Electronic supplementary material

Feasibility of novel $(H_3C)_nX(SiH_3)_{3-n}$ compounds (X = B, Al, Ga, In): structure, stability, reactivity, and Raman characterization from *ab initio* calculations

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Table S1 The lowest frequency (v_{min}) (in cm^{-1}) and molecular dipole moment (M) (in D) of the $(H_3C)_nX(SiH_3)_{3-n}$ compounds with MP2 and PW91 (values in parenthesis).

	v_{min}	M	v_{min}	M	v_{min}	M	v_{min}	M
n	B		Al		Ga		In	
0	39.44 (63.38)	0.13 (0.08)	27.56 (8.73)	0.00 (0.00)	25.74 (20.43)	0.00 (0.05)	23.97 (10.05)	0.00 (0.04)
1	45.98 (47.25)	1.18 (1.34)	8.58 (21.14)	1.12 (1.33)	14.46 (22.12)	0.98 (1.19)	14.96 (14.00)	0.90 (1.10)
2	31.04 (39.64)	1.21 (1.41)	8.74 (13.94)	1.24 (1.40)	7.86 (14.77)	1.04 (1.24)	10.34 (10.69)	0.92 (1.13)
3	11.97 (39.97)	0.00 (0.03)	43.80 (26.69)	0.00 (0.00)	48.07 (21.34)	0.00 (0.00)	27.46 (4.45)	0.00 (0.00)

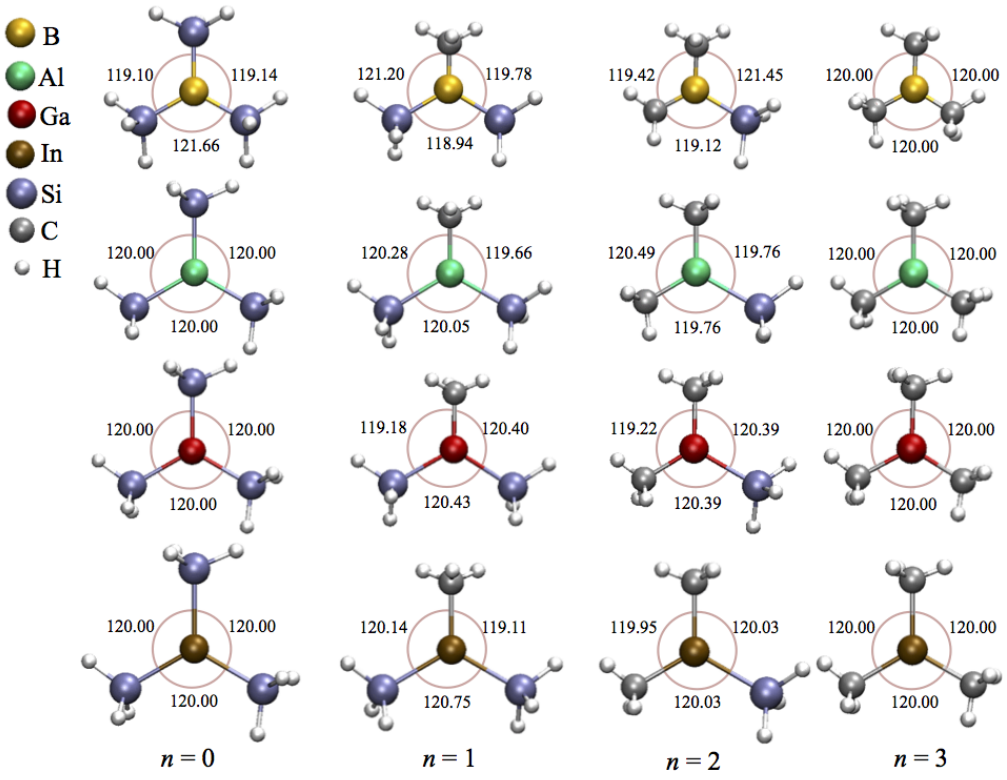


Fig. S1 Optimized angles at the MP2 level of theory for the $(H_3C)_nX(SiH_3)_{3-n}$ compounds.

Table S2 HOMO and HOMO-1 KS-MO (together with their corresponding energies in eV) calculated with PW91 for all $(H_3C)_nX(SiH_3)_{3-n}$ compounds.

