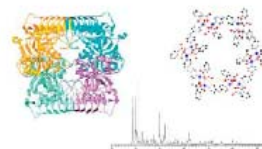


REM1017G

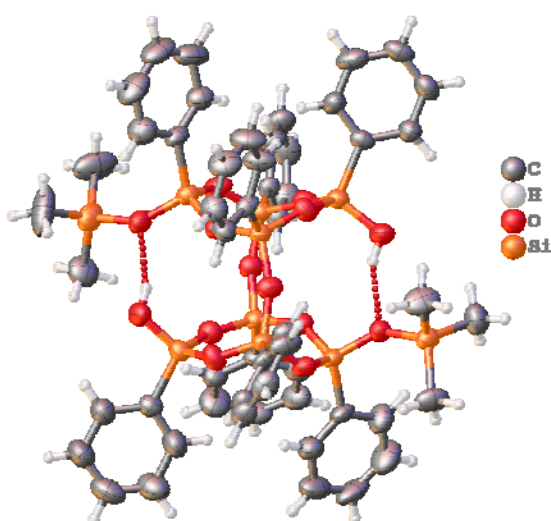


Submitted by: **Badru-Deen Barry**
Michigan State University
Solved by: **Richard J Staples**
Sample ID: **bisTMS_Ph8T8(OH)2**

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Crystal structure from crystals provided. The crystal refined as a racemic twinned crystal at a value of 0.48.

Crystal Data and Experimental



Experimental. Single colourless needle-shaped crystals of (**REM1017G**) were used as received. A suitable crystal ($0.42 \times 0.08 \times 0.07$) mm³ was selected and mounted on a nylon loop with paratone oil on a Bruker APEX-II CCD diffractometer. The crystal was kept at $T = 173(2)$ K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the XT (Sheldrick, 2015) structure solution program, using the Intrinsic Phasing solution method. The model was refined with version of **ShelXL** (Sheldrick, 2015) using Least Squares minimisation.

Crystal Data. C₅₄H₆₀O₁₄Si₁₀, $M_r = 1213.92$, tetragonal, $I-4$ (No. 82), $a = 29.6068(4)$ Å, $b = 29.6068(4)$ Å, $c = 14.0465(2)$ Å, $\alpha = \beta = \gamma = 90^\circ$, $V = 12312.6(4)$ Å³, $T = 173(2)$ K, $Z = 8$, $Z' = 1$, $\mu(\text{CuK}\alpha) = 2.524$, 46831 reflections measured, 11753 unique ($R_{\text{int}} = 0.0968$) which were used in all calculations. The final wR_2 was 0.1849 (all data) and R_1 was 0.0681 ($I > 2(I)$).

Compound	REM1017G
Formula	C ₅₄ H ₆₀ O ₁₄ Si ₁₀
$D_{\text{calc.}} / \text{g cm}^{-3}$	1.310
μ / mm^{-1}	2.524
Formula Weight	1213.92
Colour	colourless
Shape	needle
Size/mm ³	$0.42 \times 0.08 \times 0.07$
T/K	173(2)
Crystal System	tetragonal
Flack Parameter	-0.035(18)
Hooft Parameter	-0.6(5)
Space Group	$I-4$
$a/\text{\AA}$	29.6068(4)
$b/\text{\AA}$	29.6068(4)
$c/\text{\AA}$	14.0465(2)
α°	90
β°	90
γ°	90
$V/\text{\AA}^3$	12312.6(4)
Z	8
Z'	1
Wavelength/Å	1.541838
Radiation type	CuK α
$\theta_{\text{min}}^\circ$	2.110
$\theta_{\text{max}}^\circ$	72.184
Measured Refl.	46831
Independent Refl.	11753
Reflections Used	9250
R_{int}	0.0968
Parameters	712
Restraints	0
Largest Peak	0.620
Deepest Hole	-0.421
GooF	1.006
wR_2 (all data)	0.1849
wR_2	0.1692
R_1 (all data)	0.0880
R_1	0.0681

Structure Quality Indicators

Reflections:	d min (Cu) 0.81	I/ σ 8.2	R _{int} 9.68%	complete 97%
Refinement:	Shift -0.001	Max Peak 0.6	Min Peak -0.4	Goof 1.006 -0.035(18)

A colourless needle-shaped crystal with dimensions 0.42×0.08×0.07 mm³ was mounted on a nylon loop with paratone oil. Data were collected using a Bruker APEX-II CCD diffractometer equipped with an Oxford Cryosystems low-temperature device, operating at $T = 173(2)$ K.

