

Supporting Information

Bryan Carlson, Adelia J. A. Aquino, Bruce Whittlesey, Louisa J. Hope-Weeks,
Brian McNerney, William L. Hase and Clemens Krempner*

General Remarks

The manipulation of air-sensitive compounds involved standard Schlenk line and Glove box techniques. THF, THF-D₈, benzene-D₆ and n-hexane were distilled under nitrogen from alkali metals and stored over molecular sieves prior to use. Si(SiMe₂OMe)₄ [1], Ba(OtBu)₂ [2] and Sr(OtBu)₂ [2] were prepared as described in the literature. The ¹H, ¹³C and ²⁹Si NMR spectra were obtained from a Varian Unity Inova 500. All measurements, unless noted otherwise, were carried out at 300 K.

Synthetic Procedures

Bis[tris(dimethyl-methoxysilyl)silyl]magnesium [Si(SiMe₂OMe)₃]₂Mg, (Mg-2)

Upon standing a solution of MgMe₂·dioxane (20 mg, 0.14 mmol), Si(SiMe₂OMe)₄ (200 mg, 0.52 mmol) and THF (3 ml) in a Glove box for ca. 6 hours clear colorless single crystals precipitated. The crystals were washed twice with a small amount of THF and dried under vacuum to give 50 mg (31%) of the title compound. ¹H NMR (THF-D₈, 300 MHz): δ 0.41 (s, SiMe₂, 18 H), 3.48 (s, OCH₃, 9 H) ppm. ¹³C NMR (THF-D₈, 125.7MHz): δ 4.5 (SiMe₂), 52.3 (OMe) ppm. ²⁹Si NMR (THF-D₈, 99.3 MHz): δ 53.5 (SiMe₂O), -216.8 (SiSi₃) ppm. - Anal. Calc. for C₁₈H₅₄O₆Si₈Mg (615.60): C, 35.12; H, 8.84. Found: C, 33.56; H, 8.79%.

Bis[tris(dimethyl-methoxysilyl)silyl]calcium [Si(SiMe₂OMe)₃]₂Ca, (Ca-2)

Upon standing a solution of Ca(OPrⁱ)₂ (60 mg, 0.38 mmol), Si(SiMe₂OMe)₄ (283 mg, 0.74 mmol) and THF (5 ml) in a Glove box for ca. 5 days clear single crystals precipitated. The crystals were washed with a small amount of THF, centrifuged and dried under vacuum to give 112 mg (48%) of the title compound. ¹H NMR (THF-D₈, 300 MHz): δ 0.38 (s, SiMe₂, 18 H), 3.47 (s, OCH₃, 9 H) ppm. ¹³C NMR (THF-D₈, 125.7MHz): δ 3.6 (SiMe₂), 51.1 (OMe) ppm. ²⁹Si NMR (THF-D₈, 99.3 MHz, 322 K): δ 46.2 (SiMe₂O), -206.5 (SiSi₃) ppm. - Anal. Calc. for C₁₈H₅₄O₆Si₈Ca (631.38): C, 34.24; H, 8.62. Found: C, 32.18; H, 8.52%.

Bis[tris(dimethyl-methoxysilyl)silyl]strontium [Si(SiMe₂OMe)₃]₂Sr, (Sr-2)

Upon standing a solution of Sr(OBu^t)₂ (103 mg, 0.44 mmol), Si(SiMe₂OMe)₄ (334 mg, 0.87 mmol) and THF (5 ml) in a Glove box for ca. 3 days clear single crystals precipitated. The crystals were washed with THF, centrifuged and dried under vacuum to give 140 mg (48%) of the title compound. ¹H NMR (THF-D₈, 300 MHz): δ 0.37 (s, SiMe₂, 18 H), 3.46 (s, OCH₃, 9 H) ppm. ¹³C NMR (THF-D₈, 125.7MHz): δ 3.5 (SiMe₂), 50.6 (OMe) ppm. ²⁹Si NMR (THF-D₈, 99.3 MHz, 322 K): δ 42.4 (SiMe₂O), -199.4 (SiSi₃) ppm. - Anal. Calc. for C₁₈H₅₄O₆Si₈Sr (678.92): C, 31.84; H, 8.02. Found: C, 30.47; H, 8.00%.