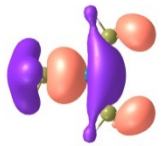
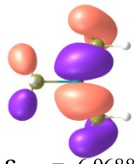
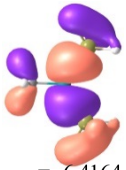
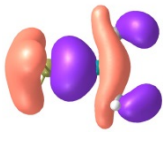
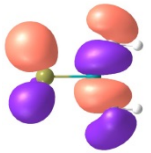
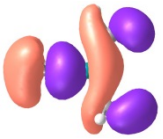
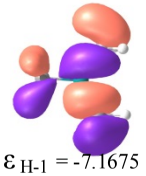
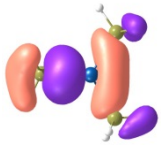
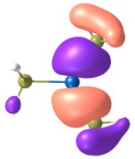
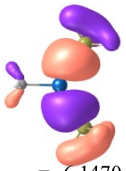
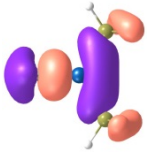
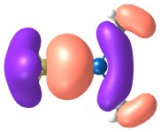
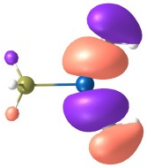
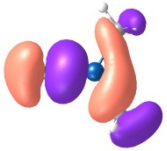
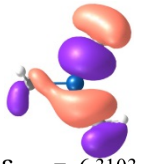
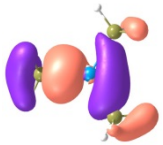
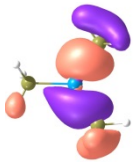
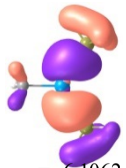
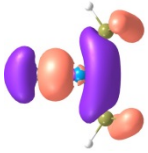
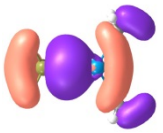
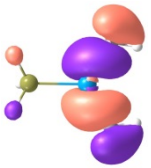
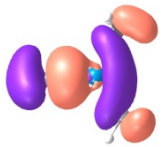
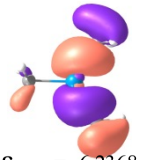
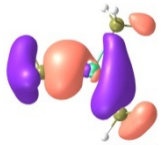
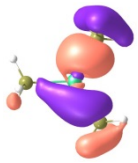
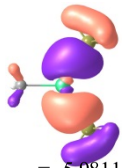
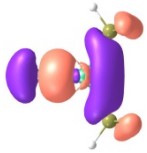
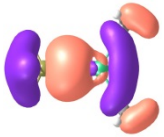
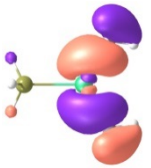
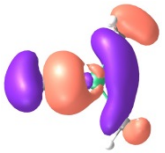
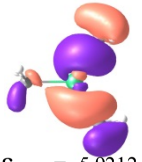
	n = 0		*n* = 1		*n* = 2		*n* = 3	
X	HOMO	HOMO-1	HOMO	HOMO-1	HOMO	HOMO-1	HOMO	HOMO-1
B	 ε_H = -6.9362	 ε_{H-1} = -6.9688	 ε_H = -6.4164	 ε_{H-1} = -7.5512	 ε_H = -6.4790	 ε_{H-1} = -7.6736	 ε_H = -7.1729	 ε_{H-1} = -7.1675
Al	 ε_H = -6.4001	 ε_{H-1} = -6.4001	 ε_H = -6.1470	 ε_{H-1} = -6.6641	 ε_H = -6.1226	 ε_{H-1} = -6.6559	 ε_H = -6.3103	 ε_{H-1} = -6.3103
Ga	 ε_H = -6.3647	 ε_{H-1} = -6.3620	 ε_H = -6.1062	 ε_{H-1} = -6.5933	 ε_H = -6.0845	 ε_{H-1} = -6.5579	 ε_H = -6.2368	 ε_{H-1} = -6.2368
In	 ε_H = -6.1770	 ε_{H-1} = -6.1797	 ε_H = -5.9811	 ε_{H-1} = -6.2722	 ε_H = -5.9158	 ε_{H-1} = -6.1715	 ε_H = -5.9212	 ε_{H-1} = -5.9212

Table S3 Bader analysis for the charge transfer (in e^-) in all $(H_3C)_nX(SiH_3)_{3-n}$ compounds with MP2 and PW91 (in parenthesis)*.

