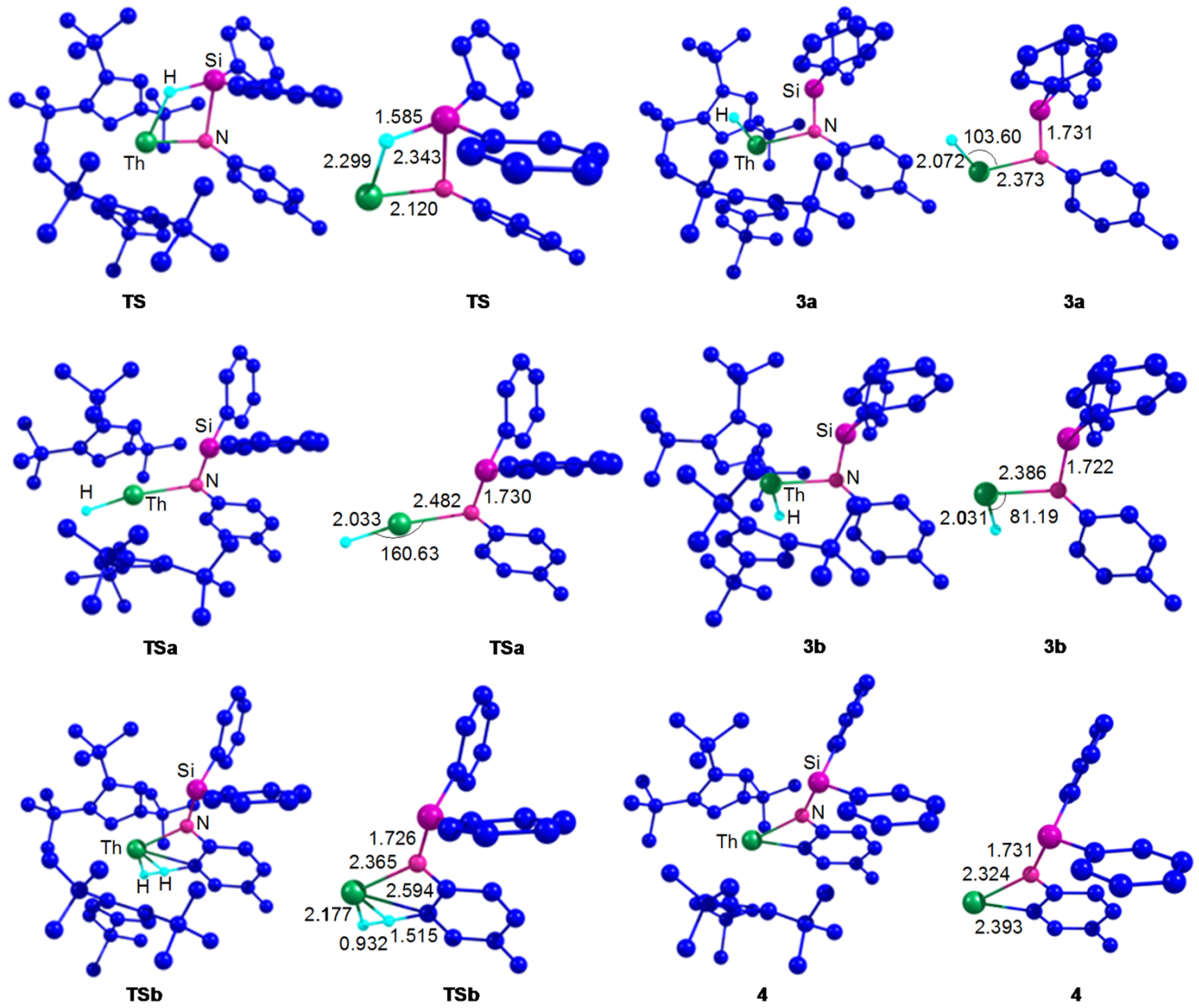


Figure S2. The structures of possible stationary points along the reaction paths (bond distances in Å and angles in deg; the hydrogen atoms have been omitted for clarity) for the reaction of **1** with Ph_2SiH_2.

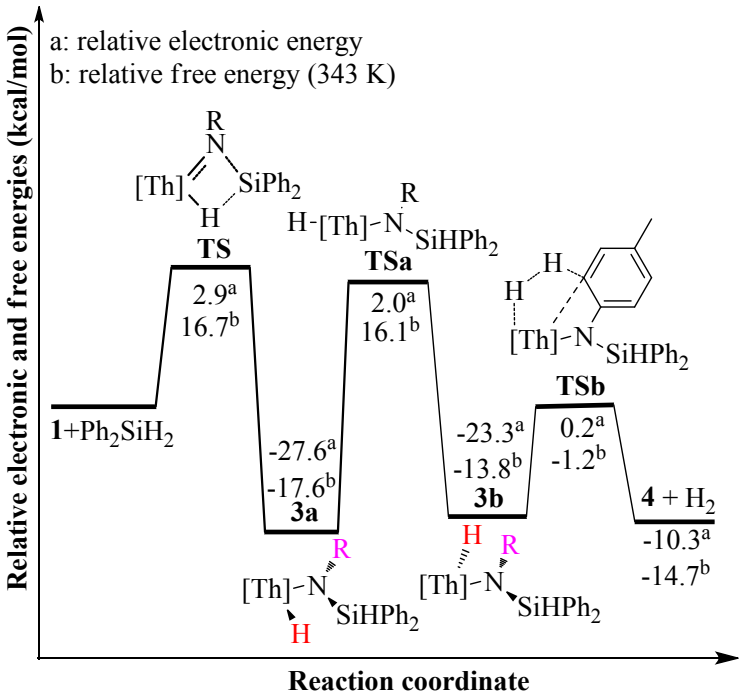


Figure S3. Energy and free energy profile (kcal/mol) for the reaction of **1** with Ph_2SiH_2, obtained with B3PW91-PCM+D3 method. [Th] = [η^5-1,2,4-$(Me_3C)_3C_5H_2$]$_2$Th. R = *p*-tolyl.

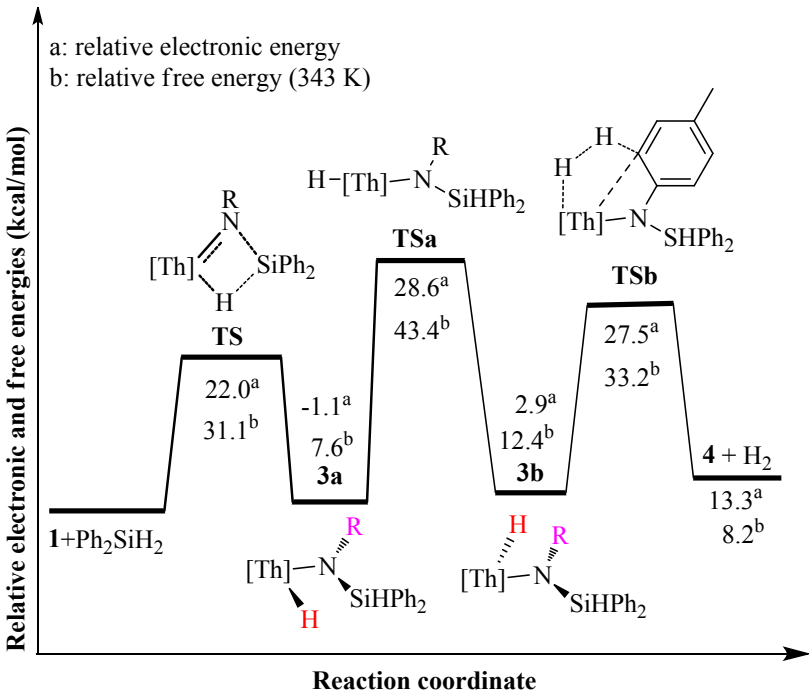


Figure S4. Energy profile (kcal/mol) for the reaction of **1** with Ph_2SiH_2, obtained with B3PW91-PCM method. [Th] = [η^5-1,2,4-$(Me_3C)_3C_5H_2$]$_2$Th. R = *p*-tolyl.

Kinetic Studies. In an attempt to evaluate the equilibrium

the conversion of **3a** to **4** was monitored by ^{1}H NMR spectroscopy in C_6D_6 solution at 343 K (Figure S5). One complication in the kinetic evaluation of this reaction arises from the limited solubility of H_2 in organic solvents, so that the equilibrium changes with the head space volume. Reproducible results were obtained with a solvent volume (0.5 mL), a headspace volume (2.2 mL) and a concentration of **3a** of 0.05 mol/l. The reaction reached equilibrium after 3h at 70 °C with a ratio of [**4**]/[**3a**] = 0.37. Unfortunately, the exact concentration of H_2 in solution cannot be determined reliably by NMR spectroscopy, which makes a precise determination of the rate constant and therefore the barrier difficult.

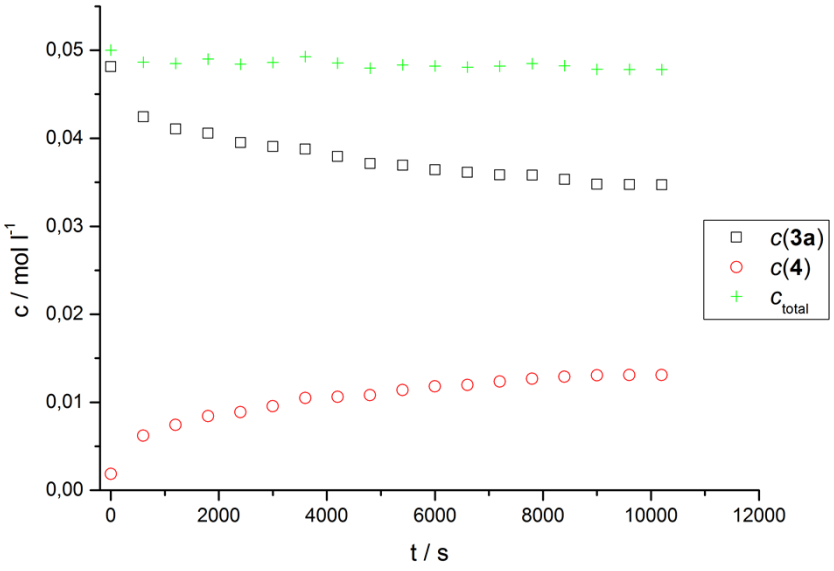
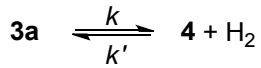


Figure S5. c *vs*. t plot for the thermal conversion of **3a** to **4** at 70 °C recorded in C_6D_6 solution.

