Electronic Supplementary Material (ESI) for Dalton Transactions.

Hetero-bimetallic alkali titanosilicates $[MOTi\{OSi(O^tBu)_3\}_3]_2$ (M = Li–Cs) with terminal Ti–O$^-$ groups.

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Materials and characterization methods

The synthesis of compounds (**AS**, **TS**, **1**–**6**) were performed under a dried dinitrogen atmosphere using Schlenk and glove-box techniques, while the synthesis of silanol **S1** did not require the use of inert atmosphere. Solvents were purchased from Sigma-Aldrich/Merck and dried before use with an MBraun SPS solvent purification system using Grubs' columns. ^{t}BuOH was dried with metallic sodium and distilled before use. $(^t BuO)_2Si(OAc)_2$ was prepared according to the literature procedure from $Si(OAc)_4$ and ^{t}BuOH.[1] C_6D_6 was and dried with a Na/K alloy and distilled before use. The NMR spectra were recorded on a Bruker Avance 300 spectrometer and ^{1}H NMR spectra were referenced to residual protons from the deuterated solvent, while ^{13}C chemical shifts are referenced to C_6D_6. ^{29}Si spectra are referenced to an external standard (TMS). FT-IR spectra were measured on a Bruker Tensor 27 using the ATR technique with a diamond window in the range of 4000–500 cm^{-1}. Negative chemical ionization mass spectrometry (NCI-MS) was carried on a Shimadzu GCMS-QP2010 Plus using direct injection in the detection range of *m*/*z* 20 – 1090. Elemental analyses (C, H, N) were determined on an Elemental vario MICRO Cube analyzer. Melting points were measured on a Büchi B-540 melting point apparatus.

1. Synthesis

Synthesis of (^{t}BuO)$_3$Si(OAc) (AS) (Route 1): To a solution of (^{t}BuO)$_2$Si(OAc)$_2$ (1.00 g, 3.42 mmol) in toluene (25 mL) was added ^{t}BuOK (0.383 g, 3.42 mmol). The mixture was stirred and heated at reflux for 2 hours. Afterwards, all volatiles were removed under reduced pressure and a yellow oil was obtained (**AS** and **TS** mixture). The crude product was dissolved in ethyl ether and colourless crystals were obtained after two days, corresponding to cyclotrisiloxanetriol **TS**. It should be noted that, despite our multiple efforts and due to **TS** solubility in **AS**, we were not able to obtained **AS** in a pure form, always was in mixture with **TS**. Nevertheless, compound **TS** could be purified by crystallization from saturated ethyl ether solution.

[(^{t}BuO)$_3$Si(μ-O)]$_3$ (TS) Yield: 0.586 g, 30%. M.p. 160–161 °C. Elemental Analysis (%) Calcd. for $C_{24}H_{54}O_9Si_3$ (570.94 gmol^{-1}): C 50.49, H 9.53; found: C 50.26, H 9.51. FT-IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2976, 2934 (w, C–H, CH_3, CH_2), 1076 (s, Si–O–C). ^{1}H NMR (300.53 MHz, $CDCl_3$, 25 °C): δ (ppm) 1.33 (s, 27H, C(C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (75.57 MHz, $CDCl_3$, 25 °C): δ (ppm) 73.5 *C*(CH$_3$)$_3$ 31.5 (C(*C*H$_3$)$_3$). ^{29}Si NMR (59.63 MHz, $CDCl_3$, 25 °C): δ (ppm) –97.9. EI-MS: *m*/*z* (%) 455 (36) [M – Me]$^+$, 499 (38) [M – C_4H_8 – Me]$^+$, 443 (100) [M – 2C_4H_8 – Me]$^+$, 387 (75) [M – 3C_4H_8 – Me]$^+$, 331 (40) [M – 4C_4H_8 – Me]$^+$, 275 (28) [M – 5C_4H_8 – Me]$^+$.

Synthesis of (^{t}BuO)$_3$Si(OAc) (AS) (Route 2): Anhydrous tert-butanol (145 mL, 1.51 mol) was added to Si(OAc)$_4$ (40.0 g, 0.151 mol). The reaction mixture was refluxed for 24 h. Afterwards, all volatiles were removed under reduced pressure, and the product was isolated as a colorless oil. Yield: 45.980 g, 99%. Elemental Analysis (%) Calcd. for $C_{14}H_{30}O_5Si$ (306.47 gmol^{-1}): C 54.87, H 9.87; found: C 54.04, H 9.76. FT-IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2976, 2934 (w, C–H, CH_3, CH_2), 1742 (m, C=O), 1071 (s, Si–O–C). ^{1}H NMR (300.53 MHz, $CDCl_3$, 25 °C): δ (ppm) 2.09 (s, 3H, OCC*H*$_3$), 1.33 (s, 27H, C(C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (75.57 MHz, $CDCl_3$, 25 °C): δ (ppm) 168.5 (O*C*CH$_3$), 70.4 *C*(CH$_3$)$_3$ 31.3 (C(*C*H$_3$)$_3$), 23.4 (OC*C*H$_3$). ^{29}Si NMR (59.63 MHz, $CDCl_3$, 25 °C): δ (ppm) –102.0. EI-MS: *m*/*z* (%) 291 (50) [M – Me]$^+$, 233 (100) [M – O^{t}Bu]$^+$.

Synthesis of (^{t}BuO)$_3$Si(OH) (S1): Compound **AS** (45.980 g, 0.150 mol) was suspended in an aqueous solution of potassium hydroxide (0.150 L, 10 M). The reaction mixture was vigorously stirred at room temperature for 6 h. Subsequently, the silanol was filtered and washed with cold water. After filtration, the product was isolated as a white powder. Yield: 39.665 g, 99%. M.p. 63–64 °C. Elemental Analysis (%) Calcd. for $C_{12}H_{28}O_4Si$ (264.43 gmol^{-1}): C 54.50, H 10.67; found: C 53.43, H 10.51. FT-IR (ATR) (cm^{-1}) $\tilde{\nu}$ 3528–3086 (w, br, O–H), 2970, 2926 (w, C–H, CH_3), 991 (s, Si–O). ^{1}H NMR (300.53 MHz, $CDCl_3$, 25 °C): δ (ppm) 3.10 (s, 1H, O*H*), 1.33 (s, 27H, C(C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (75.57 MHz, $CDCl_3$, 25 °C): δ (ppm) 73.1 *C*(CH$_3$)$_3$,

31.5 (C(CH_3)$_3$). ^{29}Si NMR (59.63 MHz, $CDCl_3$, 25 °C): δ (ppm) –90.6. EI-MS: *m*/*z* (%) 249 (100) [M – Me]$^+$, 151 (50) [M – C_4H_8 – Me]$^+$.

Synthesis of {(^{t}BuO)$_3$SiO}$_3$TiNEt$_2$ (1): A solution of **S1** (^{t}BuO)$_3$SiOH (1.00 g, 3.78 mmol) was added dropwise to a stirred cold solution of Ti(NEt$_2$)$_4$ (0.424 g, 1.26 mmol) in toluene at −78 °C. After stirring for 15 min, the solution was allowed to warm to ambient temperature (20 °C) and stirred for 8 h. All volatiles were removed under reduced pressure, and the product was isolated as a yellow powder. Yield: 1.111 g, 97%. M. p. = 148–149 °C. Elemental Analysis (%) Calcd. for $C_{40}H_{91}O_{12}NSi_3Ti$ (909.532 gmol^{-1}): C 52.78, H 10.08; found: C 52.49, H 10.01. FT-IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2972, 2930 (w, C–H, CH_3, CH_2), 1046 (s, Si–O–C), 952 (s, Si–O–C). ^{1}H NMR (300.53 MHz, C_6D_6, 25 °C): δ (ppm) 4.03 (q, 4H, $^3J_{H–H}$= 7.0 Hz, N(CH_2CH$_3$)$_2$), 1.52 (s, 81H, C(CH_3)$_3$), 1.22 (t, 6H, $^3J_{H–H}$= 7.0 Hz, N(CH$_2$CH_3)$_2$). ^{13}C{^{1}H} NMR (75.57 MHz, C_6D_6, 25 °C): δ (ppm) 73.6 (*C*(CH$_3$)$_3$), 46.4 (N(*C*H$_2$CH$_3$)$_2$), 32.1 (C(*C*H$_3$)$_3$), 14.9 (N(CH$_2$*C*H$_3$)$_2$). ^{29}Si NMR (59.63 MHz, C_6D_6): δ (ppm) –101.2.

General synthetic route for titanosilicates [{(^{t}BuO)$_3$SiO}$_3$TiOM]$_2$ (M= Li, Na, K, Rb, Cs)

The corresponding hydroxide M(OH) (M= Li, Na, K, Rb, Cs) was added to a solution of {(^{t}BuO)$_3$SiO}$_3$TiNEt$_2$ (**1**) in THF. The reaction mixture was vigorously stirred at 40°C for 2 h. Subsequently, all volatiles were removed under reduced pressure. Then, the product was purified by crystallization from a saturated hexane solution. It should be noted that yields are reported after crystallization.

[{(^{t}BuO)$_3$SiO}$_3$TiOLi]$_2$ (2): LiOH (0.010 g, 0.44 mmol); **1** (0.400 g, 0.44 mmol); stirring for 2 h. Yield: 0.160 g, 42%. M.p. >300 °C (dec.). Elemental Analysis (%) Calcd $C_{72}H_{162}O_{26}Si_6Li_2Ti_2$ (1720.925 gmol^{-1}): C 50.21, H 9.48; found: C 49.41, H 9.27. IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2972, 2931 (w, C–H, CH_3), 1049 (s, Si–O), 962 (s, Si–O–Ti). ^{1}H NMR (C_6D_6, 300.53 MHz, 25°C): δ (ppm) 1.59 (s, CH_3). NCI-MS: *m*/*z* (%) 854 (100) [M – Li]$^-$.

[{(^{t}BuO)$_3$SiO}$_3$TiONa]$_2$ (3): NaOH (0.011 g, 0.27 mmol); **1** (0.250 g, 0.27 mmol); stirring for 2 h. Yield: 0.110 g, 46%. M.p. >300 °C (dec.). IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2972, 2931 (w, C–H, CH_3), 1057 (s, Si–O), 967 (s, Si–O–Ti). Elemental Analysis (%) $C_{72}H_{162}O_{26}Si_6Na_2Ti_2$ (1754.27 gmol^{-1}): C 49.30, H 9.31; found: C 48.36, H 9.15. ^{1}H NMR (C_6D_6, 300.53 MHz, 25°C): δ (ppm) 1.58 (s, CH_3). NCI-MS: *m*/*z* (%) 854 (100) [M – Na]$^-$.

[{(^{t}BuO)$_3$SiO}$_3$TiOK]$_2$ (4): KOH (0.012 g, 0.22 mmol); **1** (0.200 g, 0.22 mmol); stirring for 2 h. Yield 0.115 g, 58%. M.p. >300 °C (dec.). Elemental Analysis (%) for $C_{72}H_{162}O_{26}Si_6K_2Ti_2$ (1786.48 gmol^{-1}): C 48.41, H 9.14; found: C 48.43, H 9.16. FT-IR (ATR) (cm^{-1}) 2972, 2930 (w, C–H, CH_3), 1046 (s, Si–O), 967 (s, Si–O–Ti). ^{1}H

NMR (C_6D_6, 300.53 MHz, 25 °C) δ (ppm) 1.57 (s, CH_3). NCI-MS: *m*/*z* (%) 854 (100) [M – K]$^-$.

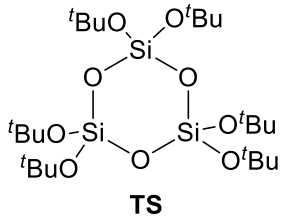
[{(^{t}BuO)$_3$SiO}$_3$TiORb]$_2$ (5): RbOH (0.022 g, 0.22 mmol); **1** (0.200 g, 0.22 mmol); stirring for 2 h. Yield 0.101 g, 48%. M.p. >300 °C (dec.). FT-IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2972, 2931 (w, C–H, CH_3), 1049 (s, Si–O), 964 (s, Si–O–Ti). Elemental Analysis (%) for $C_{72}H_{162}O_{26}Si_6Rb_2Ti_2$ (1879.22 gmol^{-1}): C 46.02, H 8.69; found: C 45.64, H 8.70. ^{1}H NMR (C_6D_6, 300.53 MHz, 25 °C) δ ppm: 1.56 (s, CH_3). NCI-MS: *m*/*z* (%) 854 (100) [M – Rb]$^-$.

[{(^{t}BuO)$_3$SiO}$_3$TiOCs]$_2$ (6): CsOH (0.033 g, 0.22 mmol); **1** (0.200 g, 0.22 mmol); stirring for 2 h. Yield 0.098 g, 45%. M.p. >300 °C (dec.). FT-IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2972, 2930 (w, C–H, CH_3), 1050 (s, Si–O), 968 (s, Si–O–Ti). Elemental Analysis (%) $C_{72}H_{162}O_{26}Si_6Cs_2Ti_2$ (1974.09 gmol^{-1}): C 43.81, H 8.21; found: C 41.48, H 7.71. ^{1}H NMR (C_6D_6, 300.53 MHz, 25°C) δ ppm: 1.56 (s, CH_3). NCI-MS: *m*/*z* (%) 854 (100) [M – Cs]$^-$.

{(^{t}BuO)$_3$SiO}$_3$TiO^{t}Bu (7): A solution of ^{t}BuOH (0.5 M in THF, 0.4 mL) was added dropwise to a stirred cold solution of **1** (0.200 g, 0.22 mmol) in THF. After stirring for 2 hours, all volatiles were removed under reduced pressure, and the product was isolated as a white powder. Yield: 0.194 g, 97%. M. p. = 274–276 °C. Elemental Analysis (%) Calcd. for $C_{40}H_{91}O_{13}Si_3Ti$ (911.26 gmol^{-1}): C 52.72, H 9.95; found: C 51.77, H 9.65. FT-IR (ATR) (cm^{-1}) $\tilde{\nu}$ 2973, 2930 (w, C–H, CH_3, CH_2), 1055 (s, Si–O–C), 904 (s, Si–O–C). ^{1}H NMR (300.53 MHz, C_6D_6, 25 °C): δ (ppm) 1.55 (s, 9H, for TiOC(CH_3)$_3$), 1.53 (s, 81H, for SiOC(CH_3)$_3$. ^{13}C{^{1}H} NMR (75.57 MHz, C_6D_6, 25 °C): δ (ppm) 86.8 (TiO*C*(CH$_3$)$_3$), 72.7 SiO*C*(CH$_3$)$_3$, 32.2 (TiOC(*C*H$_3$)$_3$), 32.1 (SiOC(*C*H$_3$)$_3$). ^{29}Si NMR (59.63 MHz, C_6D_6): δ (ppm) –101.5.

2. NMR spectra of compounds TS, AS, S1, 1–7

^{1}H NMR (300 MHz, $CDCl_3$)



TS

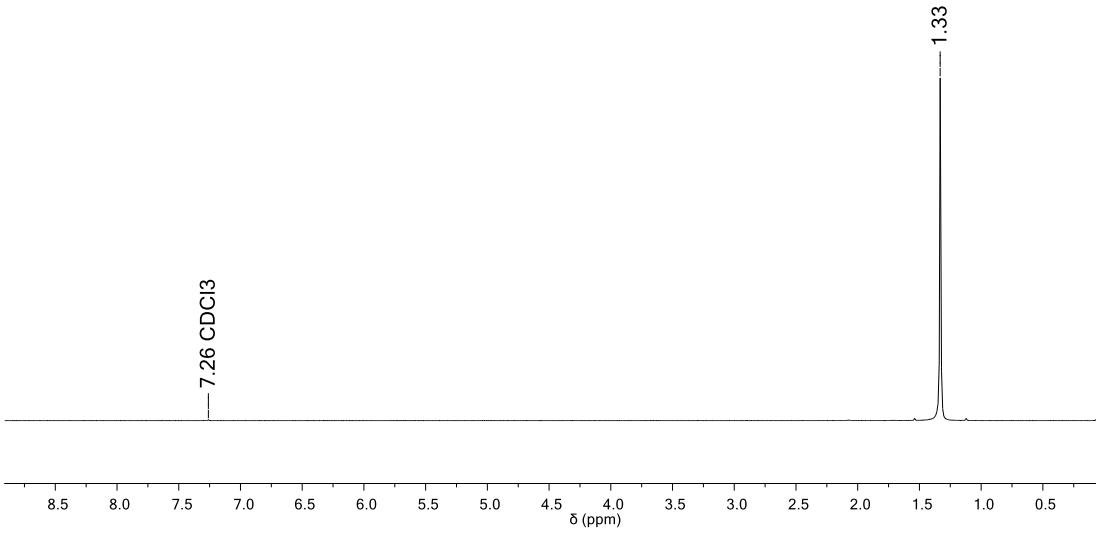


Figure S1. ^{1}H NMR spectrum of compound **TS**.

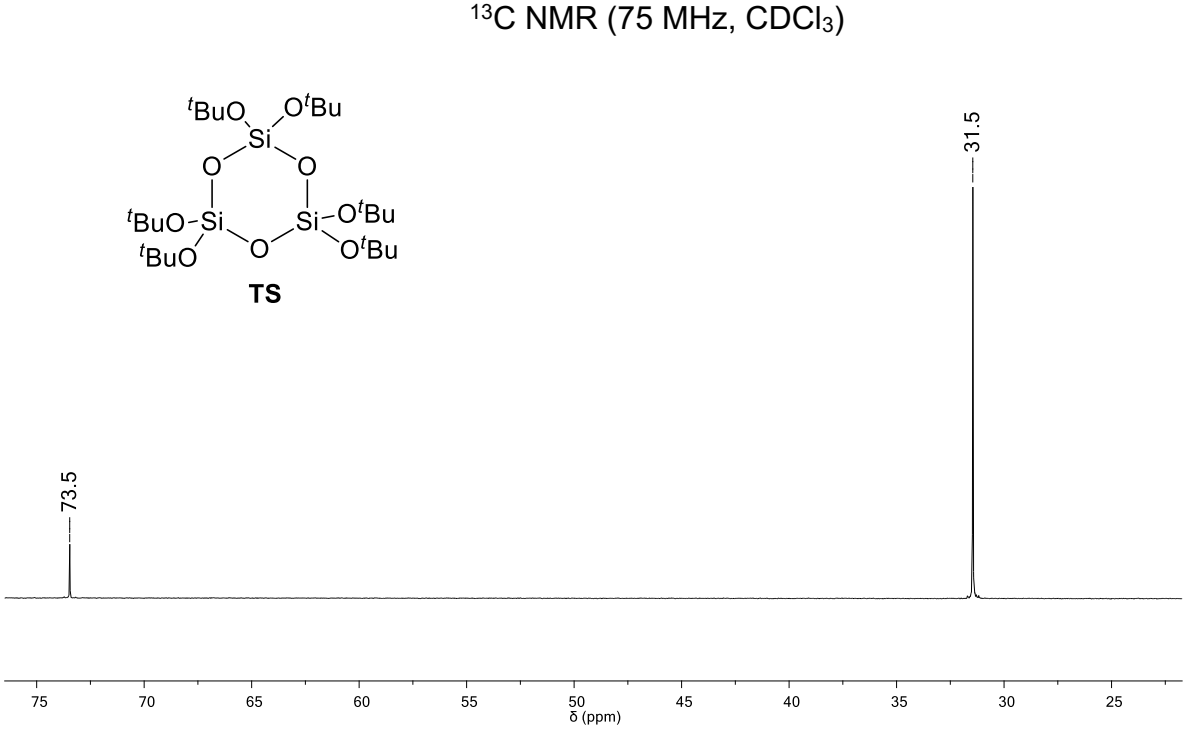


Figure S2. ^{13}C NMR spectrum of compound **TS**.