	B			Al			Ga			In		
n	B	Si	C	Al	Si	C	Ga	Si	C	In	Si	C
0	-2.91 (-3.01)	+0.97 (+1.00)	---	+2.92 (+2.91)	-0.97 (-0.97)	---	+0.52 (+0.32)	-0.17 (-0.11)	---	+0.55 (+2.39)	-0.18 (-0.79)	---
1	-0.90 (-0.93)	+0.96 (+0.98)	-1.02 (-1.03)	+2.92 (+2.91)	-0.97 (-0.97)	-0.98 (-0.97)	+0.91 (+0.68)	-0.21 (-0.14)	-0.49 (-0.39)	+0.83 (+2.62)	-0.21 (-1.12)	-0.41 (-0.31)
2	+1.07 (+1.07)	+0.95 (+0.96)	-1.01 (-1.01)	+2.92 (+2.91)	-0.96 -0.97)	-0.98 (-0.97)	+1.26 (+1.04)	-0.25 (-0.21)	-0.50 (-0.42)	+1.12 (+2.92)	-0.24 (-2.21)	-0.44 (-0.35)
3	+2.96 (+2.95)	---	-0.98 (-0.98)	+2.92 (+2.91)	---	-0.98 (-0.97)	+1.53 (+1.38)	---	-0.51 (-0.46)	+1.36 (+1.10)	---	-0.45 (-0.36)