However, to get a rough approximation of reaction kinetics we analyzed the data in the following manner.[7]



Assuming that H_2 is still completely dissolved in solution c(**4**) = c(H_2) and that c_e represents the equilibrium concentration of **3a**, the kinetics can be described by the following equation:

$$\ln \frac{ax_e + x(a - x_e)}{a(x_e - x)} = k \frac{(2a - x_e)}{x_e} t$$

where a = c_0(**3a**), x = c_0(**3a**)- c_t(**3a**), x_e = c_0(**3a**) – c_e(**3a**).

Figure S6 shows the data presented in Figure S5 analyzed by this approximation. The linear fit is of reasonable quality and a value of k = 5.88(2) x 10^{-5} s^{-1} can be derived from this analysis which corresponds to a barrier $\Delta G^{\ddagger}$(**3a**→ **4** + H_2; 343 K) = 26.8 kcal·mol^{-1}.

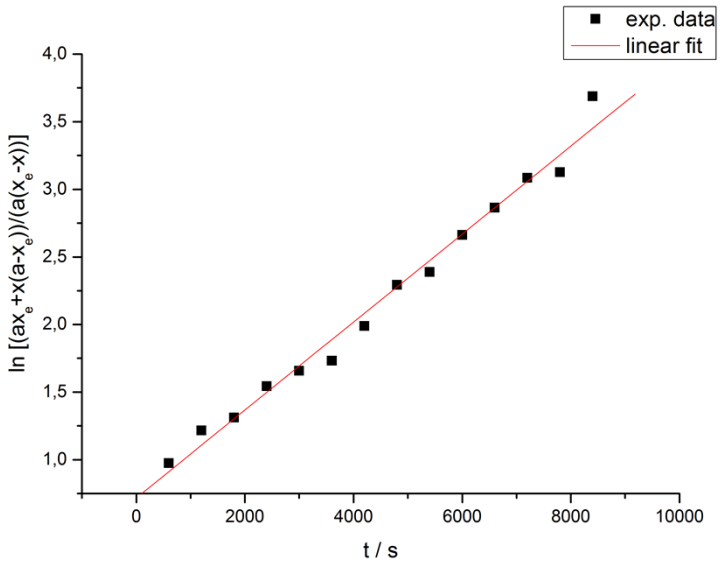


Figure S6. $\ln \frac{ax_e + x(a - x_e)}{a(x_e - x)}$ *vs.* t plot (R^2 = 0.985).

Considering the problems arising from the low solubility of H_2, the absolute value of $\Delta G^{\ddagger}$(**3a** → **4** + H_2; 343 K) = 26.8 kcal·mol^{-1} has to be treated with caution. Nevertheless, this value is consistent with the overall computed reaction profile.

References

1 G. M. Sheldrick, *SADABS, Program for Empirical Absorption Correction of Area Detector Data;* University of Göttingen, Göttingen, Germany, 1996.

2 (*a*) G. M. Sheldrick, *SHELXL-97, Program for the Refinement of Crystal Structure from Diffraction Data;* University of Göttingen, Göttingen, Germany, 1997; (*b*) G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112-122.

3 SQUEEZE: P. V. D. Sluis and A. L. Spek, *Acta Crystallogr., Sect. A: Found. Crystallogr.*, 1990, **46**, 194-201.

4 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision A.02*, Gaussian, Inc.: Wallingford CT, 2009.

5 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.

6 W. Kuechle, M. Dolg, H. Stoll and H. Preuss, *Mol. Phys.*, 1991, **74**, 1245-1263.

7 A. A. Frost and R. G. Pearson, *Kinetics and Mechanism*, 2nd edition, Wiley & Sons, New York, 1961, pp. 186-187.

Table S4. The optimized Cartesian Coordinates (in Å) of stationary points for the studied reactions, obtained with B3PW91-PCM+D3 method.

Species	Cartesian coordinates							
1	C	-1.37285	2.39150	-1.00772	H	-2.66727	-2.29338	-3.90783
	C	-1.25230	2.61902	-2.52585	H	-0.96032	-2.66196	-3.69284
	C	-2.50104	2.08213	-3.25208	C	-2.45366	-4.31257	-2.03043
	H	-3.41085	2.60501	-2.93690	H	-1.56470	-4.85564	-2.36138
	H	-2.64727	1.00850	-3.08484	H	-3.24886	-4.47622	-2.76958
	H	-2.38570	2.22997	-4.33212	H	-2.77481	-4.74868	-1.07790
	C	-0.04628	1.87604	-3.13730	C	0.34578	-2.66882	-0.75267
	H	0.10604	2.17342	-4.18224	C	1.40256	-2.87814	-1.85572
	H	-0.22698	0.79092	-3.15290	C	1.51715	-1.68646	-2.82776
	H	0.88369	2.05040	-2.59447	H	0.58904	-1.47778	-3.36026
	C	-1.18166	4.12066	-2.85515	H	2.29078	-1.88274	-3.58075
	H	-2.02806	4.65008	-2.40332	H	1.81544	-0.78360	-2.27981
	H	-1.22453	4.27063	-3.94133	C	1.11784	-4.17513	-2.63220
	H	-0.26427	4.58719	-2.49634	H	0.19403	-4.12516	-3.21107
	C	-0.55883	2.81129	0.11227	H	1.03715	-5.02457	-1.94415
	C	0.63678	3.76919	0.26769	H	1.93454	-4.38115	-3.33540
	C	1.71349	3.66346	-0.81942	C	2.80015	-3.03651	-1.22506
	H	2.52800	4.36305	-0.59541	H	3.53563	-3.21144	-2.01923
	H	1.34432	3.91434	-1.81456	H	2.84029	-3.89139	-0.54052
	H	2.13140	2.65331	-0.83830	H	3.10662	-2.13385	-0.68735
	C	0.07927	5.20811	0.31877	C	0.73526	-2.57895	0.61287
	H	-0.63583	5.31150	1.14344	H	1.75773	-2.56748	0.96476
	H	-0.43728	5.48320	-0.60437	C	-0.39737	-2.49994	1.45322
	H	0.89413	5.92603	0.47981	C	-0.38042	-2.53980	2.97563
	C	1.36354	3.51129	1.60459	C	0.30540	-1.28966	3.55839
	H	1.69661	2.47073	1.66801	H	0.40597	-1.37057	4.64775
	H	0.73691	3.74213	2.47281	H	-0.27359	-0.37301	3.36452
	H	2.24712	4.15659	1.66922	H	1.30573	-1.15499	3.13270
	C	-1.22965	2.34530	1.28205	C	-1.80420	-2.64448	3.53400
	H	-0.89087	2.52756	2.29397	H	-2.29871	-3.55773	3.18352
	C	-2.44501	1.70519	0.94858	H	-2.42233	-1.79109	3.23493
	C	-3.57779	1.35184	1.89675	H	-1.78126	-2.66994	4.62974
	C	-4.58728	2.51783	1.86503	C	0.41574	-3.78202	3.41772
	H	-4.10521	3.45525	2.16476	H	0.41537	-3.87158	4.51148
	H	-5.42465	2.32595	2.54866	H	1.45735	-3.72497	3.08357
	H	-4.99109	2.65411	0.85551	H	-0.02414	-4.69300	2.99637
	C	-3.06943	1.18782	3.33432	C	-1.51798	-2.52597	0.59413
	H	-2.30576	0.40652	3.40364	H	-2.54612	-2.53539	0.92730
	H	-3.89351	0.91058	4.00200	C	3.11660	0.40619	0.29932
	H	-2.63302	2.11795	3.71428	C	3.74930	0.25926	1.55747
	C	-4.29411	0.06757	1.46039	H	3.12154	0.10665	2.43258
	H	-4.72077	0.16490	0.45642	C	5.13240	0.30751	1.68844
	H	-5.11380	-0.17199	2.14849	H	5.57640	0.18581	2.67646
	H	-3.60325	-0.78067	1.44541	C	5.96969	0.51068	0.58375
	C	-2.50777	1.71575	-0.45904	C	7.46578	0.60121	0.74003
	H	-3.33516	1.32225	-1.03464	H	7.78937	1.62815	0.96238
	C	-1.10557	-2.61773	-0.76772	H	7.98594	0.29065	-0.17354
	C	-2.17378	-2.80608	-1.85891	H	7.82437	-0.03236	1.56002
	C	-3.49475	-2.13224	-1.43233	C	5.35352	0.66083	-0.66539
	H	-3.94188	-2.59543	-0.54805	H	5.97342	0.81864	-1.54752
	H	-4.22946	-2.21047	-2.24212	C	3.97125	0.61446	-0.81000
	H	-3.34796	-1.06723	-1.21266	H	3.52154	0.73232	-1.79353
	C	-1.82052	-2.19005	-3.21873	N	1.75642	0.34382	0.16580
	H	-1.61060	-1.11711	-3.12147	Th	-0.24319	-0.02051	0.06280