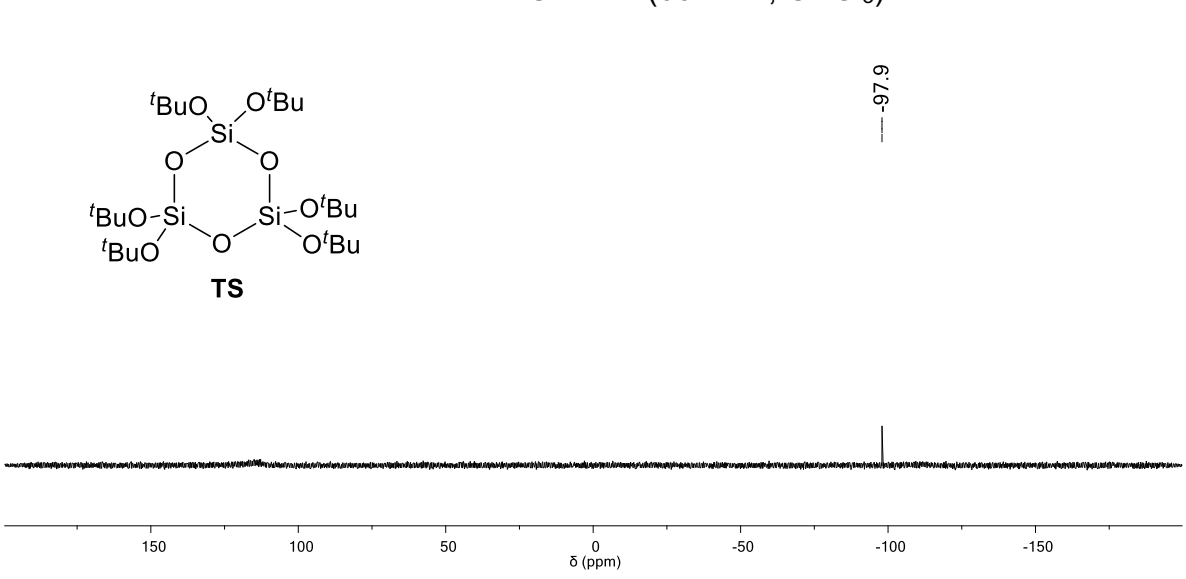


Figure S3. ^{29}Si NMR spectrum of compound **TS**.

^{1}H NMR (300 MHz, $CDCl_3$)

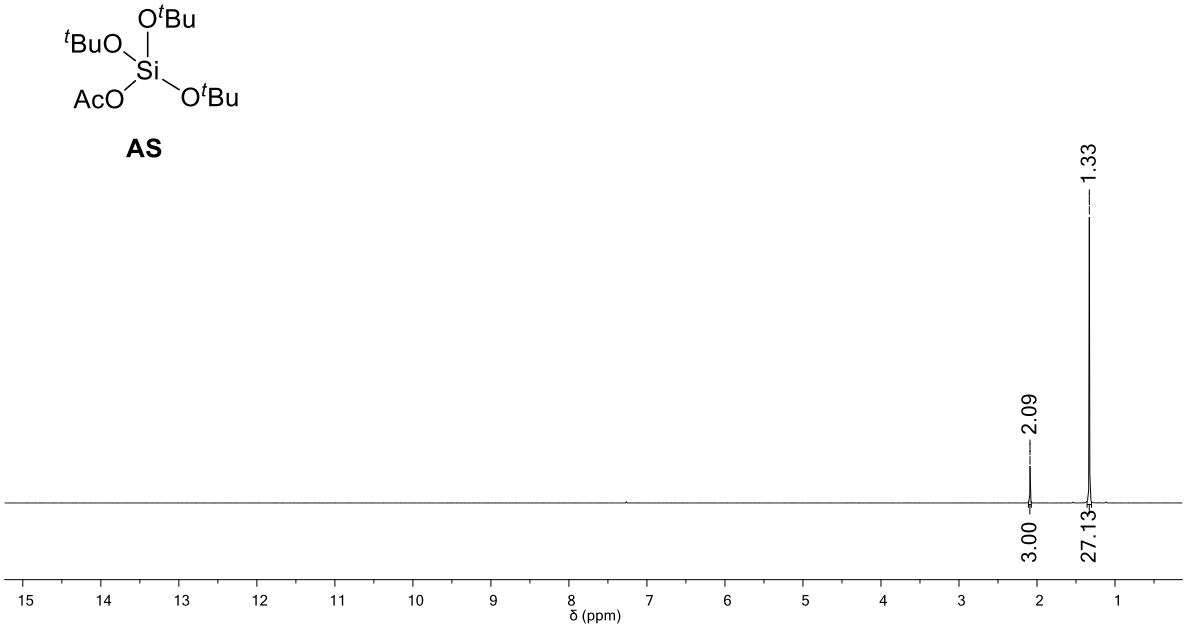


Figure S4. ^{1}H NMR spectrum of compound **AS**.

^{13}C NMR (75 MHz, $CDCl_3$)

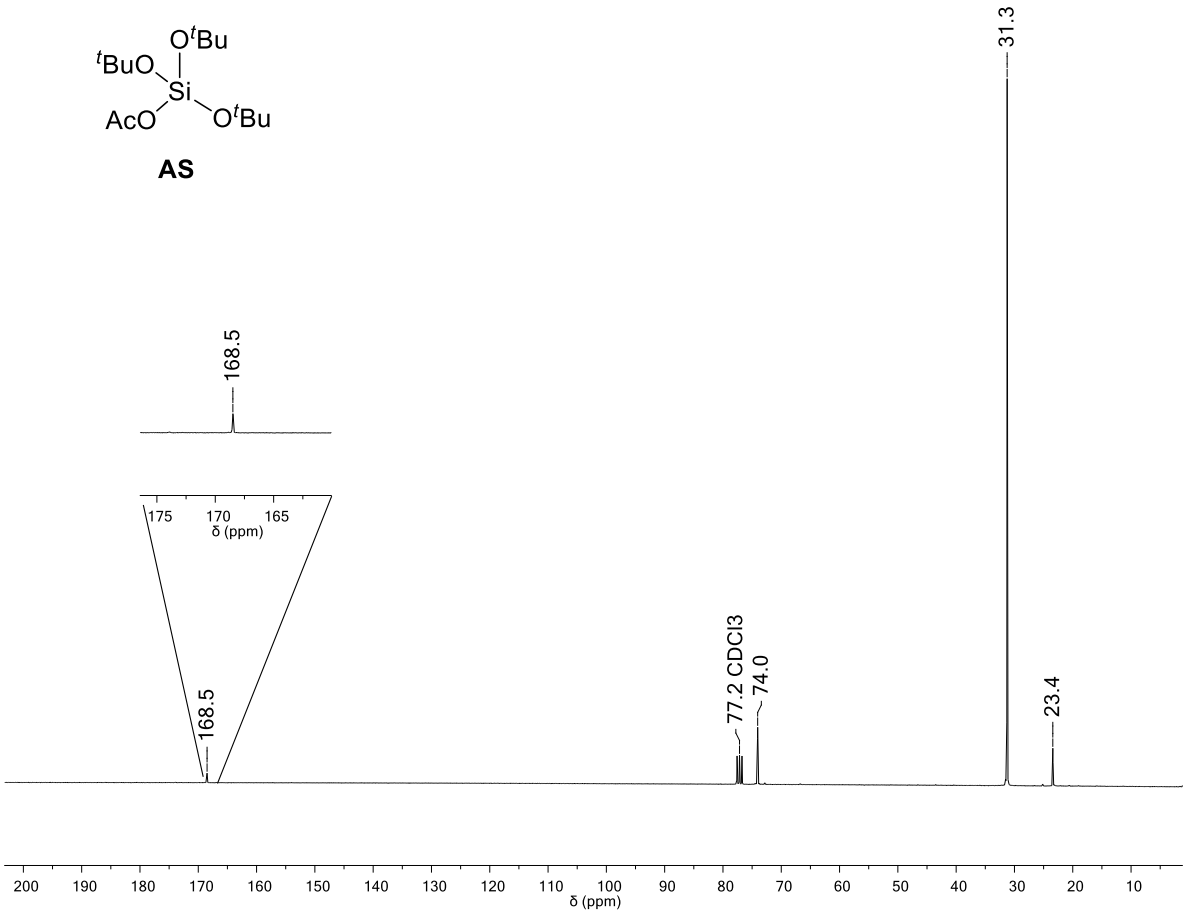


Figure S5. ^{13}C NMR spectrum of compound **AS**.

^{29}Si NMR (60 MHz, $CDCl_3$)

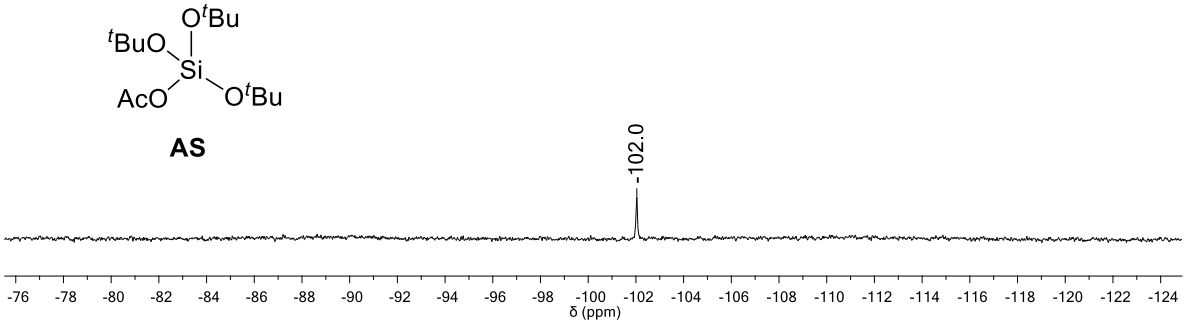


Figure S6. ^{29}Si NMR spectrum of compound **AS**.

^{1}H NMR (300 MHz, $CDCl_3$)

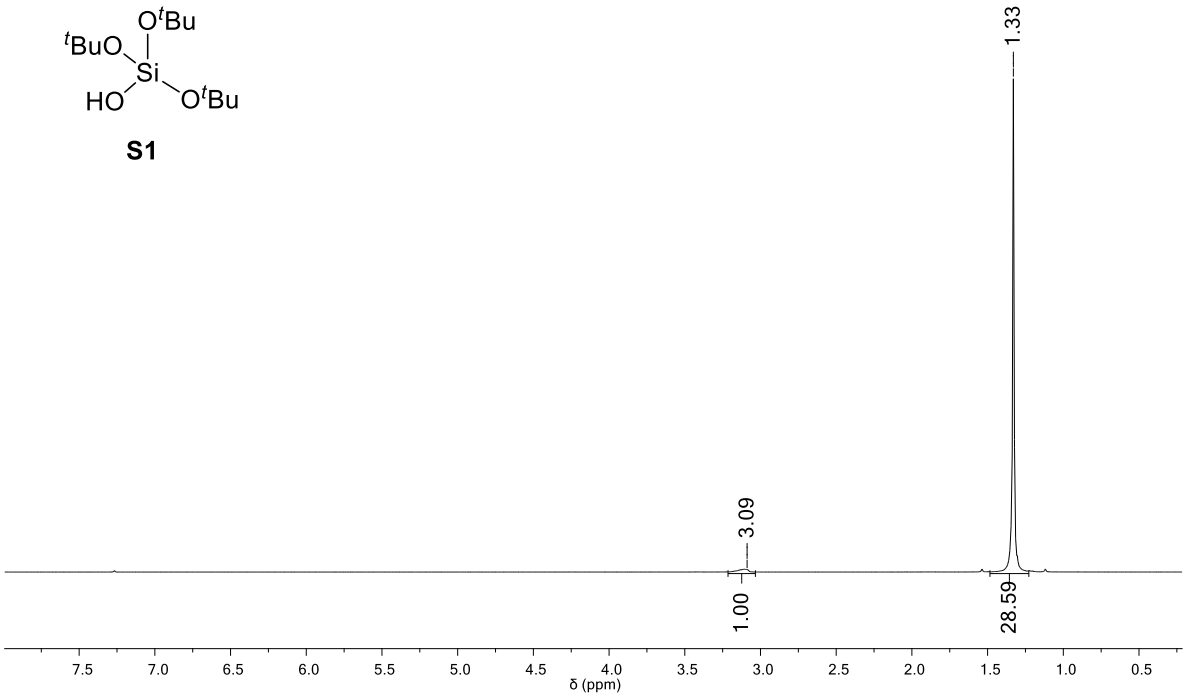


Figure S7. ^{1}H NMR spectrum of compound **S1**.

^{13}C NMR (75 MHz, $CDCl_3$)

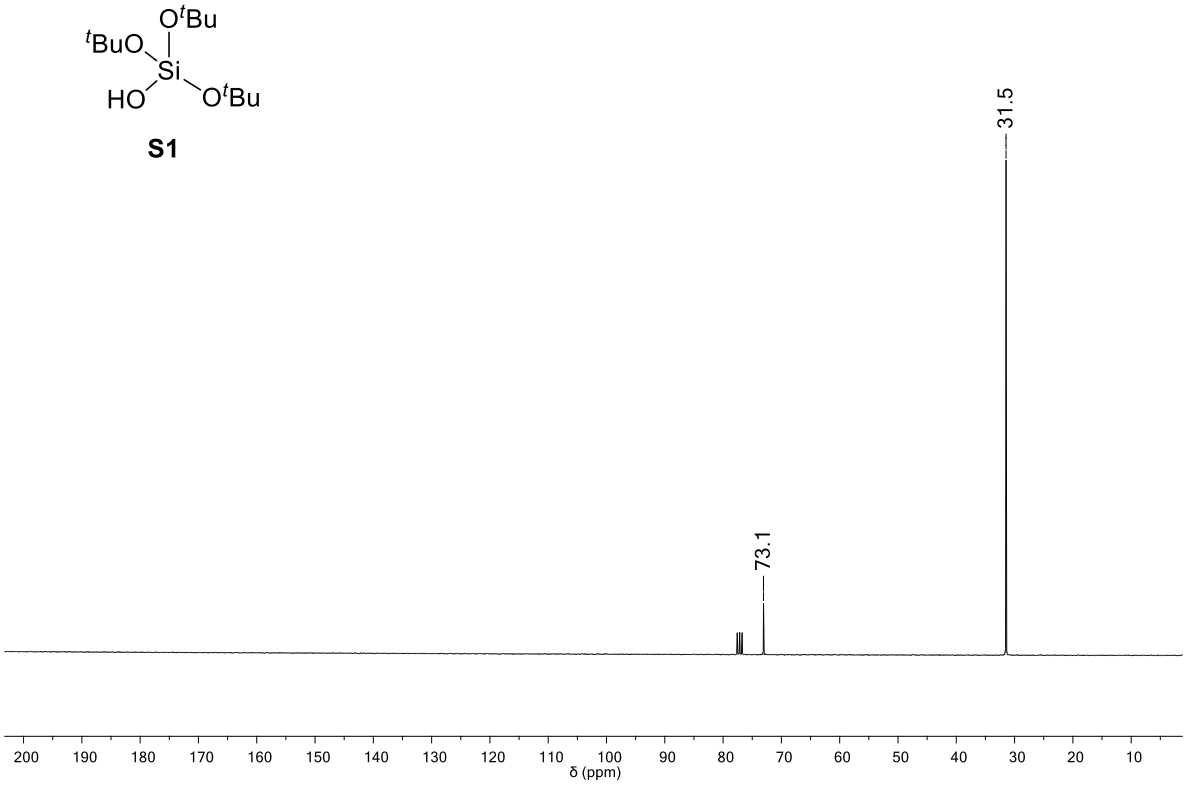


Figure S8. ^{13}C NMR spectrum of compound **S1**.

^{29}Si NMR (60 MHz, $CDCl_3$)

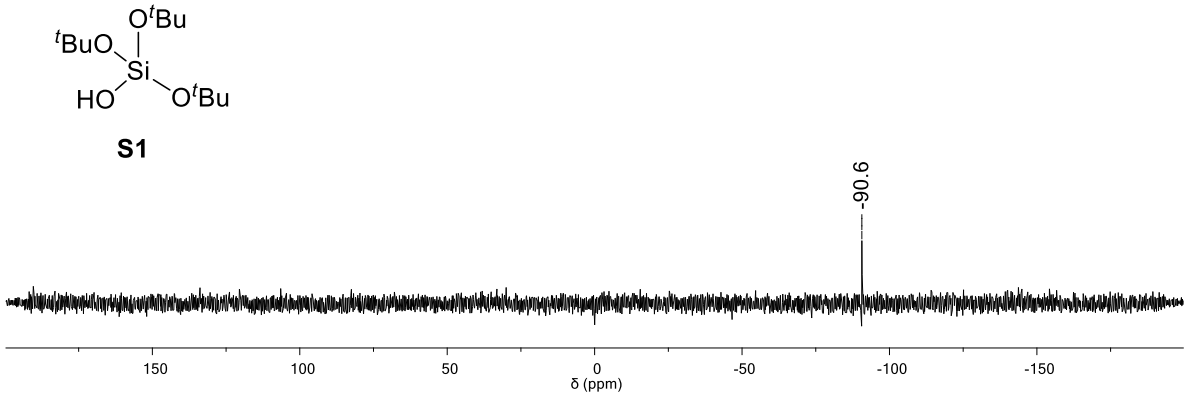


Figure S9. ^{29}Si NMR spectrum of compound **S1**.

^{1}H NMR (300 MHz, C_6D_6)

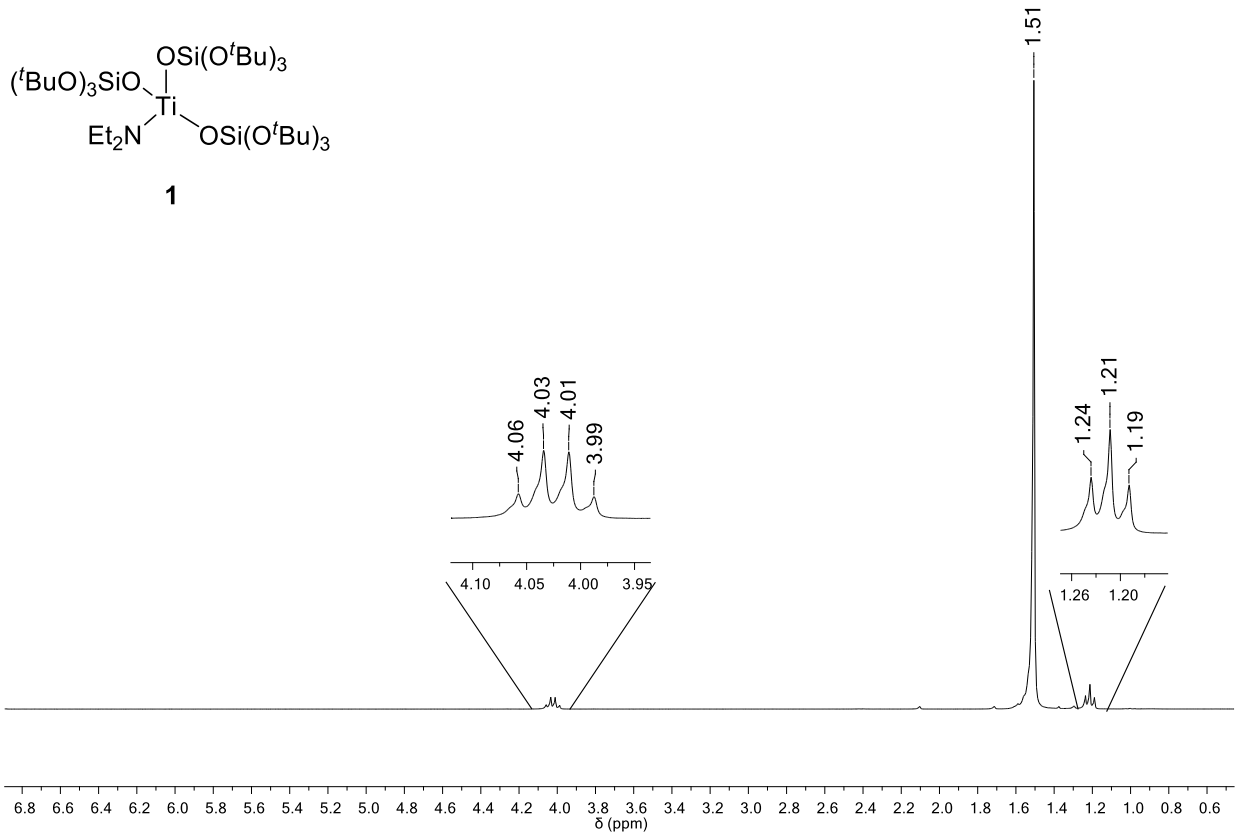


Figure S10. ^{1}H NMR spectrum of compound **1**.