*Atomic charges with hydrogens summed into heavy atoms

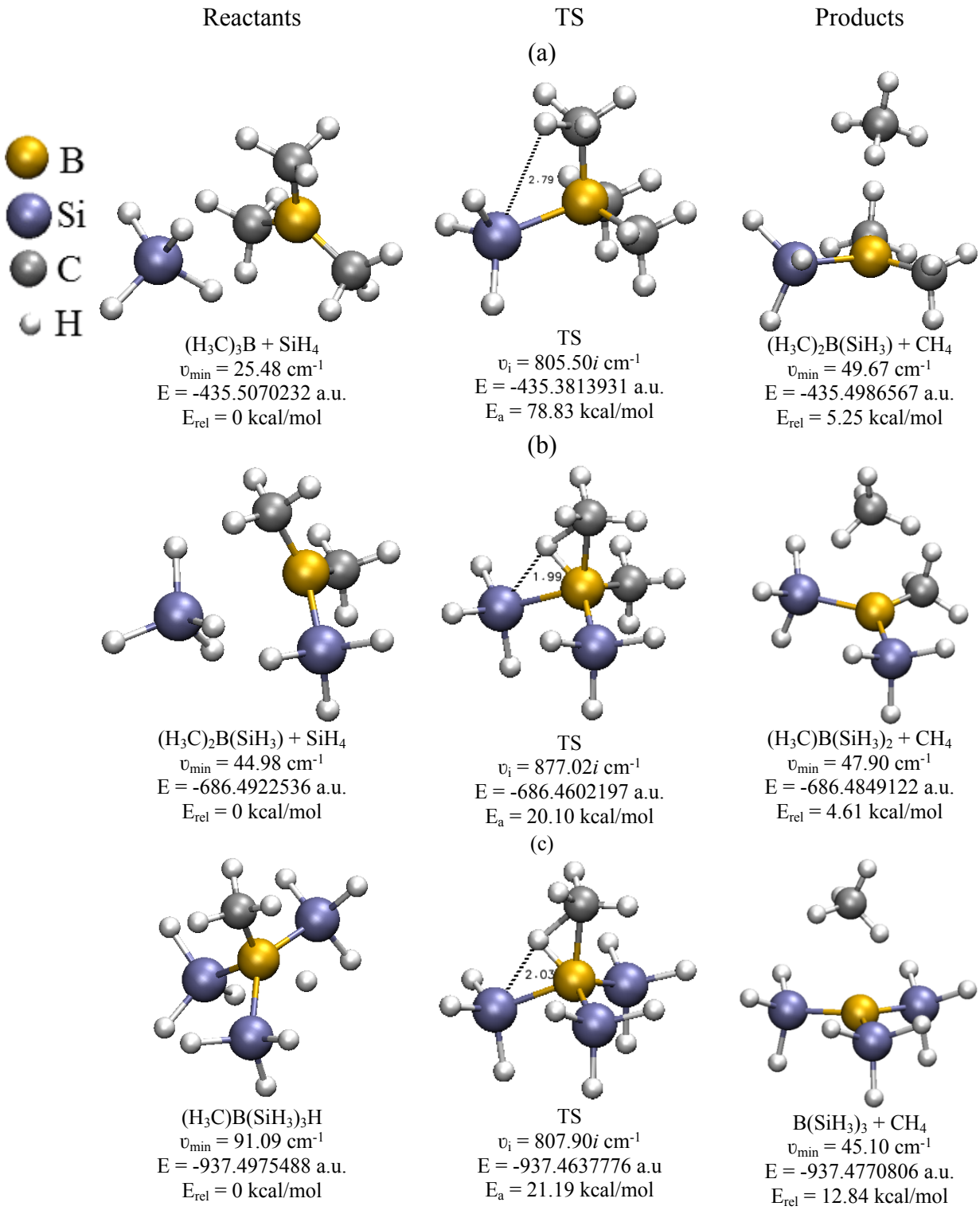


Fig. S2: Reactants, TS (one imaginary frequency), and products of the reactions with silane calculated with MP2/STQN: (a) Ia → IIa, (b) IIIa → IVa, and (c) reaction Va → VIa for X = B. In step (Va → VIa) it is observed a formation of an adduct involving the H atom, characterized as an energy minimum.

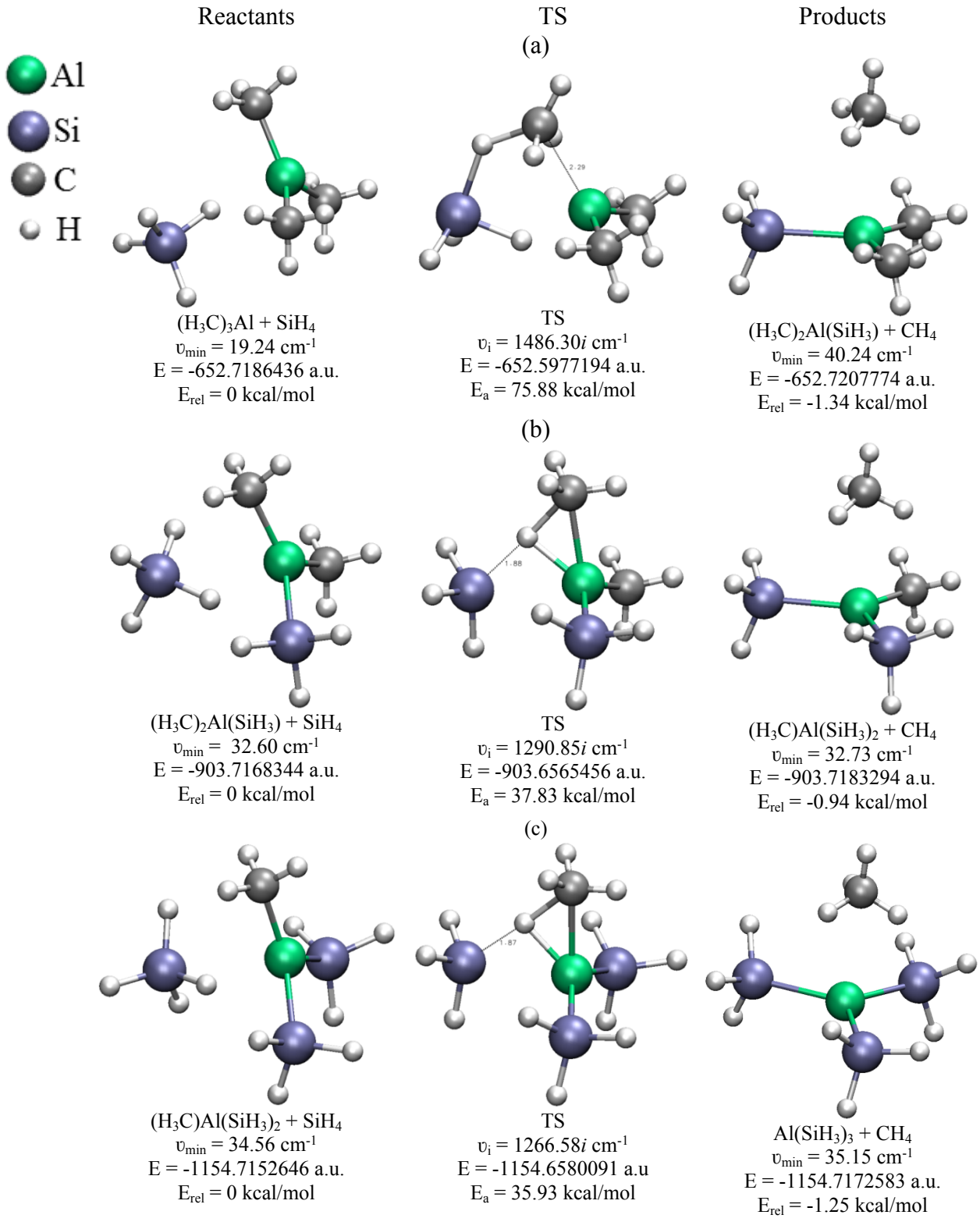


Fig. S3 Reactants, TS (one imaginary frequency), and products of the reactions with silane calculated with MP2/STQN: (a) Ib → IIb, (b) IIIb → IVb, and (c) reaction Vb → VIb for X = Al.

