Supporting information to the manuscript:

Thermodynamics of the condensation of the $(Me_3Sn)_8Si_8O_{20}$ building block with M–X (M = B, Al, Si, P, Ti, V, Zn, Sn, Sb, X = Cl, Me, Et) precursors by DFT-D3 calculations

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S1. Additional figures

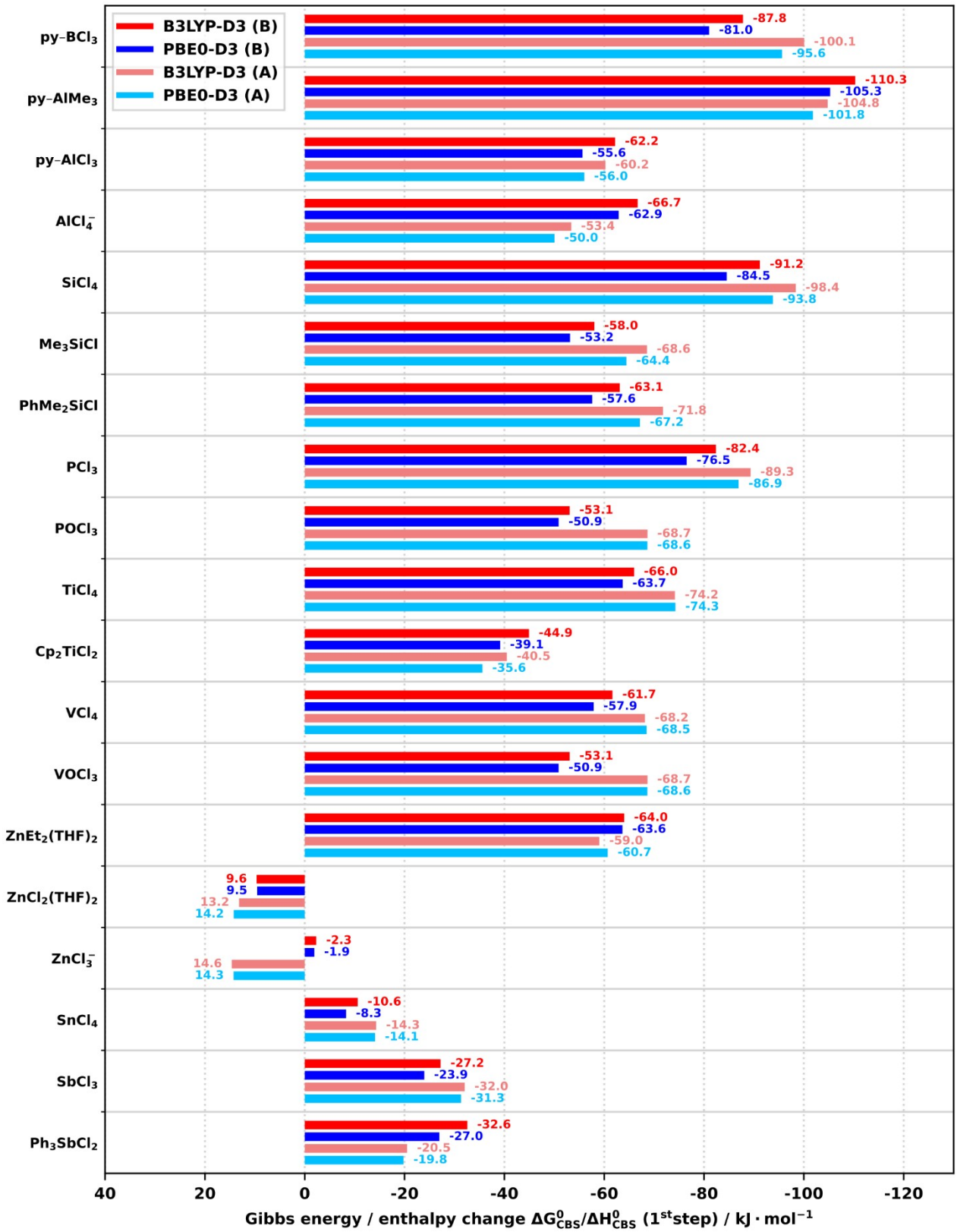

Fig. S1 Gibbs energy change of the first step of the condensation of studied precursors with models A (light) and B (dark) of CUBE at 0 K, as calculated by B3LYP-D3/CBS (red) and PBE0-D3/CBS (blue).

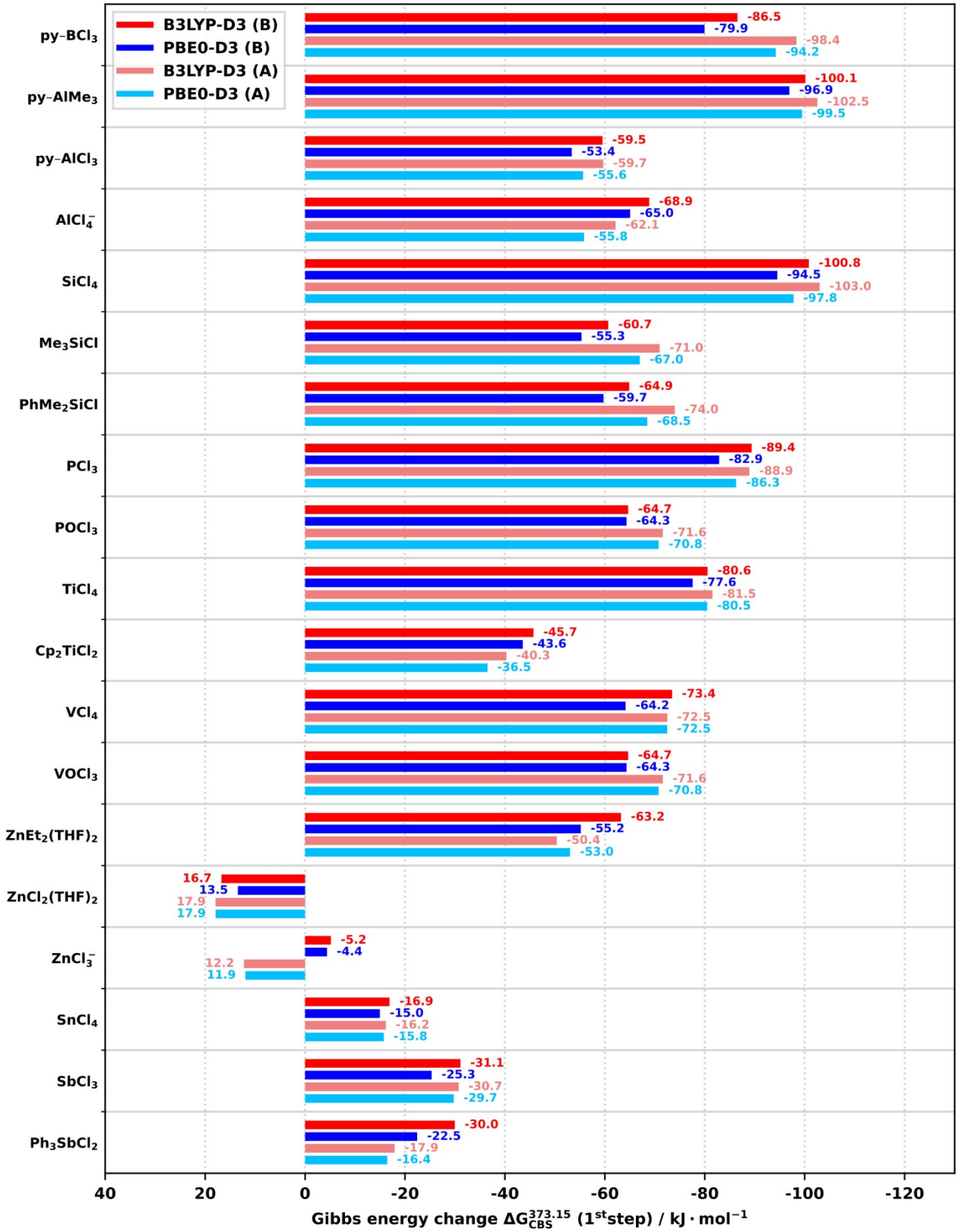

Fig. S2 Gibbs energy change of the first step of the condensation of studied precursors with models A (light) and B (dark) of CUBE at 373.15 K, as calculated by B3LYP-D3/CBS (red) and PBE0-D3/CBS (blue).

S2. Thermodynamic parameters of the model reactions

Table S1 Calculated electronic energy change and thermodynamic parameters for reaction 1A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 1A: py–$BCl_{3-x}(OSiH_3)_x$ + $Me_3SnOSiH_3$ → py–$BCl_{2-x}(OSiH_3)_{1+x}$ + $SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–102.63	–100.06	–100.20	–4.88	–98.86	–100.23	–5.01	–98.74	–100.35	–5.36	–98.35
1	–87.96	–84.25	–85.46	–19.80	–80.05	–85.53	–20.05	–79.55	–85.73	–20.65	–78.03
2	–80.19	–79.78	–79.59	2.06	–80.15	–79.62	1.95	–80.20	–79.70	1.71	–80.34
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–106.33	–103.75	–103.89	–4.88	–102.55	–103.92	–5.01	–102.43	–104.04	–5.36	–102.04
1	–92.13	–88.43	–89.63	–19.80	–84.22	–89.70	–20.05	–83.72	–89.90	–20.65	–82.20
2	–84.70	–84.29	–84.10	2.06	–84.66	–84.13	1.95	–84.71	–84.21	1.71	–84.85
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–98.04	–95.64	–95.74	–4.07	–94.63	–95.77	–4.18	–94.53	–95.88	–4.49	–94.20
1	–85.14	–81.42	–82.71	–20.65	–77.07	–82.79	–20.90	–76.56	–82.98	–21.50	–74.96
2	–79.48	–78.88	–78.66	3.28	–79.56	–78.69	3.18	–79.64	–78.78	2.92	–79.87
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–102.59	–100.19	–100.29	–4.07	–99.17	–100.32	–4.18	–99.07	–100.42	–4.49	–98.75
1	–90.15	–86.44	–87.73	–20.65	–82.09	–87.80	–20.90	–81.57	–88.00	–21.50	–79.97
2	–84.68	–84.09	–83.87	3.28	–84.76	–83.90	3.18	–84.85	–83.98	2.92	–85.07

Table S2 Calculated electronic energy change and thermodynamic parameters for reaction 2A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 2A: py–$AlMe_{3-x}(OSiH_3)_x$ + $Me_3SnOSiH_3$ → py–$AlMe_{2-x}(OSiH_3)_{1+x}$ + $SnMe_4$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–107.59	–104.78	–105.26	–7.23	–103.29	–105.32	–7.43	–103.11	–105.49	–7.92	–102.53
1	–104.14	–101.33	–101.80	–11.77	–98.58	–101.85	–11.95	–98.29	–102.00	–12.39	–97.37
2	–96.24	–94.41	–94.43	10.47	–97.29	–94.48	10.31	–97.55	–94.61	9.93	–98.31
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–107.85	–105.05	–105.53	–7.23	–103.56	–105.59	–7.43	–103.37	–105.75	–7.92	–102.80
1	–104.65	–101.83	–102.31	–11.77	–99.09	–102.36	–11.95	–98.80	–102.51	–12.39	–97.88
2	–95.40	–93.57	–93.59	10.47	–96.45	–93.64	10.31	–96.71	–93.76	9.93	–97.47
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–104.78	–101.83	–102.33	–7.55	–100.26	–102.39	–7.77	–100.07	–102.56	–8.30	–99.47
1	–101.60	–98.79	–99.18	–9.70	–96.54	–99.24	–9.88	–96.29	–99.39	–10.33	–95.53
2	–94.27	–91.68	–91.95	5.87	–93.56	–92.01	5.66	–93.70	–92.18	5.16	–94.11
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–106.29	–103.34	–103.84	–7.55	–101.77	–103.90	–7.77	–101.58	–104.07	–8.30	–100.98
1	–103.22	–100.41	–100.81	–9.70	–98.16	–100.86	–9.88	–97.92	–101.02	–10.33	–97.16
2	–94.31	–91.72	–91.99	5.87	–93.60	–92.05	5.66	–93.74	–92.22	5.16	–94.15

Table S3 Calculated electronic energy change and thermodynamic parameters for reaction 3A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 3A: py–$AlMe_{3-x}(OSiH_3)_x(THF)$ + $Me_3SnOSiH_3$ → py–$AlMe_{2-x}(OSiH_3)_{1+x}(THF)$ + $SnMe_4$											
x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–120.59	–114.63	–117.45	–45.93	–104.90	–117.57	–46.38	–103.75	–117.89	–47.32	–100.23
1	–112.88	–109.43	–110.03	–14.87	–105.97	–110.08	–15.05	–105.59	–110.24	–15.52	–104.44
2	–115.83	–113.34	–114.47	–19.39	–109.18	–114.54	–19.60	–108.69	–114.68	–20.03	–107.20
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–121.46	–115.50	–118.32	–45.93	–105.77	–118.44	–46.38	–104.62	–118.76	–47.32	–101.10
1	–114.12	–110.67	–111.27	–14.87	–107.21	–111.32	–15.05	–106.83	–111.48	–15.52	–105.69
2	–115.66	–113.17	–114.31	–19.39	–109.01	–114.37	–19.60	–108.52	–114.51	–20.03	–107.04
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–116.48	–110.64	–113.33	–44.30	–101.23	–113.45	–44.74	–100.12	–113.77	–45.68	–96.72
1	–109.80	–106.18	–106.89	–16.59	–102.36	–106.95	–16.79	–101.94	–107.12	–17.32	–100.66
2	–112.79	–110.34	–111.27	–15.35	–107.07	–111.33	–15.57	–106.69	–111.47	–16.00	–105.50
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–118.72	–112.88	–115.57	–44.30	–103.47	–115.69	–44.74	–102.35	–116.01	–45.68	–98.96
1	–112.45	–108.82	–109.53	–16.59	–105.00	–109.59	–16.79	–104.59	–109.77	–17.32	–103.31
2	–113.78	–111.33	–112.26	–15.35	–108.06	–112.32	–15.57	–107.68	–112.46	–16.00	–106.49

Table S4 Calculated electronic energy change and thermodynamic parameters for reaction 4A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 4A: py–$AlCl_{3-x}(OSiH_3)_x$ + $Me_3SnOSiH_3$ → py–$AlCl_{2-x}(OSiH_3)_{1+x}$ + $SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–60.93	–60.25	–60.07	–1.00	–59.79	–60.08	–1.03	–59.77	–60.11	–1.14	–59.69
1	–55.41	–55.80	–54.99	16.33	–59.45	–54.98	16.36	–59.86	–54.97	16.38	–61.09
2	–52.94	–52.10	–52.05	1.80	–52.54	–52.07	1.71	–52.58	–52.15	1.48	–52.70
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–62.09	–61.41	–61.23	–1.00	–60.95	–61.24	–1.03	–60.93	–61.27	–1.14	–60.85
1	–57.13	–57.53	–56.71	16.33	–61.17	–56.70	16.36	–61.58	–56.70	16.38	–62.81
2	–55.37	–54.54	–54.48	1.80	–54.98	–54.51	1.71	–55.02	–54.59	1.48	–55.14
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–56.64	–56.01	–55.82	–0.47	–55.69	–55.83	–0.49	–55.68	–55.86	–0.58	–55.64
1	–52.02	–52.22	–51.54	12.03	–54.83	–51.54	12.05	–55.13	–51.54	12.06	–56.04
2	–50.08	–48.90	–48.97	0.39	–49.08	–49.00	0.29	–49.09	–49.09	0.02	–49.10
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–58.22	–57.59	–57.40	–0.47	–57.27	–57.41	–0.49	–57.26	–57.44	–0.58	–57.22
1	–53.92	–54.12	–53.45	12.03	–56.73	–53.44	12.05	–57.03	–53.44	12.06	–57.94
2	–52.80	–51.62	–51.69	0.39	–51.80	–51.72	0.29	–51.81	–51.81	0.02	–51.82

Table S5 Calculated electronic energy change and thermodynamic parameters for reaction 5A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 5A: py–$AlCl_{3-x}(OSiH_3)_x(THF)$ + $Me_3SnOSiH_3$ → py–$AlCl_{2-x}(OSiH_3)_{1+x}(THF)$ + $SnMe_3Cl$											
x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–56.16	–55.41	–55.01	3.56	–55.98	–55.03	3.50	–56.07	–55.08	3.32	–56.32
1	–58.51	–54.92	–56.82	–35.89	–47.02	–56.90	–36.18	–46.11	–57.13	–36.85	–43.38
2	–59.66	–58.68	–58.95	–4.21	–57.80	–58.99	–4.35	–57.70	–59.09	–4.65	–57.36
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–57.70	–56.95	–56.55	3.56	–57.52	–56.57	3.50	–57.61	–56.63	3.32	–57.87
1	–60.94	–57.35	–59.25	–35.89	–49.45	–59.33	–36.18	–48.55	–59.56	–36.85	–45.81
2	–61.77	–60.79	–61.06	–4.21	–59.91	–61.10	–4.35	–59.80	–61.20	–4.65	–59.47
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–50.52	–49.77	–49.36	3.23	–50.24	–49.38	3.19	–50.33	–49.43	3.02	–50.56
1	–53.61	–50.83	–52.42	–31.14	–43.91	–52.49	–31.38	–43.14	–52.66	–31.91	–40.76
2	–55.67	–54.40	–54.79	–6.19	–53.10	–54.83	–6.34	–52.94	–54.95	–6.69	–52.45
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–52.76	–52.01	–51.60	3.23	–52.49	–51.62	3.19	–52.57	–51.67	3.02	–52.80
1	–56.80	–54.01	–55.61	–31.14	–47.10	–55.67	–31.38	–46.32	–55.85	–31.91	–43.94
2	–58.52	–57.25	–57.64	–6.19	–55.95	–57.69	–6.34	–55.80	–57.80	–6.69	–55.31