^{13}C NMR (75 MHz, C_6D_6)

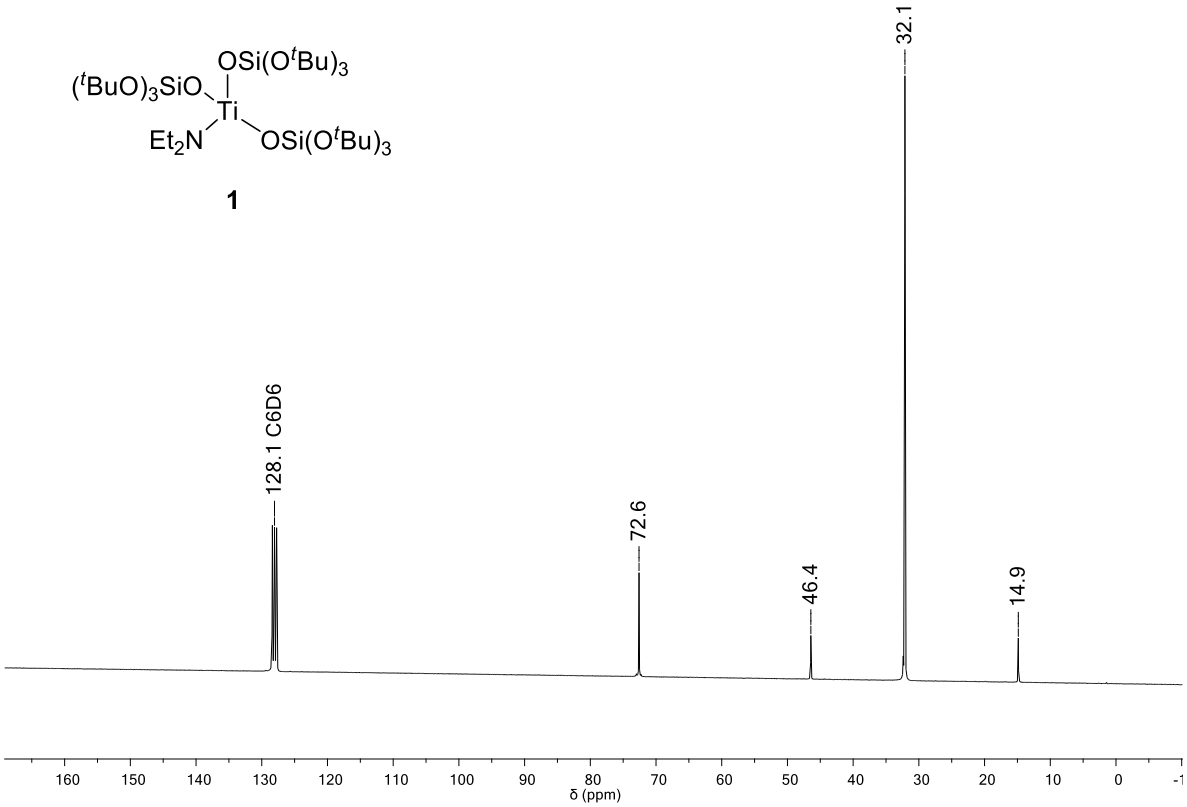


Figure S11. ^{13}C NMR spectrum of compound **1**.

^{29}Si NMR (60 MHz, C_6D_6)

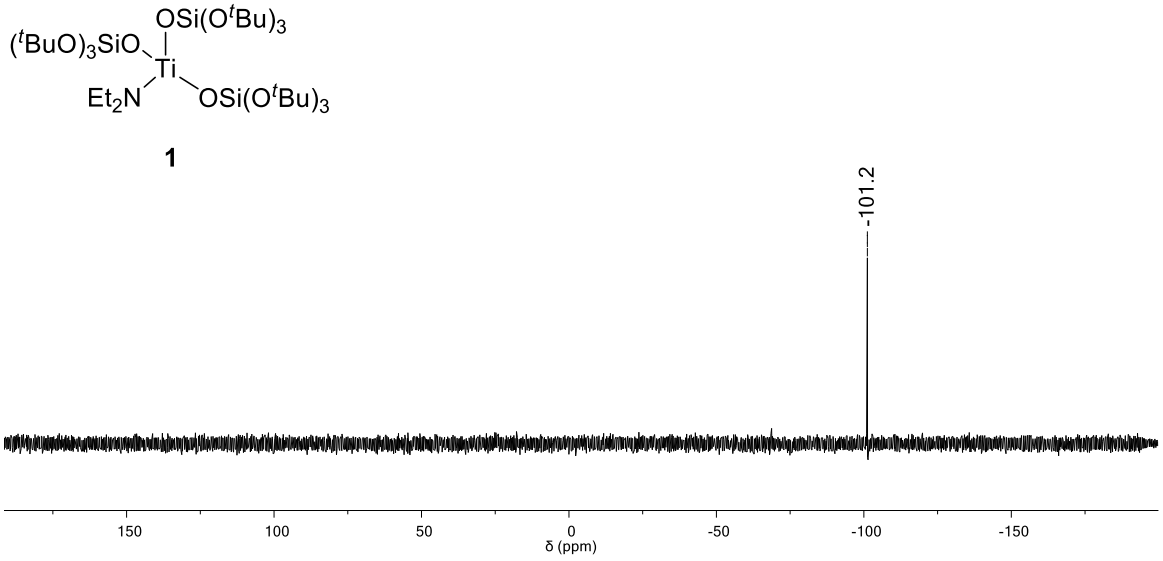
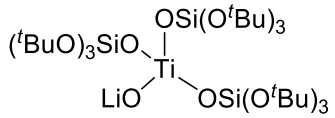


Figure S12. ^{29}Si NMR spectrum of compound **1**.

^{1}H NMR (300 MHz, C_6D_6)



2

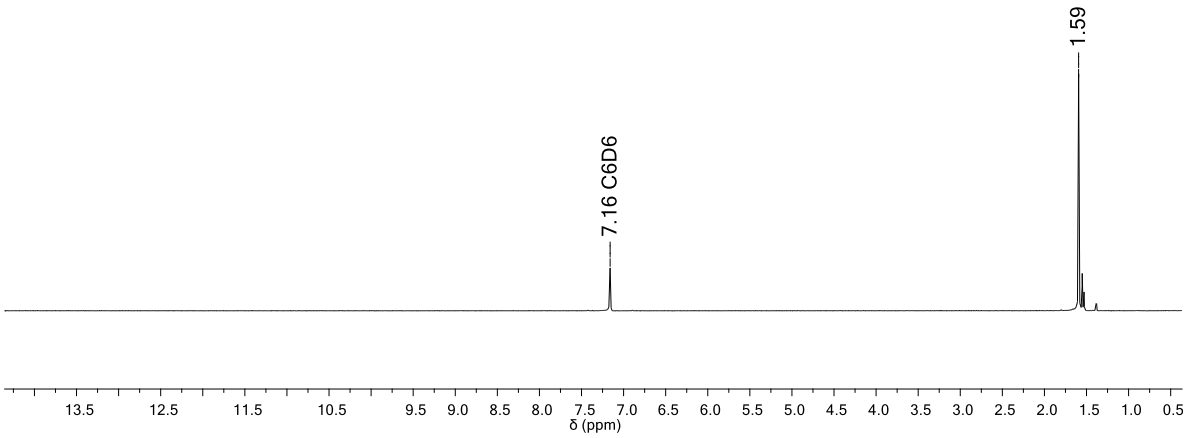
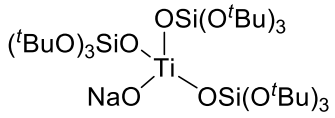


Figure S13. ^{1}H NMR spectrum of compound **2**. *Due to higher solubility of the impurities, when compared to the titanosilicate **2**, their signals are visible, but their intensities do not correspond to the real concentration in the sample.

^{1}H NMR (300 MHz, C_6D_6)



3

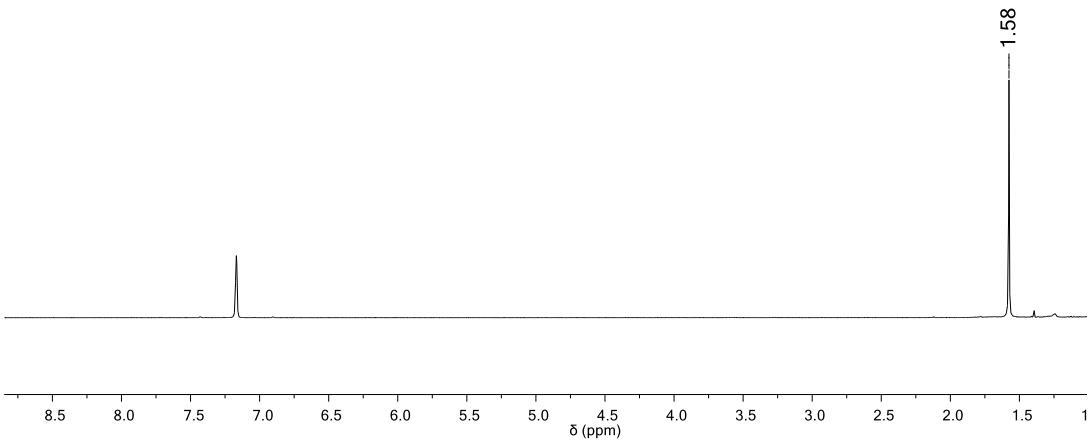


Figure S14. ^{1}H NMR spectrum of compound **3**.

^{1}H NMR (300 MHz, C_6D_6)

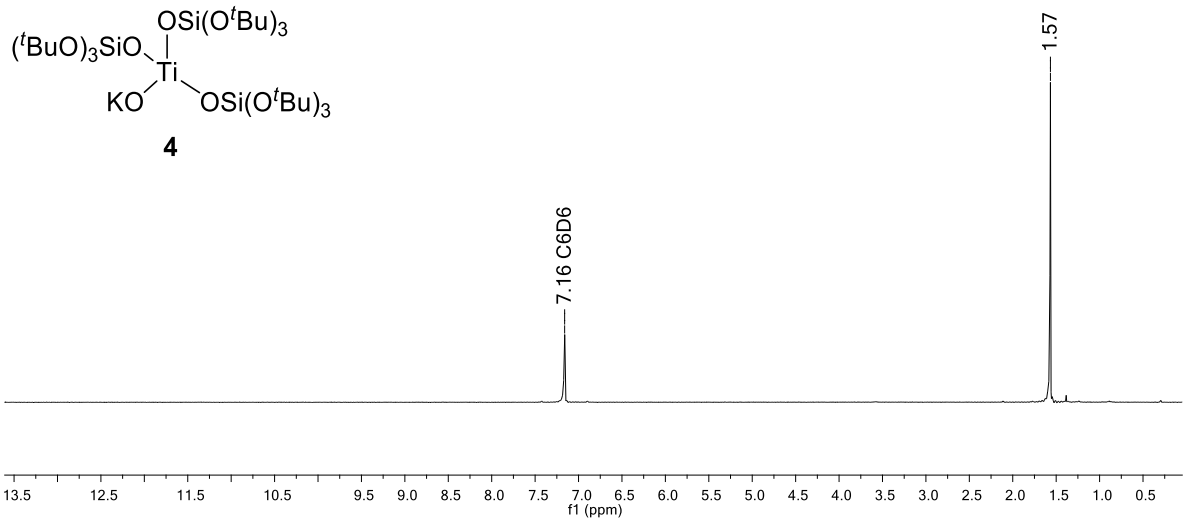


Figure S15. ^{1}H NMR spectrum of compound **4**.

^{1}H NMR (300 MHz, C_6D_6)

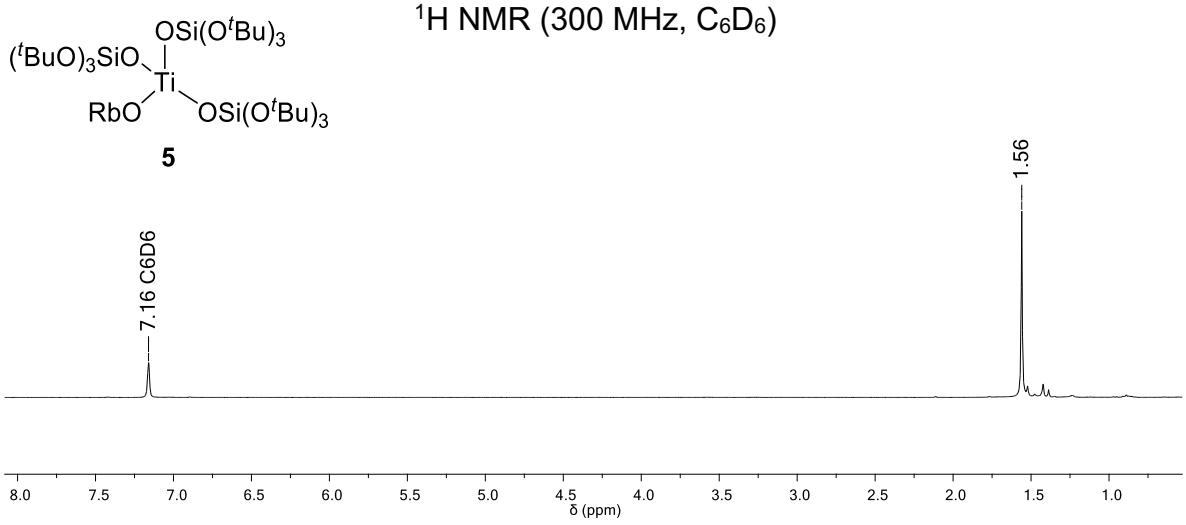


Figure S16. ^{1}H NMR spectrum of compound **5**.

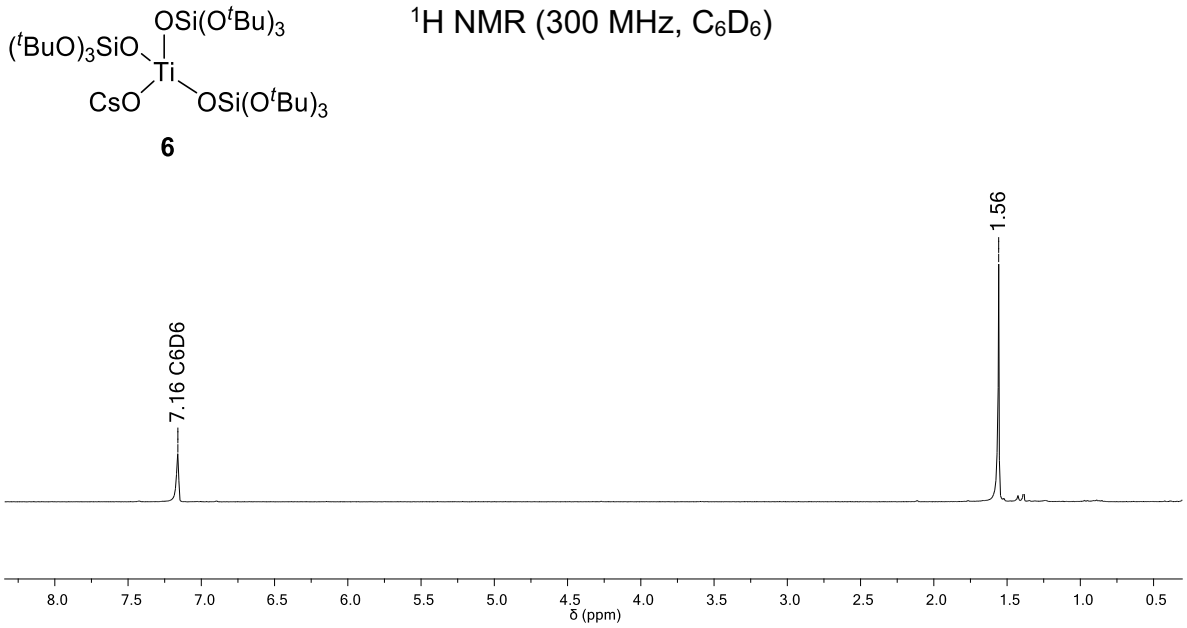


Figure S17. ^{1}H NMR spectrum of compound **6**.

^{1}H NMR (300 MHz, C_6D_6)

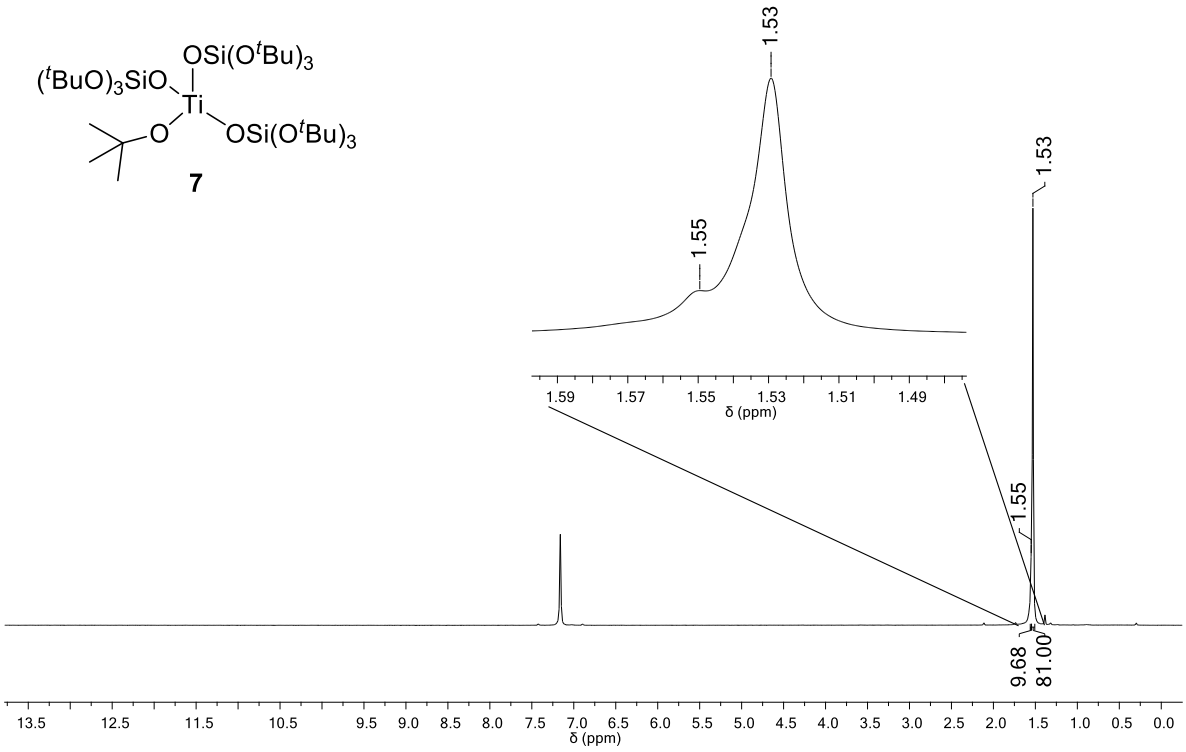


Figure S18. ^{1}H NMR spectrum of compound **7**.