Bis[tris(dimethyl-methoxysilyl)silyl]barium [Si(SiMe₂OMe)₃]₂Ba, (Ba-2)

Upon standing a solution of Ba(OBu^t)₂ (113 mg, 0.4 mmol), Si(SiMe₂OMe)₄ (300 mg, 0.78 mmol) and THF (5 ml) in a Glove box for ca. 3 days clear colorless single crystals precipitated. The crystals were washed with THF, centrifuged and dried under vacuum to give 193 mg (68%) of the title compound. ¹H NMR (THF-D₈, 300 MHz): δ 0.34 (s, SiMe₂, 18 H), 3.46 (s, OCH₃, 9 H) ppm. ¹³C NMR (THF-D₈, 125.7MHz): δ 3.7 (SiMe₂), 50.1 (OMe) ppm. ²⁹Si NMR (THF-D₈, 99.3 MHz, 322 K): δ 38.9 (SiMe₂O), -190.0 (SiSi₃) ppm. - Anal. Calc. for C₁₈H₅₄O₆Si₈Ba (728.63): C, 29.67; H, 7.47. Found: C, 28.27; H, 7.31%.

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[2] W. Weiss and D. Dawidowski, *D. Ger. Patent* 2002, 6 pp.

X-Ray studies

Bis[tris(dimethyl-methoxysilyl)silyl]magnesium [Si(SiMe₂OMe)₃]₂Mg, (Mg-2)

A colorless block/needle-like specimen of C₁₈H₅₄MgO₆Si₈, approximate dimensions 0.13 mm x 0.15 mm x 0.18 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. X-ray intensity data were measured on a Bruker Apex II automated X-ray diffractometer equipped with a CCD detector. A total of 1464 frames were collected. The total exposure time was 4.07 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 15332 reflections to a maximum θ angle of 24.08° (0.87 Å resolution), of which 2727 were independent (average redundancy 5.622, completeness = 100.0%, $R_{\text{int}} = 7.13\%$, $R_{\text{sig}} = 5.00\%$) and 2041 (74.84%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 9.8056(10)$ Å, $b = 12.7931(13)$ Å, $c = 13.7123(14)$ Å, $\beta = 95.4620(10)^\circ$, volume = 1712.3(3) Å³, are based upon the refinement of the XYZ-centroids of 41 reflections above $20 \sigma(I)$ with $6.786^\circ < 2\theta < 36.15^\circ$. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.905. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9381 and 0.9537.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/n 1, with $Z = 2$ for the formula unit, C₁₈H₅₄MgO₆Si₈. The final anisotropic full-matrix least-squares refinement on F^2 with 161 variables converged at $R1 = 3.79\%$, for the observed data and $wR2 = 8.20\%$ for all data. The goodness-of-fit was 1.043.