Ph_2SiH_2	Si	0.00998	2.35094	0.01929	H	-0.49910	-3.40636	-0.03385
	H	-1.18696	2.90916	0.71604	C	0.17962	3.01657	-1.72753
	H	1.21257	2.78856	0.78869	C	1.02316	4.10331	-2.00929
	C	-0.16650	0.48239	-0.00494	C	-0.54153	2.44501	-2.78957
	C	0.54701	-0.29675	-0.93149	C	1.13649	4.60939	-3.30414
	C	-1.00766	-0.17709	0.90583	C	-0.43028	2.94644	-4.08571
	C	0.43071	-1.68605	-0.94254	C	0.40852	4.03129	-4.34417
	C	-1.12602	-1.56688	0.89958	H	1.60488	4.55906	-1.21009
	C	-0.40559	-2.32318	-0.02497	H	-1.18834	1.58951	-2.60476
	H	1.19175	0.18807	-1.66201	H	1.79630	5.45052	-3.50238
	H	-1.58353	0.39992	1.62711	H	-0.99499	2.48951	-4.89472
	H	0.98953	-2.27168	-1.66845	H	0.49810	4.42198	-5.35482
	H	-1.78387	-2.05885	1.61186				
TS	C	3.31499	1.32229	-0.07655	C	-1.00252	-5.03426	-1.41988
	C	2.42501	2.05634	-0.94048	H	-0.35399	-4.95345	-2.29253
	C	1.35121	2.53465	-0.12508	H	-1.93400	-5.50772	-1.75412
	H	0.54331	3.16929	-0.46624	H	-0.52107	-5.70519	-0.69894
	C	1.55755	2.16706	1.22394	C	-1.97374	-2.73697	-1.79596
	C	2.72211	1.36819	1.22175	H	-2.18193	-1.77159	-1.33214
	H	3.19937	0.99272	2.11520	H	-2.92405	-3.14422	-2.16163
	C	4.80865	0.93323	-0.15748	H	-1.34391	-2.55252	-2.66657
	C	5.13280	-0.20051	0.83431	C	-2.37979	-3.96641	0.30653
	H	4.53472	-1.08853	0.61700	H	-1.99153	-4.64541	1.07475
	H	4.95683	0.08075	1.87576	H	-3.24690	-4.44774	-0.16143
	H	6.19100	-0.47448	0.75096	H	-2.73986	-3.05573	0.79106
	C	5.37543	0.46852	-1.50757	C	1.62023	-2.45058	3.19104
	H	6.45258	0.29491	-1.39539	C	0.45170	-2.06529	4.10747
	H	5.25532	1.19539	-2.30862	H	-0.37727	-2.77643	4.02701
	H	4.93131	-0.47295	-1.83310	H	0.05588	-1.07424	3.86752
	C	5.59979	2.18259	0.29968	H	0.78094	-2.05462	5.15328
	H	5.29162	2.48453	1.30680	C	2.81499	-1.53812	3.47917
	H	5.43203	3.03372	-0.36608	H	3.14595	-1.65631	4.51822
	H	6.67675	1.96973	0.31897	H	2.54678	-0.49074	3.32845
	C	2.55685	2.47065	-2.41214	H	3.66406	-1.76904	2.82859
	C	2.60236	1.24331	-3.33767	C	2.02715	-3.90603	3.50766
	H	2.67511	1.54851	-4.38918	H	2.29675	-4.01015	4.56682
	H	1.67650	0.66056	-3.22832	H	2.88852	-4.21033	2.90203
	H	3.44053	0.58211	-3.12094	H	1.20178	-4.59390	3.29202
	C	3.78335	3.38231	-2.61405	C	-2.45021	-0.16012	1.18287
	H	3.69653	4.27040	-1.97739	C	-2.30914	0.05138	2.57438
	H	3.83268	3.71711	-3.65782	H	-1.39666	0.51382	2.93414
	H	4.73126	2.90195	-2.37826	C	-3.29956	-0.30341	3.48241
	C	1.35252	3.31519	-2.85755	H	-3.13193	-0.12299	4.54345
	H	1.26950	4.24107	-2.27748	C	-4.50320	-0.88202	3.06314
	H	0.41246	2.76720	-2.77459	C	-4.65338	-1.10214	1.68954
	H	1.47393	3.59507	-3.91072	H	-5.56737	-1.56514	1.31979
	C	0.93645	2.81286	2.45218	C	-3.66137	-0.76135	0.77486
	C	1.76443	4.08136	2.75020	H	-3.81838	-0.97228	-0.27442
	H	2.81573	3.83046	2.93483	C	-5.59602	-1.22407	4.04140
	H	1.37062	4.59712	3.63570	H	-6.28260	-0.37882	4.18950
	H	1.72487	4.77490	1.90269	H	-5.18825	-1.48424	5.02496
	C	-0.51618	3.22191	2.20591	H	-6.19776	-2.07104	3.69249
	H	-0.59639	3.97134	1.41308	N	-1.42080	0.17517	0.31209
	H	-0.95227	3.65411	3.11434	Si	-1.80561	1.40568	-1.64408
	H	-1.12469	2.37028	1.90063	Th	0.63607	-0.19874	-0.04127
	C	1.01849	1.88781	3.67186	H	-0.40938	0.69477	-1.88354
	H	0.53488	0.92551	3.47779	C	-2.39945	2.88611	-0.62414
	H	0.51939	2.34487	4.53429	C	-1.96297	4.16030	-1.02634
	H	2.05551	1.68447	3.96097	C	-3.30876	2.82082	0.44492

	C	1.30956	-2.94387	-0.54899	C	-2.38013	5.31745	-0.36754
	C	-0.06702	-3.05860	-0.12207	C	-3.74886	3.97452	1.09083
	C	-0.09218	-2.67498	1.24652	C	-3.27680	5.22657	0.69591
	H	-0.98129	-2.64318	1.85952	H	-1.28585	4.25256	-1.87234
	C	1.21184	-2.42779	1.72531	H	-3.67136	1.86068	0.79258
	C	2.06291	-2.56804	0.60494	H	-2.01073	6.28809	-0.69045
	H	3.14093	-2.49518	0.64090	H	-4.45588	3.89241	1.91296
	C	2.01816	-3.22860	-1.88177	H	-3.61062	6.12496	1.20963
	C	3.29792	-2.38286	-1.97836	C	-3.18341	0.41128	-2.45149
	H	3.07146	-1.31370	-1.89328	C	-2.88744	-0.34587	-3.59629
	H	3.78003	-2.53391	-2.95133	C	-4.52987	0.53672	-2.08022
	H	4.03285	-2.63479	-1.20911	C	-3.88720	-0.99787	-4.31386
	C	2.44944	-4.70661	-1.94854	C	-5.53838	-0.10973	-2.79674
	H	2.99027	-4.90586	-2.88285	C	-5.21858	-0.88749	-3.90865
	H	1.60048	-5.38999	-1.89502	H	-1.85485	-0.43220	-3.93159
	H	3.11709	-4.93922	-1.11111	H	-4.79962	1.14185	-1.21894
	C	1.18582	-2.85038	-3.11679	H	-3.62960	-1.59022	-5.18870
	H	0.84503	-1.80613	-3.05763	H	-6.57479	-0.00314	-2.48525
	H	0.30649	-3.47878	-3.24739	H	-6.00290	-1.39495	-4.46508
	H	1.79439	-2.94542	-4.02387	H	-1.45143	2.23442	-2.87130
	C	-1.32009	-3.67356	-0.77546				
3a	C	2.54287	2.40476	0.09468	C	0.11170	-4.86158	-2.11570
	C	1.25963	2.92399	-0.31639	H	0.59227	-4.53534	-3.03751
	C	0.37622	2.71912	0.78709	H	-0.71916	-5.52107	-2.39680
	H	-0.65935	3.03078	0.81574	H	0.83823	-5.45442	-1.54744
	C	1.05727	2.14821	1.88047	C	-1.41223	-2.84517	-2.06735
	C	2.37925	1.92351	1.42906	H	-1.92528	-2.14430	-1.40644
	H	3.18597	1.55428	2.04655	H	-2.17320	-3.47999	-2.53901
	C	3.96791	2.51146	-0.47512	H	-0.93059	-2.25968	-2.84830
	C	4.81575	1.30966	-0.01530	C	-1.21587	-4.35153	-0.12078
	H	4.35971	0.37104	-0.33946	H	-0.59597	-5.05172	0.45162
	H	4.94050	1.26982	1.07022	H	-2.05009	-4.91890	-0.55030
	H	5.81861	1.36976	-0.45409	H	-1.64517	-3.62133	0.56756
	C	4.07855	2.54277	-2.00384	C	2.99783	-2.46564	2.30623
	H	5.13652	2.54168	-2.29315	C	2.03944	-2.74081	3.47136
	H	3.62659	3.42782	-2.44920	H	1.48214	-3.67157	3.31903
	H	3.61036	1.66276	-2.44936	H	1.31079	-1.93430	3.59665
	C	4.61963	3.78221	0.11322	H	2.59853	-2.83468	4.40969
	H	4.63372	3.73290	1.20800	C	3.88409	-1.26094	2.63657
	H	4.07821	4.68797	-0.17096	H	4.47630	-1.45116	3.54019
	H	5.65483	3.87849	-0.23949	H	3.27699	-0.37011	2.81032
	C	0.83069	3.82412	-1.49385	H	4.57858	-1.04078	1.81942
	C	0.84305	3.13334	-2.86864	C	3.90078	-3.70423	2.12373
	H	0.63959	3.87077	-3.65657	H	4.44603	-3.92548	3.05068
	H	0.07097	2.36076	-2.91270	H	4.63333	-3.53903	1.32573
	H	1.79036	2.64591	-3.09092	H	3.30290	-4.58282	1.85628
	C	1.71019	5.09164	-1.51653	C	-2.26242	-1.21985	1.26335
	H	1.70901	5.57568	-0.53292	C	-1.73747	-1.65998	2.49299
	H	1.31417	5.80690	-2.24832	H	-0.77139	-1.28239	2.81732
	H	2.74577	4.88998	-1.78833	C	-2.41797	-2.57585	3.28784
	C	-0.60649	4.34299	-1.28531	H	-1.96628	-2.90186	4.22314
	H	-0.69791	4.94962	-0.37744	C	-3.66723	-3.08294	2.91117
	H	-1.33656	3.53358	-1.22828	C	-4.20528	-2.62779	1.70206
	H	-0.88713	4.97441	-2.13660	H	-5.17300	-3.00283	1.37378
	C	0.55269	2.12010	3.31295	C	-3.52651	-1.72017	0.89586
	C	0.89154	3.48453	3.94596	H	-3.95808	-1.42616	-0.05785
	H	1.97386	3.65798	3.94190	C	-4.41582	-4.05305	3.78709
	H	0.53840	3.52703	4.98468	H	-3.73080	-4.67360	4.37548
	H	0.41606	4.29774	3.38642	H	-5.04982	-4.72159	3.19411