Table S6 Calculated electronic energy change and thermodynamic parameters for reaction 6A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 6A: $[AlCl_{4-x}(OSiH_3)_x]^-$ + $Me_3SnOSiH_3$ → $[AlCl_{3-x}(OSiH_3)_{1+x}]^-$ + $SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–52.65	–53.39	–52.57	25.66	–59.58	–52.57	25.65	–60.22	–52.60	25.58	–62.14
1	–52.33	–52.22	–52.05	–5.17	–50.64	–52.07	–5.23	–50.51	–52.13	–5.40	–50.11
2	–44.59	–44.67	–44.31	7.99	–46.49	–44.32	7.93	–46.69	–44.39	7.75	–47.28
3	–47.49	–46.91	–47.23	–10.97	–44.24	–47.27	–11.08	–43.96	–47.36	–11.38	–43.12
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–54.52	–55.25	–54.43	25.66	–61.44	–54.43	25.65	–62.08	–54.46	25.58	–64.00
1	–54.23	–54.13	–53.96	–5.17	–52.55	–53.98	–5.23	–52.42	–54.04	–5.40	–52.02
2	–48.67	–48.75	–48.39	7.99	–50.57	–48.41	7.93	–50.77	–48.47	7.75	–51.36
3	–50.21	–49.63	–49.95	–10.97	–46.96	–49.98	–11.08	–46.68	–50.08	–11.38	–45.84
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–49.44	–50.05	–49.37	17.36	–54.11	–49.37	17.35	–54.54	–49.39	17.29	–55.84
1	–49.36	–49.41	–49.10	4.60	–50.36	–49.12	4.55	–50.48	–49.17	4.39	–50.81
2	–41.96	–41.99	–41.69	3.26	–42.58	–41.70	3.22	–42.66	–41.75	3.06	–42.89
3	–45.75	–45.40	–45.61	–7.02	–43.70	–45.64	–7.11	–43.52	–45.72	–7.36	–42.97
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–51.28	–51.89	–51.21	17.36	–55.95	–51.21	17.35	–56.38	–51.23	17.29	–57.68
1	–51.18	–51.23	–50.92	4.60	–52.18	–50.94	4.55	–52.30	–50.99	4.39	–52.63
2	–46.09	–46.12	–45.81	3.26	–46.70	–45.83	3.22	–46.79	–45.88	3.06	–47.02
3	–48.28	–47.93	–48.14	–7.02	–46.22	–48.17	–7.11	–46.05	–48.25	–7.36	–45.50

Table S7 Calculated electronic energy change and thermodynamic parameters for reaction 7A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 7A: $SiCl_{4-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow SiCl_{3-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–99.64	–98.38	–97.83	13.82	–101.60	–97.83	13.79	–101.95	–97.87	13.69	–102.98
1	–100.19	–98.51	–98.43	1.81	–98.93	–98.45	1.75	–98.97	–98.50	1.59	–99.10
2	–95.47	–93.38	–93.47	–2.48	–92.80	–93.51	–2.59	–92.73	–93.61	–2.89	–92.53
3	–90.71	–86.52	–88.17	–29.37	–80.14	–88.25	–29.67	–79.41	–88.49	–30.37	–77.15
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–100.69	–99.42	–98.87	13.82	–102.65	–98.88	13.79	–102.99	–98.92	13.69	–104.03
1	–101.01	–99.33	–99.25	1.81	–99.75	–99.27	1.75	–99.79	–99.32	1.59	–99.92
2	–97.58	–95.49	–95.59	–2.48	–94.91	–95.62	–2.59	–94.85	–95.72	–2.89	–94.64
3	–91.62	–87.43	–89.08	–29.37	–81.05	–89.16	–29.67	–80.32	–89.40	–30.37	–78.06
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–94.93	–93.79	–93.26	12.07	–96.56	–93.27	12.07	–96.87	–93.28	12.01	–97.77
1	–95.39	–93.30	–93.52	–3.91	–92.45	–93.55	–4.00	–92.36	–93.62	–4.22	–92.05
2	–91.89	–90.26	–90.05	5.82	–91.63	–90.07	5.74	–91.78	–90.15	5.50	–92.20
3	–86.89	–83.06	–84.67	–32.65	–75.75	–84.75	–32.90	–74.94	–84.95	–33.50	–72.44
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–96.51	–95.37	–94.84	12.07	–98.14	–94.85	12.07	–98.44	–94.86	12.01	–99.35
1	–97.08	–95.00	–95.22	–3.91	–94.15	–95.24	–4.00	–94.05	–95.32	–4.22	–93.74
2	–93.97	–92.34	–92.13	5.82	–93.72	–92.15	5.74	–93.86	–92.23	5.50	–94.28
3	–88.14	–84.31	–85.92	–32.65	–77.00	–85.99	–32.90	–76.18	–86.19	–33.50	–73.69

Table S8 Calculated electronic energy change and thermodynamic parameters for reaction 8A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 8A: $Me_3SiCl + Me_3SnOSiH_3 \rightarrow Me_3SiOSiH_3 + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–69.32	–68.56	–68.34	7.06	–70.27	–68.35	7.01	–70.44	–68.40	6.86	–70.96
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–71.51	–70.75	–70.53	7.06	–72.46	–70.54	7.01	–72.63	–70.59	6.86	–73.15
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–65.33	–64.44	–64.28	7.27	–66.26	–64.30	7.21	–66.45	–64.35	7.05	–66.98
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–67.72	–66.83	–66.66	7.27	–68.65	–66.68	7.21	–68.83	–66.73	7.05	–69.36

Table S9 Calculated electronic energy change and thermodynamic parameters for reaction 9A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 9A: $PhMe_2SiCl + Me_3SnOSiH_3 \rightarrow PhMe_2SiOSiH_3 + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–72.03	–71.77	–71.38	7.04	–73.30	–71.38	7.02	–73.48	–71.41	6.94	–74.00
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–74.15	–73.88	–73.49	7.04	–75.42	–73.50	7.02	–75.59	–73.53	6.94	–76.12
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–67.60	–67.17	–66.89	4.29	–68.06	–66.90	4.27	–68.17	–66.93	4.19	–68.49
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–70.33	–69.89	–69.61	4.29	–70.79	–69.62	4.27	–70.89	–69.65	4.19	–71.21

Table S10 Calculated electronic energy change and thermodynamic parameters for reaction 10A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 10A: $PCl_{3-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow PCl_{2-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–90.91	–89.32	–89.42	–1.31	–89.07	–89.43	–1.35	–89.03	–89.46	–1.41	–88.93
1	–82.54	–79.61	–80.56	–15.64	–76.28	–80.61	–15.82	–75.89	–80.74	–16.21	–74.69
2	–72.37	–70.88	–71.51	–9.76	–68.85	–71.55	–9.90	–68.60	–71.64	–10.17	–67.85
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–93.13	–91.55	–91.65	–1.31	–91.29	–91.66	–1.35	–91.26	–91.68	–1.41	–91.15
1	–83.56	–80.62	–81.57	–15.64	–77.29	–81.62	–15.82	–76.90	–81.75	–16.21	–75.70
2	–73.96	–72.48	–73.10	–9.76	–70.44	–73.14	–9.90	–70.19	–73.23	–10.17	–69.44
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–88.42	–86.93	–87.05	–2.03	–86.50	–87.06	–2.06	–86.45	–87.08	–2.11	–86.29
1	–81.39	–78.41	–79.42	–16.57	–74.89	–79.47	–16.75	–74.48	–79.60	–17.14	–73.20
2	–72.59	–71.53	–71.94	–6.21	–70.24	–71.97	–6.31	–70.09	–72.03	–6.50	–69.60
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–90.83	–89.34	–89.46	–2.03	–88.91	–89.47	–2.06	–88.86	–89.49	–2.11	–88.70
1	–82.82	–79.83	–80.84	–16.57	–76.32	–80.89	–16.75	–75.90	–81.02	–17.14	–74.63
2	–74.79	–73.73	–74.14	–6.21	–72.44	–74.17	–6.31	–72.29	–74.23	–6.50	–71.80

Table S11 Calculated electronic energy change and thermodynamic parameters for reaction 11A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 11A: $POCl_{3-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow POCl_{2-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–111.60	–109.38	–109.41	1.08	–109.70	–109.43	0.99	–109.73	–109.50	0.79	–109.80
1	–109.39	–106.33	–106.82	–4.95	–105.46	–106.87	–5.16	–105.34	–107.03	–5.63	–104.93
2	–106.44	–104.29	–104.51	0.96	–104.77	–104.56	0.78	–104.79	–104.69	0.38	–104.84
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–113.54	–111.32	–111.35	1.08	–111.64	–111.37	0.99	–111.67	–111.44	0.79	–111.73
1	–111.08	–108.01	–108.50	–4.95	–107.15	–108.56	–5.16	–107.02	–108.72	–5.63	–106.62
2	–108.80	–106.64	–106.86	0.96	–107.13	–106.92	0.78	–107.15	–107.05	0.38	–107.19
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–110.19	–108.11	–108.15	0.59	–108.31	–108.17	0.52	–108.32	–108.22	0.35	–108.35
1	–108.36	–105.61	–105.93	–0.37	–105.83	–105.98	–0.55	–105.82	–106.12	–0.97	–105.76
2	–110.27	–107.21	–108.28	–18.99	–103.09	–108.34	–19.20	–102.62	–108.50	–19.67	–101.16
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–112.31	–110.23	–110.26	0.59	–110.42	–110.28	0.52	–110.44	–110.34	0.35	–110.47
1	–110.70	–107.95	–108.27	–0.37	–108.17	–108.32	–0.55	–108.16	–108.46	–0.97	–108.10
2	–113.27	–110.21	–111.28	–18.99	–106.09	–111.34	–19.20	–105.62	–111.50	–19.67	–104.16

Table S12 Calculated electronic energy change and thermodynamic parameters for reaction 12A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 12A: $TiCl_{4-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow TiCl_{3-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–73.40	–74.17	–73.22	22.22	–79.29	–73.17	22.37	–79.84	–73.06	22.72	–81.54
1	–65.51	–65.66	–65.22	4.42	–66.42	–65.19	4.52	–66.53	–65.12	4.72	–66.88
2	–58.91	–59.26	–58.59	11.15	–61.64	–58.57	11.23	–61.92	–58.52	11.38	–62.77
3	–52.52	–53.24	–52.45	15.46	–56.68	–52.43	15.53	–57.06	–52.39	15.66	–58.23
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–75.28	–76.04	–75.09	22.22	–81.16	–75.05	22.37	–81.72	–74.93	22.72	–83.41
1	–67.48	–67.63	–67.19	4.42	–68.40	–67.16	4.52	–68.51	–67.09	4.72	–68.85
2	–60.78	–61.13	–60.46	11.15	–63.50	–60.44	11.23	–63.78	–60.39	11.38	–64.63
3	–54.60	–55.32	–54.53	15.46	–58.75	–54.51	15.53	–59.14	–54.46	15.66	–60.31
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–73.62	–74.27	–73.42	18.87	–78.57	–73.38	19.02	–79.05	–73.26	19.36	–80.49
1	–65.78	–66.04	–65.52	7.80	–67.65	–65.50	7.89	–67.85	–65.42	8.11	–68.45
2	–59.13	–59.57	–58.89	14.04	–62.72	–58.87	14.13	–63.08	–58.81	14.29	–64.14
3	–52.78	–53.46	–52.70	13.75	–56.46	–52.68	13.83	–56.81	–52.64	13.97	–57.85
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–75.88	–76.53	–75.68	18.87	–80.83	–75.64	19.02	–81.31	–75.52	19.36	–82.75
1	–67.94	–68.20	–67.68	7.80	–69.81	–67.65	7.89	–70.01	–67.58	8.11	–70.61
2	–61.19	–61.62	–60.94	14.04	–64.78	–60.92	14.13	–65.13	–60.86	14.29	–66.19
3	–55.02	–55.70	–54.94	13.75	–58.70	–54.92	13.83	–59.04	–54.87	13.97	–60.09

Table S13 Calculated electronic energy change and thermodynamic parameters for reaction 13A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 13A: $Cp_2TiCl_{2-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow Cp_2TiCl_{1-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–39.34	–40.49	–40.24	0.14	–40.28	–40.22	0.20	–40.28	–40.16	0.39	–40.31
1	–31.45	–33.01	–32.58	0.77	–32.79	–32.55	0.87	–32.81	–32.47	1.11	–32.88
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–41.87	–43.02	–42.77	0.14	–42.80	–42.75	0.20	–42.81	–42.69	0.39	–42.83
1	–34.38	–35.94	–35.50	0.77	–35.72	–35.48	0.87	–35.74	–35.40	1.11	–35.81
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–34.37	–35.59	–35.15	3.60	–36.13	–35.12	3.69	–36.22	–35.06	3.87	–36.50
1	–28.17	–29.93	–29.21	8.92	–31.65	–29.19	9.03	–31.88	–29.11	9.25	–32.56
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–38.34	–39.57	–39.12	3.60	–40.11	–39.10	3.69	–40.20	–39.04	3.87	–40.48
1	–32.04	–33.80	–33.08	8.92	–35.52	–33.05	9.03	–35.75	–32.98	9.25	–36.43

Table S14 Calculated electronic energy change and thermodynamic parameters for reaction 14A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 14A: $VCl_{4-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow VCl_{3-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–67.21	–68.16	–67.37	13.68	–71.10	–67.31	13.86	–71.45	–67.17	14.28	–72.50
1	–65.56	–65.03	–64.89	1.49	–65.30	–64.88	1.53	–65.33	–64.85	1.61	–65.45
2	–46.45	–45.88	–46.10	–5.40	–44.63	–46.11	–5.43	–44.49	–46.12	–5.46	–44.09
3	–39.10	–38.38	–38.80	–10.89	–35.83	–38.81	–10.91	–35.56	–38.83	–10.96	–34.74
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–69.15	–70.09	–69.30	13.68	–73.04	–69.25	13.86	–73.38	–69.11	14.28	–74.44
1	–67.36	–66.83	–66.69	1.49	–67.10	–66.68	1.53	–67.13	–66.65	1.61	–67.25
2	–49.07	–48.49	–48.72	–5.40	–47.24	–48.73	–5.43	–47.11	–48.74	–5.46	–46.70
3	–41.85	–41.13	–41.55	–10.89	–38.58	–41.56	–10.91	–38.30	–41.57	–10.96	–37.48
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–67.66	–68.50	–67.79	12.40	–71.18	–67.75	12.57	–71.50	–67.61	12.98	–72.45
1	–66.28	–65.86	–65.68	2.67	–66.41	–65.67	2.71	–66.48	–65.63	2.82	–66.68
2	–47.22	–46.49	–46.82	–8.10	–44.61	–46.83	–8.14	–44.41	–46.85	–8.20	–43.79
3	–39.63	–38.35	–39.13	–17.88	–34.24	–39.14	–17.94	–33.80	–39.19	–18.07	–32.44
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–69.96	–70.80	–70.09	12.40	–73.48	–70.04	12.57	–73.79	–69.91	12.98	–74.75
1	–68.12	–67.69	–67.51	2.67	–68.24	–67.50	2.71	–68.31	–67.47	2.82	–68.52
2	–49.89	–49.16	–49.49	–8.10	–47.28	–49.50	–8.14	–47.08	–49.52	–8.20	–46.46
3	–42.21	–40.92	–41.70	–17.88	–36.82	–41.72	–17.94	–36.37	–41.76	–18.07	–35.02

Table S15 Calculated electronic energy change and thermodynamic parameters for reaction 15A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 15A: $VOCl_{3-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow VOCl_{2-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–68.64	–68.67	–68.29	8.86	–70.71	–68.27	8.91	–70.93	–68.21	9.10	–71.61
1	–61.42	–60.51	–60.65	–4.13	–59.52	–60.65	–4.14	–59.42	–60.66	–4.15	–59.11
2	–54.26	–54.71	–54.10	15.07	–58.22	–54.09	15.11	–58.60	–54.06	15.21	–59.74
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–70.78	–70.81	–70.44	8.86	–72.86	–70.42	8.91	–73.08	–70.36	9.10	–73.75
1	–63.35	–62.44	–62.58	–4.13	–61.45	–62.58	–4.14	–61.35	–62.58	–4.15	–61.04
2	–55.76	–56.21	–55.60	15.07	–59.72	–55.59	15.11	–60.10	–55.56	15.21	–61.24
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–68.73	–68.64	–68.37	6.40	–70.12	–68.36	6.45	–70.28	–68.31	6.61	–70.77
1	–61.85	–61.26	–61.20	0.87	–61.43	–61.20	0.88	–61.46	–61.18	0.91	–61.52
2	–54.39	–54.86	–54.33	10.95	–57.32	–54.32	11.00	–57.59	–54.27	11.12	–58.42
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–71.20	–71.12	–70.85	6.40	–72.60	–70.84	6.45	–72.76	–70.78	6.61	–73.25
1	–63.55	–62.96	–62.89	0.87	–63.13	–62.89	0.88	–63.15	–62.88	0.91	–63.22
2	–56.37	–56.84	–56.31	10.95	–59.30	–56.30	11.00	–59.58	–56.26	11.12	–60.40