^{13}C NMR (75 MHz, C_6D_6)

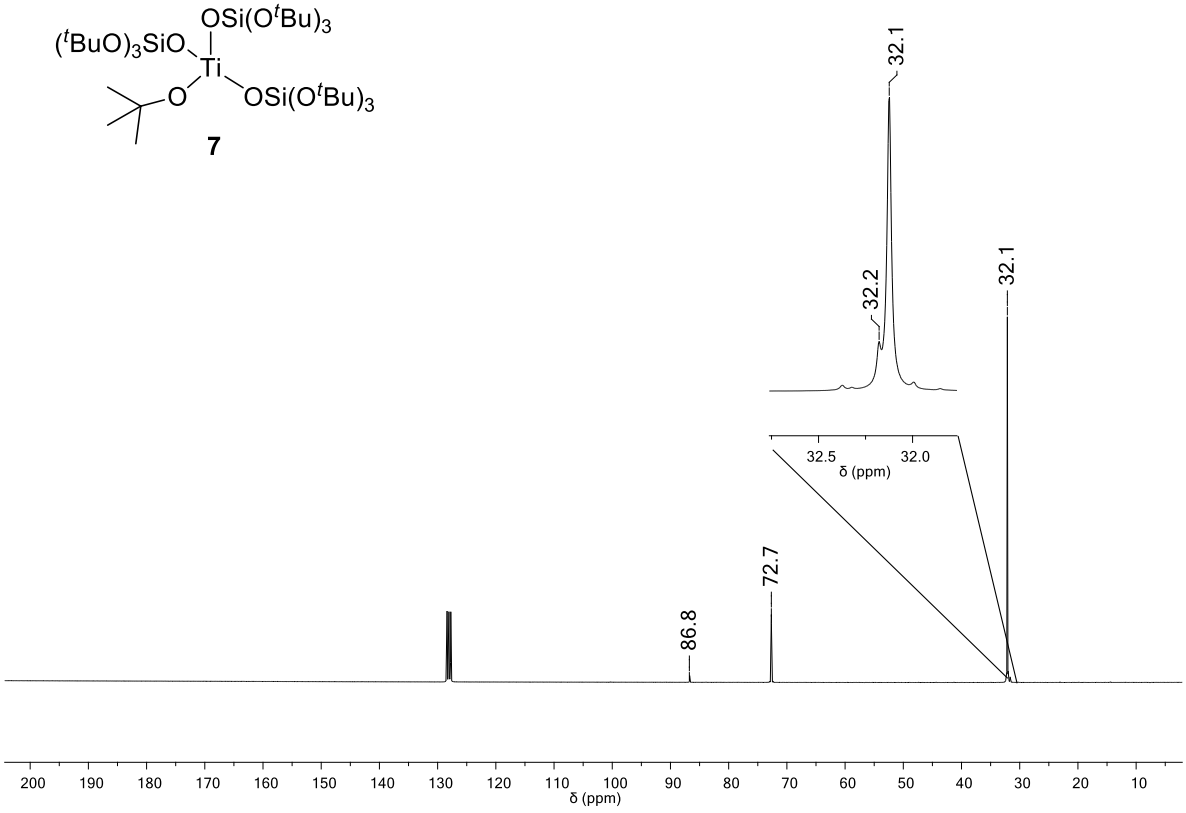


Figure S19. ^{13}C NMR spectrum of compound **7**.

^{29}Si NMR (60 MHz, C_6D_6)

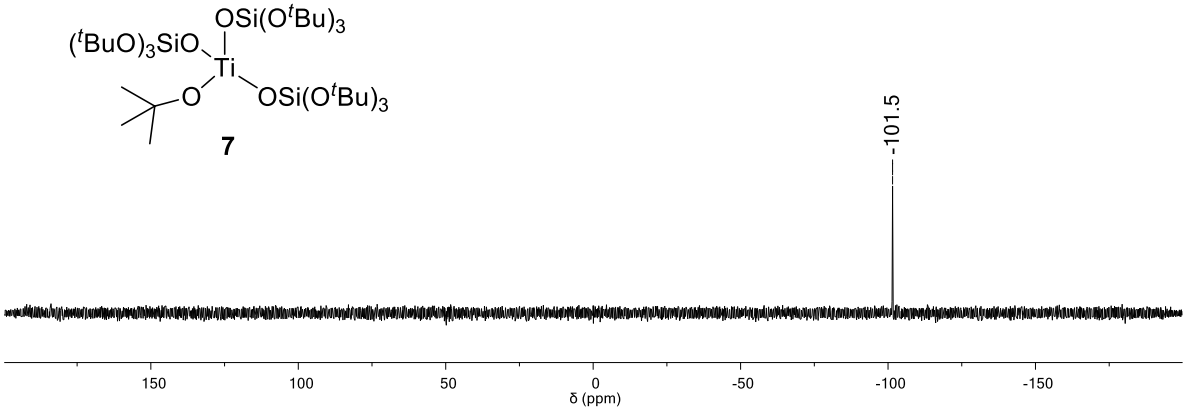


Figure S20. ^{29}Si NMR spectrum of compound **7**.

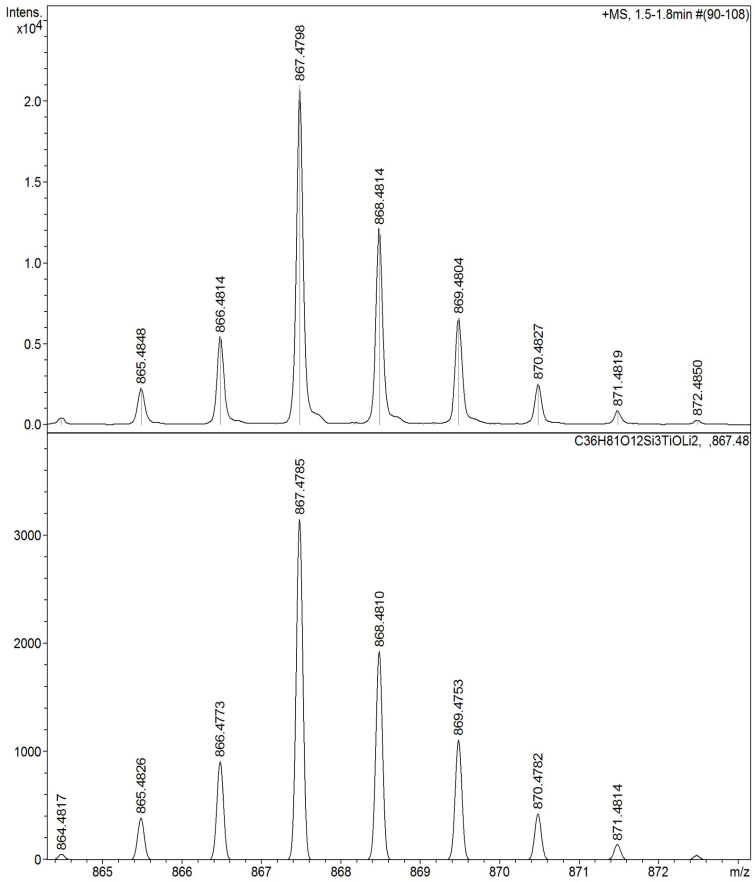


Figure S21. Experimental isotopic pattern of $[L_3TiOLi_2]^+$ (a) fragments peak in ESI-HRMS (positive mode) obtained for compound **2** (top). Simulated isotopic pattern for the later fragment (bottom). Error: 2.1 ppm.

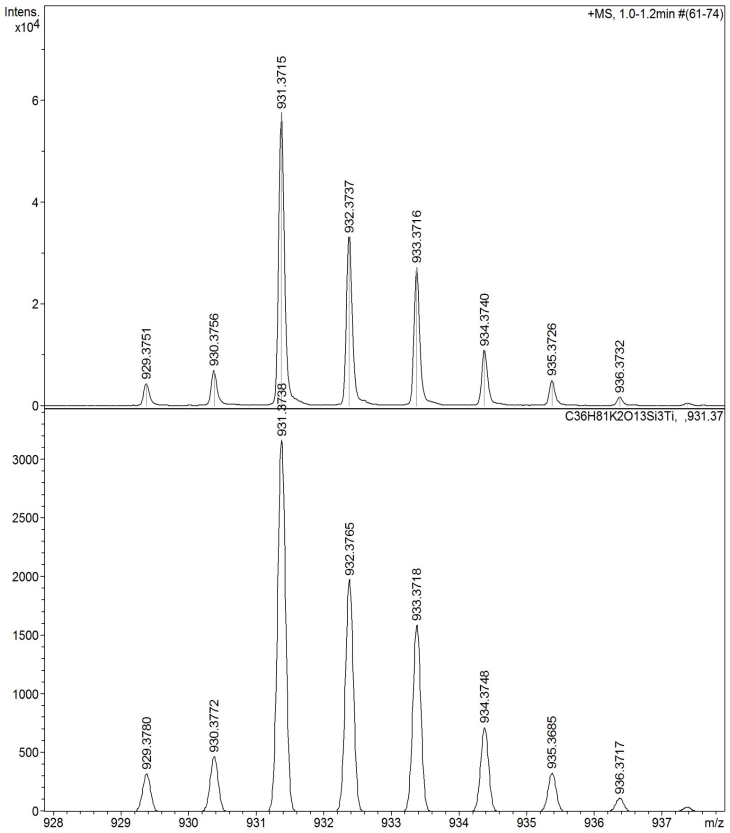


Figure S22. Experimental isotopic pattern of $[\mathbf{L_3TiOK_2}]^+$ (a) fragments peak in ESI-HRMS (positive mode) obtained for compound **2** (top). Simulated isotopic pattern for the later fragment (bottom). Error: 1.9 ppm.

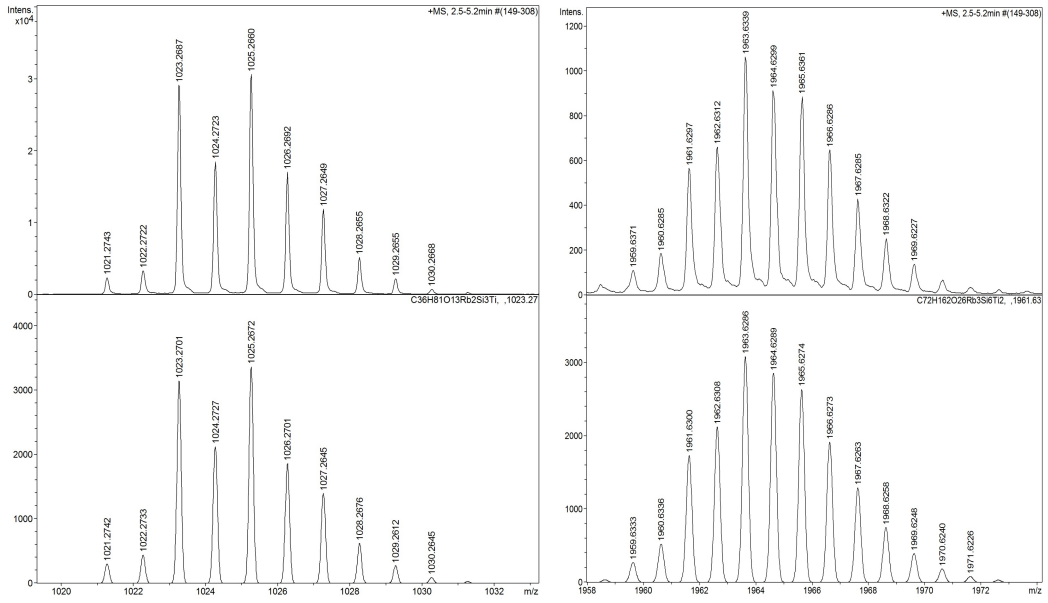


Figure S23. Experimental isotopic pattern of $[\mathbf{L_3TiORb_2}]^+$ (a) and $[\mathbf{L_6Ti_2O_2Rb_3}]^+$ (b) fragments peak in ESI-HRMS (positive mode) obtained for compound **1** (top). Simulated isotopic pattern for the later fragment (bottom). Error: 2.4 ppm in (a) and 2.6 ppm in (b).

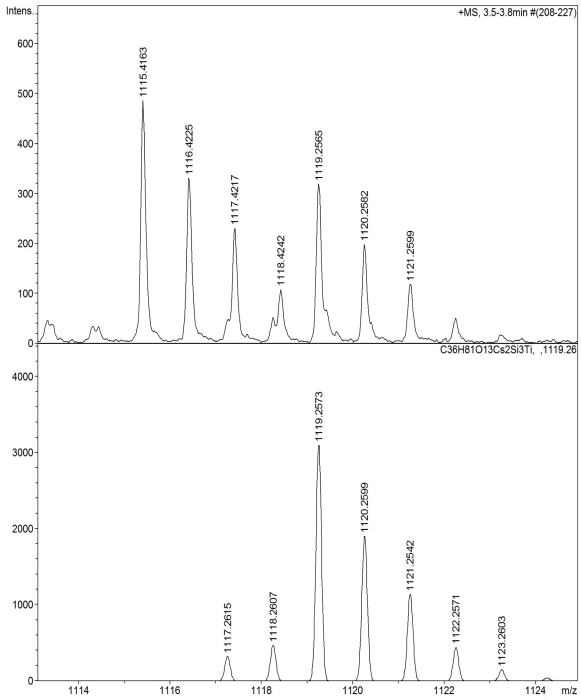


Figure S24. Experimental isotopic pattern of $[\mathbf{L_3TiOCs_2}]^+$ (a) fragments peak in ESI-HRMS (positive mode) obtained for compound **1** (top). Simulated isotopic pattern for the later fragment (bottom). Error: 0.71 ppm.

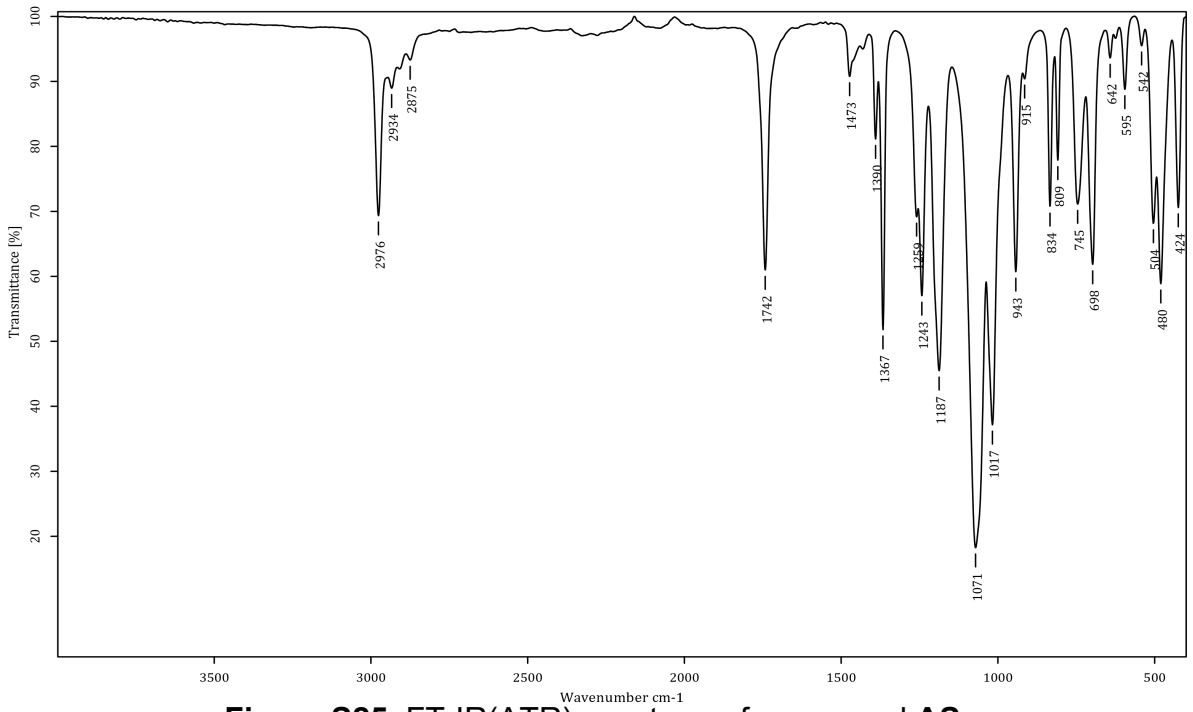


Figure S25. FT-IR(ATR) spectrum of compound **AS**.

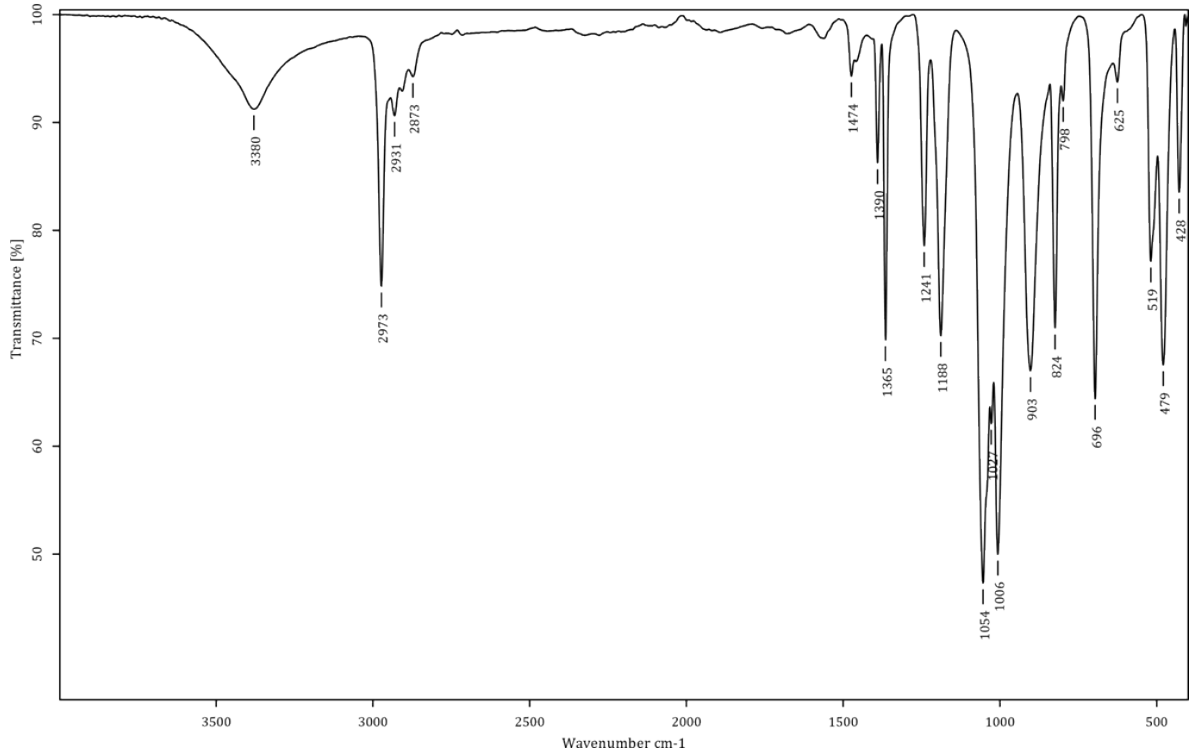


Figure S26. FT-IR(ATR) spectrum of compound **S1**.