	C	-0.96439	1.91395	3.35021	H	-5.07083	-3.52915	4.49663
	H	-1.49688	2.74394	2.87602	C	-3.42796	1.97244	0.14886
	H	-1.32040	1.83730	4.38453	C	-3.99369	3.01216	-0.60933
	H	-1.24550	1.00089	2.81766	H	-3.75502	3.10197	-1.66752
	C	1.23305	1.01824	4.12733	C	-4.86496	3.93233	-0.02949
	H	1.04911	0.03616	3.68189	H	-5.28425	4.73624	-0.62939
	H	0.84589	0.99785	5.15286	C	-5.20350	3.81449	1.31956
	H	2.31728	1.16259	4.18405	H	-5.88642	4.52844	1.77357
	C	1.93492	-2.29887	-1.32116	C	-4.67374	2.77264	2.08079
	C	0.75973	-2.87351	-0.70258	H	-4.94636	2.66819	3.12807
	C	0.96075	-2.79272	0.70354	C	-3.79237	1.86137	1.49925
	H	0.26197	-3.15797	1.44199	H	-3.39295	1.05003	2.09960
	C	2.24170	-2.27784	0.99950	N	-1.53107	-0.35228	0.44958
	C	2.81107	-1.94378	-0.24989	Si	-2.24677	0.76636	-0.66073
	H	3.82680	-1.59493	-0.38013	H	-0.96280	1.40960	-1.11686
	C	2.47418	-2.26809	-2.76268	Th	0.78086	-0.00163	0.04835
	C	3.45149	-1.09158	-2.94056	H	0.87899	0.30570	-1.99892
	H	2.93871	-0.15200	-2.71644	C	-3.00401	0.22299	-2.28880
	H	3.80258	-1.05195	-3.97864	C	-2.17667	0.07165	-3.41284
	H	4.33934	-1.16966	-2.30560	C	-4.38058	-0.00600	-2.43897
	C	3.27630	-3.56624	-3.00086	C	-2.70204	-0.32020	-4.64284
	H	3.71520	-3.56388	-4.00715	C	-4.91079	-0.40435	-3.66555
	H	2.65616	-4.46012	-2.90367	C	-4.07023	-0.56483	-4.76838
	H	4.09231	-3.64729	-2.27309	H	-1.10620	0.24761	-3.31428
	C	1.41654	-2.09019	-3.86009	H	-5.04939	0.13969	-1.59206
	H	0.86103	-1.16139	-3.69611	H	-2.04503	-0.43709	-5.50128
	H	0.70601	-2.91429	-3.91291	H	-5.97870	-0.58376	-3.76372
	H	1.91206	-2.02819	-4.83708	H	-4.48266	-0.87388	-5.72580
	C	-0.41897	-3.69192	-1.26424				
TSa	C	2.89119	2.16541	-0.03347	C	-0.89397	-4.95722	-1.61141
	C	1.69952	2.60437	-0.72466	H	-0.56314	-4.74928	-2.62985
	C	0.66269	2.68477	0.26546	H	-1.80936	-5.55833	-1.68445
	H	-0.33277	3.07164	0.09648	H	-0.12444	-5.56560	-1.12212
	C	1.17479	2.34519	1.53920	C	-2.20859	-2.81630	-1.53093
	C	2.51899	1.98984	1.32575	H	-2.50859	-1.98477	-0.89594
	H	3.20455	1.69209	2.10663	H	-3.10665	-3.40286	-1.76376
	C	4.38350	2.09542	-0.41240	H	-1.83968	-2.39697	-2.46465
	C	5.19683	1.32628	0.65054	C	-1.84032	-4.14846	0.50515
	H	4.76933	0.33490	0.82012	H	-1.21165	-4.86928	1.04069
	H	5.23845	1.86304	1.60471	H	-2.78710	-4.64619	0.26313
	H	6.23008	1.21264	0.30139	H	-2.07489	-3.31920	1.17605
	C	4.65027	1.38979	-1.74824	C	2.83717	-2.72792	2.17712
	H	5.72837	1.35232	-1.94861	C	2.48036	-1.56568	3.11560
	H	4.18309	1.89028	-2.59728	H	1.41435	-1.58273	3.36992
	H	4.27935	0.35947	-1.70586	H	2.73152	-0.60509	2.64354
	C	4.97408	3.52348	-0.41313	H	3.04340	-1.61975	4.05611
	H	4.80458	3.99701	0.56096	C	4.33098	-2.66526	1.84289
	H	4.54299	4.17132	-1.17426	H	4.92735	-2.71044	2.76226
	H	6.05762	3.47867	-0.58412	H	4.57252	-1.73462	1.32058
	C	1.45991	3.08853	-2.17393	H	4.62675	-3.50704	1.20570
	C	1.43749	1.93072	-3.19051	C	2.54213	-4.05705	2.89624
	H	1.33067	2.31564	-4.21294	H	3.16035	-4.14998	3.79856
	H	0.58248	1.26271	-3.02162	H	2.75879	-4.90873	2.24127
	H	2.35489	1.34113	-3.15623	H	1.49094	-4.12381	3.19828
	C	2.50816	4.11817	-2.63098	C	-2.12244	-0.70507	1.54845
	H	2.59204	4.93449	-1.90567	C	-1.50373	-1.01458	2.77793
	H	2.20223	4.55016	-3.59194	H	-0.47978	-0.69450	2.95079
	H	3.49667	3.68232	-2.77692	C	-2.16899	-1.69638	3.79024
	C	0.10809	3.81776	-2.27859	H	-1.63807	-1.91579	4.71522

	H	0.06690	4.68457	-1.61016	C	-3.50487	-2.08949	3.65150
	H	-0.72878	3.16300	-2.03782	C	-4.14309	-1.75194	2.45312
	H	-0.03960	4.17236	-3.30570	H	-5.18562	-2.02910	2.30648
	C	0.57932	2.67263	2.90032	C	-3.47678	-1.08496	1.43048
	C	1.02081	4.11406	3.23390	H	-4.00737	-0.88074	0.50516
	H	2.11372	4.19097	3.26835	C	-4.21423	-2.86009	4.73357
	H	0.62055	4.42534	4.20782	H	-4.06663	-3.94240	4.61577
	H	0.65587	4.81317	2.47287	H	-5.29436	-2.67683	4.71557
	C	-0.94651	2.62203	2.88083	H	-3.84390	-2.58977	5.72904
	H	-1.35786	3.32734	2.15380	C	-3.08609	2.39960	-0.05986
	H	-1.35337	2.88480	3.86529	C	-3.28995	3.50408	-0.90476
	H	-1.30524	1.62547	2.61597	H	-2.87937	3.50236	-1.91222
	C	1.11031	1.73906	3.99655	C	-4.02283	4.61206	-0.48249
	H	0.83213	0.69739	3.81220	H	-4.15320	5.46207	-1.14793
	H	0.69265	2.02448	4.96954	C	-4.59607	4.62346	0.78959
	H	2.20168	1.78187	4.07999	H	-5.17252	5.48391	1.12055
	C	1.32923	-2.69367	-1.31612	C	-4.43561	3.52221	1.63005
	C	0.16057	-2.96280	-0.49900	H	-4.88912	3.51902	2.61823
	C	0.59991	-2.86144	0.84954	C	-3.68520	2.42437	1.20975
	H	-0.03289	-3.02008	1.71165	H	-3.56151	1.58085	1.88218
	C	1.99479	-2.66303	0.91329	N	-1.40781	-0.07324	0.53375
	C	2.42639	-2.54855	-0.42084	Si	-2.15534	0.89291	-0.69154
	H	3.45418	-2.39770	-0.71806	H	-0.93999	1.24913	-1.49709
	C	1.61122	-2.74366	-2.82870	Th	1.02953	-0.13283	0.07019
	C	2.69881	-1.71528	-3.20367	H	3.03219	-0.33922	0.35596
	H	2.36923	-0.69029	-2.99862	C	-3.27528	0.21943	-2.05693
	H	2.91224	-1.77038	-4.27812	C	-2.73476	-0.05722	-3.32175
	H	3.64155	-1.87815	-2.67545	C	-4.66163	0.07017	-1.89329
	C	2.16596	-4.13545	-3.19691	C	-3.53234	-0.51186	-4.37107
	H	2.39668	-4.18710	-4.26915	C	-5.46641	-0.39257	-2.93281
	H	1.45812	-4.93333	-2.96286	C	-4.90096	-0.69235	-4.17329
	H	3.08783	-4.33559	-2.63911	H	-1.66902	0.08106	-3.49376
	C	0.40526	-2.40980	-3.71378	H	-5.12610	0.33292	-0.94430
	H	-0.01455	-1.43183	-3.45035	H	-3.08694	-0.72498	-5.33988
	H	-0.39518	-3.14551	-3.64185	H	-6.53640	-0.51019	-2.77930
	H	0.71463	-2.36516	-4.76519	H	-5.52755	-1.05148	-4.98592
	C	-1.17450	-3.67491	-0.80380				
3b	C	-2.91735	1.92599	0.04959	C	0.62146	-4.74367	2.23610
	C	-1.69772	2.59497	0.44220	H	0.16328	-4.41499	3.16995
	C	-0.85225	2.60999	-0.71320	H	1.52245	-5.31176	2.49910
	H	0.12286	3.08025	-0.75735	H	-0.07818	-5.42538	1.73865
	C	-1.50723	2.02745	-1.81947	C	1.94238	-2.60429	2.02454
	C	-2.74251	1.56366	-1.32014	H	2.33969	-1.87816	1.31531
	H	-3.50621	1.09932	-1.92739	H	2.79061	-3.14683	2.46094
	C	-4.35696	1.87264	0.60918	H	1.46072	-2.04849	2.82646
	C	-5.07560	0.59929	0.11804	C	1.81434	-4.20017	0.15628
	H	-4.53320	-0.29803	0.42840	H	1.24737	-4.97902	-0.36672
	H	-5.18443	0.56619	-0.96902	H	2.71549	-4.66632	0.57251
	H	-6.08450	0.55205	0.54467	H	2.14196	-3.45538	-0.57256
	C	-4.54648	1.89068	2.13255	C	-2.66920	-2.92449	-2.18797
	H	-5.62047	1.89527	2.35514	C	-1.71798	-3.07144	-3.38137
	H	-4.12039	2.76670	2.61828	H	-1.03248	-3.91636	-3.24914
	H	-4.12617	1.00298	2.60524	H	-1.12417	-2.16140	-3.51030
	C	-5.10716	3.08673	0.01258	H	-2.29147	-3.24956	-4.29912
	H	-5.07853	3.05667	-1.08198	C	-3.68927	-1.82294	-2.49420
	H	-4.65989	4.03321	0.32952	H	-4.27638	-2.07676	-3.38570
	H	-6.15839	3.08235	0.32982	H	-3.17428	-0.87727	-2.67892
	C	-1.34947	3.42247	1.69112	H	-4.38764	-1.67782	-1.66304
	C	-1.29983	2.56190	2.96510	C	-3.41749	-4.25775	-1.98102