Table S16 Calculated electronic energy change and thermodynamic parameters for reaction 16A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 16A: $ZnEt_{2-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow ZnEt_{1-x}(OSiH_3)_{1+x} + SnMe_3Et$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–28.66	–26.61	–27.31	–11.46	–24.18	–17.42	–11.55	–13.98	–27.41	–11.76	–23.02
1	12.93	13.04	12.54	–6.41	14.29	2.62	–6.41	4.53	12.56	–6.35	14.93
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–26.18	–24.13	–24.83	–11.46	–21.70	–14.94	–11.55	–11.50	–24.93	–11.76	–20.54
1	17.81	17.92	17.41	–6.41	19.17	7.50	–6.41	9.41	17.44	–6.35	19.81
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–29.98	–28.04	–28.65	–9.59	–26.03	–28.68	–9.68	–25.79	–28.75	–9.90	–25.06
1	9.63	9.73	9.35	–3.82	10.40	9.36	–3.81	10.49	9.37	–3.76	10.77
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–28.18	–26.24	–26.86	–9.59	–24.24	–26.88	–9.68	–24.00	–26.96	–9.90	–23.26
1	13.44	13.55	13.17	–3.82	14.21	13.17	–3.81	14.31	13.19	–3.76	14.59

Table S17 Calculated electronic energy change and thermodynamic parameters for reaction 17A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 17A: $ZnEt_{2-x}(OSiH_3)_x(THF) + Me_3SnOSiH_3 \rightarrow ZnEt_{1-x}(OSiH_3)_{1+x}(THF) + SnMe_3Et$											
x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–45.48	–44.18	–45.06	–13.33	–41.42	–45.09	–13.41	–41.09	–45.14	–13.56	–40.08
1	–14.43	–12.22	–13.04	–10.38	–10.21	–13.07	–10.48	–9.95	–13.14	–10.68	–9.15
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–44.22	–42.91	–43.80	–13.33	–40.16	–43.82	–13.41	–39.83	–43.87	–13.56	–38.81
1	–10.95	–8.74	–9.56	–10.38	–6.73	–9.59	–10.48	–6.47	–9.66	–10.68	–5.67
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–46.36	–45.39	–45.91	–0.91	–45.67	–45.94	–0.98	–45.64	–45.98	–1.11	–45.56
1	–18.01	–15.29	–16.41	–22.58	–10.24	–16.44	–22.70	–9.67	–16.52	–22.94	–7.96
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–45.60	–44.63	–45.16	–0.91	–44.91	–45.18	–0.98	–44.88	–45.22	–1.11	–44.81
1	–15.35	–12.64	–13.76	–22.58	–7.59	–13.79	–22.70	–7.02	–13.87	–22.94	–5.31

Table S18 Calculated electronic energy change and thermodynamic parameters for reaction 18A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 18A: $ZnEt_{2-x}(OSiH_3)_x(THF)_2 + Me_3SnOSiH_3 \rightarrow ZnEt_{1-x}(OSiH_3)_{1+x}(THF)_2 + SnMe_3Et$											
x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–63.03	–59.03	–60.87	–28.02	–53.22	–60.93	–28.23	–52.52	–61.09	–28.69	–50.38
1	–38.92	–34.81	–36.90	–31.37	–28.33	–36.97	–31.61	–27.54	–37.13	–32.09	–25.15
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–62.15	–58.16	–60.00	–28.02	–52.34	–60.06	–28.23	–51.64	–60.21	–28.69	–49.50
1	–36.21	–32.10	–34.19	–31.37	–25.62	–34.26	–31.61	–24.84	–34.42	–32.09	–22.45
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–64.49	–60.71	–62.37	–24.94	–55.56	–62.43	–25.14	–54.93	–62.57	–25.59	–53.03
1	–40.75	–36.83	–38.71	–25.97	–31.62	–38.78	–26.20	–30.97	–38.93	–26.67	–28.98
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–63.85	–60.07	–61.73	–24.94	–54.92	–61.79	–25.14	–54.29	–61.94	–25.59	–52.39
1	–38.76	–34.84	–36.72	–25.97	–29.63	–36.79	–26.20	–28.98	–36.95	–26.67	–26.99

Table S19 Calculated electronic energy change and thermodynamic parameters for reaction 19A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 19A: $ZnCl_{2-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow ZnCl_{1-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	12.77	11.83	11.72	23.80	5.22	11.64	23.51	4.63	11.37	22.72	2.89
1	13.51	13.27	13.61	5.60	12.08	13.62	5.65	11.94	13.65	5.75	11.51
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	12.85	11.91	11.80	23.80	5.30	11.72	23.51	4.71	11.45	22.72	2.97
1	12.78	12.54	12.88	5.60	11.35	12.89	5.65	11.21	12.93	5.75	10.78
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	13.45	12.55	12.44	24.97	5.61	12.35	24.68	4.99	12.09	23.89	3.17
1	14.67	14.45	14.78	4.60	13.52	14.79	4.65	13.41	14.83	4.75	13.05
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	13.18	12.28	12.16	24.97	5.34	12.08	24.68	4.72	11.81	23.89	2.90
1	13.30	13.08	13.41	4.60	12.16	13.43	4.65	12.04	13.46	4.75	11.69

Table S20 Calculated electronic energy change and thermodynamic parameters for reaction 20A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 20A: $ZnCl_{2-x}(OSiH_3)_x(THF) + Me_3SnOSiH_3 \rightarrow ZnCl_{1-x}(OSiH_3)_{1+x}(THF) + SnMe_3Cl$											
x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	13.11	12.37	12.66	1.77	12.18	12.68	1.82	12.13	12.71	1.92	11.99
1	16.77	16.85	16.98	–2.06	17.55	16.98	–2.08	17.60	16.96	–2.14	17.76
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	12.33	11.59	11.88	1.77	11.40	11.90	1.82	11.35	11.93	1.92	11.21
1	14.94	15.02	15.16	–2.06	15.72	15.15	–2.08	15.77	15.13	–2.14	15.93
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	14.07	13.30	13.62	2.92	12.83	13.64	2.97	12.75	13.67	3.08	12.52
1	17.74	18.00	18.01	–5.68	19.56	18.00	–5.70	19.70	17.98	–5.77	20.14
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	12.65	11.88	12.21	2.92	11.41	12.22	2.97	11.33	12.26	3.08	11.11
1	15.22	15.48	15.49	–5.68	17.04	15.49	–5.70	17.18	15.46	–5.77	17.62

Table S21 Calculated electronic energy change and thermodynamic parameters for reaction 21A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 21A: $ZnCl_{2-x}(OSiH_3)_x(THF)_2 + Me_3SnOSiH_3 \rightarrow ZnCl_{1-x}(OSiH_3)_{1+x}(THF)_2 + SnMe_3Cl$											
x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	13.64	13.17	13.25	–12.61	16.69	13.26	–12.57	17.01	13.29	–12.48	17.95
1	15.99	16.35	15.77	–13.49	19.45	15.75	–13.57	19.79	15.69	–13.74	20.81
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	11.51	11.04	11.12	–12.61	14.57	11.13	–12.57	14.88	11.16	–12.48	15.82
1	14.19	14.55	13.97	–13.49	17.65	13.95	–13.57	17.99	13.89	–13.74	19.01
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	14.62	14.22	14.33	–9.63	16.96	14.35	–9.59	17.20	14.37	–9.50	17.92
1	17.20	16.99	16.69	–8.92	19.12	16.67	–8.96	19.34	16.64	–9.06	20.02
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	11.84	11.44	11.55	–9.63	14.18	11.56	–9.59	14.42	11.59	–9.50	15.14
1	14.80	14.59	14.29	–8.92	16.72	14.28	–8.96	16.95	14.24	–9.06	17.62

Table S22 Calculated electronic energy change and thermodynamic parameters for reaction 22A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 22A: $[ZnCl_{3-x}(OSiH_3)_x]^-$ + $Me_3SnOSiH_3$ → $[ZnCl_{2-x}(OSiH_3)_{1+x}]^-$ + $SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	16.26	14.63	15.11	7.73	13.00	15.12	7.75	12.81	15.13	7.80	12.22
1	18.33	17.46	17.53	2.39	16.88	17.53	2.37	16.82	17.51	2.32	16.64
2	19.49	16.72	17.84	18.73	12.72	17.87	18.83	12.25	17.94	19.05	10.83
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	14.05	12.43	12.91	7.73	10.80	12.91	7.75	10.60	12.93	7.80	10.02
1	16.50	15.62	15.69	2.39	15.04	15.69	2.37	14.98	15.67	2.32	14.80
2	16.64	13.86	14.99	18.73	9.87	15.01	18.83	9.40	15.09	19.05	7.98
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	15.77	14.25	14.70	7.48	12.65	14.70	7.50	12.46	14.71	7.53	11.90
1	17.92	17.15	17.17	0.89	16.93	17.17	0.88	16.90	17.15	0.82	16.84
2	19.34	16.68	17.79	18.55	12.72	17.81	18.65	12.25	17.89	18.87	10.85
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	13.52	12.01	12.45	7.48	10.41	12.46	7.50	10.22	12.47	7.53	9.66
1	16.04	15.27	15.29	0.89	15.04	15.28	0.88	15.02	15.26	0.82	14.96
2	16.18	13.52	14.63	18.55	9.56	14.65	18.65	9.09	14.73	18.87	7.69

Table S23 Calculated electronic energy change and thermodynamic parameters for reaction 23A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 23A: $SnCl_{4-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow SnCl_{3-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)											
0	–14.10	–14.31	–13.95	5.92	–15.56	–13.93	5.98	–15.71	–13.87	6.14	–16.17
1	–13.76	–12.85	–13.18	–8.20	–10.94	–13.18	–8.20	–10.73	–13.18	–8.19	–10.12
2	–13.13	–11.89	–12.49	–15.70	–8.20	–12.50	–15.74	–7.81	–12.52	–15.81	–6.62
3	–12.77	–12.78	–12.80	–1.44	–12.41	–12.80	–1.42	–12.37	–12.76	–1.30	–12.27
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–11.94	–12.15	–11.79	5.92	–13.40	–11.77	5.98	–13.55	–11.72	6.14	–14.01
1	–11.35	–10.43	–10.76	–8.20	–8.52	–10.76	–8.20	–8.32	–10.76	–8.19	–7.70
2	–11.67	–10.43	–11.03	–15.70	–6.74	–11.04	–15.74	–6.35	–11.06	–15.81	–5.16
3	–13.49	–13.50	–13.53	–1.44	–13.13	–13.52	–1.42	–13.10	–13.48	–1.30	–13.00
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)											
0	–13.92	–14.09	–13.75	5.34	–15.21	–13.73	5.40	–15.34	–13.68	5.54	–15.75
1	–14.11	–13.34	–13.63	–6.48	–11.86	–13.63	–6.48	–11.70	–13.62	–6.46	–11.21
2	–13.33	–11.90	–12.58	–18.03	–7.66	–12.60	–18.08	–7.21	–12.63	–18.19	–5.85
3	–13.10	–13.42	–13.29	1.74	–13.76	–13.27	1.80	–13.81	–13.22	1.96	–13.95
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)											
0	–11.78	–11.95	–11.61	5.34	–13.06	–11.59	5.40	–13.20	–11.54	5.54	–13.61
1	–11.23	–10.46	–10.75	–6.48	–8.98	–10.75	–6.48	–8.82	–10.74	–6.46	–8.33
2	–11.62	–10.19	–10.87	–18.03	–5.95	–10.89	–18.08	–5.50	–10.92	–18.19	–4.14
3	–13.52	–13.84	–13.70	1.74	–14.18	–13.69	1.80	–14.23	–13.64	1.96	–14.37

Table S24 Calculated electronic energy change and thermodynamic parameters for reaction 24A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 24A: $SbCl_{3-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow SbCl_{2-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // B3LYP–D3/CBS(D, T, Q)											
0	–32.56	–32.04	–32.20	–3.94	–31.13	–32.20	–3.92	–31.03	–32.16	–3.82	–30.74
1	–30.03	–29.25	–29.61	–8.56	–27.27	–29.61	–8.57	–27.06	–29.61	–8.55	–26.42
2	–25.67	–25.31	–25.43	0.04	–25.44	–25.43	0.03	–25.44	–25.43	0.03	–25.44
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)											
0	–29.87	–29.35	–29.51	–3.94	–28.43	–29.50	–3.92	–28.34	–29.47	–3.82	–28.05
1	–27.13	–26.35	–26.71	–8.56	–24.37	–26.71	–8.57	–24.16	–26.70	–8.55	–23.52
2	–22.83	–22.46	–22.58	0.04	–22.59	–22.59	0.03	–22.60	–22.59	0.03	–22.60
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // PBE0–D3/CBS(D, T, Q)											
0	–31.84	–31.29	–31.50	–4.74	–30.21	–31.50	–4.72	–30.09	–31.47	–4.64	–29.74
1	–29.94	–29.16	–29.56	–9.23	–27.04	–29.56	–9.23	–26.81	–29.55	–9.21	–26.12
2	–26.29	–25.74	–26.02	–3.74	–24.99	–26.03	–3.77	–24.90	–26.04	–3.81	–24.62
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)											
0	–29.29	–28.75	–28.96	–4.74	–27.66	–28.95	–4.72	–27.54	–28.92	–4.64	–27.19
1	–26.79	–26.02	–26.41	–9.23	–23.89	–26.41	–9.23	–23.66	–26.40	–9.21	–22.97
2	–23.37	–22.83	–23.10	–3.74	–22.08	–23.11	–3.77	–21.99	–23.12	–3.81	–21.70

Table S25 Calculated electronic energy change and thermodynamic parameters for reaction 25A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 25A: $Ph_3SbCl_{2-x}(OSiH_3)_x + Me_3SnOSiH_3 \rightarrow Ph_3SbCl_{1-x}(OSiH_3)_{1+x} + SnMe_3Cl$

x	ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // B3LYP–D3/CBS(D, T, Q)											
0	–21.35	–20.51	–21.02	–8.21	–18.78	–21.04	–8.28	–18.57	–21.08	–8.41	–17.94
1	–27.06	–26.14	–27.22	–23.24	–20.87	–27.25	–23.35	–20.29	–27.31	–23.51	–18.53
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)											
0	–20.86	–20.03	–20.54	–8.21	–18.29	–20.55	–8.28	–18.09	–20.60	–8.41	–17.46
1	–28.04	–27.13	–28.21	–23.24	–21.86	–28.24	–23.35	–21.28	–28.29	–23.51	–19.52
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // PBE0–D3/CBS(D, T, Q)											
0	–20.64	–19.80	–20.37	–10.54	–17.49	–20.39	–10.61	–17.23	–20.44	–10.75	–16.43
1	–27.00	–26.21	–27.25	–20.81	–21.56	–27.28	–20.92	–21.04	–27.32	–21.06	–19.46
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)											
0	–20.91	–20.07	–20.64	–10.54	–17.76	–20.66	–10.61	–17.50	–20.71	–10.75	–16.70
1	–28.61	–27.82	–28.86	–20.81	–23.17	–28.89	–20.92	–22.65	–28.93	–21.06	–21.07

Table S26 Calculated electronic energy change and thermodynamic parameters for reaction 26A at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 26A: $Cl^- + Me_3SnOSiH_3 \rightarrow SnMe_3Cl + H_3SiO^-$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
52.46	45.39	44.03	40.95	32.85	43.77	40.02	31.83	42.95	37.57	28.93
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
43.35	36.28	34.92	40.95	23.73	34.65	40.02	22.72	33.84	37.57	19.82
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
47.31	40.52	39.11	40.14	28.14	38.84	39.20	27.15	38.02	36.74	24.31
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
38.75	31.97	30.55	40.14	19.59	30.28	39.20	18.59	29.46	36.74	15.75

Table S27 Calculated electronic energy change and thermodynamic parameters for reaction 1B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 1B: py–BCl_3 + $Me_3SnOSi(OSiH_3)_3$ → py–$BCl_2OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–88.83	–87.81	–87.25	–1.87	–86.74	–87.26	–1.89	–86.69	–87.31	–2.05	–86.55
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–93.97	–92.95	–92.40	–1.87	–91.89	–92.40	–1.89	–91.84	–92.46	–2.05	–91.69
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–82.42	–81.03	–80.65	–1.87	–80.14	–80.66	–1.92	–80.09	–80.74	–2.13	–79.94
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–88.66	–87.27	–86.89	–1.87	–86.38	–86.90	–1.92	–86.33	–86.98	–2.13	–86.18