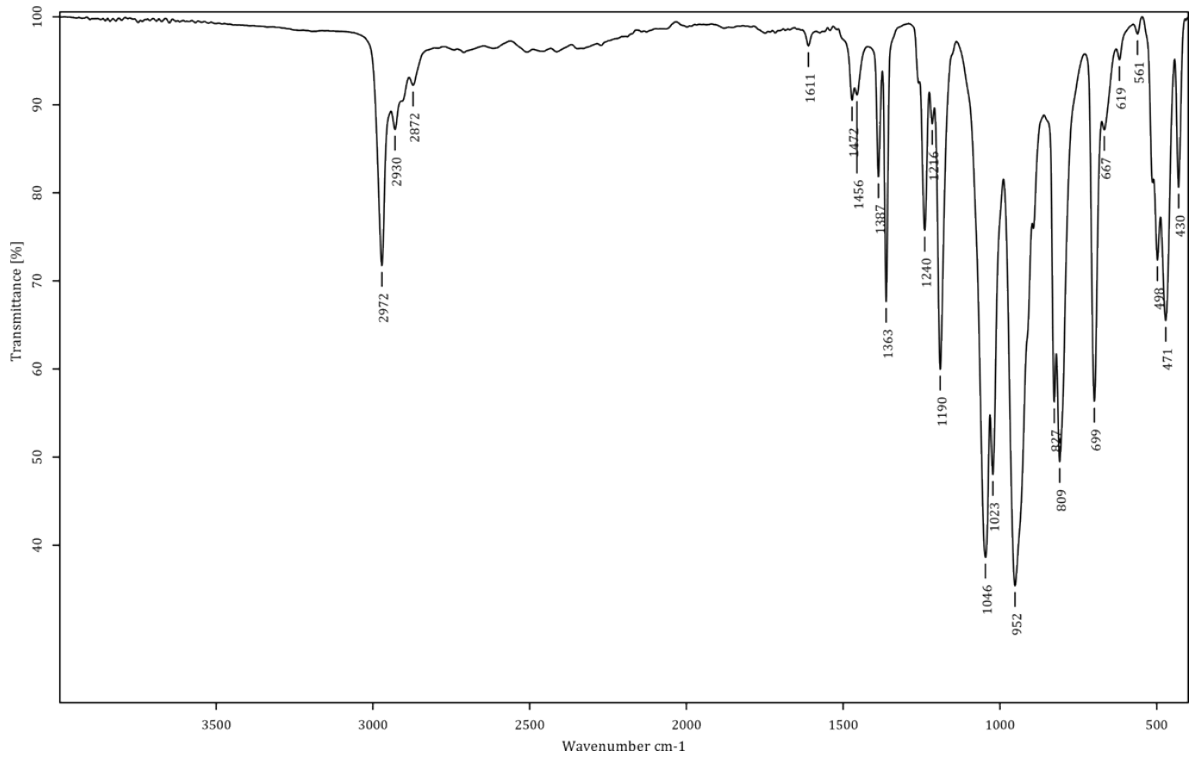


Figure S27. FT-IR(ATR) spectrum of compound **1**.

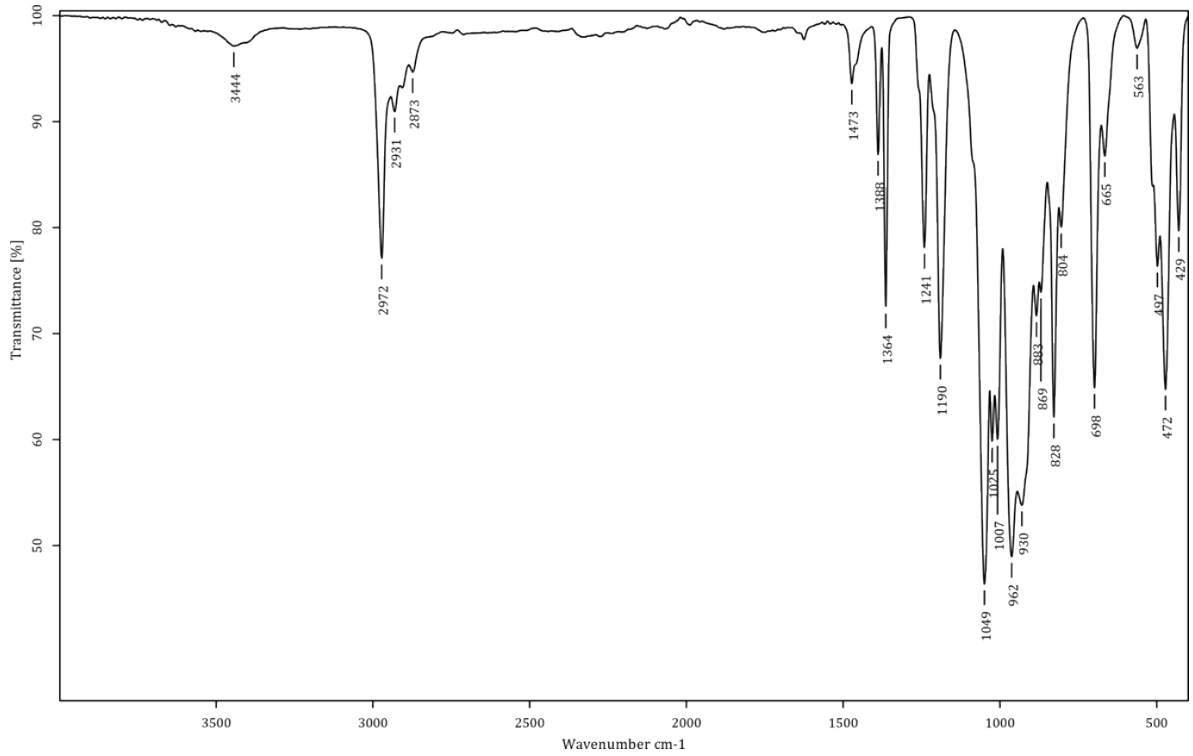


Figure S28. FT-IR(ATR) spectrum of compound **2**.

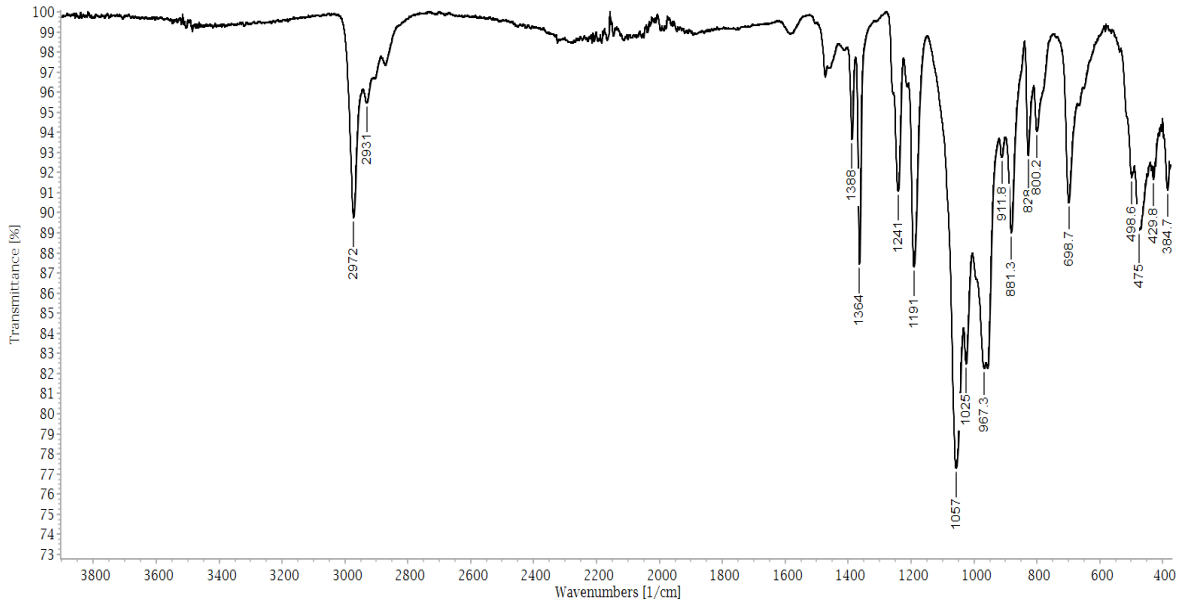


Figure S29. FT-IR(ATR) spectrum of compound **3**.

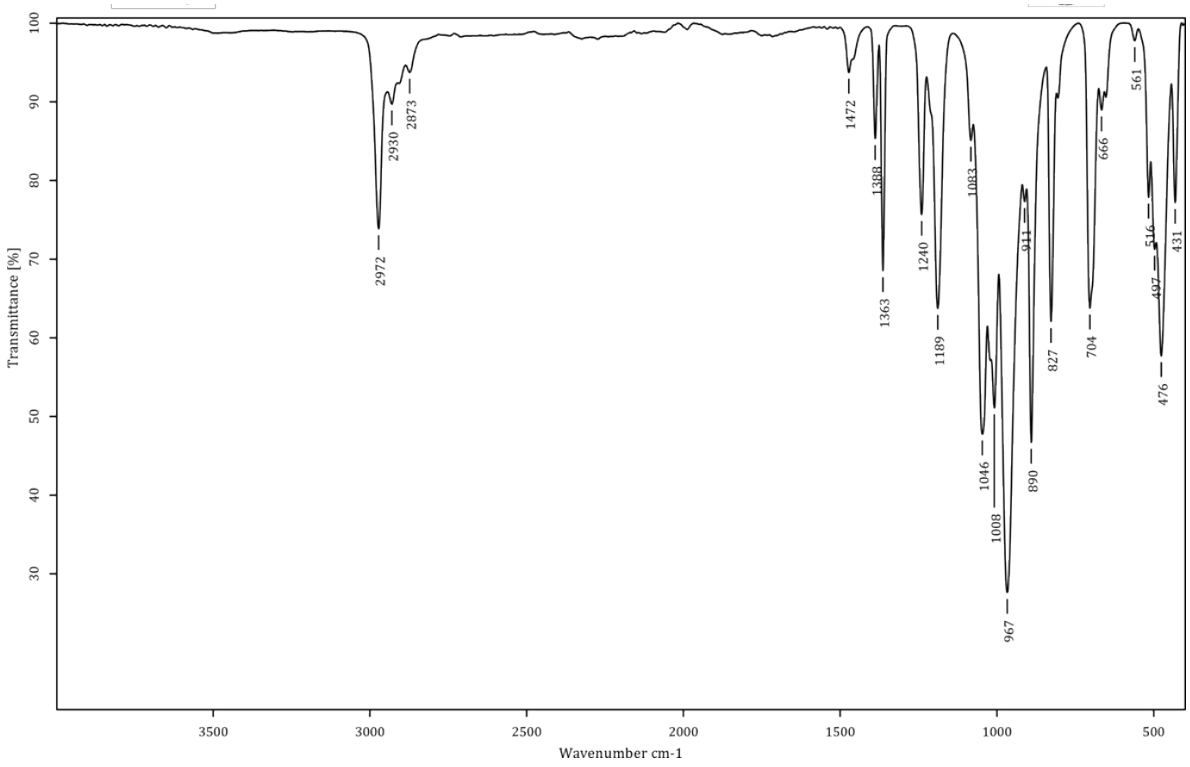


Figure S30. FT-IR(ATR) spectrum of compound **4**.

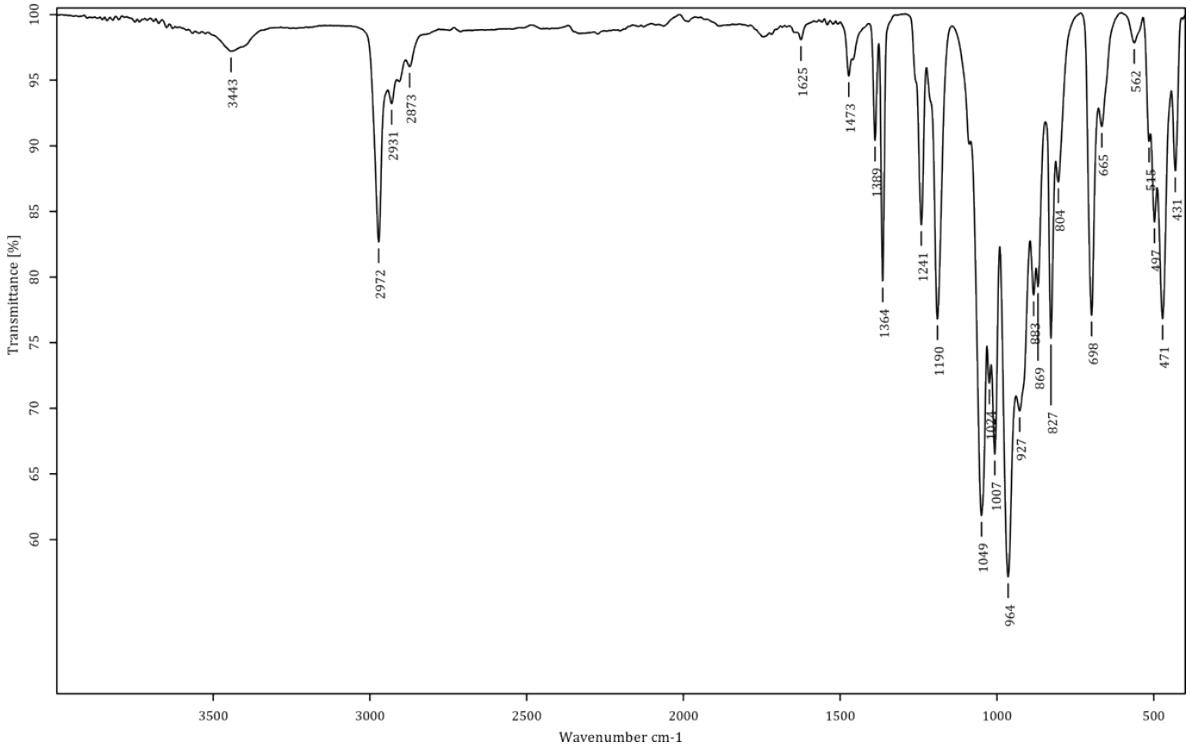


Figure S31. FT-IR(ATR) spectrum of compound **5**.

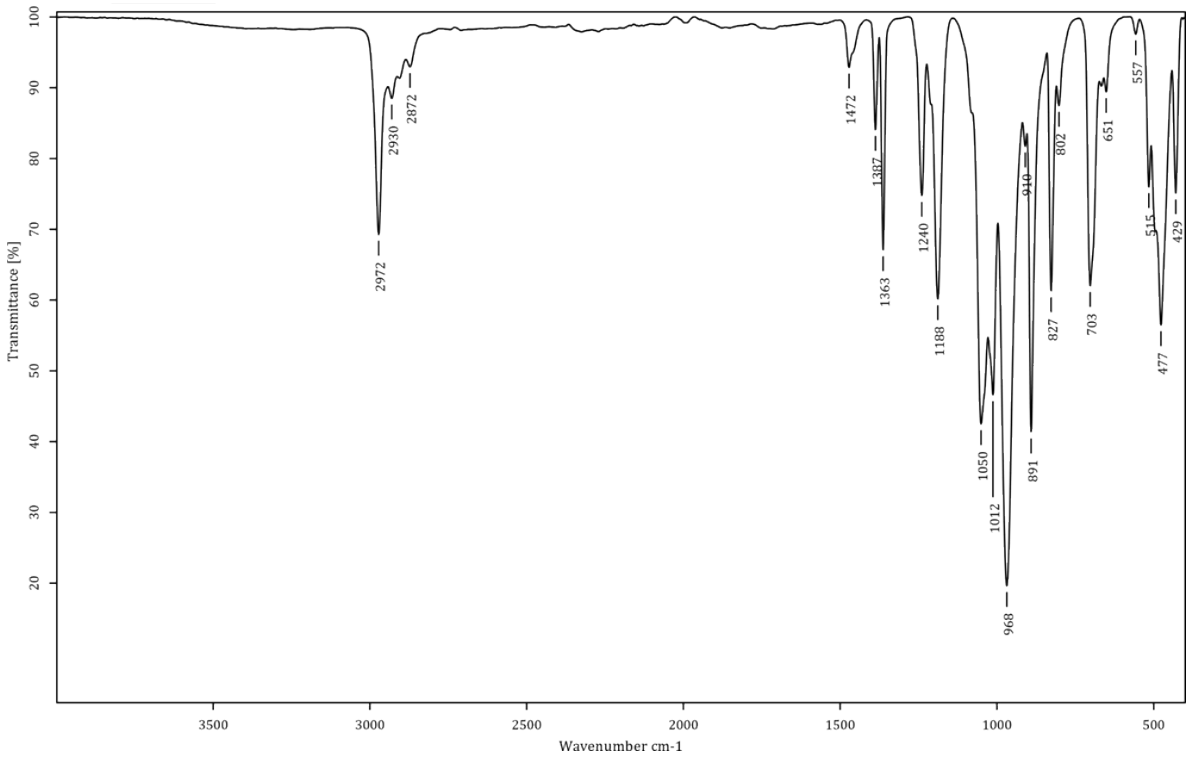


Figure S32. FT-IR(ATR) spectrum of compound **6**.

3. Molecular structure of $[(^tBuO)_3Si(\mu\text{-}O)]_3$ (TS)

Compound **TS** crystallizes in the triclinic space group $P\bar{1}$. It is noteworthy, that this compound crystallized as a non-merohedral twin. In Figure S33, the molecular structure is shown. In this compound, the SiO_4 units have a distorted tetrahedral geometry with angles ranging from 104.84(8)–113.77(8)°. Selected bond lengths and angles are listed in Table S1 and crystallographic parameters are summarized in Table S2.

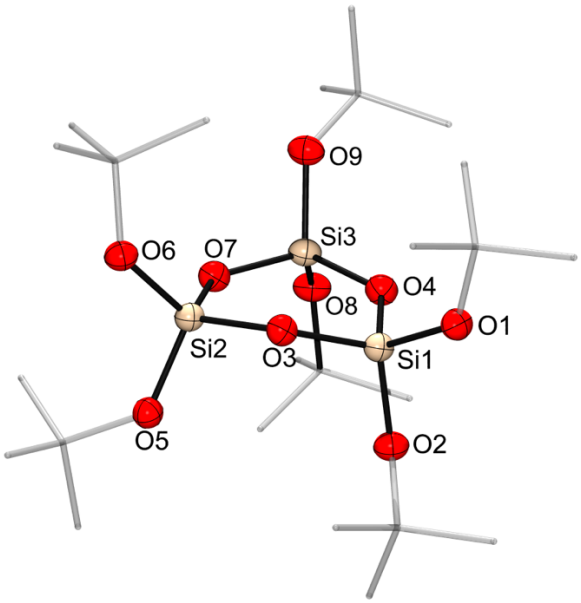
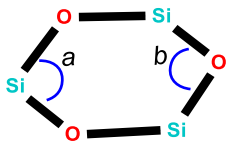


Figure S33. Molecular structure of compound **TS** with thermal ellipsoids set at 50% probability level. Carbon-bound hydrogen atoms and thermal ellipsoids of the carbon atoms were eliminated for the sake of clarity.

Table S1. Selected bond distances (Å) and angles (deg) for **TS**.



	TS
Si–OSi (range)	1.6254(10)–1.6353(10)
Si–OC (range)	1.6078(10)–1.6321(10)
O–Si–O (range)	104.80(5)–113.68(5)
O–Si–O (angle *a* range)	106.18(5)–107.27(5)
Si–O–Si (angle *b* range)	128.19(6)–132.10(6)

4. Crystallographic information for compounds 1–7

Table S2. Selected crystallographic data for compound **TS**.