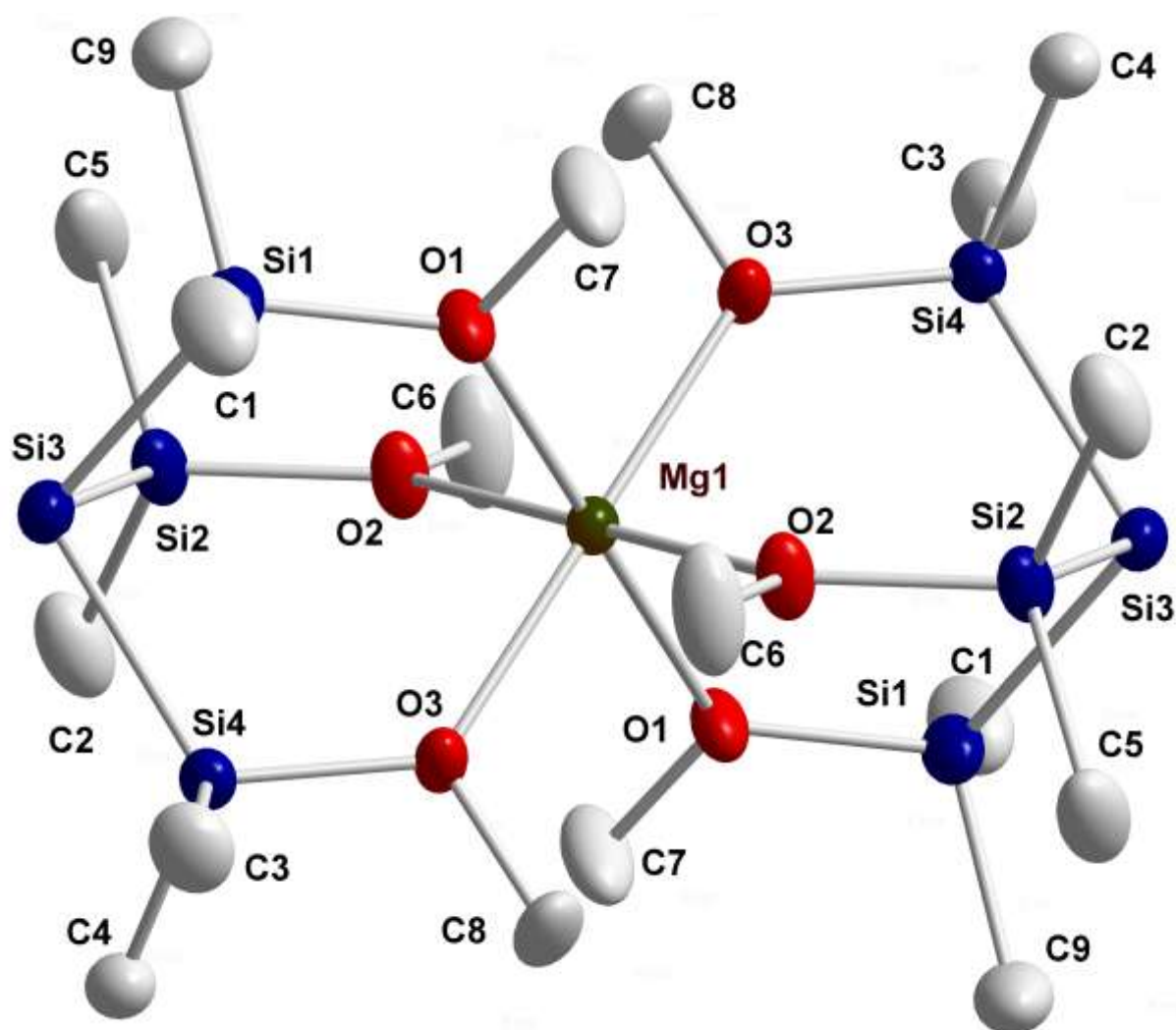


Fig. 1. Molecular structure of Mg-2 in the crystal; selected bond lengths [Å] and angles [°]: C1 Si1 1.870(3), C2 Si2 1.872(3), C3 Si4 1.874(3), C4 Si4 1.874(3), C5 Si2 1.876(3), C6 O2 1.447(3), C7 O1 1.451(3), C8 O3 1.465(3), C9 Si1 1.873(3), Mg1 O2 2.1403(18), Mg1 O3 2.1448(18), Mg1 O1 2.1701(18), O1 Si1 1.725(2), O2 Si2 1.730(2), O3 Si4 1.7198(19), Si1 Si3 2.3005(12), Si2 Si3 2.3009(12), Si3 Si4 2.2988(11), O1 Mg1 O1 180.0, O2 Mg1 O2 180.0, O3 Mg1 O3 180.0, O2 Mg1 O3 86.09(7), O2 Mg1 O1 85.43(7), O2 Mg1 O1 94.56(7), O3 Mg1 O1 94.77(7), O3 Mg1 O1 85.23(7), C7 O1 Si1 114.92(18), C6 O2 Si2 114.95(17), C8 O3 Si4 113.90(17), C7 O1 Mg1 117.53(17), C6 O2 Mg1 117.13(17), C8 O3 Mg1 116.83(17), Si1 O1 Mg1 127.54(10), Si2 O2 Mg1 127.92(10), Si4 O3 Mg1 129.25(10), Si4 Si3 Si1 98.45(4), Si4 Si3 Si2 98.02(4), Si1 Si3 Si2 98.34(4), O1 Si1 Si3 113.34(8), O2 Si2 Si3 113.29(7), O3 Si4 Si3 112.33(7)

Bis[tris(dimethyl-methoxysilyl)silyl]calcium [Si(SiMe₂OMe)₃]₂Ca, (Ca-2)