Table S28 Calculated electronic energy change and thermodynamic parameters for reaction 2B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 2B: py–$AlMe_3$ + $Me_3SnOSi(OSiH_3)_3$ → py–$AlMe_2OSi(OSiH_3)_3$ + $SnMe_4$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–113.71	–110.30	–111.43	–30.15	–103.19	–111.48	–30.35	–102.43	–111.64	–30.81	–100.14
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–113.91	–110.50	–111.63	–30.15	–103.39	–111.68	–30.35	–102.64	–111.84	–30.81	–100.34
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–108.44	–105.26	–106.15	–24.59	–99.44	–106.21	–24.78	–98.82	–106.37	–25.26	–96.94
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–110.00	–106.82	–107.71	–24.59	–101.00	–107.77	–24.78	–100.38	–107.92	–25.26	–98.50

Table S29 Calculated electronic energy change and thermodynamic parameters for reaction 4B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 4B: py–$AlCl_3$ + $Me_3SnOSi(OSiH_3)_3$ → py–$AlCl_2OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–62.45	–62.18	–61.67	–5.75	–60.10	–61.68	–5.76	–59.96	–61.71	–5.87	–59.52
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–63.93	–63.66	–63.15	–5.75	–61.58	–63.15	–5.76	–61.43	–63.19	–5.87	–61.00
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–56.29	–55.64	–55.29	–5.11	–53.89	–55.30	–5.16	–53.76	–55.36	–5.34	–53.37
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–58.28	–57.62	–57.27	–5.11	–55.87	–57.28	–5.16	–55.75	–57.34	–5.34	–55.35

Table S30 Calculated electronic energy change and thermodynamic parameters for reaction 6B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 6B: $[AlCl_4]^-$ + $Me_3SnOSi(OSiH_3)_3$ → $[AlCl_3OSi(OSiH_3)_3]^-$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–65.58	–66.70	–66.23	7.04	–68.16	–66.23	7.04	–68.33	–66.24	7.02	–68.86
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–70.02	–71.13	–70.67	7.04	–72.59	–70.67	7.04	–72.77	–70.68	7.02	–73.30
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–62.40	–62.91	–62.65	6.43	–64.41	–62.66	6.39	–64.57	–62.70	6.28	–65.05
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–65.91	–66.41	–66.16	6.43	–67.91	–66.17	6.39	–68.08	–66.21	6.28	–68.55

Table S31 Calculated electronic energy change and thermodynamic parameters for reaction 7B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 7B: $SiCl_4$ + $Me_3SnOSi(OSiH_3)_3$ → $SiCl_3OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–89.87	–91.20	–89.40	30.61	–97.76	–89.36	30.75	–98.52	–89.27	31.00	–100.84
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–90.38	–91.71	–89.91	30.61	–98.27	–89.87	30.75	–99.04	–89.79	31.00	–101.36
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–83.95	–84.55	–82.98	30.83	–91.41	–82.96	30.93	–92.18	–82.91	31.07	–94.50
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–84.95	–85.55	–83.99	30.83	–92.41	–83.96	30.93	–93.18	–83.92	31.07	–95.51

Table S32 Calculated electronic energy change and thermodynamic parameters for reaction 8B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 8B: $Me_3SiCl + Me_3SnOSi(OSiH_3)_3 \rightarrow Me_3SiOSi(OSiH_3)_3 + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–59.37	–58.04	–58.04	7.17	–60.00	–58.07	7.06	–60.17	–58.17	6.76	–60.69
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–61.51	–60.17	–60.17	7.17	–62.13	–60.20	7.06	–62.31	–60.30	6.76	–62.83
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–55.03	–53.16	–53.37	5.30	–54.81	–53.41	5.16	–54.95	–53.53	4.79	–55.32
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–57.30	–55.44	–55.64	5.30	–57.09	–55.68	5.16	–57.22	–55.81	4.79	–57.59

Table S33 Calculated electronic energy change and thermodynamic parameters for reaction 9B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 9B: $PhMe_2SiCl + Me_3SnOSi(OSiH_3)_3 \rightarrow PhMe_2SiOSi(OSiH_3)_3 + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–63.30	–63.11	–62.53	6.32	–64.26	–62.54	6.27	–64.41	–62.60	6.11	–64.88
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–65.43	–65.24	–64.66	6.32	–66.39	–64.67	6.27	–66.54	–64.73	6.11	–67.01
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–58.24	–57.59	–57.12	7.06	–59.05	–57.14	6.99	–59.23	–57.22	6.75	–59.74
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–61.06	–60.41	–59.94	7.06	–61.87	–59.96	6.99	–62.05	–60.04	6.75	–62.56

Table S34 Calculated electronic energy change and thermodynamic parameters for reaction 10B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 10B: PCl_3 + $Me_3SnOSi(OSiH_3)_3$ → $PCl_2OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–80.61	–82.39	–80.69	23.17	–87.02	–80.62	23.42	–87.60	–80.45	23.92	–89.38
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–83.83	–85.61	–83.91	23.17	–90.24	–83.84	23.42	–90.82	–83.67	23.92	–92.60
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–75.65	–76.53	–75.16	20.58	–80.78	–75.10	20.78	–81.30	–74.98	21.14	–82.87
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–79.08	–79.96	–78.58	20.58	–84.21	–78.53	20.78	–84.72	–78.41	21.14	–86.30

Table S35 Calculated electronic energy change and thermodynamic parameters for reaction 11B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 11B: $POCl_3$ + $Me_3SnOSi(OSiH_3)_3$ → $POCl_2OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–101.65	–103.21	–101.20	29.69	–109.30	–101.13	29.92	–110.05	–100.99	30.35	–112.31
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–104.69	–106.25	–104.24	29.69	–112.35	–104.18	29.92	–113.10	–104.03	30.35	–115.36
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–97.84	–98.57	–96.88	26.74	–104.18	–96.83	26.92	–104.85	–96.73	27.22	–106.89
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–101.18	–101.91	–100.22	26.74	–107.52	–100.17	26.92	–108.19	–100.07	27.22	–110.23

Table S36 Calculated electronic energy change and thermodynamic parameters for reaction 12B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 12B: $TiCl_4 + Me_3SnOSi(OSiH_3)_3 \rightarrow TiCl_3OSi(OSiH_3)_3 + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–62.31	–65.99	–63.41	45.78	–75.92	–63.31	46.12	–77.07	–63.07	46.86	–80.55
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–63.89	–67.57	–64.99	45.78	–77.50	–64.89	46.12	–78.64	–64.65	46.86	–82.13
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–60.88	–63.69	–61.40	43.22	–73.20	–61.32	43.50	–74.29	–61.13	44.08	–77.58
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–62.58	–65.39	–63.10	43.22	–74.91	–63.02	43.50	–75.99	–62.83	44.08	–79.28

Table S37 Calculated electronic energy change and thermodynamic parameters for reaction 13B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 13B: $Cp_2TiCl_2 + Me_3SnOSi(OSiH_3)_3 \rightarrow Cp_2TiClOSi(OSiH_3)_3 + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–43.11	–44.92	–43.78	5.17	–45.19	–43.76	5.25	–45.32	–43.70	5.43	–45.73
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–45.59	–47.40	–46.26	5.17	–47.67	–46.24	5.25	–47.80	–46.18	5.43	–48.21
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–37.05	–39.15	–37.80	15.46	–42.02	–37.78	15.53	–42.41	–37.74	15.64	–43.57
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–41.14	–43.24	–41.88	15.46	–46.11	–41.87	15.53	–46.49	–41.83	15.64	–47.66

Table S38 Calculated electronic energy change and thermodynamic parameters for reaction 14B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 14B: VCl_4 + $Me_3SnOSi(OSiH_3)_3$ → $VCl_3OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–58.35	–61.65	–59.16	38.14	–69.58	–59.06	38.48	–70.53	–58.82	39.19	–73.45
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–59.45	–62.76	–60.26	38.14	–70.68	–60.16	38.48	–71.63	–59.92	39.19	–74.55
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–56.24	–57.88	–56.35	20.84	–62.04	–56.28	21.07	–62.56	–56.12	21.54	–64.16
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–58.26	–59.90	–58.37	20.84	–64.06	–58.30	21.07	–64.58	–58.14	21.54	–66.18

Table S39 Calculated electronic energy change and thermodynamic parameters for reaction 15B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 15B: $VOCl_3$ + $Me_3SnOSi(OSiH_3)_3$ → $VOCl_2OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–50.28	–53.07	–50.76	37.13	–60.90	–50.68	37.42	–61.83	–50.48	38.01	–64.66
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–53.58	–56.38	–54.06	37.13	–64.21	–53.98	37.42	–65.14	–53.79	38.01	–67.97
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–48.55	–50.87	–48.63	41.95	–60.09	–48.56	42.20	–61.14	–48.40	42.68	–64.33
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–51.42	–53.74	–51.50	41.95	–62.96	–51.43	42.20	–64.01	–51.27	42.68	–67.20

Table S40 Calculated electronic energy change and thermodynamic parameters for reaction 18B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 18B: $ZnEt_2(THF)_2 + Me_3SnOSi(OSiH_3)_3 \rightarrow ZnEtOSi(OSiH_3)_3(THF)_2 + SnMe_3Et$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–66.60	–64.00	–64.39	–3.07	–63.55	–64.41	–3.14	–63.48	–64.47	–3.31	–63.24
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–67.48	–64.88	–65.27	–3.07	–64.43	–65.29	–3.14	–64.35	–65.35	–3.31	–64.11
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–69.00	–63.65	–65.35	–27.09	–57.95	–65.43	–27.37	–57.27	–65.65	–28.05	–55.19
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–69.39	–64.04	–65.74	–27.09	–58.34	–65.82	–27.37	–57.66	–66.05	–28.05	–55.58

Table S41 Calculated electronic energy change and thermodynamic parameters for reaction 21B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 21B: $ZnCl_2(THF)_2 + Me_3SnOSi(OSiH_3)_3 \rightarrow ZnClOSi(OSiH_3)_3(THF)_2 + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
8.95	9.63	9.52	–19.32	14.79	9.50	–19.39	15.28	9.44	–19.55	16.74
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
5.22	5.91	5.79	–19.32	11.07	5.77	–19.39	11.55	5.72	–19.55	13.01
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
9.55	9.55	9.82	–9.74	12.48	9.81	–9.76	12.72	9.79	–9.82	13.45
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
4.99	4.98	5.25	–9.74	7.91	5.24	–9.76	8.15	5.22	–9.82	8.89

Table S42 Calculated electronic energy change and thermodynamic parameters for reaction 22B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 22B: $[ZnCl_3]^-$ + $Me_3SnOSi(OSiH_3)_3$ → $[ZnCl_2OSi(OSiH_3)_3]^-$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–0.04	–2.31	–1.72	9.24	–4.24	–1.70	9.30	–4.47	–1.65	9.46	–5.18
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–6.61	–8.88	–8.29	9.24	–10.81	–8.27	9.30	–11.04	–8.22	9.46	–11.75
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–0.48	–1.92	–1.62	7.40	–3.64	–1.62	7.40	–3.82	–1.61	7.42	–4.38
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–6.66	–8.10	–7.80	7.40	–9.82	–7.80	7.40	–10.00	–7.79	7.42	–10.56

Table S43 Calculated electronic energy change and thermodynamic parameters for reaction 23B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 23B: $SnCl_4$ + $Me_3SnOSi(OSiH_3)_3$ → $SnCl_3OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
–8.67	–10.60	–9.04	21.03	–14.78	–8.99	21.19	–15.31	–8.88	21.53	–16.91
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–6.85	–8.78	–7.22	21.03	–12.96	–7.17	21.19	–13.49	–7.06	21.53	–15.09
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
–6.93	–8.28	–6.85	21.72	–12.79	–6.82	21.84	–13.33	–6.75	22.06	–14.98
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–5.21	–6.56	–5.14	21.72	–11.07	–5.10	21.84	–11.62	–5.03	22.06	–13.26

Table S44 Calculated electronic energy change and thermodynamic parameters for reaction 24B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 24B: $SbCl_3$ + $Me_3SnOSi(OSiH_3)_3$ → $SbCl_2OSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // B3LYP–D3/CBS(D, T, Q)										
–25.57	–27.22	–26.10	13.30	–29.74	–26.06	13.44	–30.07	–25.95	13.77	–31.09
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)										
–22.99	–24.64	–23.52	13.30	–27.16	–23.48	13.44	–27.49	–23.37	13.77	–28.51
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // PBE0–D3/CBS(D, T, Q)										
–23.54	–23.95	–23.43	5.09	–24.83	–23.42	5.15	–24.95	–23.38	5.27	–25.34
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)										
–21.10	–21.51	–20.99	5.09	–22.39	–20.98	5.15	–22.51	–20.94	5.27	–22.90

Table S45 Calculated electronic energy change and thermodynamic parameters for reaction 25B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 25B: Ph_3SbCl_2 + $Me_3SnOSi(OSiH_3)_3$ → $Ph_3SbClOSi(OSiH_3)_3$ + $SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // B3LYP–D3/CBS(D, T, Q)										
–32.34	–32.57	–32.20	–5.99	–30.57	–32.21	–6.02	–30.41	–32.23	–6.07	–29.96
B3LYP–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)										
–33.57	–33.80	–33.43	–5.99	–31.80	–33.44	–6.02	–31.64	–33.45	–6.07	–31.19
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb) // PBE0–D3/CBS(D, T, Q)										
–27.04	–26.98	–26.83	–11.72	–23.63	–26.84	–11.76	–23.34	–26.88	–11.87	–22.45
PBE0–D3/cc–pVTZ + aug–cc–pVTZ–PP(Sn, Sb)										
–29.66	–29.60	–29.45	–11.72	–26.25	–29.46	–11.76	–25.95	–29.50	–11.87	–25.07

Table S46 Calculated electronic energy change and thermodynamic parameters for reaction 26B at 0, 273.15, 298.15, and 373.15 K in vacuum.

Reaction 26B: $Cl^- + Me_3SnOSi(OSiH_3)_3 \rightarrow (H_3SiO)_3SiO^- + SnMe_3Cl$

ΔE kJ mol^{-1}	$\Delta H^0 = \Delta G^0$ kJ mol^{-1}	$\Delta H^{273.15}$ kJ mol^{-1}	$\Delta S^{273.15}$ J K^{-1} mol^{-1}	$\Delta G^{273.15}$ kJ mol^{-1}	$\Delta H^{298.15}$ kJ mol^{-1}	$\Delta S^{298.15}$ J K^{-1} mol^{-1}	$\Delta G^{298.15}$ kJ mol^{-1}	$\Delta H^{373.15}$ kJ mol^{-1}	$\Delta S^{373.15}$ J K^{-1} mol^{-1}	$\Delta G^{373.15}$ kJ mol^{-1}
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // B3LYP-D3/CBS(D, T, Q)										
12.87	6.03	4.84	74.36	–15.47	4.62	73.60	–17.32	3.93	71.54	–22.76
B3LYP-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–1.97	–8.81	–10.00	74.36	–30.31	–10.21	73.60	–32.16	–10.90	71.54	–37.60
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn) // PBE0-D3/CBS(D, T, Q)										
6.06	0.24	–1.33	70.20	–20.50	–0.56	69.37	–21.25	–2.30	67.17	–27.36
PBE0-D3/cc-pVTZ + aug-cc-pVTZ-PP(Sn)										
–7.41	–13.22	–14.79	70.20	–33.96	–14.02	69.37	–34.71	–15.76	67.17	–40.83

S3. Energy components by structure

Table S47 Electronic energies for all calculated structures. (Basis set legend: *x*Z = cc-pV*x*Z + aug-cc-pV*x*Z-PP(Sn), *x* = D, T, Q)

Geometry	Electronic energy (Hartree)					CBS exponent
	E_{DZ} *method/DZ*	E_{TZ} *method/TZ*	E_{QZ} *method/QZ*	E_{CBS} *Halkier et al.*[1]	B_{CBS} *Halkier et al.*[1]	α_{CBS} *Halkier et al.*[1]
THF						
B3LYP-D3/TZ	–232.3256252	–232.4064742	–232.4254148	–232.4312095	1.9238085	1.451
PBE0-D3/TZ	–232.1981588	–232.2675774	–232.2855734	–232.2918713	1.3944269	1.350
Cl^-						
B3LYP-D3/TZ	–460.1977034	–460.2287652	–460.2388053	–460.2436004	0.4393040	1.129
PBE0-D3/TZ	–460.0995104	–460.1259218	–460.1347641	–460.1392144	0.3542295	1.094
$Me_3SnOSiH_3$						
B3LYP-D3/TZ	–700.4555289	–700.5692931	–700.5928243	–700.5989608	3.3525076	1.576
PBE0-D3/TZ	–700.2692879	–700.3684432	–700.3907172	–700.3971705	2.5342145	1.493
$Me_3SnOSi(OSiH_3)_3$						
B3LYP-D3/TZ	–1798.3282545	–1798.5928271	–1798.6507069	–1798.6669148	7.0761937	1.520
PBE0-D3/TZ	–1797.7322886	–1797.9717071	–1798.0266144	–1798.0429539	5.9067398	1.473
$SnMe_4$						
B3LYP-D3/TZ	–373.8224018	–373.9070386	–373.9218514	–373.9249938	3.3493227	1.743
PBE0-D3/TZ	–373.7524602	–373.8228709	–373.8366982	–373.8400771	2.2719245	1.628
$SnMe_3Cl$						
B3LYP-D3/TZ	–794.1511313	–794.2336245	–794.2490704	–794.2526288	2.8950979	1.675
PBE0-D3/TZ	–794.0029952	–794.0744222	–794.0889907	–794.0927234	2.1568894	1.590
$SnMe_3Et$						
B3LYP-D3/TZ	–413.1085438	–413.2062299	–413.2239430	–413.2278663	3.6290997	1.707
PBE0-D3/TZ	–413.0177039	–413.0985511	–413.1151288	–413.1194049	2.4188395	1.585
H_3SiO^-						
B3LYP-D3/TZ	–366.4870413	–366.5479233	–366.5640989	–366.5699516	1.1745307	1.325