Data were measured using ϕ and ω scans of 1.00° per frame for 330.00 s using CuK α radiation (sealed tube, 40 kV, 30 mA). The total number of runs and images was based on the strategy calculation from the program COSMO (BRUKER, V1.61, 2009). The actually achieved resolution was $\Theta = 72.184$.

Cell parameters were retrieved using the SAINT (Bruker, V8.34A, after 2013) software and refined using SAINT (Bruker, V8.34A, after 2013) on 6860 reflections, 15 % of the observed reflections. Data reduction was performed using the SAINT (Bruker, V8.34A, after 2013) software which corrects for Lorentz polarisation. The final completeness is 99.50 out to 72.184 in Θ . A multi-scan absorption correction was performed using SADABS-2012/1 (Bruker, 2012) was used for absorption correction. $wR_2(\text{int})$ was 0.0876 before and 0.0747 after correction. The Ratio of minimum to maximum transmission is 0.7468. The $\lambda/2$ correction factor is 0.0015. The absorption coefficient μ of this material is 2.524 mm⁻¹ at this wavelength ($\lambda = 1.54178\text{\AA}$) and the minimum and maximum transmissions are 0.5628 and 0.7536.. SADABS-2012/1 (Bruker, 2012) was used for absorption correction. $wR_2(\text{int})$ was 0.0876 before and 0.0747 after correction. The Ratio of minimum to maximum transmission is 0.7468. The $\lambda/2$ correction factor is 0.0015.

The structure was solved in the space group $I-4$ (# 82) by Intrinsic Phasing using the XT (Sheldrick, 2015) structure solution program. The structure was refined by Least Squares using version 2014/6 of XL (Sheldrick, 2008) incorporated in Olex2 (Dolomanov et al., 2009). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 8 and Z' is 1.

The Flack parameter was refined to -0.035(18). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in -0.6(5). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

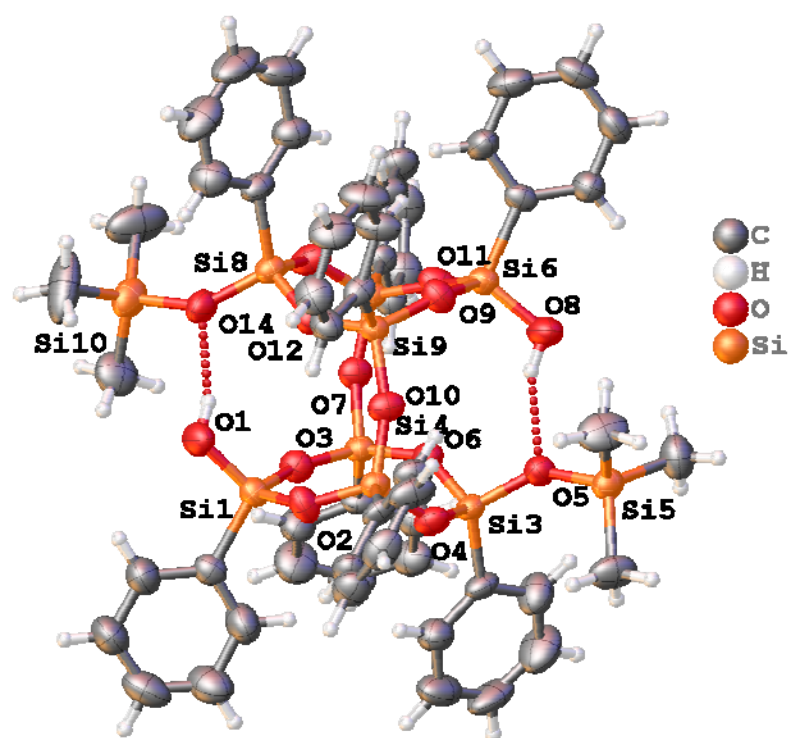


Figure 1:

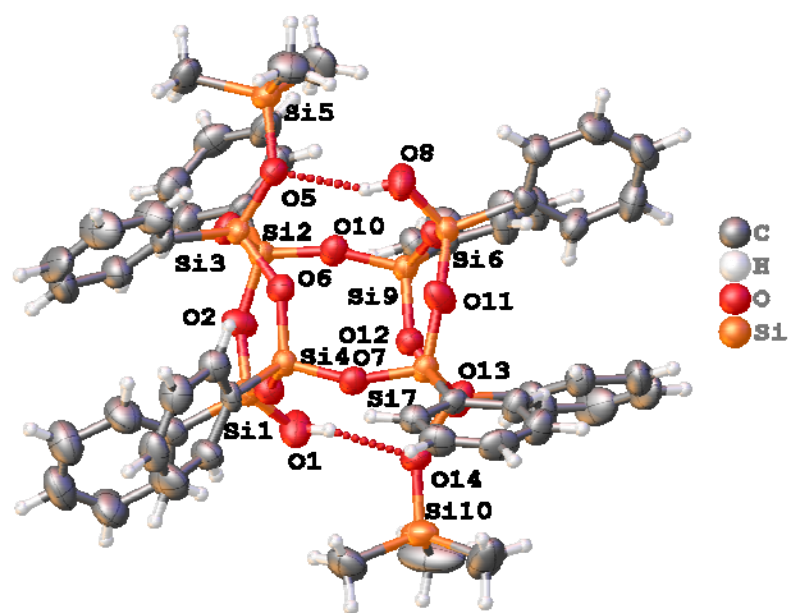


Figure 2:

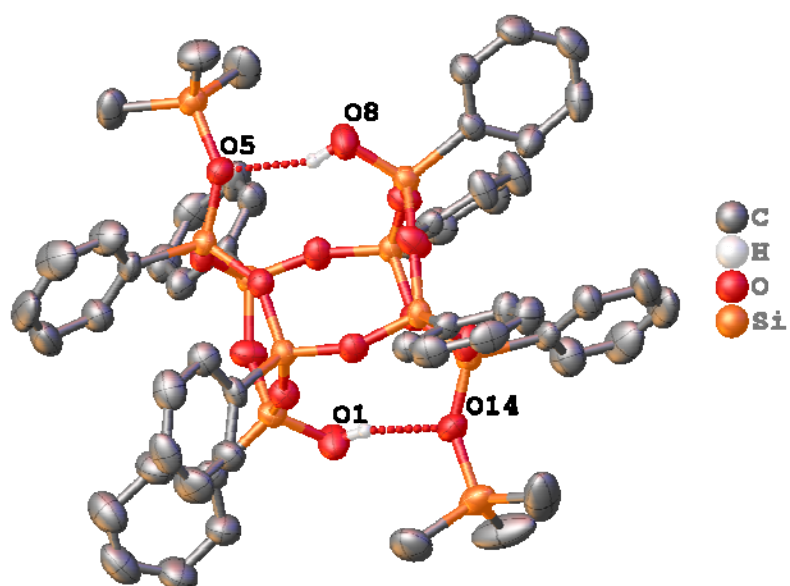


Figure 3: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ° are present in **REM1017G**: O1–O14: 2.887 Å, O8–O5: 2.846 Å.