	TS
Empirical formula	$C_{24}H_{54}O_9Si_3$
Formula mass (g/mol)	570.94
T (K)	100(2)
Crystal size (mm^3)	0.562 x 0.348 x 0.104
Space group	$P\bar{1}$.
a (Å)	10.6208(6)
b (Å)	11.9586(6) Å
c (Å)	14.0651(8) Å
α(°)	100.242(2)
β(°)	109.429(2)
γ(°)	90.071(2)
V (Å)	1654.32(16)
Z	2
$\rho_{calc.}$ ($g \cdot cm^{-3}$)	1.146
μ (mm^{-1})	1.673
F(000)	624
θ range for data collection (º)	3.393 to 70.117
No. of reflections	6116
No. of independent reflections (R_{int})	6116 [$R_{(int)}$ = 0.0395]
No. of data/restr./param.	6116 / 0 / 344
Goodnes-on-fit (GOF) on F^2	1.068
R_1,[a] wR_2[b] ($I > 2\sigma(I)$)	0.0314, 0.0873
R_1,[a] wR_2[b] (all data)	0.0336, 0.0892
Largest diff. peak/hole ($e \cdot Å^{-3}$)	0.254 / −0.312
CCDC	2156304

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum(F_o^2)^2]^{1/2}$

Table S3. Selected crystallographic data for compounds **1**–**3**.

	1	**2**	**3**
Empirical formula	$C_{40}H_{91}O_{12}NSi_3Ti$	$C_{72}H_{162}O_{26}Si_6Ti_2Li_2$	$C_{72}H_{162}O_{26}Si_6Ti_2Na_2$
Formula mass (g/mol)	910.3	1722.23	1754.33
T (K)	100(2)	100(2)	100(2)
Crystal size (mm^3)	0.426 x 0.389 x 0.356	0.483 x 0.201 x 0.146	0.425 x 0.348 x 0.268
Space group	$P2_1/n$	$P\bar{1}$.	$C2/c$
a (Å)	13.5226(8)	13.5666(5)	13.4625(5)
b (Å)	21.9475(13)	13.5671(5)	23.7520(9)
c (Å)	19.2826(12)	31.5352(12)	31.8025(12)
α(°)	90	91.934(2)	90
β(°)	105.4661(11)	100.4481(19)	99.8591(8)
γ(°)	90	116.7479(17)°	90
V (Å)	5515.6(6)	5053.1(3)	10019.0(7)
Z	4	2	4
$\rho_{calc.}$ ($g \cdot cm^{-3}$)	1.096	1.132	1.163
μ (mm^{-1})	0.270	2.538	0.303
F(000)	1992	1872	3808
θ range for data collection (º)	1.652 to 26.099	1.437 a 72.022	1.715 a 26.099
No. of reflections	82469	86288	74582
No. of independent reflections (R_{int})	10935 (0.0313)	19114 (0.0414)	9927 (0.0220)
No. of data/restr./param.	10935 / 487 / 714	19114 / 4327 / 1861	9927 / 927 / 815
Goodnes-on-fit (GOF) on F^2	1.030	1.023	1.064
R_1,[a] wR_2[b] ($I > 2\sigma(I)$)	0.0320, 0.0834	0.0524, 0.1314	0.0293, 0.0748
R_1,[a] wR_2[b] (all data)	0.0389, 0.0884	0.0580, 0.1353	0.0322, 0.0767
Largest diff. peak/hole ($e \cdot Å^{-3}$)	0.490 / −0.379	0.849 / −0.685	0.571 / −0.279
CCDC	2156311	2156307	2156306

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum(F_o^2)^2]^{1/2}$

Table S4. Selected crystallographic data for compounds **4**–**6**.

	4	**5**	**6**
Empirical formula	$C_{72}H_{162}O_{26}Si_6Ti_2K_2$	$C_{72}H_{162}O_{26}Si_6Rb_2Ti_2$	$C_{72}H_{162}O_{26}Si_6Cs_2Ti_2$
Formula mass (g/mol)	1786.55	1879.29	1974.17
T (K)	100(2)	100(2)	100(2)
Crystal size (mm^3)	0.280 x 0.199 x 0.125	0.439 x 0.241 x 0.182	0.611 x 0.526 x 0.270
Space group	$P2_1/n$	$P2_1/n$	$P2_1/c$
a (Å)	13.9466(4)	13.8809(5)	35.3441(14)
b (Å)	22.9279(6)	23.1419(8)	17.2885(8)
c (Å)	16.8771(4)	16.9695(6)	26.0710(14)
α(°)	90	90	90
β(°)	108.6892(5)°	107.9833(8)	101.1948(6)°
γ(°)	90	90	90
V (Å)	5112.2(2)	5184.8(3)	15627.5(13)
Z	2	2	6
$\rho_{calc.}$ ($g \cdot cm^{-3}$)	1.161	1.204	1.259
μ (mm^{-1})	0.370	1.217	0.972
F(000)	1936	2008	6240
θ range for data collection (º)	1.655 to 27.101	1.882 to 30.507	1.592 a 26.087
No. of reflections	58214	89116	231333
No. of independent reflections (R_{int})	11278 (0.0328)	15821 (0.0304)	30915 (0.0261)
No. of data/restr./param.	11278 / 432 / 641	15821 / 1540 / 735	30915 / 2695 / 2226
Goodnes-on-fit (GOF) on F^2	1.037	1.039	1.141
R_1,[a] wR_2[b] ($I > 2\sigma(I)$)	0.0376, 0.0971	0.0321, 0.0830	0.0321, 0.0706
R_1,[a] wR_2[b] (all data)	0.0447, 0.1018	0.0433, 0.0886	0.0365, 0.0728
Largest diff. peak/hole ($e \cdot Å^{-3}$)	0.630 / −0.478	1.736 / −0.477	1.358 / −0.775
CCDC	2156305	2156308	2156310

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum(F_o^2)^2]^{1/2}$

Table S5. Selected crystallographic data for compound **7**.

	7
Empirical formula	$C_{40}H_{90}O_{13}Si_3Ti$
Formula mass (g/mol)	911.28
T (K)	100(2)
Crystal size (mm^3)	0.423 x 0.339 x 0.232
Space group	*P*bca
a (Å)	22.2645(10)
b (Å)	21.7564(10)
c (Å)	22.6575(10)
α(°)	90
β(°)	90
γ(°)	90
V (Å)	10975.2(9)
Z	8
$\rho_{calc.}$ ($g \cdot cm^{-3}$)	1.103
μ (mm^{-1})	0.272
F(000)	3984
θ range for data collection (º)	1.798 to 26.401
No. of reflections	86645
No. of independent reflections (R_{int})	11236 [$R_{(int)}$ = 0.0271]
No. of data/restr./param.	11236 / 1367 / 810
Goodnes-on-fit (GOF) on F^2	1.032
R_1,[a] wR_2[b] ($I > 2\sigma(I)$)	0.0280, 0.0726
R_1,[a] wR_2[b] (all data)	0.0351, 0.0779
Largest diff. peak/hole ($e \cdot Å^{-3}$)	0.360 / −0.341
CCDC	2156309

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum(F_o^2)^2]^{1/2}$

Table S6. Selected bond distances (Å) and angles (°) for compound **1**.

	1
Ti(1)–O(1)	1.8366(10)
Ti(1)–O(5)	1.7975(10)
Ti(1)–O(9)	1.8131(9)
Ti(1)–N(1)	1.8560(12)
Si–O (range)	1.6155(10)–1.6272(11)
O(1)–Ti(1)–O(5)	111.01(5)
O(1)–Ti(1)–O(9)	107.86(5)
O(5)–Ti(1)–O(9)	113.32(5)
O(1)–Ti(1)–N(1)	110.76(5)
O(5)–Ti(1)–N(1)	105.03(5)
O(9)–Ti(1)–N(1)	108.86(5)
O–Si–O (range)	104.72(5)–114.18(6)

Table S7. Selected bond distances (Å) and angles (°) for compounds **2** and **3**.

	2	**3**
Si–O(Ti) (range)	1.582(4)–1.606(3)	1.6005(10)–1.6031(10)
Si–O(C) (range)	1.607(4)–1.659(3)	1.616(6)–1.6559(9)
Ti–OM	1.705(2)	1.6828(9)
Ti–OSi (range)	1.817(2)–1.862(2)	1.8382(9)–1.8643(9)
M–O(Ti) (range)	1.676(7)–1.933(5)	2.2802(10)–2.4175(11)
M–O(Si) (range)	1.899(6)–1.965(6)	2.4293(11)–2.5655(11)
O–Si–O (range)	104.26(12)–115.03(14)	104.1(2)–115.5(2)
O–Ti–O (range)	102.93(13)–114.45(18)	105.67(4)–113.80(5)
Si–O–Ti (range)	146.62(17)–163.48(14)	147.86(6)–175.37(7)
Ti–O–M (range)	89.6(3)–157.3(2)	98.59(4)–162.26(6)
M–O–M	82.6(2)	92.21(4)

Table S8. Selected bond distances (Å) and angles (°) for compounds **4**–**6**.

	4	**5**	**6**
Si–O(Ti) (range)	1.5977(12)–1.5995(12)	1.5962(10)–1.5998(11)	1.5957(17)–1.617(3)
Si–O(C) (range)	1.6205(12)–1.6450(12)	1.6198(10)–1.6379(11)	1.6187(17)–1.642(2)
Ti–OM	1.6737(11)	1.6723(10)	1.6703(17)
Ti–OSi (range)	1.8419(11)–1.8637(12)	1.8450(10)–1.8646(10)	1.8404(18)–1.8695(15)
M–O(Ti) (range)	2.6478(12)–2.6547(13)	2.7748(11)–2.7979(11)	2.8940(15)–3.1233(16)
M–O(Si) (range)	2.8699(13)–3.0428(12)	2.9947(11)–3.1181(10)	3.1903(17)–3.6804(17)
M···H	2.802–3.112	2.927–3.099	3.283–3.513
O–Si–O (range)	103.20(6)–113.72(7)	103.64(5)–113.92(6)	103.20(11)–115.27(13)
O–Ti–O (range)	108.29(6)–111.30(5)	108.23(5)–110.81(5)	105.44(7)–113.46(7)
Si–O–Ti (range)	150.24(8)–174.21(8)	155.21(8)–178.05(7)	143.16(10)–169.74(11)
Ti–O–M (range)	118.66(6)–123.35(6)	82.87(4)–121.14(5)	83.33(6)–122.67(9)
M–O–M	99.92(4)	99.31(3)	109.22(5)
C–H···M	100.80–117.03	113.14–117.55	117.95–126.80

Table S9. Selected bond distances (Å) and angles (°) for compound **7**.

	7
Ti(1)–O(1)	1.8147(9)
Ti(1)–O(5)	1.8116(9)
Ti(1)–O(9)	1.7975(9)
Ti(1)–O(13)	1.747(5)
Si–O (range)	1.6133(9)–1.6257(9)
O(13)–Ti(1)–O(9)	113.9(5)
O(13)–Ti(1)–O(5)	108.5(7)
O(5)–Ti(1)–O(9)	109.26(4)
O(1)–Ti(1)–O(13)	108.1(4)
O(5)–Ti(1)–O(1)	110.04(4)
O(9)–Ti(1)–O(1)	107.19(4)
O–Si–O (range)	105.25(5)–113.86(5)

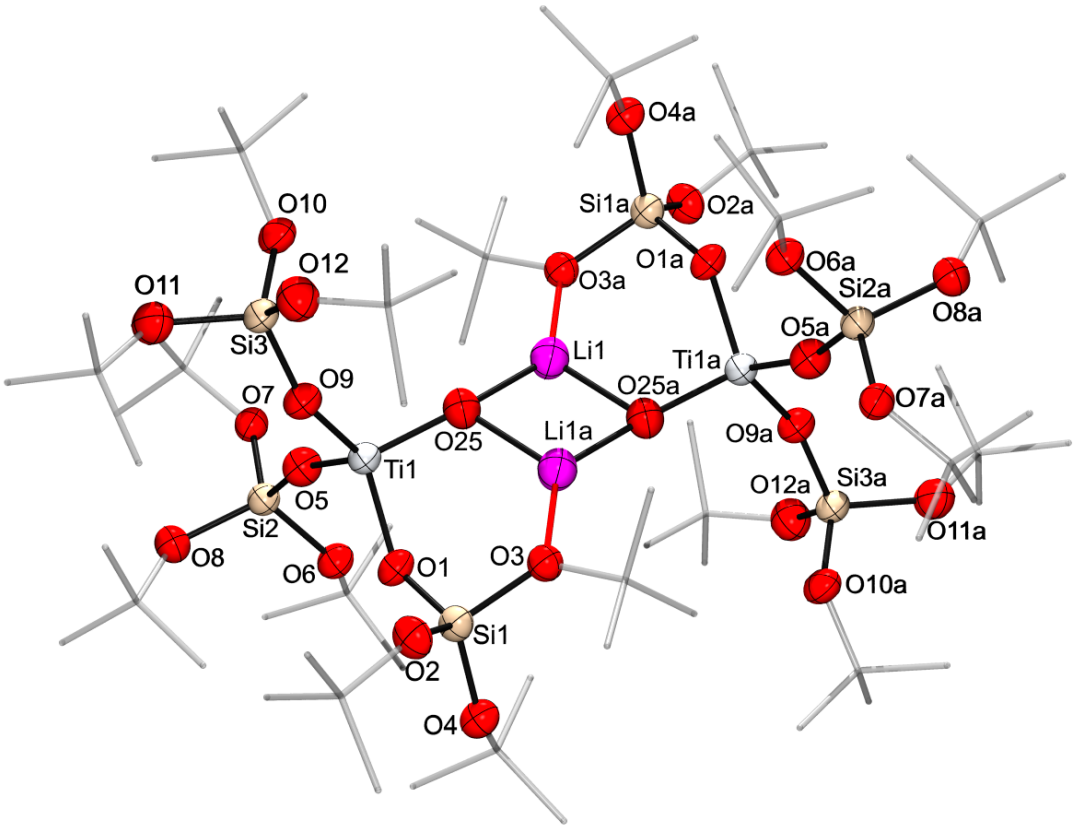


Figure S34. Molecular structure of compound **2** with thermal ellipsoids set at 50% probability level. Carbon-bound hydrogen atoms and thermal ellipsoids of the carbon atoms were eliminated for the sake of clarity.

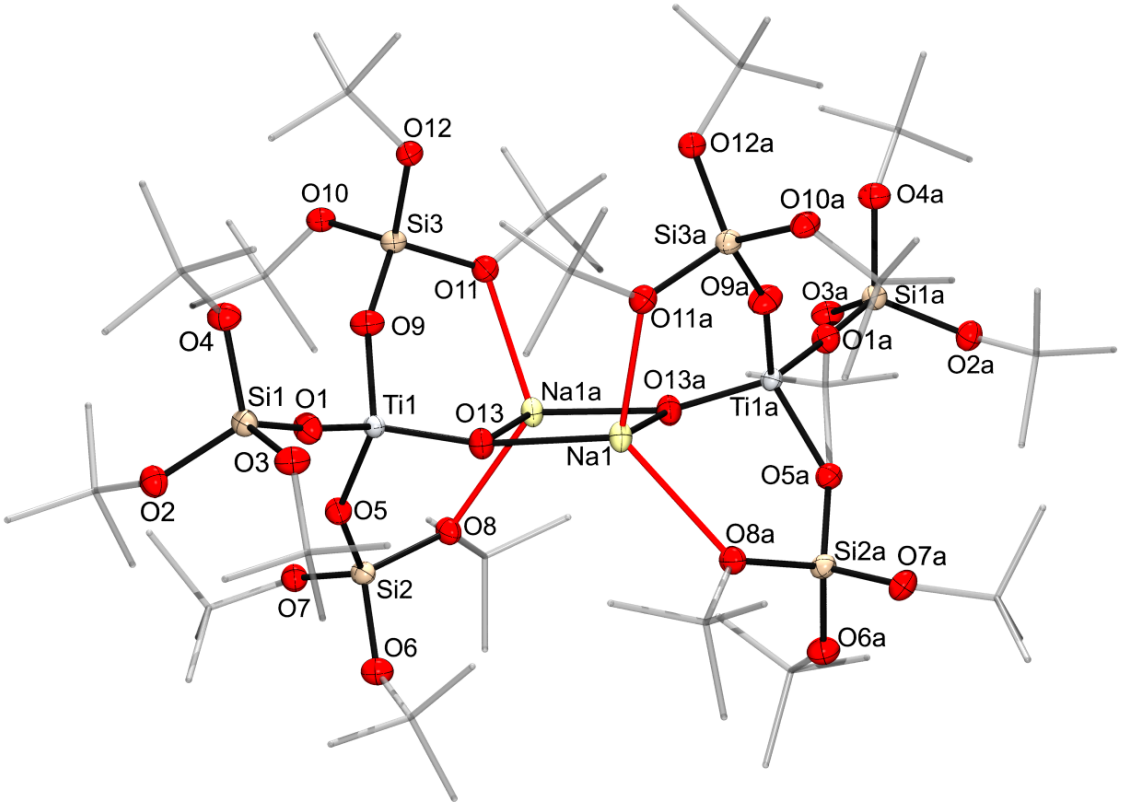


Figure S35. Molecular structure of compound **3** with thermal ellipsoids set at 50% probability level. Carbon-bound hydrogen atoms and thermal ellipsoids of the carbon atoms were eliminated for the sake of clarity.

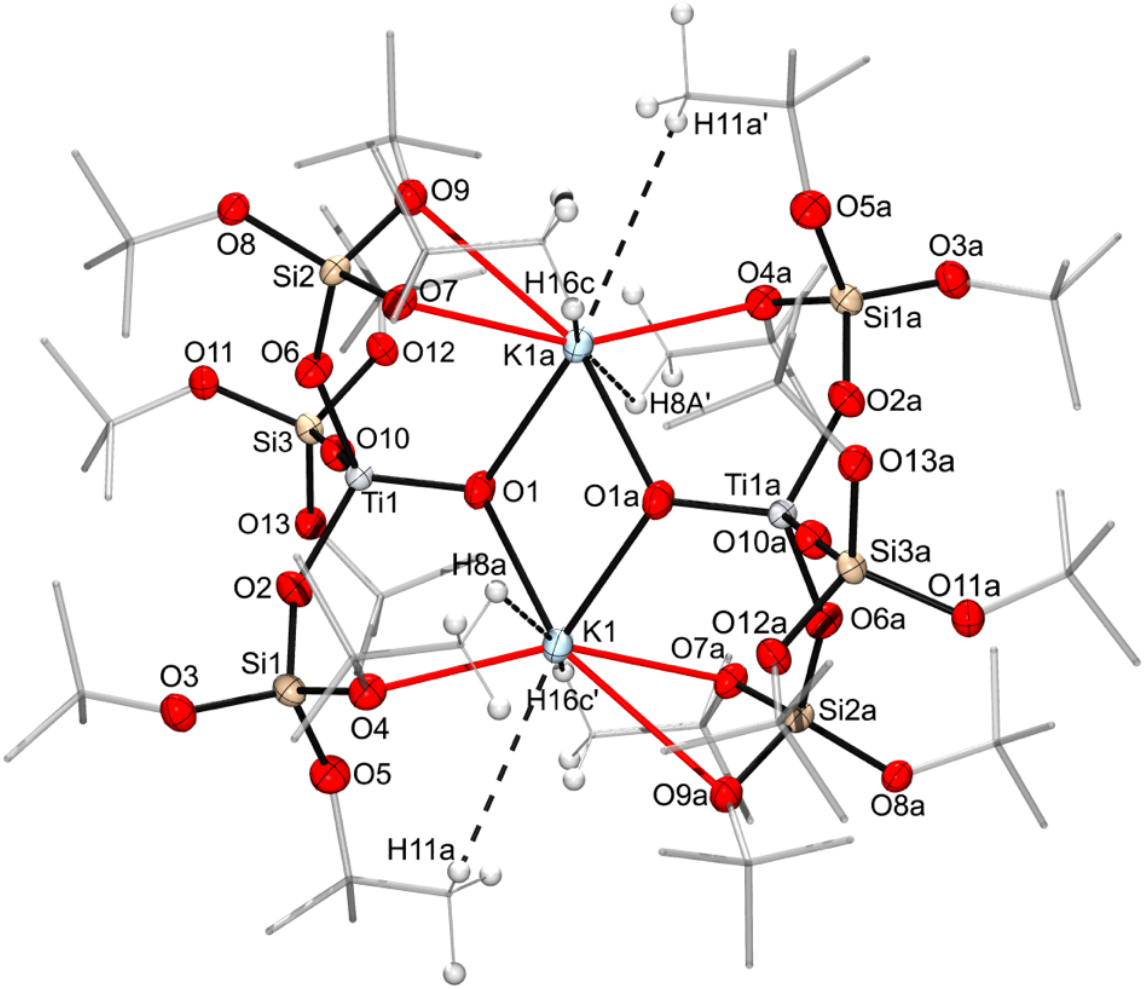


Figure S36. Molecular structure of compound **4** with thermal ellipsoids set at 50% probability level. Carbon-bound hydrogen atoms and thermal ellipsoids of the carbon atoms were eliminated for the sake of clarity.