	H	-1.12944	3.18583	3.85192	H	-3.96676	-4.53743	-2.88951
	H	-0.46770	1.84983	2.90426	H	-4.13557	-4.18082	-1.15608
	H	-2.21629	1.99421	3.12469	H	-2.71420	-5.06390	-1.74179
	C	-2.34645	4.58986	1.84169	C	2.45953	-0.96532	-1.28484
	H	-2.34358	5.20314	0.93331	C	2.01483	-1.50945	-2.50553
	H	-2.05360	5.22888	2.68444	H	0.99506	-1.30145	-2.81710
	H	-3.37124	4.26723	2.01527	C	2.84497	-2.31091	-3.28048
	C	0.02547	4.10579	1.55461	H	2.45777	-2.72361	-4.21094
	H	0.05043	4.80313	0.71065	C	4.16110	-2.59910	-2.89660
	H	0.83984	3.39289	1.42454	C	4.61144	-2.04365	-1.69548
	H	0.23507	4.67827	2.46602	H	5.62630	-2.24724	-1.35814
	C	-1.11080	2.20050	-3.27750	C	3.78622	-1.24578	-0.90765
	C	-1.52553	3.63521	-3.67087	H	4.16327	-0.87006	0.04033
	H	-2.60584	3.77579	-3.54634	C	5.05927	-3.44682	-3.75896
	H	-1.27072	3.83630	-4.71955	H	4.50235	-4.25758	-4.24272
	H	-1.01387	4.37544	-3.04490	H	5.86898	-3.89722	-3.17433
	C	0.40278	2.05668	-3.46280	H	5.52454	-2.85318	-4.55781
	H	0.94806	2.80097	-2.87428	C	3.04098	2.41611	-0.26634
	H	0.67705	2.20119	-4.51556	C	3.49943	3.53193	0.45431
	H	0.73691	1.06276	-3.14806	H	3.34850	3.58038	1.53104
	C	-1.83189	1.21360	-4.20068	C	4.15421	4.58036	-0.18910
	H	-1.55530	0.18583	-3.94967	H	4.49342	5.44147	0.38143
	H	-1.55487	1.40756	-5.24434	C	4.38056	4.51834	-1.56542
	H	-2.92160	1.30971	-4.12592	H	4.89555	5.33301	-2.06875
	C	-1.49768	-2.45363	1.39254	C	3.95471	3.40629	-2.29208
	C	-0.28719	-2.92133	0.75544	H	4.13957	3.34902	-3.36179
	C	-0.56207	-2.96040	-0.63895	C	3.28754	2.36545	-1.64668
	H	0.15200	-3.24758	-1.39669	H	2.96003	1.50233	-2.21820
	C	-1.91070	-2.64292	-0.90147	N	1.59632	-0.21023	-0.47773
	C	-2.46919	-2.30270	0.34838	Si	2.14858	1.01737	0.59545
	H	-3.51473	-2.07509	0.51025	H	0.78061	1.41660	1.10962
	C	-1.95402	-2.33691	2.85623	Th	-0.76766	-0.15045	-0.15780
	C	-3.01651	-1.23152	2.98290	H	-0.73332	-0.48252	-2.16144
	H	-2.61357	-0.26556	2.65458	C	3.06152	0.67283	2.20320
	H	-3.32492	-1.11714	4.02901	C	2.34608	0.45579	3.38986
	H	-3.91914	-1.43554	2.40153	C	4.46427	0.66324	2.27086
	C	-2.61604	-3.66342	3.28148	C	2.99739	0.20379	4.59580
	H	-2.98600	-3.59638	4.31297	C	5.12491	0.40631	3.47130
	H	-1.92006	-4.50310	3.22252	C	4.39140	0.17059	4.63516
	H	-3.46521	-3.88958	2.62693	H	1.25889	0.48230	3.37524
	C	-0.85653	-1.95549	3.85650	H	5.04977	0.87061	1.37688
	H	-0.38799	-1.00445	3.57735	H	2.41983	0.03430	5.50116
	H	-0.07149	-2.70486	3.94346	H	6.21161	0.39594	3.50109
	H	-1.29504	-1.82503	4.85325	H	4.90550	-0.02859	5.57210
	C	0.99743	-3.57417	1.30546				
TSb	C	2.36677	2.35724	-0.85220	C	-0.30745	-5.16678	-0.93693
	C	0.98103	2.70439	-1.09542	H	-0.25635	-5.02237	-2.01854
	C	0.34735	2.75339	0.18326	H	-1.10141	-5.89853	-0.74096
	H	-0.69161	3.00508	0.34719	H	0.64547	-5.59906	-0.60965
	C	1.28040	2.51029	1.21478	C	-1.91176	-3.23694	-0.67330
	C	2.50196	2.22680	0.56018	H	-2.29532	-2.52215	0.05494
	H	3.43879	2.05219	1.07376	H	-2.67600	-4.01248	-0.80872
	C	3.64857	2.41321	-1.70727	H	-1.80459	-2.71075	-1.61584
	C	4.68276	1.39728	-1.19247	C	-0.86148	-4.24439	1.29179
	H	4.29227	0.37753	-1.26678	H	-0.04289	-4.83742	1.71553
	H	4.97384	1.57063	-0.15433	H	-1.77133	-4.85481	1.33856
	H	5.59530	1.45466	-1.79780	H	-1.02549	-3.36329	1.92146
	C	3.49728	2.10324	-3.20163	C	3.93810	-2.25918	1.44030
	H	4.48641	2.12140	-3.67520	C	3.56081	-2.33277	2.92538