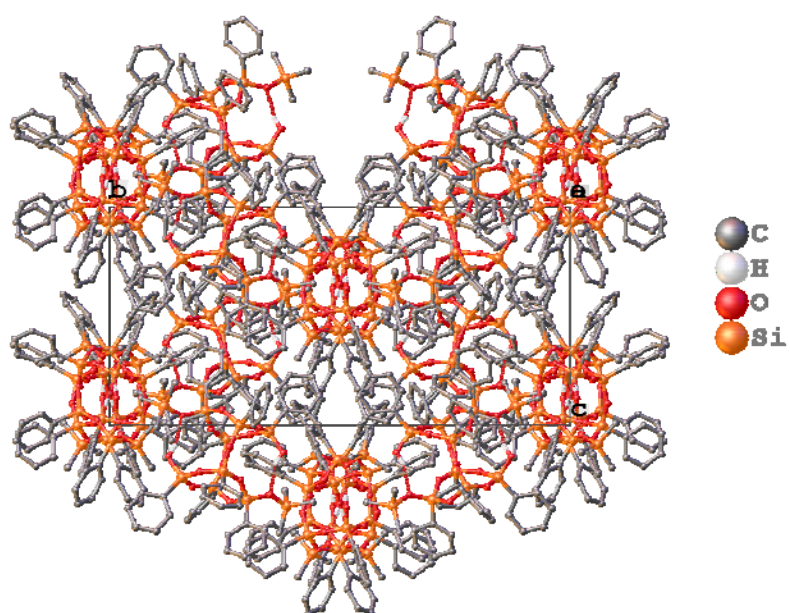
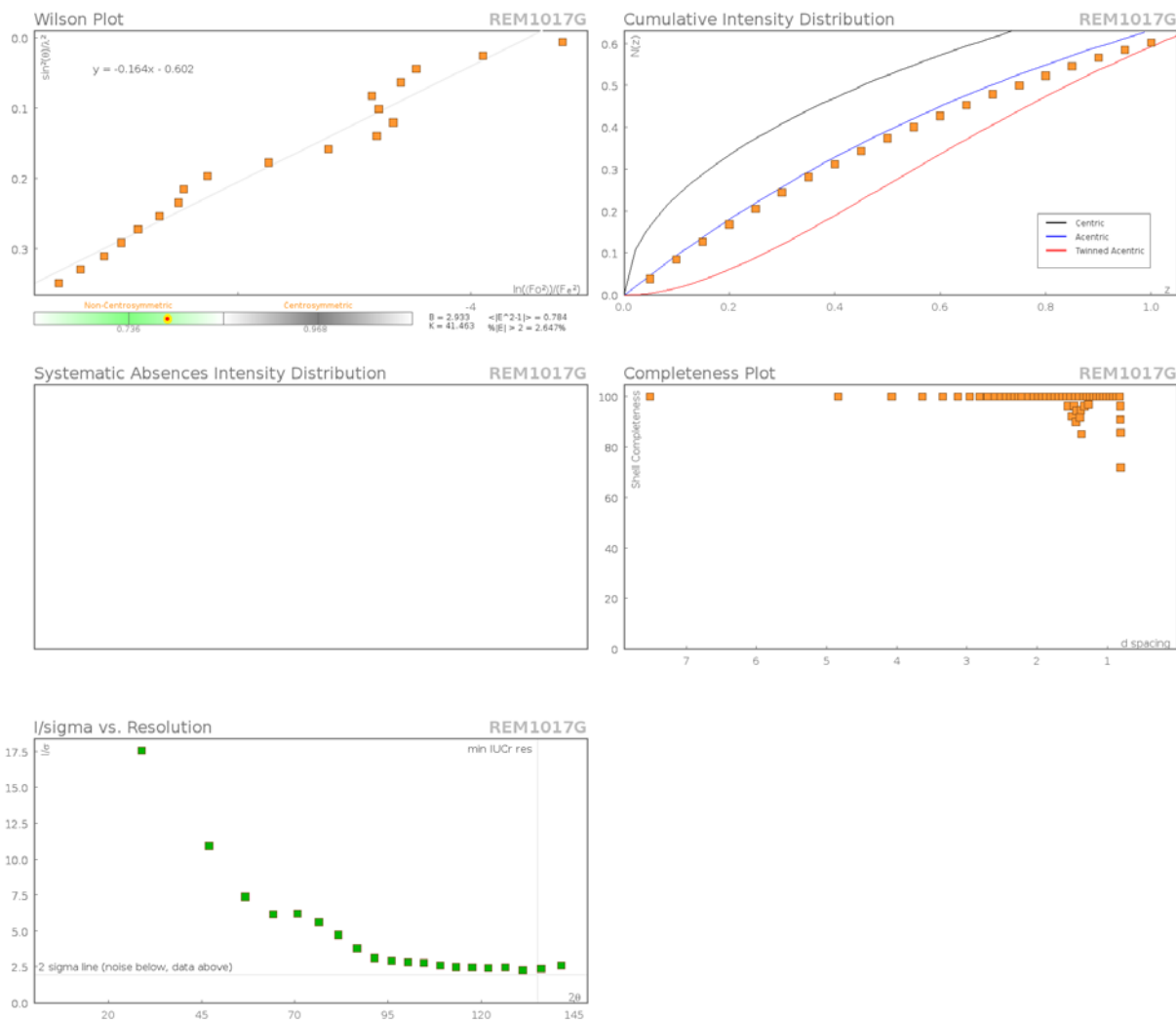