X-ray intensity data were measured on a Bruker Apex II automated X-ray diffractometer equipped with a CCD detector. The total exposure time was 4.07 hours. The frames were integrated with the Bruker SAINT software package and data were corrected for Lorentz and polarization effects with SAINT V7.53A (Bruker AXS) using a narrow-frame integration algorithm. This yielded a total of 16495 reflections out to a maximum θ angle of 24.66° (0.85 Å resolution), of which 1589 were independent (average redundancy 10.381, completeness = 100.0%, $R_{\text{int}} = 2.99\%$, $R_{\text{sig}} = 1.39\%$) and 1365 (85.90%) had intensities greater than $2\sigma(F^2)$. The final cell constants were $a = 16.731(4)$ Å, $b = 12.770(3)$ Å, $c = 16.848(4)$ Å, volume = $3599.7(13)$ Å³, which were based upon the refinement of the XYZ-centroids of 5277 reflections above $20 \sigma(I)$ with $4.788^\circ < 2\theta < 43.60^\circ$. The calculated minimum and maximum transmission coefficients (based on crystal size) were 0.8141 and 0.8858. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group Cmca (No. 64 in the International Tables for X-ray Crystallography), with $Z = 4$ for the formula unit C₁₈H₅₄CaO₆Si₈. The final anisotropic full-matrix least-squares refinement on F^2 with 178 variables converged at $R_1 = 3.57\%$, for the observed data and $wR_2 = 9.69\%$ for all data. The goodness-of-fit was 1.007.

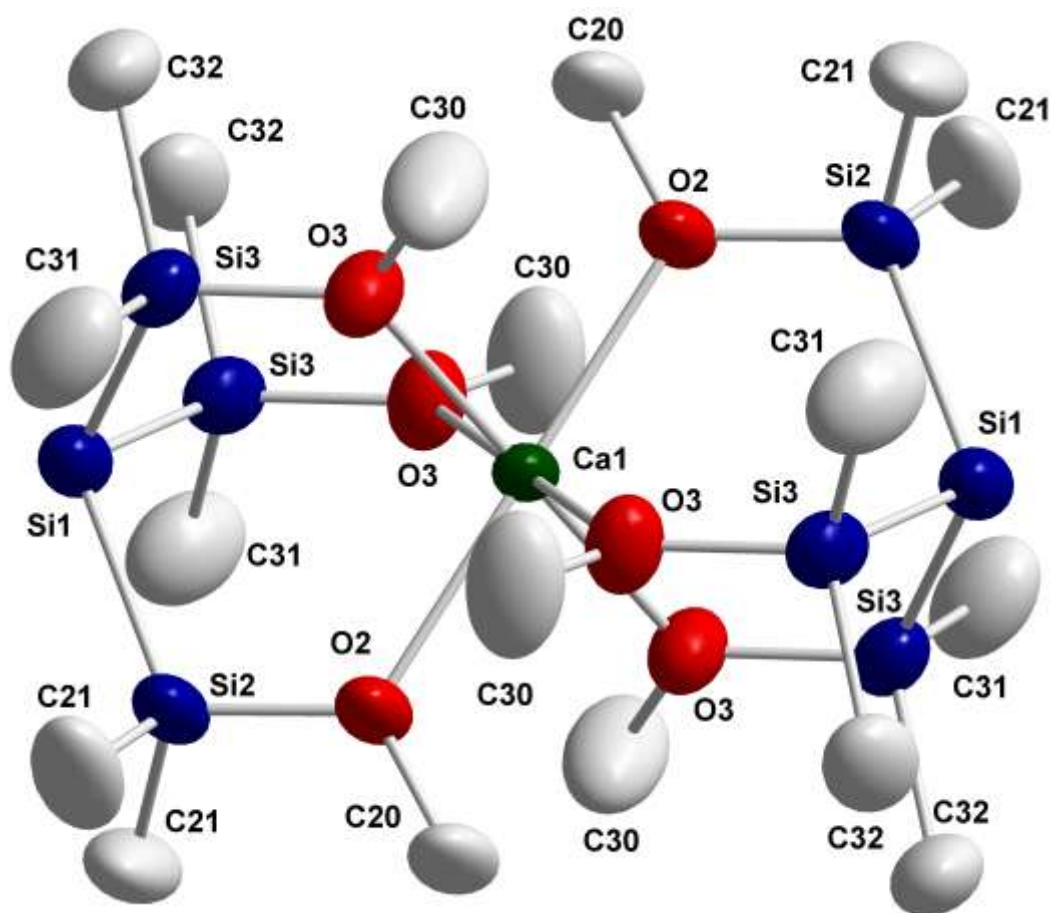


Fig. 2. Molecular structure of Ca-2 in the crystal; selected bond lengths [\AA] and angles [$^\circ$]: Ca1 O2 2.361(3), Ca1 O3 2.394(2), Si1 Si2 2.2971(14), Si1 Si3 2.2991(11), Si2 O2 1.705(3), Si3 O3 1.704(2), O2 C20 1.460(6), O3 C30 1.432(5), O2 Ca1 O2 180.00, O3 Ca1 O3 180.00(9), O3 Ca1 O3 98.62(10), O3 Ca1 O3 81.38(10), O2 Ca1 O3 98.36(6), O2 Ca1 O3 81.64(6), Si2 Si1 Si3 104.64(3), Si2 Si1 Si3 104.64(3), Si3 Si1 Si3 105.42(6), O2 Si2 Si1 112.80(10), O3 Si3 Si1 113.18(8), Si2 O2 Ca1 120.24(13), Si3 O3 Ca1 119.42(10).