PBE0-D3/TZ	–366.3508981	–366.4051835	–366.4200432	–366.4256439	0.9975449	1.296
$(H_3SiO)_3SiO^-$						
B3LYP-D3/TZ	–1464.3820514	–1464.5887178	–1464.6377407	–1464.6529855	4.8150904	1.439
PBE0-D3/TZ	–1463.8367694	–1464.0260274	–1464.0722222	–1464.0871384	4.2024526	1.410
py–BCl_3						
B3LYP-D3/TZ	–1653.6357393	–1653.7603599	–1653.7915528	–1653.8019673	2.6532162	1.385
PBE0-D3/TZ	–1653.1781163	–1653.2878485	–1653.3175098	–1653.3284974	2.0581779	1.308
py–BCl_2OSiH_3						
B3LYP-D3/TZ	–1559.9798499	–1560.1365257	–1560.1749246	–1560.1873908	3.4551782	1.406
PBE0-D3/TZ	–1559.4827212	–1559.6209431	–1559.6573054	–1559.6702862	2.7102134	1.335
py–$BCl(OSiH_3)_2$						
B3LYP-D3/TZ	–1466.3185514	–1466.5072840	–1466.5527765	–1466.5672247	4.2800035	1.423
PBE0-D3/TZ	–1465.7822647	–1465.9493005	–1465.9922748	–1466.0071610	3.3976795	1.358
py–$B(OSiH_3)_3$						
B3LYP-D3/TZ	–1372.6558233	–1372.8752144	–1372.9276398	–1372.9441008	5.0485305	1.431
PBE0-D3/TZ	–1372.0812649	–1372.2755764	–1372.3250120	–1372.3418808	4.0264113	1.369
py–$BCl_2OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–2657.8465622	–2658.1553538	–2658.2278464	–2658.2500859	7.3217189	1.449
PBE0-D3/TZ	–2656.9381851	–2657.2189016	–2657.2877478	–2657.3101190	6.1836110	1.405
py–$AlCl_3$						
B3LYP-D3/TZ	–1871.3140754	–1871.4494076	–1871.4840217	–1871.4959176	2.7796570	1.363
PBE0-D3/TZ	–1870.7856782	–1870.9057497	–1870.9378649	–1870.9495910	2.2912490	1.319
py–$AlCl_3$(THF)						
B3LYP-D3/TZ	–2103.6702624	–2103.8799997	–2103.9320079	–2103.9491566	4.5357258	1.394
PBE0-D3/TZ	–2103.0141880	–2103.1972163	–2103.2459018	–2103.2635453	3.5241982	1.324
py–$AlCl_2OSiH_3$						
B3LYP-D3/TZ	–1777.6410816	–1777.8087256	–1777.8511132	–1777.8654574	3.5097339	1.375
PBE0-D3/TZ	–1777.0728057	–1777.2219468	–1777.2614114	–1777.2756120	2.8964020	1.329
py–$AlCl_2OSiH_3$(THF)						
B3LYP-D3/TZ	–2009.9960607	–2010.2376448	–2010.2973098	–2010.3168785	5.2596247	1.398
PBE0-D3/TZ	–2009.2996405	–2009.5113317	–2009.5672010	–2009.5872326	4.1289222	1.332

py–AlCl(OSiH$_3$)$_2$						
B3LYP-D3/TZ	–1683.9660228	–1684.1661544	–1684.2162036	–1684.2328938	4.2671728	1.386
PBE0-D3/TZ	–1683.3580027	–1683.5365043	–1683.5832701	–1683.5998717	3.5237783	1.339
py–AlCl(OSiH$_3$)$_2$(THF)						
B3LYP-D3/TZ	–1916.3236489	–1916.5965230	–1916.6636180	–1916.6854945	5.9850563	1.403
PBE0-D3/TZ	–1915.5869768	–1915.8269859	–1915.8898180	–1915.9121000	4.7439609	1.340
py–AlCl$_2$OSi(OSiH$_3$)$_3$						
B3LYP-D3/TZ	–2875.5132985	–2875.8329596	–2875.9097279	–2875.9339912	7.2942510	1.426
PBE0-D3/TZ	–2874.5339738	–2874.8252309	–2874.8974507	–2874.9212625	6.2990734	1.394
py–AlMe$_3$						
B3LYP-D3/TZ	–610.2802431	–610.4188752	–610.4507042	–610.4601898	3.4136858	1.471
PBE0-D3/TZ	–609.9823763	–610.0982012	–610.1276027	–610.1376052	2.4090013	1.371
py–AlMe$_3$(THF)						
B3LYP-D3/TZ	–842.6203219	–842.8351745	–842.8847439	–842.8996101	5.2469440	1.467
PBE0-D3/TZ	–842.1943531	–842.3751948	–842.4214370	–842.4373237	3.7159859	1.364
py–AlMe$_2$OSiH$_3$						
B3LYP-D3/TZ	–936.9531387	–937.1222091	–937.1625164	–937.1751340	3.9058107	1.434
PBE0-D3/TZ	–936.5388102	–936.6842560	–936.7216586	–936.7346068	2.9607539	1.358
py–AlMe$_2$OSiH$_3$(THF)						
B3LYP-D3/TZ	–1169.2999131	–1169.5436911	–1169.6015216	–1169.6195072	5.6790137	1.439
PBE0-D3/TZ	–1168.7566647	–1168.9659847	–1169.0199974	–1169.0387818	4.2370146	1.355
py–AlMe(OSiH$_3$)$_2$						
B3LYP-D3/TZ	–1263.6244358	–1263.8243225	–1263.8730544	–1263.8887655	4.4471992	1.411
PBE0-D3/TZ	–1263.0934863	–1263.2691433	–1263.3145591	–1263.3303958	3.5440490	1.353
py–AlMe(OSiH$_3$)$_2$(THF)						
B3LYP-D3/TZ	–1495.9752618	–1496.2494103	–1496.3154843	–1496.3364661	6.2181827	1.423
PBE0-D3/TZ	–1495.3154058	–1495.5543873	–1495.6161623	–1495.6376973	4.8233884	1.353
py–AlMe$_2$OSi(OSiH$_3$)$_3$						
B3LYP-D3/TZ	–2034.8273481	–2035.1480497	–2035.2227423	–2035.2454203	7.7072236	1.457
PBE0-D3/TZ	–2034.0018194	–2034.2889326	–2034.3590938	–2034.3817837	6.3628812	1.409
py–Al(OSiH$_3$)$_3$						

B3LYP-D3/TZ	–1590.2909352	–1590.5229124	–1590.5804271	–1590.5993878	5.0178963	1.395
PBE0-D3/TZ	–1589.6433849	–1589.8506350	–1589.9044876	–1589.9233934	4.1471313	1.348
py–Al(OSiH$_3$)$_3$(THF)						
B3LYP-D3/TZ	–1822.6510940	–1822.9557162	–1823.0303381	–1823.0545487	6.7233363	1.407
PBE0-D3/TZ	–1821.8746039	–1822.1432977	–1822.2131844	–1822.2377516	5.3679722	1.347
AlCl$_4^-$						
B3LYP-D3/TZ	–2083.4171520	–2083.5003483	–2083.5229800	–2083.5314370	1.5444130	1.302
PBE0-D3/TZ	–2082.9381422	–2083.0141356	–2083.0343506	–2083.0416768	1.4631550	1.324
AlCl$_3$OSiH$_3^-$						
B3LYP-D3/TZ	–1989.7404440	–1989.8567806	–1989.8871205	–1989.8978245	2.3139550	1.344
PBE0-D3/TZ	–1989.2215000	–1989.3276878	–1989.3552730	–1989.3649540	2.1257291	1.348
AlCl$_2$(OSiH$_3$)$_2^-$						
B3LYP-D3/TZ	–1896.0640555	–1896.2131043	–1896.2510925	–1896.2640863	3.0793413	1.367
PBE0-D3/TZ	–1895.5052595	–1895.6412019	–1895.6761263	–1895.6882005	2.7718138	1.359
AlCl(OSiH$_3$)$_3^-$						
B3LYP-D3/TZ	–1802.3850551	–1802.5673110	–1802.6125024	–1802.6274023	3.9417697	1.395
PBE0-D3/TZ	–1801.7864525	–1801.9527765	–1801.9945883	–1802.0086290	3.5156839	1.381
Al(OSiH$_3$)$_4^-$						
B3LYP-D3/TZ	–1708.7081904	–1708.9221029	–1708.9746846	–1708.9918223	4.6941498	1.403
PBE0-D3/TZ	–1708.0701490	–1708.2651853	–1708.3141146	–1708.3305005	4.1366789	1.383
AlCl$_3$OSi(OSiH$_3$)$_3^-$						
B3LYP-D3/TZ	–3087.6184475	–3087.8862192	–3087.9504403	–3087.9707022	6.1239501	1.428
PBE0-D3/TZ	–3086.6888104	–3086.9365231	–3086.9965079	–3087.0156748	5.5741954	1.418
SiCl$_4$						
B3LYP-D3/TZ	–2130.2915807	–2130.3757321	–2130.3951892	–2130.4010410	2.0475058	1.464
PBE0-D3/TZ	–2129.8128997	–2129.8927819	–2129.9110936	–2129.9165398	1.9722835	1.473
SiCl$_3$OSiH$_3$						
B3LYP-D3/TZ	–2036.6309079	–2036.7497504	–2036.7771289	–2036.7853243	2.9094951	1.468
PBE0-D3/TZ	–2036.1123941	–2036.2235614	–2036.2493528	–2036.2571442	2.6891907	1.461
SiCl$_2$(OSiH$_3$)$_2$						
B3LYP-D3/TZ	–1942.9701344	–1943.1238907	–1943.1592535	–1943.1698160	3.7749314	1.470

PBE0-D3/TZ	–1942.4118091	–1942.5545587	–1942.5878187	–1942.5979222	3.4283212	1.457
$SiCl(OSiH_3)_3$						
B3LYP-D3/TZ	–1849.3082065	–1849.4967263	–1849.5397726	–1849.5525102	4.6856818	1.477
PBE0-D3/TZ	–1848.7103862	–1848.8843727	–1848.9249955	–1848.9373692	4.1637631	1.455
$Si(OSiH_3)_4$						
B3LYP-D3/TZ	–1755.6439053	–1755.8672923	–1755.9183000	–1755.9333934	5.5523335	1.477
PBE0-D3/TZ	–1755.0061387	–1755.2119627	–1755.2601681	–1755.2749110	4.8998723	1.452
$SiCl_3OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–3134.4967221	–3134.7693584	–3134.8313273	–3134.8495557	6.8295161	1.482
PBE0-D3/TZ	–3133.5675545	–3133.8224236	–3133.8811568	–3133.8987445	6.2365493	1.468
Me_3SiCl						
B3LYP-D3/TZ	–869.3698968	–869.4545393	–869.4716535	–869.4759909	2.5951127	1.599
PBE0-D3/TZ	–794.0029952	–794.0744222	–794.0889907	–794.0927234	2.1568894	1.590
$Me_3SiOSiH_3$						
B3LYP-D3/TZ	–775.6983410	–775.8174439	–775.8422186	–775.8487255	3.4756064	1.570
PBE0-D3/TZ	–700.2692879	–700.3684432	–700.3907172	–700.3971705	2.5342145	1.493
$Me_3SiOSi(OSiH_3)_3$						
B3LYP-D3/TZ	–1873.5653133	–1873.8371677	–1873.8963935	–1873.9128904	7.3232037	1.524
PBE0-D3/TZ	–1797.7322886	–1797.9717071	–1798.0266144	–1798.0429539	5.9067398	1.473
$PhMe_2SiCl$						
B3LYP-D3/TZ	–1061.0179905	–1061.1514946	–1061.1817854	–1061.1906750	3.3544591	1.483
PBE0-D3/TZ	–1060.6568737	–1060.7701015	–1060.7985146	–1060.8080330	2.4005184	1.383
$PhMe_2SiOSiH_3$						
B3LYP-D3/TZ	–967.3477227	–967.5154050	–967.5533472	–967.5644433	4.2328108	1.486
PBE0-D3/TZ	–966.9468828	–967.0909081	–967.1265263	–967.1382290	3.1286249	1.397
$PhMe_2SiOSi(OSiH_3)_3$						
B3LYP-D3/TZ	–2065.2155996	–2065.5356179	–2065.6079484	–2065.6290706	8.0937811	1.487
PBE0-D3/TZ	–2064.4043589	–2064.6906431	–2064.7590026	–2064.7804459	6.5960703	1.432
PCl_3						
B3LYP-D3/TZ	–1721.8566508	–1721.9255012	–1721.9411970	–1721.9458318	1.7159942	1.479
PBE0-D3/TZ	–1721.4697538	–1721.5366339	–1721.5516719	–1721.5560341	1.7065676	1.492

PCl_2OSiH_3						
B3LYP-D3/TZ	–1628.1947924	–1628.2966414	–1628.3199031	–1628.3267885	2.5304236	1.477
PBE0-D3/TZ	–1627.7693980	–1627.8652497	–1627.8874598	–1627.8941584	2.3236583	1.462
$PCl(OSiH_3)_2$						
B3LYP-D3/TZ	–1534.5290407	–1534.6641342	–1534.6952494	–1534.7045605	3.3086401	1.468
PBE0-D3/TZ	–1534.0654700	–1534.1908138	–1534.2204378	–1534.2296060	2.9384725	1.442
$P(OSiH_3)_3$						
B3LYP-D3/TZ	–1440.8597611	–1441.0279740	–1441.0668045	–1441.0784584	4.1040801	1.466
PBE0-D3/TZ	–1440.3583512	–1440.5133202	–1440.5501897	–1440.5617001	3.5924939	1.436
$PCl_2OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–2726.0605181	–2726.3166314	–2726.3741566	–2726.3908200	6.5472557	1.493
PBE0-D3/TZ	–2725.2238616	–2725.4640380	–2725.5188622	–2725.5350784	5.9727987	1.477
$POCl_3$						
B3LYP-D3/TZ	–1797.0723754	–1797.1799894	–1797.2033883	–1797.2098895	2.9086899	1.526
PBE0-D3/TZ	–1796.6442162	–1796.7479232	–1796.7704129	–1796.7766405	2.8158976	1.529
$POCl_2OSiH_3$						
B3LYP-D3/TZ	–1703.4169619	–1703.5589023	–1703.5900022	–1703.5987283	3.7862220	1.518
PBE0-D3/TZ	–1702.9507857	–1703.0847193	–1703.1145251	–1703.1230568	3.4784745	1.503
$POCl(OSiH_3)_2$						
B3LYP-D3/TZ	–1609.7606015	–1609.9368781	–1609.9757374	–1609.9867262	4.6531447	1.512
PBE0-D3/TZ	–1609.2564712	–1609.4209025	–1609.4579810	–1609.4687763	4.1752816	1.489
$PO(OSiH_3)_3$						
B3LYP-D3/TZ	–1516.1035159	–1516.3139844	–1516.3604409	–1516.3735998	5.5434398	1.511
PBE0-D3/TZ	–1515.5638717	–1515.7580654	–1515.8022250	–1515.8152225	4.8607154	1.481
$POCl_2OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–2801.2831269	–2801.5790677	–2801.6443893	–2801.6628912	7.7949005	1.511
PBE0-D3/TZ	–2800.4056699	–2800.6837467	–2800.7461091	–2800.7641379	7.1274591	1.495
$TiCl_4$						
B3LYP-D3/TZ	–2690.3226512	–2690.3921397	–2690.4090618	–2690.4145094	1.5489303	1.413
PBE0-D3/TZ	–2689.7806043	–2689.8486079	–2689.8644890	–2689.8693278	1.6268192	1.454
$TiCl_3OSiH_3$						