	H	2.87745	2.82164	-3.73604	H	2.94382	-3.21076	3.14495
	H	3.07870	1.10546	-3.35580	H	3.01265	-1.44001	3.24182
	C	4.25537	3.82296	-1.53581	H	4.46902	-2.40686	3.53578
	H	4.48416	4.01355	-0.48134	C	4.86137	-1.05681	1.22715
	H	3.56836	4.60412	-1.87150	H	5.74182	-1.13011	1.87773
	H	5.18547	3.91301	-2.11192	H	4.33949	-0.12257	1.45938
	C	0.25978	3.23655	-2.34783	H	5.21762	-1.00377	0.19400
	C	0.13834	2.19792	-3.47550	C	4.70873	-3.54541	1.07235
	H	-0.37751	2.63176	-4.34150	H	5.60337	-3.65366	1.69927
	H	-0.45664	1.33887	-3.14537	H	5.02418	-3.52350	0.02296
	H	1.10343	1.82823	-3.81741	H	4.07719	-4.42958	1.21637
	C	0.96389	4.51032	-2.85847	C	-1.50739	-0.52191	1.58583
	H	1.04819	5.24473	-2.04925	C	-0.27244	-0.58570	2.28415
	H	0.37641	4.96204	-3.66773	H	1.20024	-0.24788	2.14011
	H	1.96542	4.32699	-3.24681	C	-0.26223	-1.07962	3.58934
	C	-1.17157	3.68369	-1.99785	H	0.69104	-1.15574	4.11762
	H	-1.17490	4.50121	-1.26904	C	-1.42201	-1.49275	4.25642
	H	-1.77695	2.87222	-1.59509	C	-2.62808	-1.41604	3.55015
	H	-1.67225	4.04329	-2.90449	H	-3.54991	-1.74100	4.03015
	C	1.13512	2.92170	2.67591	C	-2.67804	-0.95043	2.24068
	C	1.62042	4.38811	2.73867	H	-3.62390	-0.94287	1.70762
	H	2.67502	4.46347	2.44876	C	-1.37238	-1.97844	5.68167
	H	1.51291	4.78822	3.75528	H	-2.24188	-2.59908	5.92512
	H	1.03701	5.01720	2.05661	H	-1.36034	-1.14073	6.39260
	C	-0.32114	2.86847	3.14812	H	-0.47138	-2.57391	5.87089
	H	-0.95921	3.53356	2.55670	C	-3.62272	1.92918	-0.07556
	H	-0.38789	3.19043	4.19466	C	-4.60585	2.60025	-0.82083
	H	-0.71417	1.84936	3.07932	H	-4.90587	2.21289	-1.79337
	C	1.99562	2.08627	3.63413	C	-5.20528	3.76185	-0.33695
	H	1.58802	1.08069	3.75992	H	-5.95813	4.27385	-0.93171
	H	2.01458	2.56230	4.62225	C	-4.84007	4.26655	0.91308
	H	3.03131	1.99652	3.28818	H	-5.30774	5.17218	1.29193
	C	1.42117	-2.46485	-1.40151	C	-3.87899	3.60279	1.67516
	C	0.64508	-2.95410	-0.28510	H	-3.59648	3.98433	2.65356
	C	1.43777	-2.73146	0.87340	C	-3.27714	2.44538	1.18049
	H	1.13446	-2.98667	1.87585	H	-2.53043	1.93248	1.77707
	C	2.71005	-2.22165	0.53923	N	-1.45652	-0.08184	0.25858
	C	2.67532	-2.02275	-0.85752	Si	-2.77437	0.39273	-0.75152
	H	3.52136	-1.70162	-1.45402	H	-2.12656	0.67399	-2.06537
	C	1.26884	-2.54665	-2.93087	Th	0.89800	-0.04673	0.03134
	C	1.91206	-1.31616	-3.60050	H	2.07659	-0.10199	1.86190
	H	1.39276	-0.39132	-3.31557	C	-4.16200	-0.81010	-1.19216
	H	1.83792	-1.39683	-4.69149	C	-4.11089	-1.55101	-2.38336
	H	2.97153	-1.20369	-3.35544	C	-5.30489	-0.94690	-0.38730
	C	2.02660	-3.79749	-3.42178	C	-5.13623	-2.42656	-2.73864
	H	1.95761	-3.88924	-4.51358	C	-6.33330	-1.82274	-0.73181
	H	1.62219	-4.71011	-2.97550	C	-6.24642	-2.57087	-1.90636
	H	3.08600	-3.73531	-3.14884	H	-3.25493	-1.44370	-3.04717
	C	-0.17174	-2.58983	-3.45215	H	-5.40489	-0.34525	0.51447
	H	-0.73936	-1.71236	-3.12068	H	-5.07111	-2.99323	-3.66450
	H	-0.71102	-3.48282	-3.13713	H	-7.20565	-1.91608	-0.08942
	H	-0.16401	-2.58201	-4.54889	H	-7.04691	-3.25462	-2.17832
	C	-0.60031	-3.85587	-0.17818				
4	C	2.55719	2.09844	-1.03399	C	-0.74917	-3.79654	0.15083
	C	1.20704	2.56619	-1.24910	C	-0.51298	-5.19255	-0.45941
	C	0.62666	2.75168	0.03895	H	-0.43294	-5.16310	-1.54815
	H	-0.37395	3.11965	0.21453	H	-1.34884	-5.85824	-0.20919
	C	1.56612	2.47280	1.05559	H	0.40886	-5.63717	-0.06622
	C	2.72886	2.02873	0.38360	C	-2.02656	-3.17448	-0.42671

H	3.66558	1.80362	0.87724	H	-2.36838	-2.35019	0.20006
C	3.80757	2.04032	-1.93344	H	-2.83152	-3.91925	-0.45931
C	4.84048	1.05423	-1.36355	H	-1.89882	-2.78505	-1.43149
H	4.41327	0.05106	-1.28448	C	-1.04362	-4.01261	1.64954
H	5.20882	1.34719	-0.37728	H	-0.25852	-4.59371	2.14701
H	5.71144	1.00241	-2.02739	H	-1.98132	-4.57270	1.74703
C	3.59939	1.60329	-3.38960	H	-1.17098	-3.06121	2.17705
H	4.56917	1.58792	-3.90164	C	3.79881	-2.15853	1.70068
H	2.95300	2.26926	-3.95845	C	3.35686	-1.70051	3.09693
H	3.18503	0.59364	-3.44381	H	2.61800	-2.37808	3.53630
C	4.44780	3.44606	-1.90872	H	2.91556	-0.70015	3.05939
H	4.69844	3.73041	-0.88060	H	4.21859	-1.66462	3.77454
H	3.77333	4.20786	-2.30736	C	4.89697	-1.21677	1.20692
H	5.37035	3.45877	-2.50395	H	5.75120	-1.23208	1.89466
C	0.45009	2.99534	-2.51735	H	4.52473	-0.19073	1.15098
C	0.22061	1.81972	-3.48254	H	5.26427	-1.50174	0.21545
H	-0.33639	2.14912	-4.36876	C	4.37360	-3.58648	1.80183
H	-0.38197	1.03886	-3.00169	H	5.22500	-3.61327	2.49459
H	1.15189	1.36980	-3.82295	H	4.71602	-3.93736	0.82145
C	1.17815	4.15165	-3.22939	H	3.61218	-4.28634	2.16414
H	1.33661	4.98360	-2.53372	C	-1.53003	-0.22939	1.45189
H	0.56641	4.51834	-4.06323	C	-0.28038	-0.29557	2.13166
H	2.14867	3.87020	-3.63684	C	-0.29214	-0.65801	3.48342
C	-0.93630	3.55556	-2.15023	H	0.65617	-0.74688	4.01481
H	-0.85812	4.46510	-1.54464	C	-1.46235	-0.92300	4.19837
H	-1.54353	2.83737	-1.59870	C	-2.67856	-0.83226	3.50343
H	-1.48311	3.80938	-3.06579	H	-3.61146	-1.03701	4.02677
C	1.49331	2.94755	2.49846	C	-2.72012	-0.50329	2.15661
C	2.15785	4.34074	2.53243	H	-3.67558	-0.46753	1.64246
H	3.20635	4.28154	2.21788	C	-1.43508	-1.29224	5.65861
H	2.12521	4.75917	3.54698	H	-0.40904	-1.44226	6.01218
H	1.64102	5.03285	1.85757	H	-1.99415	-2.21655	5.85168
C	0.04412	3.08338	2.98114	H	-1.88722	-0.50820	6.28066
H	-0.50956	3.81337	2.37947	C	-3.65044	2.08631	-0.18988
H	0.02574	3.43193	4.02089	C	-4.79845	2.65037	-0.76833
H	-0.47472	2.12169	2.93205	H	-5.27974	2.15355	-1.60932
C	2.25621	2.01319	3.44196	C	-5.34049	3.83851	-0.27854
H	1.78251	1.02979	3.45995	H	-6.22771	4.26300	-0.74259
H	2.25312	2.41212	4.46373	C	-4.74608	4.47988	0.80963
H	3.30211	1.89133	3.13690	H	-5.16933	5.40500	1.19364
C	1.35377	-2.63324	-1.17933	C	-3.61245	3.92691	1.40620
C	0.54075	-2.96866	-0.02974	H	-3.15020	4.41469	2.26125
C	1.33028	-2.66041	1.11158	C	-3.07260	2.74226	0.90748
H	1.01040	-2.80970	2.13006	H	-2.19556	2.31423	1.38236
C	2.61828	-2.22314	0.74361	N	-1.49819	0.07085	0.06419
C	2.61479	-2.18063	-0.66798	Si	-2.87457	0.51946	-0.88560
H	3.47039	-1.92738	-1.28166	H	-2.33143	0.74157	-2.25413
C	1.20974	-2.87439	-2.69129	Th	0.82019	-0.07998	0.01826
C	1.92046	-1.75567	-3.47398	C	-4.26531	-0.72438	-1.17075
H	1.45315	-0.78388	-3.27348	C	-4.20579	-1.58757	-2.27653
H	1.83963	-1.93555	-4.55253	C	-5.39543	-0.80355	-0.34156
H	2.98499	-1.68139	-3.23716	C	-5.20981	-2.52281	-2.52340
C	1.90873	-4.20649	-3.03350	C	-6.40464	-1.73558	-0.57956
H	1.85210	-4.40768	-4.11119	C	-6.30858	-2.60397	-1.66751
H	1.45136	-5.04659	-2.50403	H	-3.35788	-1.53076	-2.95720
H	2.96546	-4.16822	-2.74632	H	-5.50070	-0.11374	0.49403
C	-0.22643	-2.90226	-3.22824	H	-5.13708	-3.18524	-3.38273
H	-0.75805	-1.97061	-2.99867	H	-7.26845	-1.78106	0.07938
H	-0.81168	-3.73364	-2.83576	H	-7.09331	-3.33297	-1.85474

	H -0.20450 -3.00700 -4.31979	

Table S5. Frequencies of the stationary points optimized for the studied reactions, obtained with B3PW91-PCM+D3 method.