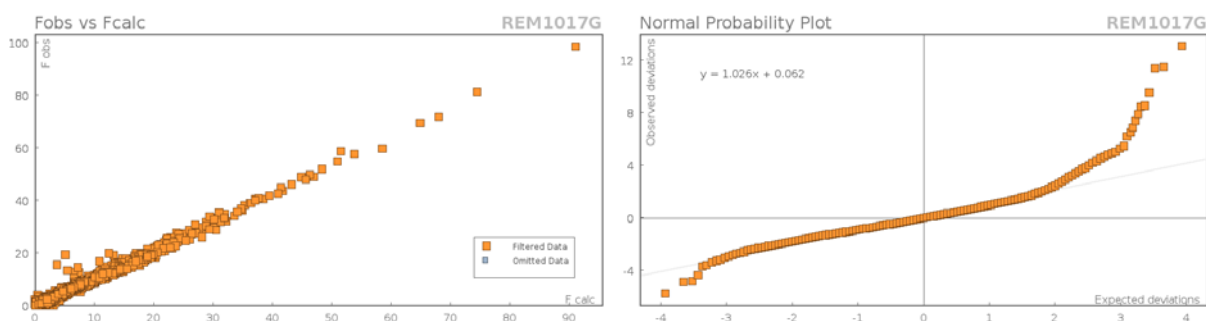