B3LYP-D3/TZ	–2596.6593643	–2596.7564798	–2596.7807296	–2596.7887999	2.0759415	1.387
PBE0-D3/TZ	–2596.0793987	–2596.1715298	–2596.1943228	–2596.2018154	2.0000899	1.397
$TiCl_2(OSiH_3)_2$						
B3LYP-D3/TZ	–2502.9925539	–2503.1178511	–2503.1494374	–2503.1600839	2.6362047	1.378
PBE0-D3/TZ	–2502.3746707	–2502.4914264	–2502.5211585	–2502.5313167	2.4155996	1.368
$TiCl(OSiH_3)_3$						
B3LYP-D3/TZ	–2409.3226617	–2409.4766689	–2409.5156469	–2409.5288547	3.2189764	1.374
PBE0-D3/TZ	–2408.6669143	–2408.8087514	–2408.8454646	–2408.8582863	2.8563485	1.352
$Ti(OSiH_3)_4$						
B3LYP-D3/TZ	–2315.6500187	–2315.8331324	–2315.8794828	–2315.8951913	3.8265617	1.374
PBE0-D3/TZ	–2314.9564460	–2315.1237286	–2315.1674049	–2315.1828378	3.3210215	1.343
$TiCl_3OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–3694.5258297	–3694.7756756	–3694.8344495	–3694.8525285	5.9036692	1.447
PBE0-D3/TZ	–3693.5348911	–3693.7697273	–3693.8254268	–3693.8427455	5.4723516	1.439
Cp_2TiCl_2						
B3LYP-D3/TZ	–2156.7845812	–2156.9321494	–2156.9684759	–2156.9803385	3.2303969	1.402
PBE0-D3/TZ	–2156.2440223	–2156.3727408	–2156.4070303	–2156.4194817	2.4724947	1.323
$Cp_2TiClOSiH_3$						
B3LYP-D3/TZ	–2063.1059933	–2063.2837652	–2063.3274351	–2063.3416561	3.9052823	1.404
PBE0-D3/TZ	–2062.5257453	–2062.6813661	–2062.7223586	–2062.7370180	3.0448773	1.334
$Cp_2Ti(OSiH_3)_2$						
B3LYP-D3/TZ	–1969.4243968	–1969.6325274	–1969.6834628	–1969.6999671	4.6011529	1.408
PBE0-D3/TZ	–1968.8048290	–1968.9875907	–1969.0353227	–1969.0521956	3.6265380	1.343
$Cp_2TiClOSi(OSiH_3)_3$						
B3LYP-D3/TZ	–3160.9809523	–3161.3087170	–3161.3866992	–3161.4110453	7.5979350	1.436
PBE0-D3/TZ	–3159.9903843	–3160.2856937	–3160.3593481	–3160.3838230	6.3246076	1.389
VCl_4						
B3LYP-D3/TZ	–2784.7934577	–2784.8651962	–2784.8828510	–2784.8886142	1.5711481	1.402
PBE0-D3/TZ	–2784.2441754	–2784.3145029	–2784.3310455	–2784.3361336	1.6619934	1.447
VCl_3OSiH_3						
B3LYP-D3/TZ	–2691.1287619	–2691.2272022	–2691.2521095	–2691.2605462	2.0585234	1.374

PBE0-D3/TZ	–2690.5416665	–2690.6351698	–2690.6585542	–2690.6663527	1.9935307	1.386
$VCl_2(OSiH_3)_2$						
B3LYP-D3/TZ	–2597.4629718	–2597.5885283	–2597.6207372	–2597.6318507	2.5662637	1.361
PBE0-D3/TZ	–2596.8381050	–2596.9551358	–2596.9854489	–2596.9960451	2.3541437	1.351
$VCl(OSiH_3)_3$						
B3LYP-D3/TZ	–2503.7894166	–2503.9428846	–2503.9822747	–2503.9958757	3.1339755	1.360
PBE0-D3/TZ	–2503.1267253	–2503.2681588	–2503.3052727	–2503.3184768	2.7846440	1.338
$V(OSiH_3)_4$						
B3LYP-D3/TZ	–2410.1116094	–2410.2944919	–2410.3411333	–2410.3571008	3.7743013	1.366
PBE0-D3/TZ	–2409.4108123	–2409.5782564	–2409.6222999	–2409.6380197	3.2839622	1.335
$VCl_3OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–3788.9960443	–3789.2470406	–3789.3065959	–3789.3251230	5.8451070	1.439
PBE0-D3/TZ	–3787.9981125	–3788.2339777	–3788.2901931	–3788.3077839	5.4515192	1.434
$VOCl_3$						
B3LYP-D3/TZ	–2399.8290512	–2399.9048580	–2399.9244034	–2399.9311936	1.5365009	1.355
PBE0-D3/TZ	–2399.3290261	–2399.4032847	–2399.4218559	–2399.4280492	1.5832557	1.386
$VOCl_2OSiH_3$						
B3LYP-D3/TZ	–2306.1645947	–2306.2674862	–2306.2942551	–2306.3036686	2.0546691	1.346
PBE0-D3/TZ	–2305.6265894	–2305.7244261	–2305.7497937	–2305.7586736	1.9646886	1.350
$VOCl(OSiH_3)_2$						
B3LYP-D3/TZ	–2212.4966534	–2212.6272836	–2212.6613651	–2212.6733958	2.5965181	1.344
PBE0-D3/TZ	–2211.9206894	–2212.0426515	–2212.0750013	–2212.0866795	2.3593253	1.327
$VO(OSiH_3)_3$						
B3LYP-D3/TZ	–2118.8257081	–2118.9841896	–2119.0256798	–2119.0403939	3.1323568	1.340
PBE0-D3/TZ	–2118.2117115	–2118.3581425	–2118.3974331	–2118.4118417	2.7797265	1.316
$VOCl_2OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–3404.0281710	–3404.2844696	–3404.3455320	–3404.3646299	5.9275785	1.434
PBE0-D3/TZ	–3403.0788507	–3403.3201556	–3403.3783087	–3403.3967731	5.4740305	1.423
$ZnCl_2$						
B3LYP-D3/TZ	–2699.7912059	–2699.8294929	–2699.8418098	–2699.8476513	0.5454236	1.134
PBE0-D3/TZ	–2699.4122533	–2699.4469993	–2699.4585706	–2699.4643482	0.4697248	1.100

$ZnCl_2(THF)$						
B3LYP-D3/TZ	–2932.1559792	–2932.2697624	–2932.2999906	–2932.3109264	2.1954140	1.326
PBE0-D3/TZ	–2931.6482079	–2931.7472373	–2931.7759149	–2931.7876047	1.6622527	1.239
$ZnCl_2(THF)_2$						
B3LYP-D3/TZ	–3164.5208835	–3164.7090207	–3164.7569209	–3164.7732819	3.8936992	1.368
PBE0-D3/TZ	–3163.8836141	–3164.0460195	–3164.0915203	–3164.1092299	2.8742941	1.272
$ZnClOSiH_3$						
B3LYP-D3/TZ	–2606.0918256	–2606.1602662	–2606.1805628	–2606.1891194	1.1062863	1.216
PBE0-D3/TZ	–2605.6746449	–2605.7360002	–2605.7550709	–2605.7636718	0.9215032	1.169
$ZnClOSiH_3(THF)$						
B3LYP-D3/TZ	–2838.4570136	–2838.6007353	–2838.6386664	–2838.6522665	2.8031900	1.332
PBE0-D3/TZ	–2837.9109760	–2838.0364386	–2838.0723205	–2838.0866932	2.1482794	1.252
$ZnClOSiH_3(THF)_2$						
B3LYP-D3/TZ	–3070.8220555	–3071.0403050	–3071.0956315	–3071.1144196	4.5495137	1.372
PBE0-D3/TZ	–3070.1463975	–3070.3355313	–3070.3879816	–3070.4081086	3.4030234	1.283
$ZnClOSi(OSiH_3)_3(THF)_2$						
B3LYP-D3/TZ	–4168.6977917	–4169.0662334	–4169.1555668	–4169.1841595	8.2732203	1.417
PBE0-D3/TZ	–4167.6125359	–4167.9414052	–4168.0262895	–4168.0558214	6.6538882	1.354
$ZnCl_3^-$						
B3LYP-D3/TZ	–3160.1009106	–3160.1581955	–3160.1762573	–3160.1845747	0.8415753	1.154
PBE0-D3/TZ	–3159.6242818	–3159.6748280	–3159.6914284	–3159.6995466	0.6977930	1.113
$ZnCl_2OSiH_3^-$						
B3LYP-D3/TZ	–3066.4008778	–3066.4885125	–3066.5141318	–3066.5247155	1.4490041	1.230
PBE0-D3/TZ	–3065.8858261	–3065.9636976	–3065.9875049	–3065.9979885	1.2000075	1.185
$ZnCl(OSiH_3)_2^-$						
B3LYP-D3/TZ	–2972.6994013	–2972.8178980	–2972.8511207	–2972.8640643	2.0947810	1.272
PBE0-D3/TZ	–2972.1459691	–2972.2516088	–2972.2826710	–2972.2956087	1.7307573	1.224
$Zn(OSiH_3)_3^-$						
B3LYP-D3/TZ	–2878.9981342	–2879.1472301	–2879.1878041	–2879.2029739	2.7659813	1.301
PBE0-D3/TZ	–2878.4064139	–2878.5394681	–2878.5774839	–2878.5926904	2.2818512	1.253
$ZnCl_2OSi(OSiH_3)_3^-$						

B3LYP-D3/TZ	–4164.2810979	–4164.5199172	–4164.5792579	–4164.5988777	5.1470629	1.392
PBE0-D3/TZ	–4163.3557260	–4163.5746511	–4163.6306855	–4163.6499613	4.4913483	1.363
$ZnEt_2$						
B3LYP-D3/TZ	–1937.6927916	–1937.7617511	–1937.7774784	–1937.7821250	1.7174882	1.478
PBE0-D3/TZ	–1937.4249014	–1937.4795564	–1937.4940329	–1937.4992489	1.0597387	1.329
$ZnEt_2$(THF)						
B3LYP-D3/TZ	–2170.0380770	–2170.1835719	–2170.2171362	–2170.2272010	3.5537465	1.467
PBE0-D3/TZ	–2169.6415354	–2169.7616636	–2169.7931524	–2169.8043388	2.3694020	1.339
$ZnEt_2(THF)_2$						
B3LYP-D3/TZ	–2402.3856300	–2402.6069768	–2402.6582116	–2402.6736427	5.3756020	1.463
PBE0-D3/TZ	–2401.8599206	–2402.0450456	–2402.0933416	–2402.1103885	3.6800941	1.344
$ZnEtOSiH_3$						
B3LYP-D3/TZ	–2225.0509543	–2225.1347855	–2225.1565247	–2225.1641358	1.6830702	1.350
PBE0-D3/TZ	–2224.6887640	–2224.7601817	–2224.7804248	–2224.7884324	1.2405489	1.261
$ZnEtOSiH_3$(THF)						
B3LYP-D3/TZ	–2457.4042212	–2457.5634775	–2457.6027586	–2457.6156196	3.4747779	1.400
PBE0-D3/TZ	–2456.9131322	–2457.0489237	–2457.0859134	–2457.0997617	2.5151427	1.300
$ZnEtOSiH_3(THF)_2$						
B3LYP-D3/TZ	–2689.7591119	–2689.9937133	–2690.0505623	–2690.0687438	5.2730430	1.417
PBE0-D3/TZ	–2689.1391239	–2689.3392570	–2689.3929926	–2689.4127164	3.7950536	1.315
$ZnEtOSi(OSiH_3)_3(THF)_2$						
B3LYP-D3/TZ	–3787.6338007	–3788.0192759	–3788.1100787	–3788.1380595	9.0875754	1.446
PBE0-D3/TZ	–3786.6047204	–3786.9446323	–3787.0308871	–3787.0602176	7.0737857	1.371
$Zn(OSiH_3)_2$						
B3LYP-D3/TZ	–2512.3923815	–2512.4910656	–2512.5191416	–2512.5303055	1.7039822	1.257
PBE0-D3/TZ	–2511.9366696	–2512.0249541	–2512.0513123	–2512.0625313	1.4119928	1.209
$Zn(OSiH_3)_2$(THF)						
B3LYP-D3/TZ	–2744.7570302	–2744.9307120	–2744.9761293	–2744.9922112	3.4392812	1.341
PBE0-D3/TZ	–2744.1724898	–2744.3246639	–2744.3675532	–2744.3843853	2.6675077	1.266
$Zn(OSiH_3)_2(THF)_2$						
B3LYP-D3/TZ	–2977.1223299	–2977.3705671	–2977.4333814	–2977.4546605	5.1902379	1.374

PBE0-D3/TZ	–2976.4080862	–2976.6239137	–2976.6833844	–2976.7060043	3.9237737	1.289
$SnCl_4$						
B3LYP-D3/TZ	–2055.0839674	–2055.1645784	–2055.1826880	–2055.1879352	2.0600080	1.493
PBE0-D3/TZ	–2054.7009330	–2054.7813667	–2054.7990251	–2054.8039923	2.1382694	1.516
$SnCl_3OSiH_3$						
B3LYP-D3/TZ	–1961.3934385	–1961.5047950	–1961.5313339	–1961.5396377	2.5740159	1.434
PBE0-D3/TZ	–1960.9723416	–1961.0798743	–1961.1056300	–1961.1137418	2.4647995	1.429
$SnCl_2(OSiH_3)_2$						
B3LYP-D3/TZ	–1867.7022787	–1867.8447843	–1867.8798029	–1867.8912117	3.1287740	1.404
PBE0-D3/TZ	–1867.2431066	–1867.3781715	–1867.4121443	–1867.4235612	2.8522665	1.380
$SnCl(OSiH_3)_3$						
B3LYP-D3/TZ	–1774.0115142	–1774.1848958	–1774.2281588	–1774.2425433	3.7105532	1.388
PBE0-D3/TZ	–1773.5144017	–1773.6766172	–1773.7185036	–1773.7330843	3.2798332	1.354
$Sn(OSiH_3)_4$						
B3LYP-D3/TZ	–1680.3211316	–1680.5257027	–1680.5767584	–1680.5937383	4.3766037	1.388
PBE0-D3/TZ	–1679.7859120	–1679.9757882	–1680.0251677	–1680.0425228	3.7942248	1.347
$SnCl_3OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–3059.2623425	–3059.5263916	–3059.5872776	–3059.6055246	6.4544383	1.467
PBE0-D3/TZ	–3058.4305980	–3058.6806361	–3058.7390529	–3058.7568615	5.9773127	1.454
$SbCl_3$						
B3LYP-D3/TZ	–1620.8363945	–1620.9003549	–1620.9142760	–1620.9181489	1.7257699	1.525
PBE0-D3/TZ	–1620.5443784	–1620.6079920	–1620.6214607	–1620.6250784	1.8001832	1.552
$SbCl_2OSiH_3$						
B3LYP-D3/TZ	–1527.1525841	–1527.2474006	–1527.2698902	–1527.2768832	2.2093818	1.439
PBE0-D3/TZ	–1526.8225707	–1526.9131694	–1526.9348391	–1526.9416515	2.0815248	1.431
$SbCl(OSiH_3)_2$						
B3LYP-D3/TZ	–1433.4672607	–1433.5934020	–1433.6244877	–1433.6346535	2.7563288	1.401
PBE0-D3/TZ	–1433.0992747	–1433.2173938	–1433.2473347	–1433.2575010	2.4625927	1.372
$Sb(OSiH_3)_3$						
B3LYP-D3/TZ	–1339.7805618	–1339.9377667	–1339.9774023	–1339.9907646	3.3067235	1.378
PBE0-D3/TZ	–1339.3749357	–1339.5203164	–1339.5584231	–1339.5719597	2.8676702	1.339

$SbCl_2OSi(OSiH_3)_3$						
B3LYP-D3/TZ	–2625.0215290	–2625.2683141	–2625.3251609	–2625.3421745	6.0429989	1.468
PBE0-D3/TZ	–2624.2812374	–2624.5133117	–2624.5676565	–2624.5842736	5.5262868	1.452
Ph_3SbCl_2						
B3LYP-D3/TZ	–1855.2089288	–1855.4554438	–1855.5139025	–1855.5320748	5.7462921	1.439
PBE0-D3/TZ	–1854.6178855	–1854.8306234	–1854.8863240	–1854.9060809	4.2039351	1.340
$Ph_3SbClOSiH_3$						
B3LYP-D3/TZ	–1761.5217383	–1761.7990588	–1761.8655603	–1761.8865377	6.3438862	1.428
PBE0-D3/TZ	–1760.8925480	–1761.1326075	–1761.1958055	–1761.2183881	4.7014839	1.335
$Ph_3Sb(OSiH_3)_2$						
B3LYP-D3/TZ	–1667.8376938	–1668.1454077	–1668.2196020	–1668.2431751	6.9746801	1.422
PBE0-D3/TZ	–1667.1705772	–1667.4375236	–1667.5079117	–1667.5331179	5.2144232	1.333
$Ph_3SbClOSi(OSiH_3)_3$						
B3LYP-D3/TZ	–2859.3996810	–2859.8274308	–2859.9278624	–2859.9586780	10.1402538	1.449
PBE0-D3/TZ	–2858.3591600	–2858.7392033	–2858.8346219	–2858.8666103	8.0499649	1.382

Table S48 Thermal corrections for all calculated structures. (Basis set legend: TZ = cc-pVTZ + aug-cc-pVTZ-PP(Sn))