Bis[tris(dimethyl-methoxysilyl)silyl]strontium [Si(SiMe₂OMe)₃]₂Sr, (Sr-2)

A cubic-like specimen of C₁₈H₆O₆Si₈Sr, approximate dimensions 0.16 mm x 0.19 mm x 0.36 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. X-ray intensity data were measured on a Bruker Apex II automated X-ray diffractometer equipped with a CCD detector. The total exposure time was 8.13 hours. The frames were integrated with the Bruker SAINT software package using a Intensity data were corrected for Lorentz and polarization effects with SAINT V7.53A (Bruker AXS) using a narrow-frame integration algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 11755 reflections to a maximum θ angle of 20.99° (0.99 Å resolution), of which 1259 were independent (average redundancy 11.391, completeness = 99.9%, $R_{\text{int}} = 3.98\%$, $R_{\text{sig}} = 1.74\%$) and 1044 (84.69%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 16.8439(16)$ Å, $b = 12.8565(12)$ Å, $c = 16.9429(16)$ Å, volume = 3669.0(6) Å³, are based upon the refinement of the XYZ-centroids of 5813 reflections above $20 \sigma(I)$ with $4.652^\circ < 2\theta < 41.86^\circ$. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.3908 and 0.6305. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group Cmca (No. 64 in the International Tables for X-ray Crystallography) with $Z = 4$ for the formula unit, C₁₈H₆O₆Si₈Sr. The final anisotropic full-matrix least-squares refinement on F^2 with 155 variables converged at $R1 = 3.49\%$, for the observed data and $wR2 = 9.50\%$ for all data. The goodness-of-fit was 1.028.