Figure 4: Packing diagram of REM1017G.

Data Plots: Diffraction Data



Data Plots: Refinement and Data



Reflection Statistics

Total reflections (after filtering)	46831	Unique reflections	11753
Completeness	0.965	Mean I/σ	8.18
hkl_{max} collected	(36, 36, 17)	hkl_{min} collected	(-36, -36, -17)
hkl_{max} used	(36, 36, 17)	hkl_{min} used	(-36, 0, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.77
d_{max} used	20.94	d_{min} used	0.81
Friedel pairs	10649	Friedel pairs merged	0

Inconsistent equivalents	2	R_{int}	0.0968
R_{sigma}	0.0794	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	0
Multiplicity	(20359, 7089, 2572, 962, 146)	Maximum multiplicity	11
Removed systematic absences	0	Filtered off (Shel/OMIT)	0

Images of the Crystal on the Diffractometer



Table 1: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **REM1017G**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Atom	x	y	z	U_{eq}
Si1	6570.2(7)	5130.5(7)	2630.2(16)	35.9(4)
Si2	7259.9(7)	4383.4(6)	2178.8(14)	32.6(4)
Si3	7983.4(7)	5047.9(7)	1594.2(14)	33.6(4)
Si4	7467.0(7)	5704.9(7)	2912.7(14)	31.6(4)
Si5	8847.9(8)	4484.1(8)	1340.0(16)	42.5(5)
Si6	8460.7(7)	4848.0(7)	4692.0(14)	34.7(4)
Si7	7829.9(7)	5689.9(7)	5011.1(14)	34.1(4)
Si8	7084.9(7)	5065.0(7)	5674.0(14)	34.4(4)
Si9	7541.6(7)	4352.7(6)	4364.1(14)	30.9(4)
Si10	6179.4(11)	5592.4(9)	5873(2)	58.9(7)
O1	6275(2)	5012(3)	3561(5)	55.2(16)
O2	6802(2)	4677(2)	2203(5)	50.2(15)
O3	6971(2)	5484.2(19)	2879(4)	42.0(12)
O4	7619(2)	4639(2)	1500(4)	44.7(13)
O5	8480.3(19)	4848(2)	1823(4)	42.1(12)
O6	7844.1(19)	5354.7(19)	2504(4)	39.0(12)
O7	7598.4(19)	5806.8(18)	4010(4)	39.9(12)
O8	8778(2)	4858(3)	3750(5)	56.0(16)
O9	8060(2)	4483.8(19)	4604(4)	43.6(13)
O10	7473(2)	4337.7(18)	3229(4)	42.6(13)
O11	8235(2)	5339(2)	4876(5)	52.2(16)
O12	7204.0(19)	4738.0(19)	4783(4)	38.7(12)
O13	7452(2)	5465(2)	5714(4)	50.1(15)
O14	6586(2)	5252(2)	5442(4)	49.0(14)
C1	6172(3)	5354(3)	1734(6)	41.8(17)
C2	5709(4)	5366(4)	1899(8)	63(3)
C3	5404(4)	5516(5)	1211(10)	78(3)
C4	5576(5)	5674(4)	350(10)	76(3)
C5	6015(5)	5673(5)	166(10)	78(4)
C6	6320(4)	5517(4)	886(9)	70(3)
C7	7131(3)	3813(2)	1714(5)	36.1(16)
C8	6807(3)	3752(3)	1016(6)	48(2)
C9	6705(4)	3322(4)	681(8)	58(2)
C10	6924(4)	2954(3)	1061(8)	58(3)
C11	7236(4)	3007(3)	1752(7)	62(3)
C12	7354(4)	3437(3)	2065(6)	50(2)
C13	7976(3)	5395(3)	496(5)	42.2(18)
C14	7584(4)	5458(4)	-1(7)	57(2)
C15	7565(5)	5765(4)	-752(8)	77(4)
C16	7942(5)	6000(4)	-1007(8)	80(4)
C17	8349(5)	5932(4)	-535(10)	84(4)

Atom	x	y	z	U_{eq}
C18	8367(4)	5632(4)	210(9)	66(3)
C19	7457(3)	6246(3)	2248(5)	36.4(16)
C20	7055(3)	6487(3)	2177(7)	52(2)
C21	7049(5)	6900(4)	1718(10)	75(3)
C22	7424(4)	7073(3)	1302(8)	62(3)
C23	7822(4)	6828(3)	1334(8)	58(2)
C24	7841(3)	6415(3)	1803(7)	49(2)
C25	9411(4)	4749(4)	1483(10)	71(3)
C26	8810(5)	3947(3)	2016(9)	74(3)
C27	8696(4)	4388(4)	73(7)	66(3)
C28	8067(3)	6215(3)	5536(6)	36.9(16)
C29	8125(3)	6604(3)	4995(6)	41.6(17)
C30	8329(3)	6983(3)	5396(8)	55(2)
C31	8467(3)	6976(3)	6309(8)	56(2)
C32	8425(4)	6595(4)	6860(7)	58(2)
C33	8219(4)	6217(3)	6466(7)	52(2)
C34	8835(3)	4680(3)	5695(6)	37.6(16)
C35	9304(3)	4646(3)	5591(7)	48(2)
C36	9566(3)	4504(4)	6341(8)	58(2)
C37	9388(4)	4386(3)	7194(7)	58(2)
C38	8930(4)	4422(4)	7304(7)	66(3)
C39	8654(3)	4565(3)	6567(6)	50(2)
C40	7098(3)	4767(3)	6845(6)	42.3(18)
C41	7439(4)	4829(3)	7483(7)	55(2)
C42	7442(5)	4606(4)	8354(8)	78(4)
C43	7096(5)	4322(4)	8569(8)	79(4)
C44	6746(5)	4259(4)	7949(10)	80(4)
C45	6744(4)	4479(4)	7105(8)	64(3)
C46	6021(4)	5984(4)	4908(10)	74(3)
C47	5696(5)	5241(5)	6221(16)	120(8)
C48	6426(7)	5905(5)	6925(10)	108(6)
C49	7412(3)	3795(2)	4882(6)	38.4(17)
C50	7629(4)	3640(3)	5688(7)	55(2)
C51	7516(5)	3226(4)	6106(8)	72(3)
C52	7183(4)	2974(3)	5711(8)	64(3)
C53	6968(4)	3108(3)	4896(8)	60(2)
C54	7076(3)	3524(3)	4492(7)	46.2(19)