Geometry/method	ZPE_{corr}	273.15 K			298.15 K			373.15 K		
		H_{corr}	S_{corr}	G_{corr}	H_{corr}	S_{corr}	G_{corr}	H_{corr}	S_{corr}	G_{corr}
	kJ mol^{-1}	kJ mol^{-1}	J K^{-1} mol^{-1}	kJ mol^{-1}	kJ mol^{-1}	J K^{-1} mol^{-1}	kJ mol^{-1}	kJ mol^{-1}	J K^{-1} mol^{-1}	kJ mol^{-1}
THF										
B3LYP-D3/TZ	305.59	319.14	294.44	238.71	321.03	301.08	231.27	327.79	321.20	207.93
PBE0-D3/TZ	307.45	320.93	293.69	240.71	322.81	300.28	233.28	329.51	320.23	210.01
Cl$^-$										
B3LYP-D3/TZ	0.00	5.68	151.26	–35.64	6.20	153.08	–39.44	7.76	157.74	–51.10
PBE0-D3/TZ	0.00	5.68	151.26	–35.64	6.20	153.08	–39.44	7.76	157.74	–51.10
$Me_3SnOSiH_3$										
B3LYP-D3/TZ	359.88	391.10	462.04	264.90	395.46	477.28	253.15	409.83	520.19	215.73
PBE0-D3/TZ	360.95	392.00	459.71	266.43	396.35	474.94	254.75	410.73	517.84	217.49
$Me_3SnOSi(OSiH_3)_3$										
B3LYP-D3/TZ	541.96	594.90	651.71	416.89	602.72	679.09	400.25	628.67	756.53	346.37
PBE0-D3/TZ	541.64	594.81	653.36	416.35	602.65	680.82	399.67	628.69	758.51	345.65
$SnMe_4$										
B3LYP-D3/TZ	376.07	402.99	410.85	290.76	406.82	424.27	280.32	419.48	462.05	247.07
PBE0-D3/TZ	377.76	404.52	409.28	292.72	408.34	422.66	282.32	420.98	460.39	249.19
$SnMe_3Cl$										
B3LYP-D3/TZ	285.43	311.26	413.04	198.44	314.74	425.25	187.96	326.11	459.19	154.77
PBE0-D3/TZ	286.77	312.35	409.84	200.41	315.83	422.01	190.01	327.18	455.88	157.06
$SnMe_3Et$										
B3LYP-D3/TZ	452.85	482.15	431.08	364.40	486.42	446.05	353.43	500.66	488.53	318.37
PBE0-D3/TZ	454.72	483.90	430.11	366.42	488.17	445.05	355.48	502.39	487.48	320.49
H_3SiO^-										
B3LYP-D3/TZ	67.38	77.10	241.20	11.21	78.22	245.12	5.13	81.97	256.31	–13.68
PBE0-D3/TZ	67.40	77.13	241.26	11.23	78.25	245.21	5.14	82.02	256.44	–13.67
$(H_3SiO)_3SiO^-$										
B3LYP-D3/TZ	249.70	281.29	464.28	154.47	285.93	480.51	142.66	301.38	526.61	104.87

PBE0-D3/TZ	249.05	280.75	464.97	153.75	286.41	481.26	142.92	300.91	527.53	104.06
py–BCl_3										
B3LYP-D3/TZ	261.29	284.96	402.18	175.10	288.60	414.94	164.88	301.92	451.67	133.37
PBE0-D3/TZ	263.04	286.59	400.97	177.07	290.21	413.66	166.88	302.45	450.16	134.47
py–BCl_2OSiH_3										
B3LYP-D3/TZ	338.32	367.24	446.29	245.33	371.72	461.97	233.98	387.92	507.31	198.62
PBE0-D3/TZ	339.63	368.54	446.77	246.50	373.00	462.40	235.14	388.17	507.63	198.75
py–$BCl(OSiH_3)_2$										
B3LYP-D3/TZ	416.47	449.58	475.48	319.70	454.85	493.95	307.58	473.87	547.65	269.51
PBE0-D3/TZ	417.52	450.61	475.99	320.60	455.88	494.43	308.46	473.87	548.08	269.35
py–$B(OSiH_3)_3$										
B3LYP-D3/TZ	491.33	530.03	526.53	386.21	536.14	547.93	372.78	558.08	610.36	330.33
PBE0-D3/TZ	492.30	531.08	529.15	386.54	537.19	550.54	373.04	558.12	612.95	329.40
py–$BCl_2OSi(OSiH_3)_3$										
B3LYP-D3/TZ	518.85	570.17	638.97	395.64	578.14	666.89	379.31	605.99	746.96	327.26
PBE0-D3/TZ	519.30	570.82	642.62	395.29	578.79	670.55	378.87	605.65	750.65	325.54
py–$AlCl_3$										
B3LYP-D3/TZ	253.13	280.00	438.36	160.26	283.90	452.01	149.13	296.86	490.67	113.76
PBE0-D3/TZ	254.40	281.27	438.09	161.60	285.16	451.71	150.48	298.08	490.28	115.13
py–$AlCl_3$(THF)										
B3LYP-D3/TZ	567.03	606.76	538.28	459.73	612.90	559.78	446.00	633.72	621.86	401.67
PBE0-D3/TZ	569.67	609.31	537.75	462.43	615.43	559.17	448.71	636.16	621.00	404.44
py–$AlCl_2OSiH_3$										
B3LYP-D3/TZ	328.26	360.72	486.36	227.87	365.47	503.01	215.50	381.40	550.53	175.97
PBE0-D3/TZ	329.22	361.74	487.50	228.58	366.49	504.15	216.18	382.42	551.66	176.57
py–$AlCl_2OSiH_3$(THF)										
B3LYP-D3/TZ	642.23	687.76	590.83	526.37	694.75	615.31	511.29	718.51	686.18	462.46
PBE0-D3/TZ	644.59	690.12	590.86	528.72	697.09	615.29	513.64	720.80	685.98	464.82
py–$AlCl(OSiH_3)_2$										
B3LYP-D3/TZ	402.32	440.98	551.69	290.29	446.61	571.40	276.25	465.56	627.91	231.25
PBE0-D3/TZ	403.20	441.86	549.40	291.79	447.50	569.13	277.81	466.45	625.67	232.98

py–AlCl(OSiH$_3$)$_2$(THF)										
B3LYP-D3/TZ	720.27	769.29	603.94	604.32	777.07	631.16	588.88	803.61	710.33	538.56
PBE0-D3/TZ	721.56	770.96	609.59	604.45	778.74	636.84	588.86	805.30	716.02	538.11
py–AlCl$_2$OSi(OSiH$_3$)$_3$										
B3LYP-D3/TZ	509.93	564.43	671.28	381.07	572.65	700.09	363.92	600.16	782.14	308.30
PBE0-D3/TZ	509.92	564.73	676.50	379.95	572.98	705.37	362.67	600.53	787.57	306.65
py–AlMe$_3$										
B3LYP-D3/TZ	518.74	550.91	457.46	425.95	555.96	475.18	414.29	573.13	526.36	376.71
PBE0-D3/TZ	520.65	552.99	459.75	427.41	558.06	477.50	415.69	575.25	528.78	377.94
py–AlMe$_3$(THF)										
B3LYP-D3/TZ	832.39	878.15	575.35	720.99	885.43	600.84	706.29	910.35	675.15	658.42
PBE0-D3/TZ	835.52	881.44	578.21	723.50	888.71	603.68	708.72	913.63	677.96	660.65
py–AlMe$_2$OSiH$_3$										
B3LYP-D3/TZ	505.35	541.34	501.42	404.38	546.86	520.76	391.60	565.58	576.58	350.43
PBE0-D3/TZ	506.79	542.92	502.63	405.63	548.46	522.01	392.82	567.21	577.93	351.55
py–AlMe$_2$OSiH$_3$(THF)										
B3LYP-D3/TZ	822.15	869.41	580.61	710.82	877.08	607.47	695.96	903.41	685.96	647.44
PBE0-D3/TZ	824.56	872.07	584.34	712.46	879.75	611.23	697.52	906.08	689.73	648.71
py–AlMe(OSiH$_3$)$_2$										
B3LYP-D3/TZ	491.97	531.80	540.83	384.07	537.79	561.83	370.28	558.08	622.32	325.86
PBE0-D3/TZ	492.79	532.82	543.36	384.40	538.83	564.41	370.55	559.16	625.04	325.92
py–AlMe(OSiH$_3$)$_2$(THF)										
B3LYP-D3/TZ	809.40	860.37	616.93	691.86	868.52	645.44	676.08	896.40	728.57	624.53
PBE0-D3/TZ	811.38	862.48	618.19	693.62	870.62	646.71	677.80	898.51	729.85	626.16
py–AlMe$_2$OSi(OSiH$_3$)$_3$										
B3LYP-D3/TZ	688.03	745.10	668.17	562.59	754.09	699.65	545.49	784.39	790.02	489.59
PBE0-D3/TZ	687.71	745.57	679.24	560.03	754.60	710.89	542.65	785.03	801.64	485.90
py–Al(OSiH$_3$)$_3$										
B3LYP-D3/TZ	477.60	521.72	602.48	357.15	528.19	625.15	341.80	550.06	690.39	292.44
PBE0-D3/TZ	478.57	522.62	599.67	358.82	529.10	622.36	343.54	550.99	687.64	294.39
py–Al(OSiH$_3$)$_3$(THF)										

B3LYP-D3/TZ	795.69	849.84	648.72	672.64	858.44	678.85	656.04	887.90	766.67	601.81
PBE0-D3/TZ	797.02	851.49	653.27	673.05	860.10	683.43	656.34	889.57	771.29	601.76
$AlCl_4^-$										
B3LYP-D3/TZ	15.17	34.06	359.82	–64.23	36.43	368.13	–73.33	43.77	390.09	–101.79
PBE0-D3/TZ	15.42	34.23	359.37	–63.93	36.59	367.64	–73.02	43.91	389.52	–101.44
$AlCl_3OSiH_3^-$										
B3LYP-D3/TZ	88.89	113.99	434.48	–4.69	117.22	445.81	–15.70	127.55	476.66	–50.31
PBE0-D3/TZ	88.99	113.96	426.60	–2.57	117.19	437.92	–13.38	127.51	468.76	–47.41
$AlCl_2(OSiH_3)_2^-$										
B3LYP-D3/TZ	163.44	194.11	478.30	63.46	198.19	492.61	51.32	211.47	532.26	12.86
PBE0-D3/TZ	163.12	193.86	481.07	62.46	197.95	495.40	50.25	211.25	535.11	11.58
$AlCl(OSiH_3)_3^-$										
B3LYP-D3/TZ	237.81	274.23	535.28	128.02	279.17	552.58	114.42	295.39	601.01	71.13
PBE0-D3/TZ	237.28	273.78	534.20	127.86	278.73	551.55	114.29	295.01	600.12	71.07
$Al(OSiH_3)_4^-$										
B3LYP-D3/TZ	312.84	354.34	573.31	197.73	360.11	593.53	183.15	379.24	650.63	136.46
PBE0-D3/TZ	311.80	353.57	577.05	195.94	359.36	597.36	181.26	378.58	654.72	134.28
$AlCl_3OSi(OSiH_3)_3^-$										
B3LYP-D3/TZ	270.59	317.05	605.52	151.65	323.75	629.01	136.21	345.67	694.44	86.54
PBE0-D3/TZ	269.78	316.44	609.32	150.00	323.16	632.85	134.47	345.13	698.43	84.51
$SiCl_4$										
B3LYP-D3/TZ	18.96	36.29	344.83	–57.90	38.53	352.69	–66.62	45.55	373.66	–93.88
PBE0-D3/TZ	19.40	36.62	344.04	–57.35	38.84	351.84	–66.06	45.82	372.68	–93.25
$SiCl_3OSiH_3$										
B3LYP-D3/TZ	94.68	117.95	407.64	6.60	121.05	418.51	–3.72	131.05	448.35	–36.25
PBE0-D3/TZ	94.72	117.93	405.98	7.04	121.03	416.84	–3.25	131.02	446.65	–35.65
$SiCl_2(OSiH_3)_2$										
B3LYP-D3/TZ	170.81	199.55	458.45	74.33	203.51	472.29	62.69	216.45	510.93	25.80
PBE0-D3/TZ	170.99	199.45	451.94	76.00	203.39	465.76	64.52	216.33	504.38	28.12
$SiCl(OSiH_3)_3$										
B3LYP-D3/TZ	247.35	281.39	504.96	143.46	286.18	521.73	130.63	302.03	569.04	89.70

PBE0-D3/TZ	246.81	280.94	507.64	142.28	285.74	524.43	129.38	301.62	571.83	88.24
$Si(OSiH_3)_4$										
B3LYP-D3/TZ	326.00	363.79	524.59	220.50	369.36	544.09	207.13	387.98	599.66	164.22
PBE0-D3/TZ	324.82	362.81	524.86	219.44	368.40	544.46	206.07	387.12	600.28	163.12
$SiCl_3OSi(OSiH_3)_3$										
B3LYP-D3/TZ	274.17	320.40	614.10	152.66	327.02	637.28	137.01	348.70	702.00	86.75
PBE0-D3/TZ	273.67	320.04	618.39	151.13	326.66	641.59	135.38	348.37	706.37	84.79
Me_3SiCl										
B3LYP-D3/TZ	295.29	316.62	354.22	219.87	319.81	365.37	210.87	330.38	396.92	182.27
PBE0-D3/TZ	295.98	317.39	354.77	220.48	320.58	365.96	211.47	331.19	397.61	182.82
$Me_3SiOSiH_3$										
B3LYP-D3/TZ	370.50	397.45	410.27	285.38	401.49	424.41	274.95	415.02	464.78	241.59
PBE0-D3/TZ	371.06	398.09	411.91	285.58	402.14	426.10	275.10	415.72	466.61	241.61
$Me_3SiOSi(OSiH_3)_3$										
B3LYP-D3/TZ	553.16	601.60	600.05	437.69	609.09	626.27	422.36	634.14	701.02	372.55
PBE0-D3/TZ	552.72	601.51	603.59	436.64	609.03	629.94	421.22	634.20	705.02	371.12
$PhMe_2SiCl$										
B3LYP-D3/TZ	437.72	465.95	429.87	348.53	470.40	445.46	337.59	485.57	490.69	302.47
PBE0-D3/TZ	439.34	467.62	430.11	350.13	472.07	445.71	339.18	487.25	490.95	304.05
$PhMe_2SiOSiH_3$										
B3LYP-D3/TZ	512.44	546.45	485.91	413.72	551.76	504.51	401.34	569.91	558.63	361.46
PBE0-D3/TZ	513.96	547.98	484.27	415.70	553.30	502.90	403.36	571.47	557.09	363.59
$PhMe_2SiOSi(OSiH_3)_3$										
B3LYP-D3/TZ	694.44	750.36	674.86	566.02	759.13	705.57	548.77	788.83	794.13	492.49
PBE0-D3/TZ	694.87	751.19	680.69	565.26	759.99	711.51	547.86	789.77	800.33	491.13
PCl_3										
B3LYP-D3/TZ	12.39	26.74	315.99	–59.57	28.53	322.26	–67.55	34.09	338.88	–92.36
PBE0-D3/TZ	13.02	27.15	314.18	–58.67	28.91	320.36	–66.60	34.41	336.80	–91.27
PCl_2OSiH_3										
B3LYP-D3/TZ	88.42	108.07	363.68	8.73	110.72	372.94	–0.48	119.26	398.46	–29.42
PBE0-D3/TZ	88.69	108.16	362.03	9.28	110.79	371.23	0.11	119.31	396.65	–28.71

$PCl(OSiH_3)_2$										
B3LYP-D3/TZ	165.81	189.91	397.03	81.46	193.37	409.15	71.38	204.79	443.25	39.39
PBE0-D3/TZ	165.86	189.79	395.33	81.80	193.24	407.42	71.77	204.65	441.47	39.91
$P(OSiH_3)_3$										
B3LYP-D3/TZ	241.75	270.62	436.27	151.45	274.90	451.28	140.35	289.25	494.08	104.88
PBE0-D3/TZ	241.09	270.09	439.00	150.18	274.38	454.04	139.01	288.76	496.92	103.33
$PCl_2OSi(OSiH_3)_3$										
B3LYP-D3/TZ	267.14	310.30	577.82	152.46	316.49	599.52	137.74	336.80	660.14	90.47
PBE0-D3/TZ	267.01	310.10	578.28	152.14	316.29	599.95	137.41	336.59	660.56	90.10
$POCl_3$										
B3LYP-D3/TZ	25.21	41.01	327.32	–48.40	43.10	334.66	–56.68	50.70	354.37	–81.54
PBE0-D3/TZ	25.99	41.58	325.75	–47.40	43.65	333.00	–55.63	50.18	352.51	–81.36
$POCl_2OSiH_3$										
B3LYP-D3/TZ	101.88	123.05	377.39	19.96	125.98	387.68	10.39	136.52	416.16	–18.77
PBE0-D3/TZ	102.25	123.27	376.21	20.51	126.20	386.45	10.98	135.70	414.82	–19.09
$POCl(OSiH_3)_2$										
B3LYP-D3/TZ	179.39	205.47	421.43	90.35	209.21	434.55	79.65	222.60	471.52	46.65
PBE0-D3/TZ	179.18	205.35	425.71	89.07	209.10	438.83	78.26	221.49	475.80	43.94
$PO(OSiH_3)_3$										
B3LYP-D3/TZ	256.00	287.25	471.39	158.49	291.81	487.36	146.50	308.07	532.90	109.22
PBE0-D3/TZ	256.42	286.99	456.60	162.27	291.54	472.55	150.65	306.81	518.08	113.48
$POCl_2OSi(OSiH_3)_3$										
B3LYP-D3/TZ	280.18	325.10	595.67	162.39	331.59	618.42	147.21	353.91	682.06	99.40
PBE0-D3/TZ	280.13	325.00	596.01	162.20	331.49	618.74	147.02	352.81	682.35	98.19
$TiCl_4$										
B3LYP-D3/TZ	15.00	34.18	365.75	–65.72	36.55	374.05	–74.97	44.88	395.96	–102.87
PBE0-D3/TZ	15.24	34.36	365.40	–65.45	36.72	373.66	–74.69	44.02	395.50	–103.56
$TiCl_3OSiH_3$										
B3LYP-D3/TZ	88.69	114.22	436.96	–5.14	117.49	448.45	–16.21	128.95	479.67	–50.04
PBE0-D3/TZ	88.77	114.21	434.15	–4.38	117.48	445.61	–15.38	127.93	476.81	–49.99
$TiCl_2(OSiH_3)_2$										