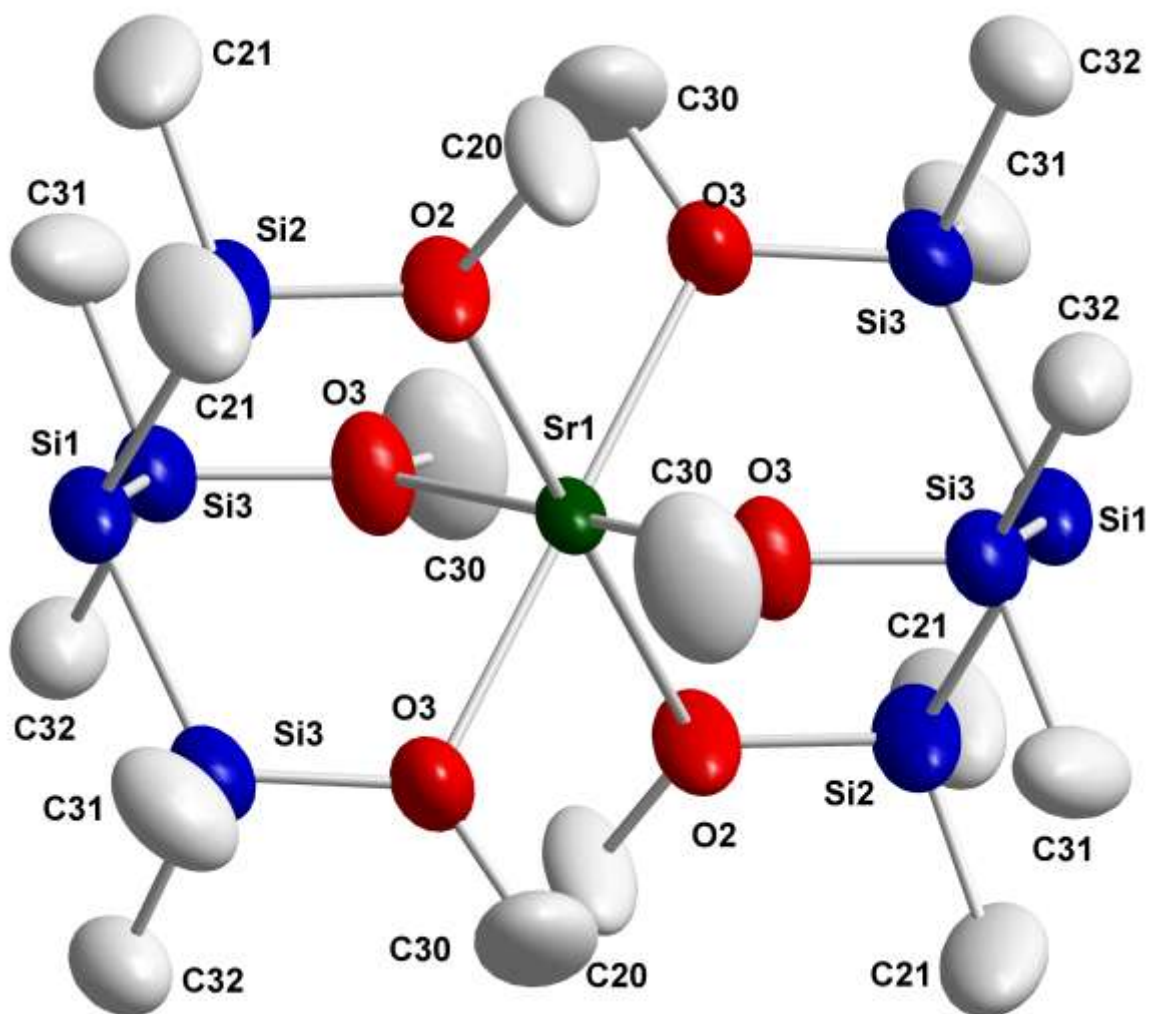


Fig. 3. Molecular structure of Sr-2 in the crystal; selected bond lengths [\AA] and angles [$^\circ$]: Sr1 O2 2.493(4), Sr1 O3 2.521(4), Si1 Si3 2.2946(18), Si1 Si2 2.308(3), Si2 O2 1.695(5), Si3 O3 1.697(3), Si2 C21 1.861(13), Si3 C31 1.861(10), Si3 C32 1.866(9), O2 C20 1.431(11), O3 C30 1.463(7), O2 Sr1 O2 180.0, O3 Sr1 O3 180.0, O2 Sr1 O3 80.88(11), O2 Sr1 O3 99.12(11), O3 Sr1 O3 99.75(17), O3 Sr1 O3 80.25(17), Si3 Si1 Si3 108.71(10), Si3 Si1 Si2 107.33(6), O2 Si2 Si1 112.90(18), O3 Si3 Si1 113.56(15), Si3 O3 Sr1 115.79(18), Si2 O2 Sr1 116.7(2), C20 O2 Si2 121.2(6), C20 O2 Sr1 122.1(6), C30 O3 Si3 122.9(4), C30 O3 Sr1 121.3(3).

Bis[tris(dimethyl-methoxysilyl)silyl]barium [Si(SiMe₂OMe)₃]₂Ba, (Ba-2)

X-ray intensity data were measured on a Bruker Apex II automated X-ray diffractometer equipped with a CCD detector. A total of 1464 frames were collected and the total exposure time was 4.07 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 113473 reflections to a maximum θ angle of 28.83° (0.74 Å resolution), of which 23539 were independent (average redundancy 4.821, completeness = 94.6%, $R_{\text{int}} = 4.27\%$, $R_{\text{sig}} = 3.85\%$) and 16807 (71.40%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 21.499(5)$ Å, $b = 17.291(4)$ Å, $c = 26.008(6)$ Å, $\beta = 100.524(2)^\circ$, volume = 9506.4 Å³, are based upon the refinement of the XYZ-centroids of 284 reflections above $20\sigma(I)$ with $4.663^\circ < 2\theta < 48.81^\circ$. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.762. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.5877 and 0.6980.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_1/n$ (a non-standard setting of $P2_1/c$, No. 14 in the International Tables for X-ray Crystallography), with $Z = 10$ for the formula unit, $C_{18}H_{54}BaO_6Si_8$. The final anisotropic full-matrix least-squares refinement on F^2 with 790 variables converged at $R_1 = 4.61\%$, for the observed data and $wR_2 = 12.63\%$ for all data. The goodness-of-fit was 0.909.