Table 2: Anisotropic Displacement Parameters ($\times 10^4$) **REM1017G**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \dots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	33.9(10)	33.8(10)	40.0(11)	-0.3(8)	-3.4(8)	1.1(8)
Si2	38.6(10)	28.6(9)	30.7(10)	-2.8(7)	-1.0(8)	0.9(8)
Si3	35.9(10)	36.5(10)	28.2(9)	2.0(8)	2.7(8)	0.6(8)
Si4	35.9(10)	29.7(9)	29.2(9)	1.7(7)	-0.8(7)	-0.9(7)
Si5	46.4(12)	41.8(12)	39.2(11)	-0.4(9)	3.3(9)	6.4(9)
Si6	37.3(11)	34.1(10)	32.7(10)	-1.2(8)	-4.3(8)	1.6(8)
Si7	44.9(11)	28.6(9)	28.9(9)	-1.3(7)	-1.6(8)	-2.3(8)
Si8	42.3(11)	29.7(9)	31.1(9)	-0.3(7)	2.6(8)	0.5(7)
Si9	36.8(10)	26.5(9)	29.4(9)	-0.9(7)	-1.7(8)	0.7(7)
Si10	64.2(17)	49.8(14)	62.7(17)	3.3(12)	17.8(13)	16.5(12)
O1	38(3)	80(5)	48(4)	6(3)	0(3)	-11(3)
O2	38(3)	45(3)	67(4)	-9(3)	-9(3)	5(2)
O3	44(3)	37(3)	45(3)	-2(2)	-3(2)	-3(2)
O4	56(4)	47(3)	31(3)	-5(2)	1(2)	-8(3)
O5	41(3)	48(3)	37(3)	-3(2)	0(2)	4(2)
O6	42(3)	40(3)	35(3)	4(2)	2(2)	-1(2)
O7	47(3)	31(3)	41(3)	-4(2)	0(2)	2(2)
O8	50(4)	80(5)	38(3)	5(3)	-4(3)	-2(3)
O9	43(3)	35(3)	53(3)	-4(2)	-8(3)	2(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O10	59(4)	31(3)	38(3)	-2(2)	-1(3)	1(2)
O11	59(4)	37(3)	60(4)	-4(3)	-20(3)	3(3)
O12	43(3)	37(3)	36(3)	0(2)	-1(2)	4(2)
O13	68(4)	44(3)	38(3)	-2(3)	3(3)	-14(3)
O14	50(4)	55(4)	42(3)	-1(3)	8(3)	12(3)
C1	44(4)	36(4)	45(4)	-1(3)	-6(3)	2(3)
C2	51(6)	76(7)	61(6)	2(5)	-2(5)	11(5)
C3	53(6)	104(10)	76(8)	8(7)	-12(6)	12(6)
C4	82(8)	70(7)	77(8)	11(6)	-34(7)	2(6)
C5	75(8)	82(8)	76(8)	26(7)	-15(6)	-8(6)
C6	47(6)	85(8)	78(8)	15(6)	-2(5)	5(5)
C7	53(4)	30(4)	26(3)	-7(3)	8(3)	-3(3)
C8	48(5)	54(5)	42(4)	-9(4)	-2(4)	-4(4)
C9	60(6)	63(6)	53(5)	-14(5)	-3(4)	-12(5)