B3LYP-D3/TZ	162.99	194.36	490.38	60.41	198.53	504.99	47.97	213.06	545.38	9.55
PBE0-D3/TZ	162.69	194.12	491.81	59.78	198.29	506.44	47.30	211.83	546.88	7.77
$TiCl(OSiH_3)_3$										
B3LYP-D3/TZ	237.09	274.53	550.53	124.15	279.59	568.25	110.16	297.17	617.76	66.65
PBE0-D3/TZ	236.44	274.01	555.73	122.21	279.08	573.49	108.09	295.71	623.12	63.19
$Ti(OSiH_3)_4$										
B3LYP-D3/TZ	310.82	354.44	614.98	186.46	360.39	635.81	170.82	381.03	694.42	121.90
PBE0-D3/TZ	309.94	353.74	619.35	184.56	359.70	640.25	168.81	379.40	699.04	118.56
$TiCl_3OSi(OSiH_3)_3$										
B3LYP-D3/TZ	267.86	316.72	650.19	139.12	323.52	674.01	122.56	346.68	740.15	70.49
PBE0-D3/TZ	267.30	316.30	652.15	138.16	323.10	675.98	121.56	345.28	742.20	68.33
Cp_2TiCl_2										
B3LYP-D3/TZ	454.05	484.44	448.84	361.84	489.45	466.39	350.40	507.72	517.86	314.48
PBE0-D3/TZ	457.84	487.38	440.19	367.15	492.33	457.52	355.92	509.43	508.49	319.69
$Cp_2TiClOSiH_3$										
B3LYP-D3/TZ	527.35	563.39	497.97	427.37	569.29	518.62	414.66	590.62	579.24	374.48
PBE0-D3/TZ	530.79	566.25	493.66	431.41	572.10	514.13	418.81	592.29	574.31	377.98
$Cp_2Ti(OSiH_3)_2$										
B3LYP-D3/TZ	600.24	642.11	547.74	492.50	648.90	571.53	478.50	673.32	641.34	434.01
PBE0-D3/TZ	603.22	644.86	552.46	493.96	651.61	576.09	479.85	674.90	645.52	434.02
$Cp_2TiClOSi(OSiH_3)_3$										
B3LYP-D3/TZ	708.78	767.41	692.67	578.21	776.78	725.48	560.48	809.69	820.62	503.47
PBE0-D3/TZ	710.61	769.09	699.17	578.12	778.43	731.86	560.23	810.25	826.76	501.75
VCl_4										
B3LYP-D3/TZ	14.59	34.03	375.58	–68.56	36.41	383.91	–78.05	44.76	405.89	–106.70
PBE0-D3/TZ	14.88	34.25	375.17	–68.23	36.61	383.46	–77.72	43.93	405.34	–107.32
VCl_3OSiH_3										
B3LYP-D3/TZ	88.10	113.73	438.25	–5.98	117.02	449.79	–17.09	128.52	481.16	–51.02
PBE0-D3/TZ	88.23	113.77	437.45	–5.72	117.05	448.96	–16.80	127.54	480.27	–51.68
$VCl_2(OSiH_3)_2$										
B3LYP-D3/TZ	163.08	194.25	488.74	60.75	198.42	503.35	48.34	212.96	543.77	10.05

PBE0-D3/TZ	162.84	194.02	489.99	60.18	198.19	504.60	47.74	211.74	545.05	8.36
$VCl(OSiH_3)_3$										
B3LYP-D3/TZ	238.10	274.44	532.33	129.04	279.47	549.95	115.50	297.01	599.31	73.38
PBE0-D3/TZ	237.75	274.07	531.76	128.82	279.10	549.39	115.30	295.65	598.80	72.21
$V(OSiH_3)_4$										
B3LYP-D3/TZ	313.27	354.59	570.44	198.77	360.47	591.07	184.25	381.01	649.34	138.70
PBE0-D3/TZ	313.22	354.22	563.75	200.23	360.11	584.37	185.88	379.65	642.68	139.83
$VCl_3OSi(OSiH_3)_3$										
B3LYP-D3/TZ	267.81	316.86	652.39	138.66	323.67	676.23	122.05	346.84	742.42	69.81
PBE0-D3/TZ	268.11	316.60	639.53	141.91	323.40	663.34	125.62	345.56	729.50	73.35
$VOCl_3$										
B3LYP-D3/TZ	20.72	38.17	345.40	–56.17	40.39	353.15	–64.91	48.28	373.76	–91.19
PBE0-D3/TZ	21.21	38.56	344.59	–55.57	40.76	352.29	–64.28	47.62	372.79	–91.49
$VOCl_2OSiH_3$										
B3LYP-D3/TZ	95.14	118.37	403.25	8.22	121.46	414.10	–2.00	132.43	443.85	–33.20
PBE0-D3/TZ	95.48	118.56	400.86	9.07	121.65	411.67	–1.09	131.59	441.36	–33.10
$VOCl(OSiH_3)_2$										
B3LYP-D3/TZ	170.50	198.99	448.12	76.58	202.95	461.99	65.21	216.92	500.70	30.08
PBE0-D3/TZ	170.25	198.87	451.61	75.51	202.83	465.48	64.05	215.81	504.22	27.66
$VO(OSiH_3)_3$										
B3LYP-D3/TZ	244.50	278.99	512.18	139.08	283.82	529.12	126.07	300.84	576.91	85.56
PBE0-D3/TZ	243.97	278.58	512.43	138.61	283.42	529.41	125.58	299.47	577.29	84.05
$VOCl_2OSi(OSiH_3)_3$										
B3LYP-D3/TZ	274.46	321.34	621.20	151.66	327.96	644.41	135.83	350.64	709.11	86.03
PBE0-D3/TZ	273.76	320.94	630.06	148.84	327.58	653.30	132.79	349.28	718.10	81.32
$ZnCl_2$										
B3LYP-D3/TZ	6.38	18.98	277.42	–56.80	20.39	282.39	–63.80	24.75	295.40	–85.48
PBE0-D3/TZ	6.55	19.07	276.70	–56.51	20.49	281.65	–63.49	24.82	294.61	–85.11
$ZnCl_2$(THF)										
B3LYP-D3/TZ	319.63	345.09	423.29	229.47	348.63	435.71	218.73	360.49	471.10	184.70
PBE0-D3/TZ	321.37	346.74	422.24	231.40	350.26	434.59	220.69	362.06	469.76	186.76

$ZnCl_2(THF)_2$										
B3LYP-D3/TZ	632.83	671.75	544.79	522.94	677.52	565.00	509.07	697.18	623.61	464.48
PBE0-D3/TZ	635.90	674.81	545.20	525.89	680.55	565.30	512.01	700.10	623.57	467.41
$ZnClOSiH_3$										
B3LYP-D3/TZ	79.89	97.77	350.21	2.11	99.97	357.93	–6.74	107.07	379.12	–34.40
PBE0-D3/TZ	79.83	97.71	351.54	1.68	99.91	359.26	–7.20	107.01	380.45	–34.96
$ZnClOSiH_3(THF)$										
B3LYP-D3/TZ	393.34	424.49	474.05	295.00	428.92	489.56	282.95	443.82	534.01	244.55
PBE0-D3/TZ	394.78	425.94	475.03	296.19	430.36	490.49	284.11	445.21	534.80	245.65
$ZnClOSiH_3(THF)_2$										
B3LYP-D3/TZ	706.81	751.21	581.17	592.46	757.86	604.47	577.64	780.55	672.13	529.75
PBE0-D3/TZ	709.68	754.18	585.44	594.26	760.80	608.64	579.33	783.40	676.02	531.14
$ZnClOSi(OSiH_3)_3(THF)_2$										
B3LYP-D3/TZ	890.05	955.96	764.14	747.24	966.05	799.46	727.69	1000.23	901.41	663.87
PBE0-D3/TZ	890.77	957.53	778.98	744.75	967.63	814.35	724.83	1001.84	916.37	659.90
$ZnCl_3^-$										
B3LYP-D3/TZ	7.85	24.52	343.89	–69.41	26.46	350.68	–78.10	32.38	368.38	–105.08
PBE0-D3/TZ	8.07	24.63	342.72	–68.99	26.56	349.48	–77.64	32.46	367.12	–104.53
$ZnCl_2OSiH_3^-$										
B3LYP-D3/TZ	80.67	103.22	400.61	–6.20	106.03	410.46	–16.34	114.98	437.17	–48.15
PBE0-D3/TZ	80.73	103.21	400.07	–6.07	106.02	409.91	–16.20	114.96	436.61	–47.97
$ZnCl(OSiH_3)_2^-$										
B3LYP-D3/TZ	154.25	182.27	452.00	58.80	185.94	464.86	47.34	197.87	500.49	11.11
PBE0-D3/TZ	154.14	182.10	450.83	58.96	185.78	463.71	47.52	197.73	499.38	11.38
$Zn(OSiH_3)_3^-$										
B3LYP-D3/TZ	225.93	260.46	519.72	118.50	265.03	535.73	105.30	280.04	580.53	63.42
PBE0-D3/TZ	225.66	260.20	519.25	118.37	264.78	535.30	105.18	279.83	580.21	63.32
$ZnCl_2OSi(OSiH_3)_3^-$										
B3LYP-D3/TZ	262.11	306.49	591.79	144.84	312.78	613.82	129.77	333.33	675.17	81.39
PBE0-D3/TZ	261.50	305.95	593.63	143.80	312.25	615.70	128.68	332.84	677.16	80.16
$ZnEt_2$										

B3LYP-D3/TZ	337.89	358.84	360.76	260.30	361.80	371.11	251.15	371.70	400.65	222.20
PBE0-D3/TZ	339.28	360.21	360.21	261.82	363.16	370.55	252.68	373.07	400.09	223.77
$ZnEt_2(THF)$										
B3LYP-D3/TZ	650.30	684.83	482.78	552.95	690.02	500.96	540.65	707.74	553.80	501.09
PBE0-D3/TZ	653.08	687.62	483.50	555.55	692.80	501.63	543.24	710.47	554.32	503.63
$ZnEt_2(THF)_2$										
B3LYP-D3/TZ	959.47	1008.74	614.15	840.99	1016.22	640.32	825.31	1041.89	716.86	774.40
PBE0-D3/TZ	963.49	1012.94	618.09	844.11	1020.39	644.18	828.33	1045.98	720.45	777.14
$ZnEtOSiH_3$										
B3LYP-D3/TZ	246.96	269.15	380.26	165.28	282.07	390.79	165.56	282.13	420.55	125.20
PBE0-D3/TZ	247.45	269.64	380.23	165.78	272.64	390.76	156.14	282.63	420.55	125.70
$ZnEtOSiH_3(THF)$										
B3LYP-D3/TZ	558.63	594.20	500.41	457.51	599.44	518.77	444.77	617.26	571.89	403.86
PBE0-D3/TZ	560.28	596.17	512.20	456.26	601.40	530.53	443.22	619.19	583.56	401.43
$ZnEtOSiH_3(THF)_2$										
B3LYP-D3/TZ	870.49	919.86	617.09	751.30	927.35	643.31	735.54	953.01	719.83	684.41
PBE0-D3/TZ	873.50	923.17	622.76	753.06	930.64	648.92	737.16	956.23	725.23	685.61
$ZnEtOSi(OSiH_3)_3(THF)_2$										
B3LYP-D3/TZ	1051.17	1123.71	831.71	896.53	1134.70	870.22	875.25	1172.04	981.55	805.77
PBE0-D3/TZ	1055.76	1127.51	814.26	905.09	1138.45	852.58	884.25	1175.62	963.43	816.12
$Zn(OSiH_3)_2$										
B3LYP-D3/TZ	154.10	177.71	404.80	67.14	180.79	415.61	56.88	190.93	445.86	24.56
PBE0-D3/TZ	153.79	177.46	406.01	66.56	180.55	416.84	56.27	190.71	447.16	23.86
$Zn(OSiH_3)_2(THF)$										
B3LYP-D3/TZ	467.87	504.55	520.98	362.24	509.84	539.51	348.98	527.73	592.87	306.50
PBE0-D3/TZ	469.23	505.87	519.22	364.04	511.15	537.72	350.83	529.01	590.98	308.48
$Zn(OSiH_3)_2(THF)_2$										
B3LYP-D3/TZ	781.62	830.83	616.68	662.38	838.33	642.93	646.63	863.97	719.39	595.53
PBE0-D3/TZ	783.65	833.31	626.40	662.21	840.80	652.61	646.22	866.39	728.92	594.39
$SnCl_4$										
B3LYP-D3/TZ	12.38	32.69	381.59	–71.54	35.16	390.22	–81.19	42.71	412.82	–111.33

PBE0-D3/TZ	12.84	32.94	379.52	–70.73	35.38	388.09	–80.33	42.90	410.57	–110.30
$SnCl_3OSiH_3$										
B3LYP-D3/TZ	86.62	112.69	436.51	–6.54	116.04	448.23	–17.60	126.66	479.96	–52.44
PBE0-D3/TZ	86.85	112.76	434.73	–5.99	116.09	446.41	–17.00	126.69	478.07	–51.70
$SnCl_2(OSiH_3)_2$										
B3LYP-D3/TZ	161.98	193.13	477.30	62.75	197.34	492.06	50.63	210.97	532.76	12.17
PBE0-D3/TZ	161.81	192.89	478.13	62.29	197.09	492.87	50.15	210.72	533.56	11.62
$SnCl(OSiH_3)_3$										
B3LYP-D3/TZ	237.66	273.61	510.60	134.14	278.68	528.35	121.15	295.29	577.95	79.63
PBE0-D3/TZ	237.42	273.28	509.97	133.98	278.34	527.71	121.01	294.97	577.33	79.54
$Sn(OSiH_3)_4$										
B3LYP-D3/TZ	312.10	353.42	558.15	200.96	359.36	578.96	186.74	379.02	637.64	141.09
PBE0-D3/TZ	311.28	352.75	561.59	199.35	358.70	582.44	185.04	378.40	641.24	139.12
$SnCl_3OSi(OSiH_3)_3$										
B3LYP-D3/TZ	266.98	315.97	641.29	140.80	322.81	665.25	124.47	345.07	731.68	72.04
PBE0-D3/TZ	266.36	315.47	644.76	139.35	322.32	668.74	122.93	344.59	735.25	70.23
$SbCl_3$										
B3LYP-D3/TZ	8.60	24.83	343.32	–68.95	26.74	350.03	–77.62	32.61	367.57	–104.55
PBE0-D3/TZ	8.98	25.02	341.30	–68.21	26.92	347.97	–76.83	32.76	365.41	–103.60
$SbCl_2OSiH_3$										
B3LYP-D3/TZ	83.57	105.04	388.38	–1.05	107.82	398.15	–10.88	116.73	424.75	–41.76
PBE0-D3/TZ	83.71	105.00	386.43	–0.55	107.78	396.17	–10.34	116.68	422.73	–41.07
$SbCl(OSiH_3)_2$										
B3LYP-D3/TZ	158.80	185.30	428.81	68.17	188.96	441.61	57.29	200.88	477.20	22.81
PBE0-D3/TZ	158.66	185.03	427.08	68.37	188.68	439.87	57.53	200.61	475.47	23.19
$Sb(OSiH_3)_3$										
B3LYP-D3/TZ	233.62	265.40	477.85	134.87	269.91	493.67	122.73	284.84	538.22	84.01
PBE0-D3/TZ	233.39	264.95	473.22	135.69	269.47	489.03	123.66	284.41	533.62	85.29
$SbCl_2OSi(OSiH_3)_3$										
B3LYP-D3/TZ	263.49	307.94	595.29	145.34	314.23	617.31	130.17	334.79	678.68	81.53
PBE0-D3/TZ	263.44	307.58	589.91	146.44	313.86	611.93	131.42	334.43	673.31	83.18

Ph_3SbCl_2										
B3LYP-D3/TZ	721.22	769.25	616.49	600.85	777.02	643.72	585.10	803.71	723.28	533.82
PBE0-D3/TZ	725.18	772.95	613.23	605.44	780.70	640.37	589.77	807.30	719.68	538.75
$Ph_3SbClOSiH_3$										
B3LYP-D3/TZ	796.51	849.42	657.27	669.89	858.05	687.47	653.08	887.70	775.87	598.18
PBE0-D3/TZ	800.20	852.86	652.56	674.61	861.46	682.70	657.92	891.05	770.89	603.39
$Ph_3Sb(OSiH_3)_2$										
B3LYP-D3/TZ	871.88	929.10	683.02	742.53	938.56	716.15	725.04	971.17	813.35	667.67
PBE0-D3/TZ	875.17	932.26	681.62	746.07	941.71	714.71	728.62	974.27	811.78	671.35
$Ph_3SbClOSi(OSiH_3)_3$										
B3LYP-D3/TZ	977.52	1053.02	849.16	821.08	1065.13	891.54	799.31	1106.38	1014.55	727.80
PBE0-D3/TZ	980.11	1055.61	845.03	824.79	1067.72	887.43	803.13	1108.97	1010.43	731.93

S4. References

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