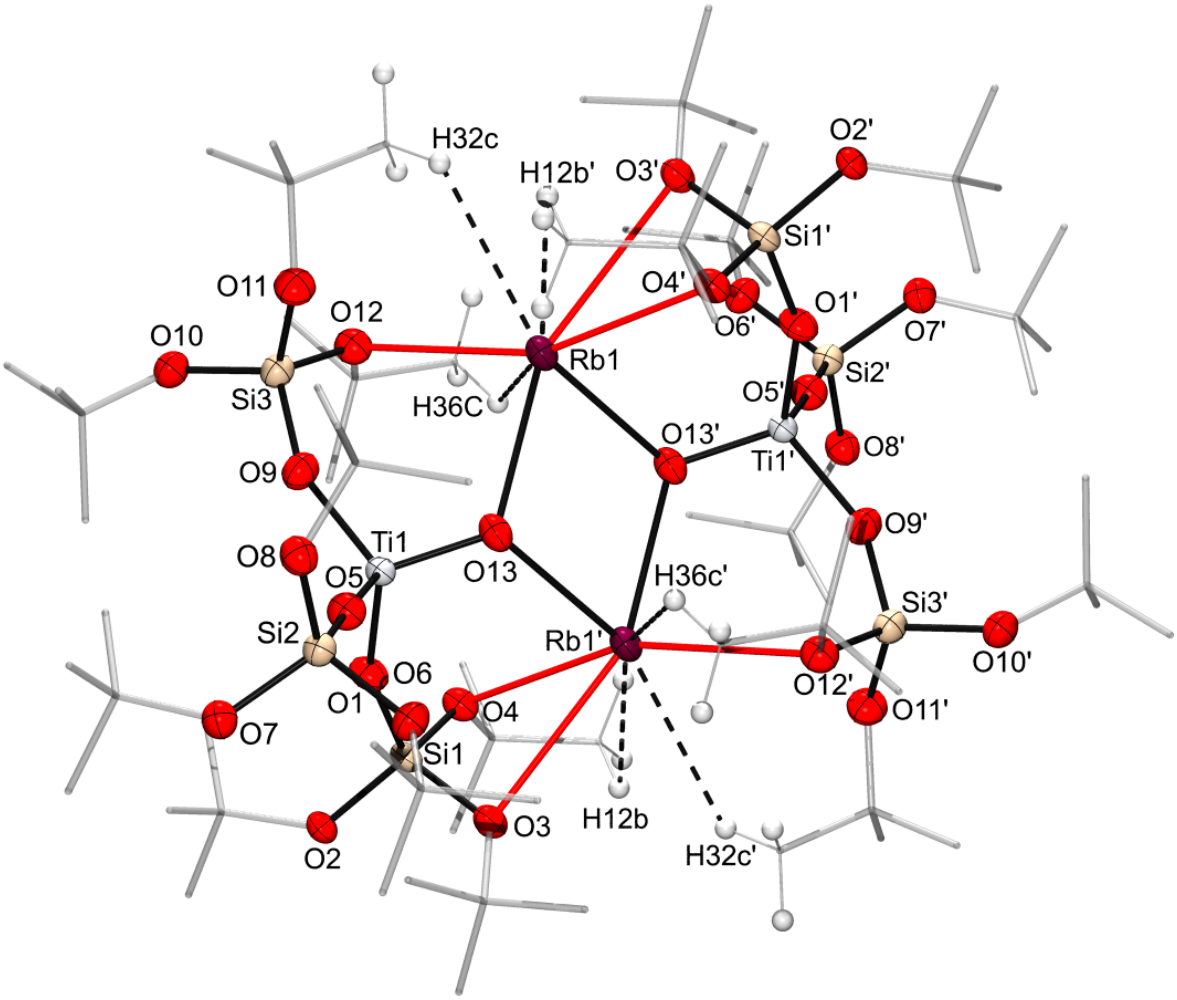


Figure S37. Molecular structure of compound **5** with thermal ellipsoids set at 50% probability level. Carbon-bound hydrogen atoms and thermal ellipsoids of the carbon atoms were eliminated for the sake of clarity.

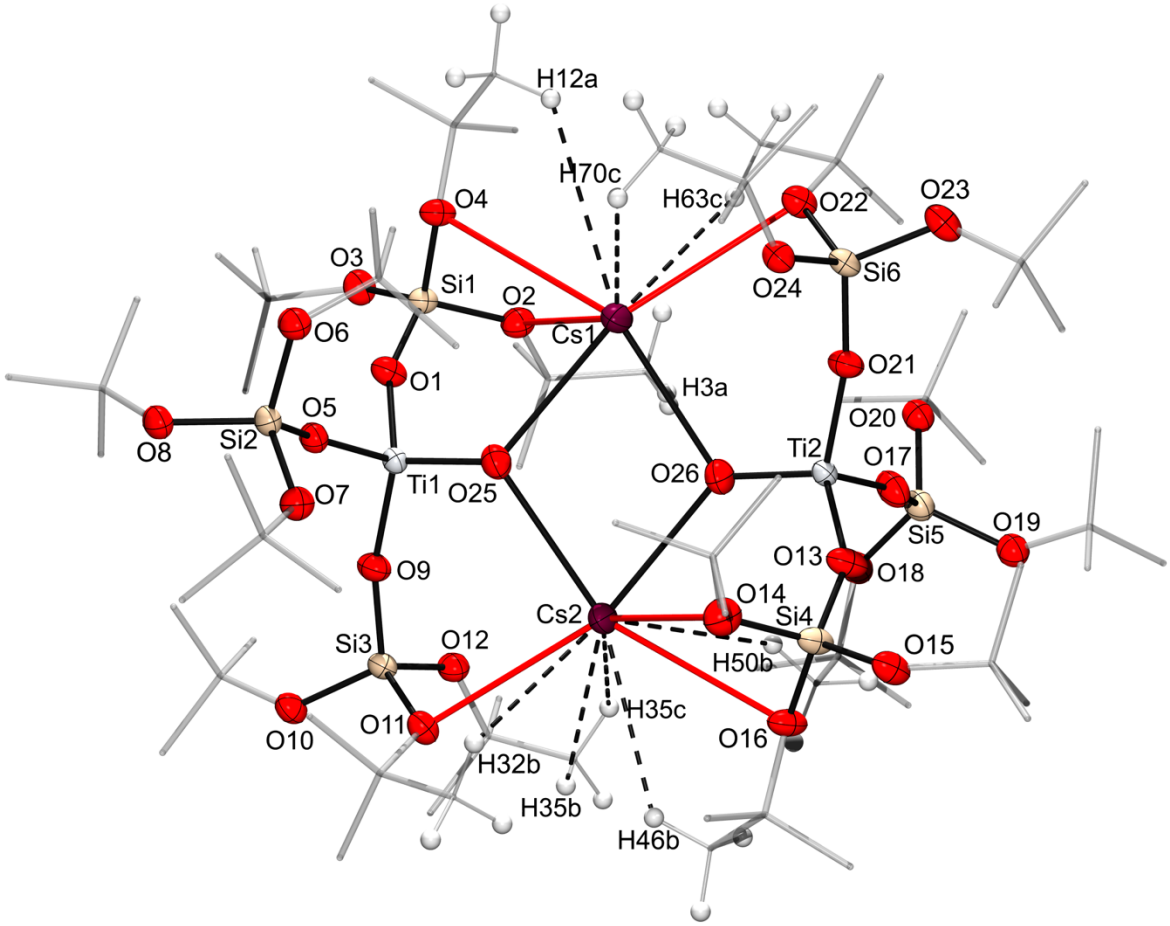


Figure S38. Molecular structure of compound **6** with thermal ellipsoids set at 50% probability level. Carbon-bound hydrogen atoms and thermal ellipsoids of the carbon atoms were eliminated for the sake of clarity.

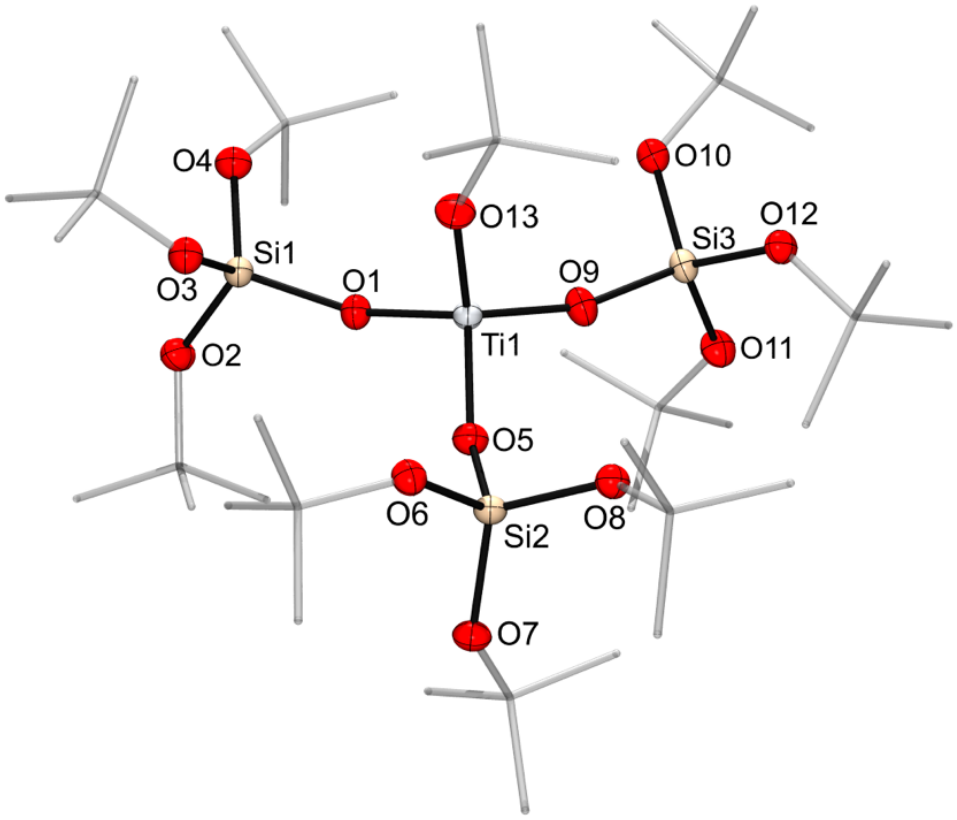


Figure S39. Molecular structure of compound **7** with thermal ellipsoids set at 50% probability level. Carbon-bound hydrogen atoms and thermal ellipsoids of the carbon atoms were eliminated for the sake of clarity.

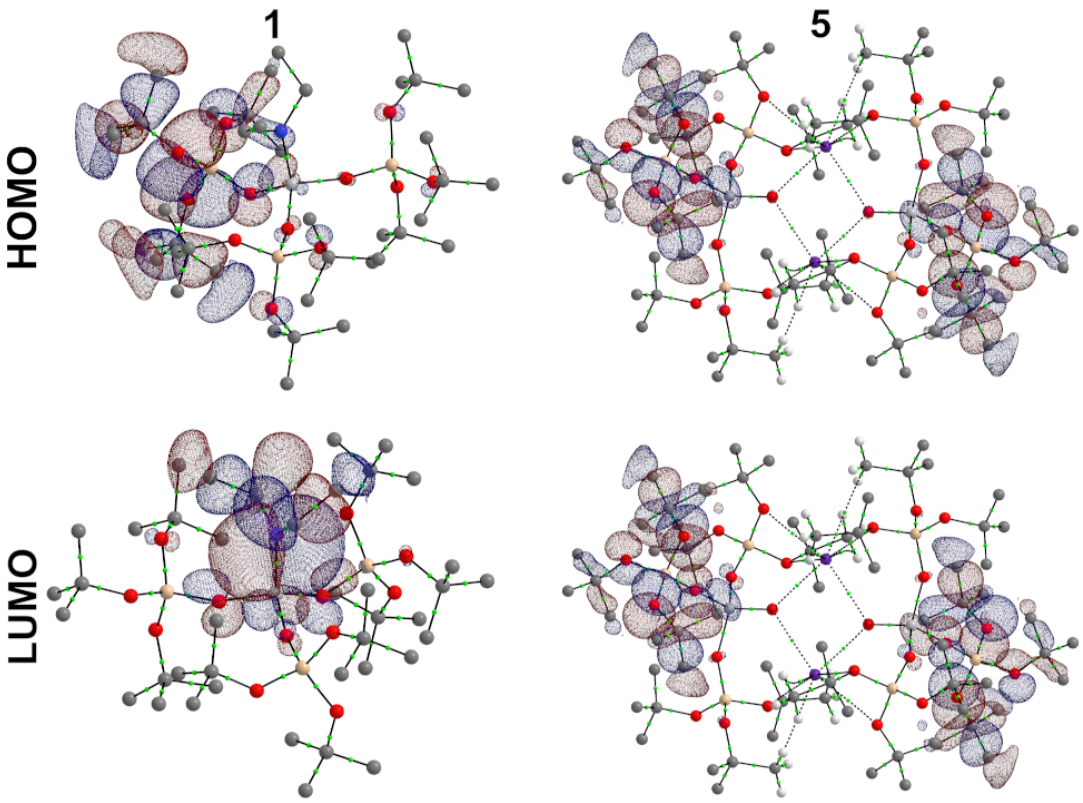


Figure S40. HOMO and LUMO orbitals for compounds **1** and **5** obtained from HAR.

5. Hirshfeld atom refinement obtained coordinates of 1 and 5.

Compound 1

Atom	x	y	z
Ti1	3.8174114837	16.1753750937	12.0786544704
Si2	2.1709977768	19.0393887352	12.8426426299
O3	3.2741780911	14.8071224499	13.1769936913
O4	3.3995515904	12.3280582003	12.1404935734
O5	5.6121943308	16.2398689996	11.9648499076
O6	7.8912486784	17.5351631188	11.4966083343
O7	3.0839369174	17.7136433917	12.7033972570
O8	2.0434637579	19.4720262472	14.4050617890
O9	2.9032708938	20.1560167081	11.9256048792
O10	0.6723092595	18.8307402685	12.2646738521
C11	4.5681671005	11.5430507182	12.4025087824
C12	5.5500190892	12.2923791333	13.2898782530
H13	6.4644049686	11.6933129688	13.4124277503
H14	5.8029070437	13.2564251490	12.8244073883

H15	5.0929041343	12.4693773394	14.2746207295
C16	4.1319506252	10.2264119754	13.0433005413
H17	5.0009042459	9.5584142934	13.1365683913
H18	3.7134651068	10.4251269702	14.0409890694
H19	3.3674289386	9.7477820177	12.4136814922
C20	5.2014585920	11.2863787653	11.0343351977
H21	6.0963775910	10.6585285970	11.1565004383
H22	4.4775584455	10.7708297990	10.3861237970
H23	5.4859481018	12.2451611501	10.5762934524
Si24	2.5900597915	13.3500801874	13.0588833031
O25	2.4283934484	12.6689046637	14.5365386176
C26	2.0287331937	13.1713280921	15.8074296169
C27	1.6407082554	11.9707375813	16.6441816325
H28	1.4668302054	12.2884539452	17.6828456303
H29	0.7213003939	11.5230425053	16.2388934878
H30	2.4520700503	11.2284129435	16.6187579096
C31	3.2302190565	13.8466548525	16.4672986389
H32	2.9445667539	14.2087508517	17.4659424325
H33	4.0522912402	13.1218458706	16.5613700657
H34	3.5586918212	14.6955035426	15.8495917983
C35	0.8930746786	14.1675483279	15.6746378251
H36	0.5714775616	14.4924648627	16.6751400627
H37	1.2358295034	15.0396405677	15.0984655829
H38	0.0481685020	13.6931466605	15.1539874737
O39	1.1883311091	13.5970456749	12.2687270852
C40	0.2476360080	12.6697129237	11.7210979812
C41	0.0787515073	11.4489600029	12.6186403023
H42	-0.6435454808	10.7557952754	12.1627785661
H43	1.0484908722	10.9431595505	12.7359930091
H44	-0.2905428529	11.7671389948	13.6047356257
C45	0.7409736589	12.2102641014	10.3536295939
H46	0.0254178120	11.4912015557	9.9282720210
H47	0.8291909935	13.0790655783	9.6847485246
H48	1.7242526110	11.7290353436	10.4612472069
C49	-1.0605497792	13.4196329325	11.5842028326
H50	-1.8183688115	12.7570179303	11.1407483662
H51	-1.3989419556	13.7508741779	12.5770624172
H52	-0.9147470112	14.2958301590	10.9353421632
Si53	7.2015014516	16.0839827167	11.7026265784
O54	7.3155381645	15.1198080845	10.4068803512
C55	8.3892964830	14.4119558890	9.7649272494
C56	7.8982995154	14.0674322999	8.3793432728
H57	8.7022114313	13.5674121035	7.8192489806
H58	7.0307745198	13.3952893291	8.4543391827
H59	7.6041948127	14.9885914523	7.8549689529
C60	8.6983980107	13.1677560610	10.5950331322
H61	9.5197284202	12.6076024216	10.1242418400