Species	Frequencies (cm^{-1})
1	8 18 31 36 38 44 60 64 66 78 82 86 93 95 98 102 108 118 123 134 137 153 154 180 185 195 202 208 213 217 225 227 232 235 240 251 262 263 273 276 277 280 288 290 291 298 302 306 311 316 326 332 337 340 347 354 357 362 365 369 374 376 389 390 393 394 399 407 410 412 419 425 442 442 448 452 472 473 486 488 490 527 536 542 566 567 573 574 579 587 594 606 612 657 660 665 694 697 710 715 720 802 805 809 829 835 836 837 839 840 843 853 861 864 940 940 943 943 944 947 948 949 949 955 957 957 958 958 962 967 970 970 972 978 979 980 984 1016 1027 1029 1033 1054 1056 1057 1058 1059 1060 1062 1065 1065 1067 1072 1075 1081 1144 1153 1160 1203 1209 1209 1212 1213 1228 1229 1239 1239 1241 1242 1244 1247 1248 1249 1251 1264 1266 1279 1281 1283 1285 1314 1323 1325 1348 1356 1390 1398 1406 1411 1413 1414 1415 1418 1419 1421 1421 1423 1425 1426 1429 1431 1434 1445 1446 1447 1453 1455 1459 1461 1464 1465 1495 1497 1500 1502 1505 1505 1506 1506 1509 1511 1512 1513 1513 1515 1516 1516 1518 1520 1520 1522 1522 1523 1524 1528 1528 1532 1535 1537 1539 1541 1542 1545 1549 1550 1552 1556 1559 1562 1568 1603 1632 1673 1695 3032 3036 3042 3045 3047 3048 3050 3051 3051 3054 3055 3056 3056 3057 3058 3059 3061 3062 3068 3095 3101 3104 3117 3117 3120 3121 3122 3123 3123 3123 3125 3126 3126 3127 3128 3129 3129 3131 3134 3135 3135 3138 3139 3144 3146 3146 3150 3152 3154 3160 3162 3163 3166 3172 3181 3185 3187 3194 3195 3195 3197 3261 3264 3273 3277
Ph_2SiH_2	13 36 55 150 160 198 242 391 400 404 422 425 476 600 629 629 696 707 711 714 723 756 777 853 872 873 937 938 960 982 984 1008 1008 1013 1013 1058 1059 1112 1114 1137 1142 1201 1201 1226 1228 1335 1339 1374 1374 1475 1478 1534 1535 1637 1639 1660 1660 2219 2225 3183 3183 3185 3186 3197 3198 3208 3208 3220 3220
TS	-164i 22 22 28 32 41 47 55 59 60 68 76 77 79 81 88 92 96 99 102 105 107 111 118 127 131 136 144 151 156 162 169 171 174 185 186 191 197 200 201 211 215 217 221 223 230 239 241 244 248 251 263 270 272 278 283 290 291 298 303 306 307 314 318 320 324 336 339 351 357 363 369 372 374 377 382 387 390 396 401 403 406 409 411 412 414 425 426 437 443 444 447 453 457 466 469 477 485 487 491 491 492 540 557 558 566 568 576 578 583 608 609 629 631 657 659 661 672 679 689 691 694 710 716 724 729 733 755 765 774 803 832 837 838 841 843 844 849 854 865 869 870 872 875 879 927 931 935 939 943 944 946 949 951 954 956 956 957 959 962 965 966 971 972 977 978 978 982 984 984 985 990 994 1000 1006 1015 1016 1017 1029 1033 1035 1056 1057 1058 1058 1059 1060 1061 1062 1065 1065 1066 1067 1069 1072 1089 1111 1115 1125 1138 1153 1157 1158 1198 1198 1206 1208 1209 1212 1225 1227 1229 1230 1231 1233 1241 1244 1248 1249 1253 1255 1256 1258 1265 1266 1277 1280 1282 1284 1291 1321 1322 1327 1334 1338 1351 1367 1373 1376 1397 1402 1410 1414 1414 1417 1417 1419 1420 1420 1423 1426 1431 1433 1433 1435 1445 1450 1452 1455 1456 1461 1462 1466 1468 1473 1475 1476 1497 1497 1499 1499 1501 1502 1505 1506 1507 1509 1509 1511 1512 1516 1517 1519 1520 1521 1522 1523 1524 1524 1525 1528 1529 1529 1532 1533 1534 1536 1538 1541 1544 1547 1548 1549 1554 1556 1557 1559 1559 1565 1581 1608 1635 1637 1656 1658 1673 1735 2046 3037 3041 3042 3049 3050 3051 3052 3055 3057 3059 3059 3061 3061 3066 3068 3069 3071 3073 3077 3101 3111 3117 3118 3118 3119 3121 3122 3124 3125 3127 3127 3129 3130 3131 3134 3137 3137 3143 3143 3150 3154 3157 3161 3162 3164 3170 3172 3174 3175 3175 3178 3179 3183 3185 3185 3189 3194 3196 3197 3198 3199 3199 3204 3205 3210 3215 3218 3219 3238 3245 3265 3268 3272 3286

	3287
3a	23 29 34 37 40 42 46 52 58 67 70 71 72 77 82 85 86 92 93 98 102 105 108 112 117 127 135 141 143 145 150 170 175 176 180 182 186 194 195 200 204 205 214 221 224 243 243 246 250 251 258 260 266 273 276 280 286 288 292 295 299 303 307 317 318 320 332 335 346 353 361 363 369 370 376 380 384 388 392 394 395 398 405 407 410 412 415 416 427 432 440 443 446 451 456 473 481 485 489 489 490 496 539 552 560 566 567 574 575 577 606 607 629 630 647 658 663 665 680 691 694 706 706 717 718 721 724 737 755 758 795 802 816 825 831 837 839 841 841 848 863 866 876 877 878 878 938 939 941 942 943 945 947 948 951 951 953 954 957 958 961 962 964 969 972 976 976 979 980 983 985 993 995 1009 1010 1013 1015 1017 1025 1030 1031 1034 1056 1057 1058 1058 1059 1060 1060 1061 1063 1063 1064 1066 1067 1070 1072 1114 1114 1137 1142 1143 1152 1155 1200 1200 1205 1207 1209 1212 1214 1227 1228 1229 1229 1241 1241 1243 1243 1247 1248 1251 1252 1253 1263 1264 1278 1278 1283 1285 1319 1323 1324 1329 1338 1342 1354 1377 1377 1395 1403 1408 1410 1411 1414 1416 1417 1418 1419 1420 1421 1422 1426 1431 1436 1437 1444 1448 1451 1455 1456 1458 1462 1468 1473 1475 1477 1488 1496 1497 1498 1500 1501 1501 1502 1504 1506 1507 1509 1510 1510 1512 1513 1515 1516 1517 1519 1520 1523 1523 1523 1525 1527 1527 1528 1529 1532 1533 1535 1535 1539 1540 1544 1546 1549 1551 1554 1555 1557 1560 1562 1620 1637 1638 1659 1660 1679 2155 3042 3042 3042 3048 3049 3053 3053 3055 3056 3057 3058 3061 3062 3063 3064 3065 3065 3067 3074 3107 3117 3118 3119 3120 3120 3121 3123 3126 3127 3130 3130 3133 3133 3134 3134 3135 3137 3137 3144 3145 3154 3161 3162 3162 3163 3163 3168 3171 3175 3178 3178 3179 3181 3183 3183 3185 3186 3191 3194 3194 3198 3205 3205 3206 3207 3211 3216 3218 3218 3218 3230 3262 3266 3279 3288
TSa	-407i 22 27 31 33 36 40 48 51 62 66 73 75 78 83 86 89 93 95 98 108 112 115 119 129 134 135 142 148 149 155 159 166 173 181 185 189 198 201 204 208 212 220 221 236 240 242 252 260 263 268 272 279 280 283 286 290 291 296 298 310 315 320 320 331 336 348 350 355 357 365 367 369 370 381 387 389 394 397 398 405 406 406 407 410 415 424 430 436 442 446 447 450 458 476 478 484 485 489 491 503 517 541 555 561 568 572 574 579 581 607 608 629 630 650 659 663 681 682 688 699 708 711 718 719 726 741 754 757 820 829 832 836 838 840 840 845 853 863 868 870 872 873 875 924 937 938 940 941 944 945 946 947 951 951 956 958 959 960 961 964 967 968 976 978 978 981 982 984 986 990 993 1005 1009 1014 1015 1018 1022 1026 1033 1046 1054 1056 1057 1059 1059 1060 1061 1064 1064 1065 1066 1067 1069 1073 1093 1099 1115 1119 1135 1138 1156 1162 1184 1199 1200 1207 1211 1213 1216 1228 1228 1231 1231 1239 1243 1244 1248 1248 1251 1252 1254 1255 1265 1266 1276 1282 1285 1286 1289 1321 1323 1336 1337 1339 1348 1376 1377 1394 1395 1401 1402 1410 1411 1413 1417 1419 1420 1420 1421 1423 1427 1435 1436 1437 1438 1441 1442 1453 1453 1457 1464 1469 1474 1474 1475 1492 1497 1497 1499 1500 1504 1504 1507 1509 1510 1511 1512 1513 1513 1515 1516 1517 1517 1518 1519 1519 1522 1524 1524 1527 1527 1531 1534 1535 1536 1538 1540 1541 1541 1543 1550 1554 1555 1557 1558 1560 1569 1602 1613 1637 1637 1637 1654 1659 1660 1702 2212 3032 3040 3040 3044 3049 3050 3052 3052 3052 3055 3055 3056 3057 3058 3058 3065 3065 3067 3068 3104 3105 3112 3117 3117 3118 3119 3119 3119 3121 3122 3123 3123 3124 3125 3126 3131 3132 3132 3132 3138 3141 3142 3147 3156 3165 3170 3172 3177 3177 3179 3179 3180 3181 3182 3184 3184 3186 3191 3193 3195 3196 3197 3204 3206 3210 3216 3218 3219 3225 3229 3230 3271 3275 3277 3278