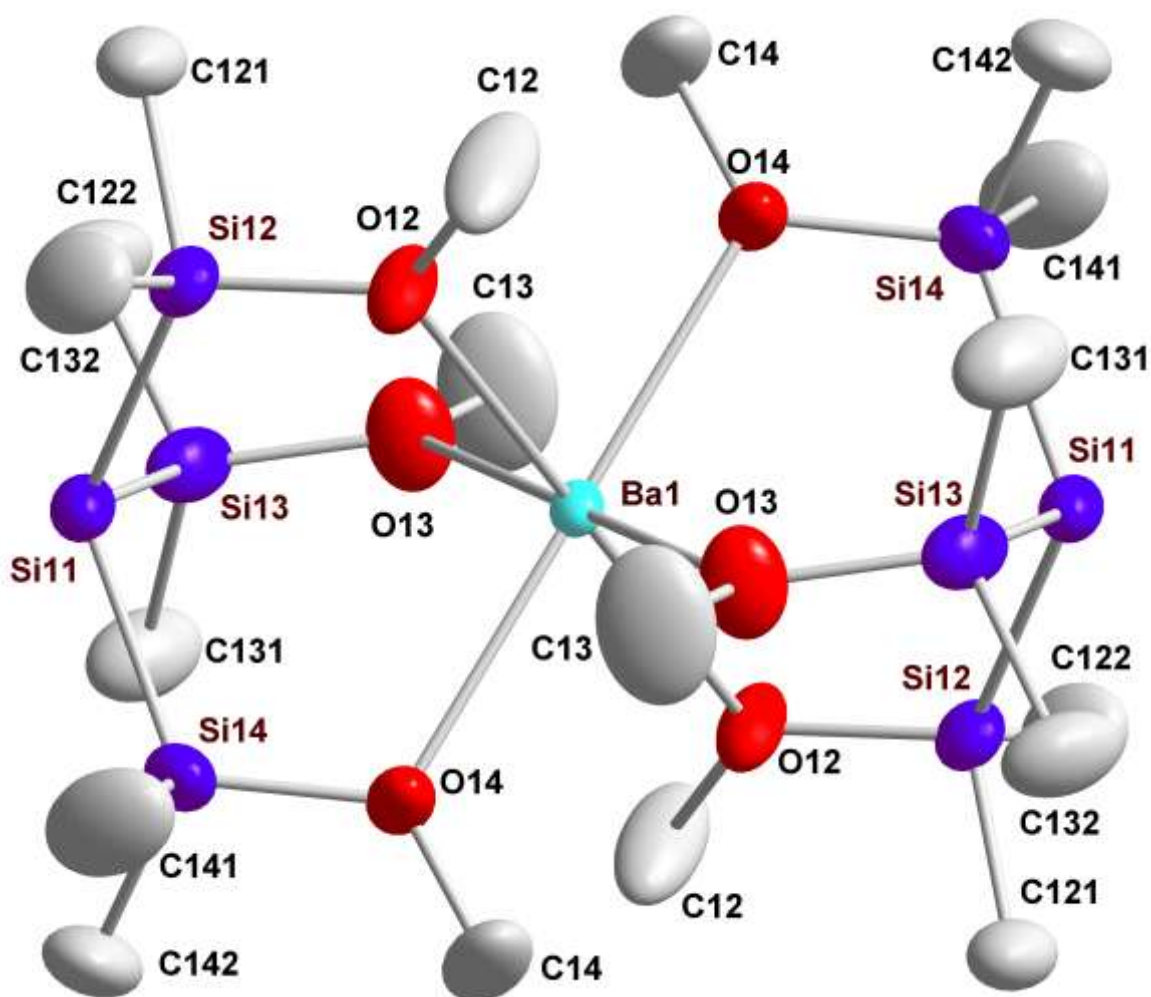


Fig. 4. Molecular structure of Ba-2 in the crystal (only one molecule is shown for clarity); selected bond lengths [Å] and angles [°]: Ba1 O12 2.637(3), Ba1 O13 2.670(3), Ba1 O14 2.680(3), Si11 Si13 2.2911(19), Si11 Si14 2.3147(17), Si11 Si12 2.3267(17), Si12 O12 1.692(3), Si13 O13 1.703(4), Si14 O14 1.691(3), O12 C12 1.446(5), O13 C13 1.434(6), O14 C14 1.442(6), O12 Ba1 O12 179.997(1), O14 Ba1 O14 179.999(1), O13 Ba1 O13 179.999(1), O12 Ba1 O13 82.80(10), O12 Ba1 O14 97.20(10), O12 Ba1 O14 97.68(10), O12 Ba1 O14 82.32(10), O13 Ba1 O14 81.99(11), O13 Ba1 O14 98.00(11), Si13 Si11 Si14 108.45(7), Si13 Si11 Si12 108.25(6), Si14 Si11 Si12 111.25(7), O12 Si12 Si11 113.59(11), O13 Si13 Si11 113.84(12), O14 Si14 Si11 114.02(12), C12 O12 Ba1 121.4(3), C13 O13 Ba1 123.7(3), C14 O14 Ba1 122.6(3), Si12 O12 Ba1 114.81(14), Si14 O14 Ba1 114.60(14), Si13 O13 Ba1 114.31(14).