H62	8.9948474713	13.4688926032	11.6106288649
H63	7.8032405221	12.5306704215	10.6480909779
C64	9.6228478995	15.2986426257	9.7046577550
H65	10.4410859929	14.7553559660	9.2093535756
H66	9.3911577430	16.2109873256	9.1354943437
H67	9.9287902760	15.5711138162	10.7255195950
O68	7.9579646312	15.3619193603	12.9364931146
C69	8.1234009336	15.8150305654	14.2984123587
C70	8.3099227479	14.5546323678	15.1281449916
H71	8.5548008693	14.8307169818	16.1643940837
H72	7.3805638458	13.9663069351	15.1152850108
H73	9.1293441134	13.9550290143	14.7050319611
C74	9.3635269487	16.6847386342	14.3540766353
H75	9.5545271849	16.9847908658	15.3949838048
H76	10.2257275957	16.1188258476	13.9715155844
H77	9.2103207105	17.5817710030	13.7361276484
C78	6.9130668726	16.5950260880	14.7883419546
H79	7.0604663324	16.8774095993	15.8412109695
H80	6.7905244715	17.5025993448	14.1790026923
H81	6.0128654517	15.9691819301	14.6991417579
C82	7.5026696386	18.6996217987	10.7498455292
C83	8.7937630483	19.4757438179	10.5193151388
H84	8.5710564271	20.4036775874	9.9721946164
H85	9.2513322013	19.7224785682	11.4887235245
H86	9.4908210599	18.8612857922	9.9306287754
C87	6.5379927114	19.5219848605	11.5798008822
H88	6.3199518142	20.4665092841	11.0598663013
H89	5.6043824998	18.9581209001	11.7227329325
H90	6.9892920453	19.7383568861	12.5593478384
C91	6.8696546157	18.3094245773	9.4210165164
H92	6.6223222179	19.2177165362	8.8519536223
H93	7.5773993724	17.6963925308	8.8437044105
H94	5.9519646699	17.7322938628	9.6074715803
C95	3.0224285449	19.4946178082	15.4524321178
C96	3.1130951077	18.1041561615	16.0687458463
H97	3.7925622621	18.1299395133	16.9334190740
H98	2.1136781227	17.7827992856	16.3972205425
H99	3.4985026188	17.3958714482	15.3205520084
C100	4.3847108046	19.9204910538	14.9222644395
H101	5.1051884444	19.9603191455	15.7525209526
H102	4.7296911636	19.1938296551	14.1719631902
H103	4.3034426203	20.9149993007	14.4592860207
C104	2.5029630849	20.5028333545	16.4720787552
H105	3.2200440470	20.5877347746	17.3018900821
H106	2.3830017829	21.4839261538	15.9893092503
H107	1.5311789897	20.1640145290	16.8604570145
C108	3.7482407464	22.2266474681	11.1823603303

H109	3.4889674163	23.2178628038	10.7820233690
H110	4.3201170748	22.3457773480	12.1144363617
H111	4.3568601848	21.6814886482	10.4458928009
C112	1.6364342072	22.1519709220	12.5255091811
H113	1.3782178769	23.1615934818	12.1733915757
H114	0.7144921053	21.5808419771	12.7094512458
H115	2.2143949680	22.2256996217	13.4585288044
C116	2.4703590087	21.4426442164	11.4663512121
C117	1.6601446659	21.2560466768	10.1872778626
H118	1.3581858563	22.2394586377	9.7977628353
H119	2.2743429343	20.7371665662	9.4365954364
H120	0.7636979111	20.6569681189	10.4051959589
C121	-0.5183170925	18.2427233144	12.8226205737
C122	-1.2263634749	19.3020268441	13.6571739002
H123	-2.1459542730	18.8769496293	14.0857323022
H124	-0.5624170152	19.6332511083	14.4692488726
H125	-1.4820673351	20.1609044379	13.0192514938
C126	-1.3808840677	17.8409195425	11.6322309862
H127	-2.3568707510	17.4822200146	11.9910969933
H128	-1.5287766573	18.7113801807	10.9761622029
H129	-0.8796033288	17.0391375280	11.0702137009
C130	-0.1680699540	17.0312350278	13.6771484733
H131	-1.0911489827	16.5820391258	14.0723045407
H132	0.3659876798	16.2913161727	13.0628987530
H133	0.4738624147	17.3455427336	14.5132906281
N134	3.2336242010	15.8949107126	10.3344593437
C135	4.0583758102	15.4527642876	9.2053045970
H136	4.0070709487	16.2110497949	8.4100869681
H137	5.1054250924	15.3853332258	9.5356696043
C138	3.6386541020	14.1111100662	8.6306483842
H139	4.3466082964	13.8115954733	7.8438243531
H140	3.6364993875	13.3546693765	9.4292678343
H141	2.6288474625	14.1952964725	8.2026257423
C142	1.8249795795	16.1492281919	10.0899242139
H143	1.3776518160	15.2669778550	9.6087460772
H144	1.3143706204	16.3040646453	11.0518516314
C145	1.6014008847	17.3670327751	9.2049457302
H146	0.5221687779	17.5187561052	9.0558206075
H147	2.0332840439	18.2557831919	9.6882673734
H148	2.0871529226	17.2067566706	8.2311096444

Compound 5

Atom	x	y	z
Rb1	6.1031577592	10.6348738580	7.3937962685
Rb2	2.5385832652	12.5070279218	8.7466862628
Ti3	4.5834033825	10.0873235559	10.9553516022

Ti4	4.0583376421	13.0545782239	5.1851309287
Si5	3.1820233847	12.9145697531	12.1804142965
Si6	5.4597176301	10.2273320262	3.9600682445
Si7	3.0353070534	7.2714173493	12.1863861872
Si8	5.6064339713	15.8704844305	3.9540963541
Si9	7.9434572809	10.1109278177	10.5540991516
Si10	0.6982837337	13.0309739621	5.5863833798
O11	4.0147291987	11.5781236804	11.9195850064
O12	4.6270118158	11.5637780995	4.2208975346
O13	3.2163011773	13.3790279689	13.7323227360
O14	5.4254398473	9.7628738110	2.4081597952
O15	3.7778780805	8.5664388989	11.6255052143
O16	4.8638629440	14.5754628809	4.5149773272
O17	3.0081892413	7.2077768042	13.8162534524
O18	5.6335517833	15.9341249756	2.3242290887
O19	6.4407714353	9.9637459561	11.0794731820
O20	2.2009695792	13.1781558232	5.0610093492
O21	8.1182885241	11.3483265327	9.4933473499
O22	0.5234525003	11.7935752471	6.6471351814
O23	4.1632780402	10.3106431930	9.3498589492
O24	4.4784629844	12.8312585868	6.7906235922
C25	4.2015685531	13.1948180548	14.7667661853
C26	4.4401724715	9.9470837250	1.3737163556
C27	4.1203828769	11.7655738849	15.2884264255
C28	4.5213581477	11.3763278950	0.8520561155
H29	4.3408602738	11.0636898308	14.4706558728
H30	4.3008807507	12.0782119491	1.6698266684
H31	4.8532890432	11.6282255843	16.0971193080
H32	3.7884519813	11.5136761955	0.0433632333
H33	3.1083866290	11.5729514199	15.6741210851
H34	5.5333543953	11.5689503594	0.4663614559
C35	5.5973317004	13.4688186057	14.2350986346
C36	3.0444093241	9.6730831741	1.9053838965
H37	5.8333026785	12.7497953404	13.4367732535
H38	2.8084383460	10.3921064390	2.7037092879
H39	5.6421157037	14.4915020142	13.8324657737
H40	2.9996253107	8.6503997652	2.3080167675
H41	6.3276533466	13.3636416879	15.0509223277
H42	2.3140876779	9.7782600919	1.0895602038
C43	3.8351414649	14.1806631806	15.8627049296
C44	4.8065995496	8.9612385992	0.2777776114
H45	3.8994667499	15.2061403692	15.4699467396
H46	4.7422742647	7.9357614101	0.6705358016
H47	2.8087789960	13.9830286954	16.2055181062
H48	5.8329620286	9.1588730845	-0.0650355650
H49	4.5318196785	14.0667493215	16.7063063050
H50	4.1099213460	9.0751524578	-0.5658237735

O51	1.6209578647	12.7676180417	11.7173445910
O52	7.0207831501	10.3742837376	4.4231379501
C53	0.4989901184	12.1342248730	12.3925009431
C54	8.1427508961	11.0076769063	3.7479815982
C55	0.9342005218	10.8530891847	13.0586187743
C56	7.7075404926	12.2888125951	3.0818637670
H57	1.3427272933	10.1669100620	12.3021372560
H58	7.2990137312	12.9749917178	3.8383452752
H59	1.7076559813	11.0742817415	13.8088458821
H60	6.9340850430	12.0676200378	2.3316366593
H61	0.0696539854	10.3836353987	13.5507291218
H62	8.5720870395	12.7582663812	2.5897534091
C63	-0.0510721039	13.1142842584	13.4259761722
C64	8.6928131185	10.0276175209	2.7145063687
H65	-0.2926965325	14.0682257017	12.9344341547
H66	8.9344375470	9.0736760776	3.2060483766
H67	-0.9608556439	12.6953561764	13.8807215476
H68	9.6025966587	10.4465456035	2.2597609938
H69	0.7040406042	13.2853599217	14.2073455527
H70	7.9377004203	9.8565418581	1.9331369887
C71	-0.5387390914	11.8789696837	11.3127028400
C72	9.1804801160	11.2629320962	4.8277797013
H73	-0.7902367008	12.8268591162	10.8144511417
H74	9.4319777251	10.3150426631	5.3260313996
H75	-0.1327174702	11.1726770190	10.5735835632
H76	8.7744584850	11.9692247603	5.5668989681
H77	-1.4446415911	11.4525527709	11.7682349050
H78	10.0863826158	11.6893490089	4.3722476362
O79	3.7857750511	14.0323235792	11.1525888976
O80	4.8559659734	9.1095782007	4.9878936436
C81	3.6288949990	15.4629556493	11.0654306112
C82	5.0128460255	7.6789461306	5.0750519203
C83	3.0412179839	16.0850103271	12.2964652654
C84	5.6005230308	7.0568914528	3.8440172756
H85	2.9528735071	17.1718522605	12.1516548645
H86	5.6888675172	5.9700495189	3.9888276667
H87	2.0449234273	15.6578105839	12.4832745500
H88	6.5968175975	7.4840911954	3.6572079913
H89	3.6946794241	15.8817685813	13.1576743718
H90	4.9470616004	7.2601331986	2.9828081594
C91	5.0367303773	16.0505288042	10.8254216322
C92	3.6050106472	7.0913729752	5.3150609086
H93	5.4778720611	15.5909387090	9.9286657336
H94	3.1638689633	7.5509630709	6.2118168077
H95	4.9602154015	17.1382014479	10.6801155113
H96	3.6815256131	6.0037003319	5.4603670301
H97	5.6749036864	15.8409741484	11.6965254494

H98	2.9668373382	7.3009276314	4.4439570917
C99	2.7582249221	15.7557011014	9.8519891478
C100	5.8835161024	7.3862006779	6.2884933936
H101	2.6082890706	16.6982706744	9.7135037972
H102	6.0334519538	6.4436311055	6.4269787441
H103	1.8615145232	15.3650656615	9.9533513856
H104	6.7802265012	7.7768361179	6.1871311558
H105	3.2314458285	15.3703883120	9.0719195875
H106	5.4102951860	7.7715134679	7.0685629438
O107	1.4833633841	7.3656048565	11.7255763919
O108	7.1583776307	15.7762969234	4.4149061395
C109	0.3337255157	6.5898882669	12.0921265199
C110	8.3080155090	16.5520135129	4.0483560113
C111	-0.3483626368	7.2096280742	13.2834555716
C112	8.9901036613	15.9322737051	2.8570269697
H113	-0.5135526295	8.2807440165	13.0952453971
H114	9.1552936438	14.8611577628	3.0452371442
H115	-1.3156109712	6.7134080065	13.4513737147
H116	9.9573519857	16.4284937733	2.6891088168
H117	0.2859309420	7.0873424749	14.1738027400
H118	8.3558100827	16.0545593044	1.9666798013
C119	0.6590697807	5.1275514043	12.2110821988
C120	7.9826712338	18.0143503753	3.9294003422
H121	0.8862455981	4.7202396930	11.2148450325
H122	7.7554954165	18.4216620865	4.9256375088
H123	1.5320062578	4.9983728844	12.8678127394
H124	7.1097347669	18.1435288951	3.2726697917
H125	-0.2029023056	4.5936641232	12.6376600619
H126	8.8446433302	18.5482376564	3.5028224694
C127	-0.6567409105	6.8638879077	10.9385664910
C128	9.2984819349	16.2780138716	5.2019160501
H129	-0.7909880108	7.9492706210	10.8205737924
H130	9.4327290356	15.1926311583	5.3199087390
H131	-0.2584978599	6.4400395853	10.0048881394
H132	8.9002388846	16.7018621945	6.1355943920
H133	-1.6259565450	6.3974433722	11.1688939287
H134	10.2676975694	16.7444584077	4.9715886023
O135	3.7626477193	5.9111349346	11.6732809678
O136	4.8790932952	17.2307668453	4.4672015735
C137	4.2673036582	5.5850667995	10.3657407773
C138	4.3744373664	17.5568349804	5.7747417641
C139	4.2516116470	4.0627924824	10.2695434296
C140	4.3901293776	19.0791092971	5.8709391017
H141	4.7051100318	3.7508849284	9.3171500965
H142	3.9366309827	19.3910168512	6.8233324449
H143	4.8252809611	3.6366174697	11.1057722038
H144	3.8164600535	19.5052843102	5.0347103272

H145	3.2131280171	3.7031228548	10.3163375635
H146	5.4286130073	19.4387789249	5.8241449778
C147	5.6921679878	6.1302896716	10.2049815150
C148	2.9495730368	17.0116121083	5.9355010164
H149	6.0826245278	5.8498337599	9.2155936485
H150	2.5591164968	17.2920680200	6.9248888923
H151	5.6778083165	7.2264015156	10.2962657620
H152	2.9639326979	15.9155002638	5.8442167693
H153	6.3377701573	5.7055858188	10.9878127047
H154	2.3039708672	17.4363159610	5.1526698362
C155	3.3929123009	6.2279484491	9.2638299524
C156	5.2488287137	16.9139533307	6.8766525789
H157	3.7839043210	5.9467533975	8.2748634365
H158	4.8578367036	17.1951483824	7.8656190949
H159	2.3569672113	5.8717096113	9.3633881699
H160	6.2847738035	17.2701921680	6.7770943609
H161	3.4159774627	7.3226150831	9.3695330703
H162	5.2257635618	15.8192866968	6.7709494706
C163	4.0477261113	6.9768208865	14.7703169959
C164	4.5940149133	16.1650808934	1.3701655454
C165	3.5876896559	7.6703835400	16.0567133749
C166	5.0540513587	15.4715182399	0.0837691564
H167	3.4740621472	8.7486947725	15.8714194407
H168	5.1676788774	14.3932070068	0.2690631007
H169	2.6226634817	7.2493958673	16.3752946891
H170	6.0190775327	15.8925059121	-0.2348121581
H171	4.3360619134	7.5110006576	16.8469894456
H172	4.3056791111	15.6309011223	-0.7065069043
C173	4.1792945814	5.4793080116	14.9880522625
C174	4.4624464432	17.6625937683	1.1524302686
H175	4.4648136033	4.9950026941	14.0425749098
H176	4.1769274212	18.1468990853	2.0979076313
H177	4.9515378908	5.2855961665	15.7470754408
H178	3.6902031338	17.8563056134	0.3934071003
H179	3.2168109674	5.0728623501	15.3321850992
H180	5.4249300570	18.0690394295	0.8082974322
C181	5.3707832131	7.5639309319	14.2988535296
C182	3.2709578115	15.5779708479	1.8416290016
H183	5.6973419882	7.0452595817	13.3854316195
H184	2.9443990364	16.0966421976	2.7550509119
H185	5.2413186130	8.6353016440	14.0857716032
H186	3.4004224115	14.5066001354	2.0547109280
H187	6.1297059012	7.4354665516	15.0846865000
H188	2.5120351232	15.7064352277	1.0557960412
O189	8.9930670814	10.3650265669	11.7683486348
O190	-0.3513260670	12.7768752124	4.3721339062
C191	8.9922399515	9.8508133773	13.1235035294

C192	-0.3504989370	13.2910884020	3.0169790120
C193	7.9686019427	10.6684167205	13.9058327094
C194	0.6731390718	12.4734850593	2.2346498219
H195	8.2159906916	11.7373736625	13.8275381032
H196	0.4257503327	11.4045281168	2.3129444379
H197	6.9649800555	10.4929962469	13.4911389073
H198	1.6767609590	12.6489055330	2.6493436337
H199	7.9869052244	10.3642818769	14.9627940107
H200	0.6548358004	12.7776199024	1.1776885306
C201	8.6306555836	8.3602433730	13.0841208763
C202	0.0110854409	14.7816584068	3.0563616650
H203	7.6426083576	8.2348371234	12.6171774701
H204	0.9991326568	14.9070646564	3.5233050709
H205	9.3851327817	7.8152877709	12.4977867212
H206	-0.7433917572	15.3266140084	3.6426958101
H207	8.6049924519	7.9619606921	14.1091635548
H208	0.0367485728	15.1799410873	2.0313189862
C209	10.4008188598	10.0692727844	13.6299919583
C210	-1.7590778353	13.0726289954	2.5104905830
H211	11.1191274549	9.8190942549	12.8353576668
H212	-2.4773864305	13.3228075244	3.3051248642
H213	10.5269574796	11.1228642453	13.9198786203
H214	-1.8852164550	12.0190375340	2.2206039108
H215	10.5806375335	9.4247153748	14.5030390154
H216	-1.9388965191	13.7171864050	1.6374435259
O217	8.2555083050	8.7719371147	9.6804156943
O218	0.3862327197	14.3699646652	6.4600668370
C219	9.4093801537	8.3826912645	8.8997007643
C220	-0.7676391290	14.7592105148	7.2407817766
C221	9.3361754479	6.8634254978	8.7839733856
C222	-0.6944344234	16.2784762821	7.3565091457
H223	8.4180044774	6.5803078658	8.2484300544
H224	0.2237365472	16.5615939135	7.8920524769
H225	10.2121868755	6.4952728295	8.2298364228
H226	-1.5704458508	16.6466289503	7.9106461181
H227	9.3255462873	6.4191369236	9.7902014327
H228	-0.6838052626	16.7227648562	6.3502811082
C229	10.7256931848	8.7997080668	9.5600077953
C230	-2.0839521602	14.3421937130	6.5804747360
H231	11.5702091398	8.4201991273	8.9660667696
H232	-2.9284681152	14.7217026520	7.1744157718
H233	10.7780951090	9.8972129112	9.6123274192
H234	-2.1363540943	13.2446888686	6.5281551222
H235	10.7748030984	8.3814201146	10.5761886832
H236	-2.1330620840	14.7604816652	5.5642938481
C237	9.3465934387	9.0181675136	7.5053244473
C238	-0.7048524142	14.1237342662	8.6351580941

H239	10.0446986423	8.7677723141	6.9505759646
H240	-1.4029576179	14.3741294653	9.1899065668
H241	9.4349491056	10.0505279927	7.5863496033
H242	-0.7932080810	13.0913737866	8.5541329280
H243	8.5701875990	8.7147773404	7.1137562668
H244	0.0715534255	14.4271244395	9.0267262640
C245	8.3163613994	12.7685436717	9.7204441976
C246	0.3253796250	10.3733581076	6.4200383438
C247	7.4501242428	13.2505900988	10.8628675754
C248	1.1916167816	9.8913116805	5.2776149659
H249	7.5964569041	14.3317581419	11.0030909663
H250	1.0452841104	8.8101436375	5.1373915651
H251	6.3934891814	13.0505495034	10.6315533174
H252	2.2482518429	10.0913522760	5.5089292235
H253	7.7304649246	12.7200257683	11.7847736361
H254	0.9112761001	10.4218760116	4.3557089050
C255	9.7886850928	13.0043602899	10.0296957111
C256	-1.1469440682	10.1375414894	6.1107868298
H257	10.4031120102	12.6229594708	9.2008331477
H258	-1.7613709855	10.5189423091	6.9396493937
H259	9.9691533067	14.0823038830	10.1540702011
H260	-1.3274122921	9.0595978969	5.9864123403
H261	10.0573137935	12.4781581797	10.9575697027
H262	-1.4155727689	10.6637436002	5.1829128286
C263	7.9336706303	13.4607181753	8.4259774777
C264	0.7080703845	9.6811836046	7.7145050631
H265	8.4404637991	13.0726288552	7.6635010792
H266	0.2012772155	10.0692729241	8.4769814521
H267	8.1166492039	14.4525806412	8.5118448548
H268	0.5250918204	8.6893211381	7.6286376766
H269	6.9331019132	13.3290411753	8.2597305250
H270	1.7086391114	9.8128606046	7.8807520158