3b	26 31 33 36 41 45 47 54 55 60 63 66 71 78 81 85 88 89 95 95 101 104 107 115 122 130 136 143 149 150 156 169 174 177 179 187 192 195 198 201 207 213 215 220 224 240 246 248 249 252 256 258 260 268 277 282 284 289 290 291 310 311 316 319 323 325 329 329 346 351 353 363 367 371 375 375 386 387 392 393 395 399 404 407 410 413 415 420 429 440 440 448 449 455 459 479 481 485 489 489 498 541 555 560 565 565 573 574 576 601 607 614 629 630 650 662 663 686 689 691 696 706 714 718 719 727 742 756 757 767 786 818 822 834 834 839 841 842 854 858 865 866 869 871 877 908 934 934 940 942 945 945 946 948 950 951 954 954 954 956 963 964 965 969 975 977 979 980 981 982 986 989 994 1006 1012 1015 1016 1019 1028 1030 1038 1051 1056 1057 1058 1058 1059 1060 1060 1062 1062 1064 1064 1065 1067 1072 1104 1115 1119 1137 1141 1151 1157 1158 1200 1200 1204 1205 1209 1213 1224 1227 1228 1229 1231 1234 1240 1242 1243 1248 1249 1249 1252 1252 1264 1265 1278 1279 1284 1286 1307 1324 1327 1336 1337 1342 1356 1374 1379 1400 1403 1404 1406 1411 1412 1414 1415 1416 1417 1418 1422 1424 1427 1428 1431 1434 1444 1445 1446 1450 1456 1460 1462 1464 1466 1474 1476 1492 1496 1500 1501 1502 1502 1503 1505 1508 1509 1509 1510 1512 1514 1514 1515 1516 1518 1520 1521 1522 1523 1524 1525 1526 1527 1529 1532 1532 1533 1535 1535 1540 1540 1543 1547 1548 1553 1555 1559 1560 1562 1564 1588 1620 1637 1638 1659 1660 1679 2173 3039 3040 3040 3047 3048 3050 3050 3051 3053 3054 3055 3056 3058 3058 3064 3065 3066 3070 3075 3105 3109 3115 3115 3117 3119 3120 3121 3123 3123 3124 3125 3126 3127 3128 3128 3132 3132 3132 3138 3147 3151 3153 3153 3159 3163 3168 3171 3172 3176 3176 3177 3180 3180 3181 3183 3188 3188 3194 3195 3197 3199 3203 3203 3206 3206 3209 3217 3221 3221 3227 3229 3246 3252 3281 3289
TSb	-715i 15 21 27 29 29 37 38 41 43 46 49 52 55 57 60 67 71 74 82 85 90 94 98 102 105 122 132 133 135 140 152 160 166 173 176 180 185 187 195 197 202 207 209 214 224 231 232 239 241 244 246 252 253 267 268 271 273 274 278 286 295 297 304 306 308 312 318 325 344 347 353 356 357 358 362 368 369 373 376 379 383 385 393 396 401 404 405 409 420 429 430 433 434 436 444 461 469 477 477 479 495 534 541 549 554 556 561 563 564 585 597 599 629 630 648 652 665 679 684 690 692 697 702 709 717 721 734 753 758 797 808 823 827 830 831 833 834 841 847 857 857 862 873 874 881 906 928 937 937 937 940 940 940 941 942 944 948 952 952 954 955 956 958 966 967 970 971 971 972 979 987 987 1000 1006 1007 1014 1014 1017 1021 1022 1048 1049 1050 1052 1053 1053 1054 1055 1057 1058 1058 1059 1060 1064 1067 1074 1108 1110 1128 1132 1137 1143 1164 1174 1190 1191 1198 1199 1203 1206 1220 1222 1224 1225 1232 1234 1236 1237 1239 1241 1241 1243 1247 1259 1262 1269 1272 1273 1276 1277 1303 1313 1317 1325 1333 1339 1374 1375 1377 1386 1401 1401 1407 1409 1411 1411 1412 1414 1415 1417 1421 1422 1422 1424 1426 1434 1441 1442 1443 1444 1452 1452 1455 1455 1473 1475 1489 1493 1497 1498 1498 1500 1501 1502 1503 1503 1505 1506 1507 1508 1509 1510 1514 1514 1516 1517 1518 1519 1520 1521 1521 1523 1523 1526 1529 1530 1531 1533 1534 1534 1535 1537 1540 1542 1543 1548 1550 1551 1552 1594 1636 1637 1653 1658 1658 1793 2134 2207 3041 3043 3046 3049 3051 3052 3052 3053 3053 3053 3055 3057 3059 3059 3060 3064 3066 3071 3072 3101 3106 3114 3118 3119 3121 3121 3122 3123 3124 3124 3125 3125 3128 3128 3128 3131 3132 3133 3135 3135 3145 3145 3146 3148 3148 3149 3157 3158 3162 3163 3163 3165 3177 3178 3179 3182 3183 3184 3184 3191 3192 3197 3201 3202 3206 3211 3215 3218 3219 3224 3246 3256 3273 3300
4	19 30 33 39 43 46 47 50 51 58 65 66 73 74

	76 86 90 90 96 100 103 109 110 116 117 131 144 147 153 163 172 178 178 180 186 192 192 199 205 208 212 215 216 222 238 243 244 248 251 255 261 261 270 275 279 281 288 294 299 303 306 313 327 330 345 349 351 358 363 363 367 369 373 378 383 386 388 391 393 400 402 407 409 410 414 414 419 433 440 444 448 452 454 460 467 476 478 485 489 490 495 535 561 565 566 570 571 575 578 606 608 631 631 661 664 674 684 692 695 696 698 702 715 719 721 735 752 756 809 809 813 818 837 839 842 844 848 855 864 867 868 874 876 894 906 939 940 941 942 943 944 945 948 949 950 955 956 956 959 963 964 970 973 977 980 980 985 986 987 990 994 1006 1009 1015 1016 1017 1029 1029 1038 1054 1056 1058 1058 1059 1060 1061 1063 1063 1064 1066 1066 1070 1075 1076 1113 1114 1134 1138 1148 1153 1178 1198 1199 1205 1207 1210 1212 1224 1224 1230 1232 1236 1238 1241 1245 1247 1247 1248 1249 1250 1251 1265 1266 1279 1280 1284 1285 1304 1323 1325 1329 1335 1340 1372 1374 1397 1400 1406 1412 1414 1415 1417 1417 1419 1422 1424 1426 1426 1428 1430 1433 1434 1435 1446 1450 1453 1454 1460 1463 1464 1467 1475 1477 1482 1494 1497 1499 1502 1503 1504 1504 1505 1507 1508 1509 1513 1513 1514 1514 1514 1517 1518 1520 1522 1523 1524 1525 1526 1527 1528 1531 1532 1533 1534 1538 1539 1543 1546 1550 1551 1557 1558 1559 1560 1564 1590 1614 1637 1638 1656 1659 1660 2233 3039 3040 3042 3048 3049 3050 3052 3052 3054 3056 3058 3059 3062 3063 3064 3066 3068 3072 3073 3099 3115 3116 3118 3119 3119 3123 3123 3123 3123 3124 3127 3127 3129 3130 3131 3132 3134 3135 3138 3145 3147 3152 3154 3155 3157 3159 3162 3164 3165 3171 3176 3176 3178 3178 3179 3180 3185 3186 3190 3190 3194 3200 3201 3205 3210 3215 3217 3221 3236 3247 3254 3257 3288 3309

Table S6. The energies, enthalpies and free energies (in au at 343[a] and 298[b]K) and corresponding relative values (in kcal/mol), obtained with B3PW91-PCM+D3 method

species	E	H	G (gas)	G (sol)
1	-1691.88739	-1690.84607[a] -1690.86129[b]	-1691.01183 -1690.99115	-1690.99641 -1690.97789
Ph_2SiH_2	-753.78890	-753.57304[a] -753.57665[b]	-753.63739 -753.62920	-753.62126 -753.61532
1+Ph_2SiH_2	-2445.67629(0.0)	-2444.41911(0.0)[a] -2444.43794(0.0)[b]	-2444.64922(0.0) -2444.62035(0.0)	-2444.61767(0.0) -2444.59321(0.0)
TS	-2445.67164(2.9)	-2444.41161(4.7)[a] -2444.43051(4.7)[b]	-2444.60688(26.6) -2444.58259(23.7)	-2444.59105(16.7) -2444.56897(15.2)
3a	-2445.72035(-27.6)	-2444.46186(-26.8)[a] -2444.48100(-27.0)[b]	-2444.66103(-7.4) -2444.63624(-10.0)	-2444.64576(-17.6) -2444.62310(-18.8)
TSa	-2445.67305(2.0)	-2444.41263(4.1)[a]	-2444.60763(26.1)	-2444.59198(16.1)
3b	-2445.71339(-23.3)	-2444.45426(-22.1)[a]	-2444.65282(-2.3)	-2444.63967(-13.8)
TSb	-2445.67595(0.2)	-2444.42519(-3.8)[a]	-2444.63261(10.4)	-2444.61961(-1.2)
4	-2444.51816	-2443.27857[a]	-2443.47522	-2443.46208
4+H_2^g	-2445.69272(-10.3)	-2444.43920(-12.6)[a]	-2444.65427(-3.2)	-2444.64117(-14.7)
4+H_2^l	-2445.69272(-10.3)	-2444.43920(-12.6)[a]	-2444.65427(-3.2)	-2444.62881(-7.0)

Table S7. The energies, enthalpies and free energies (in au at 343[a] and 298[b]K) and corresponding relative values (in kcal/mol), obtained with B3PW91-PCM method

species	E	H	G (gas)	G (sol)
1	-1691.69265	-1690.65402[a] -1690.66939[b]	-1690.82298 -1690.80189	-1690.80979 -1690.79057
Ph_2SiH_2	-753.76827	-753.55249[a] -753.55611[b]	-753.61707 -753.60885	-753.60393 -753.59757
1+Ph_2SiH_2	-2445.46092(0.0)	-2444.20651(0.0)[a] -2444.22550(0.0)[b]	-2444.44005(0.0) -2444.41074(0.0)	-2444.41372(0.0) -2444.38814(0.0)
TS	-2445.42583(22.0)	-2444.17086(22.4)[a] -2444.19002(22.3)[b]	-2444.37717(39.5) -2444.35144(37.2)	-2444.36409(31.1) -2444.34021(30.0)
3a	-2445.46275(-1.1)	-2444.20794(-0.9)[a] -2444.22727(-1.1)[b]	-2444.41439(16.1) -2444.38865(13.9)	-2444.40156(7.6) -2444.37764(6.6)
TSa	-2445.41535(28.6)	-2444.15794(30.5)[a]	-2444.35753(51.8)	-2444.34449(43.4)
3b	-2445.45628(2.9)	-2444.20116(3.4)[a]	-2444.40664(21.0)	-2444.39394(12.4)
TSb	-2445.41704(27.5)	-2444.16628(25.2)[a]	-2444.37370(41.6)	-2444.36069(33.3)
4	-2444.26508	-2443.02972[a]	-2443.23453	-2443.22162
4+H_2^g	-2445.43968(13.3)	-2444.19039(10.1)[a]	-2444.41362(16.6)	-2444.40071(8.2)
4+H_2^l	-2445.43968(13.3)	-2444.19039(10.1)[a]	-2444.41362(16.6)	-2444.38835(16.0)