Computational Details

The crystallographic structures of **Mg-2**, **Ca-2**, **Sr-2** and **Ba-2** were taken as start geometry in the quantum chemical calculations. These geometries were therefore optimized by density functional theory (DFT) and second-order Moller-Plesset perturbation theory (MP2) [1] methods using the SVP basis. In the DFT calculations the functional Becke 3-Parameter (Exchange), Lee, Yang and Parr correlation (B3LYP) was used [2]. A set of different basis set SVP [3], SVP+sp and 6-31G* [4] were taken into the calculations. The SVP+sp basis was constructed by augmenting the SVP basis with a set of s and p functions on the heavy atoms. The exponents of these additional basis functions were obtained by dividing the smallest respective exponent of the SVP basis set by a factor of three. The MP2/SVP+sp optimized geometry of each complex was taken to calculate the atomic charges with the 6-31G* basis set using natural population analysis [5]. The effective core potential basis were used for both barium and strontium complexes [6]. All calculations were carried out using the TURBOMOLE [7] and GAUSSIAN [8] suite programs.

Table 1. Calculated (B3-LYP/6-31G*) NPA charges [e] of **M-2** and $[\text{M}(\text{H}_2\text{O})_6]^{2+}$.

	Mg-2	Ca-2	Sr-2	Ba-2
M	1.701	1.619	1.299	1.288
Si1	-0.579	-0.597	-0.641	-0.687
Si	1.437	1.522	1.483	1.504
O	-0.978	-0.991	-0.975	-0.966
(Si)- CH₃	-0.438	-0.438	-0.433	-0.433
(O)- CH₃	0.326	0.324	0.324	0.323
	$[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$	$[\text{Ca}(\text{H}_2\text{O})_6]^{2+}$	$[\text{Sr}(\text{H}_2\text{O})_6]^{2+}$	$[\text{Ba}(\text{H}_2\text{O})_6]^{2+}$
M	1.427	1.656	1.687	1.869

Table 2. Calculated B3-LYP and MP2 average bond lengths [\AA] angles [$^\circ$] of $[\text{Si}(\text{SiMe}_2\text{OMe})_3]_2\text{M}$ (M-2) (M = Mg, Ca, Sr, Ba) with different basis set.

	Mg-2		Ca-2		Sr-2		Ba-2	
	MP2	B3-LYP	MP2	B3-LYP	MP2	B3-LYP	MP2	B3-LYP
Si-Si	2.313/ 2.313	2.333/ 2.333	2.314/ 2.313	2.337/ 2.337/ 2.337	2.316/ 2.319	2.338/ 2.337/ 2.339	2.318/ 2.320	2.339/ 2.338
Si-O	1.771/ 1.774	1.785/ 1.785	1.754/ 1.754	1.771/ 1.772/ 1.772	1.752/ 1.751	1.764/ 1.767/ 1.766	1.750/ 1.751	1.759/ 1.763
M-O	2.153/ 2.137	2.200/ 2.200/	2.376/ 2.365	2.431/ 2.432/ 2.434	2.522/ 2.492	2.572/ 2.586/ 2.583	2.700/ 2.68	2.744/ 2.762
M \cdots Si3	4.020/ 4.021	4.062/ 4.061	3.807/ 3.762	3.949/ 3.956/ 3.956	3.738/ 3.726	3.901/ 3.913/ 3.907	3.783/ 3.798	3.931/ 3.960
Si-O-M	126.61/ 126.89	126.96/ 126.84	118.55/ 117.89	120.57/ 120.77/ 120.72	114.61/ 115.52	117.33/ 117.51/ 117.30	112.73/ 114.32	115.36/ 115.72
Si-Si-O	113.94/ 113.94	113.61/ 113.78	113.31/ 112.88	113.76/ 113.69/ 113.71	113.70/ 112.81	114.08/ 113.98/ 114.04	114.43/ 113.50	114.72/ 114.69
Si-Si-Si	97.65/ 97.38	98.55/ 98.47	104.68/ 105.11	104.07/ 104.10/ 104.16	107.78/ 107.79	106.91/ 107.28/ 107.24	110.00/ 110.11	109.19/ 109.47

SV(P)/ SVP+sp/ SVP+sp_all

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