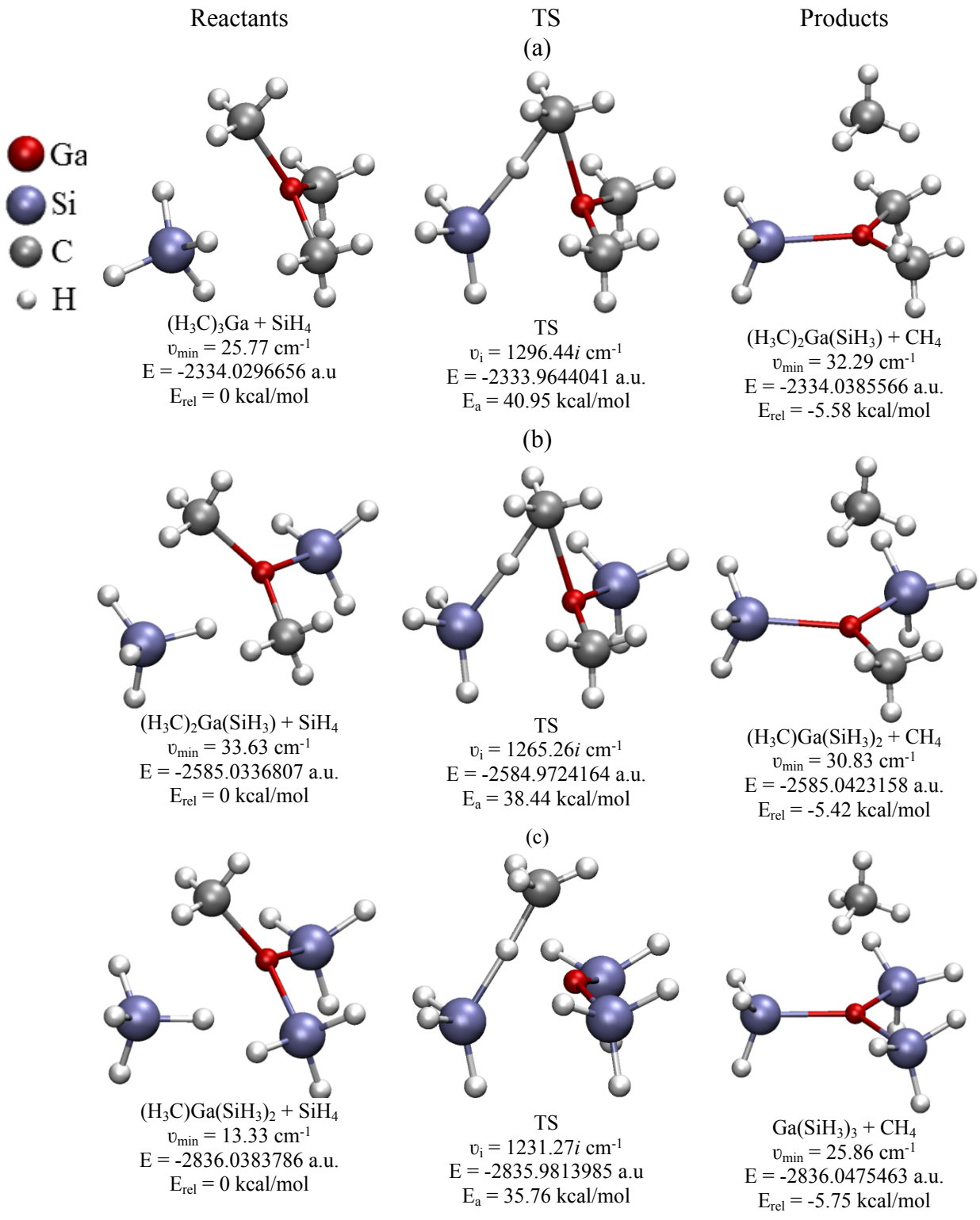


Fig. S4 Reactants, TS (one imaginary frequency), and products of the reactions with silane calculated with MP2/STQN: (a) Ic → IIc, (b) IIIc → IVc, and (c) reaction Vc → VIc for X = Ga.

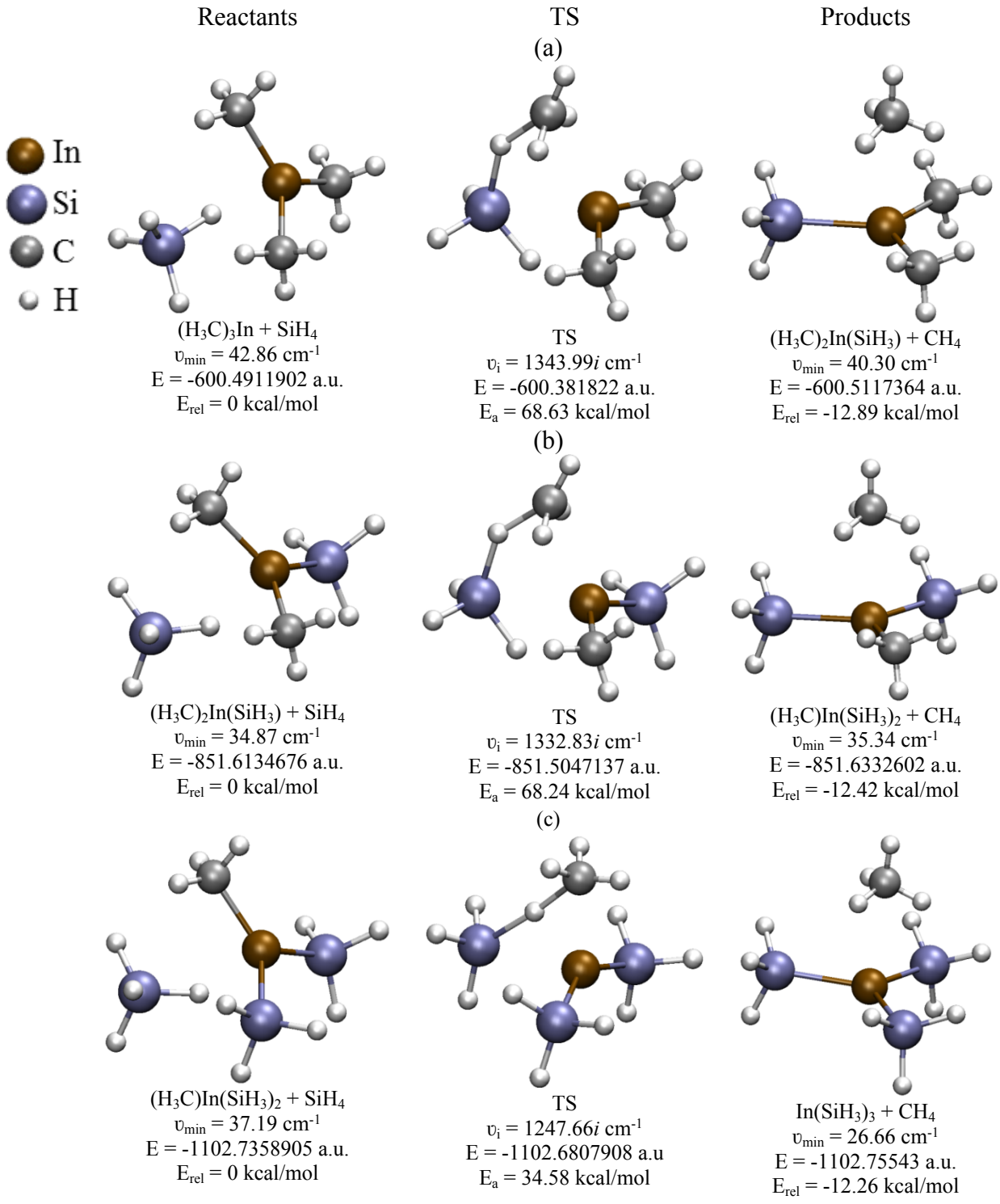


Fig. S5 Reactants, TS (one imaginary frequency), and products of the reactions with silane calculated with MP2/STQN: (a) Id → IId, (b) IIId → IVd, and (c) reaction Vd → VId for X = In.