C10	74(7)	36(4)	65(6)	-13(4)	15(5)	-11(4)
C11	105(9)	41(5)	40(5)	-6(4)	5(5)	7(5)
C12	68(6)	42(5)	39(4)	-7(3)	-4(4)	3(4)
C13	59(5)	41(4)	27(4)	6(3)	8(3)	7(4)
C14	60(6)	62(6)	49(5)	8(5)	1(4)	8(4)
C15	96(9)	84(8)	51(6)	8(6)	-13(6)	38(7)
C16	121(11)	75(8)	44(6)	26(5)	29(6)	28(7)
C17	92(9)	70(8)	91(9)	33(7)	34(8)	2(6)
C18	61(6)	63(6)	76(7)	19(6)	18(5)	1(5)
C19	49(4)	32(4)	28(3)	7(3)	-7(3)	-2(3)
C20	55(5)	48(5)	53(5)	11(4)	3(4)	9(4)
C21	86(8)	51(6)	86(8)	22(6)	2(7)	16(6)
C22	93(8)	37(5)	55(5)	14(4)	-15(5)	-9(5)
C23	65(6)	54(6)	55(5)	8(4)	-2(5)	-20(5)
C24	53(5)	43(5)	52(5)	2(4)	-2(4)	-5(4)
C25	48(5)	75(7)	90(8)	-4(6)	5(5)	3(5)
C26	120(10)	34(5)	70(7)	15(5)	3(7)	7(5)
C27	106(9)	49(5)	44(5)	-11(4)	-3(5)	10(5)
C28	41(4)	31(4)	38(4)	-7(3)	-1(3)	1(3)
C29	42(4)	36(4)	47(4)	1(3)	1(3)	-2(3)
C30	62(6)	31(4)	72(6)	3(4)	3(5)	0(4)
C31	58(5)	36(4)	75(7)	-22(4)	1(5)	-8(4)
C32	72(7)	56(6)	46(5)	-10(4)	-2(4)	-6(5)
C33	74(6)	43(5)	39(5)	-1(4)	-3(4)	-6(4)
C34	45(4)	32(4)	36(4)	-3(3)	-10(3)	1(3)
C35	44(5)	57(5)	44(5)	3(4)	-2(4)	0(4)
C36	42(5)	65(6)	66(6)	-5(5)	-12(4)	7(4)
C37	66(6)	51(5)	56(6)	0(4)	-28(5)	5(4)
C38	91(8)	70(7)	37(5)	5(5)	-3(5)	-14(6)
C39	45(5)	66(6)	39(4)	-4(4)	3(4)	-4(4)
C40	55(5)	37(4)	34(4)	9(3)	9(4)	9(3)
C41	69(6)	50(5)	46(5)	4(4)	-1(4)	5(4)
C42	110(10)	77(8)	46(6)	3(5)	-15(6)	32(7)
C43	120(11)	65(7)	51(6)	28(5)	22(7)	25(7)
C44	106(10)	55(6)	79(8)	23(6)	34(8)	1(6)
C45	73(7)	56(6)	63(6)	8(5)	-2(5)	-7(5)
C46	81(8)	52(6)	88(8)	7(6)	-5(7)	21(5)
C47	80(10)	75(9)	210(20)	37(11)	82(12)	12(7)
C48	191(19)	72(9)	60(7)	-13(6)	1(9)	41(10)
C49	52(4)	25(3)	38(4)	4(3)	9(3)	5(3)
C50	83(7)	38(4)	44(5)	3(4)	-19(5)	-11(4)
C51	107(10)	55(6)	54(6)	16(5)	-23(6)	-5(6)
C52	91(8)	38(5)	63(6)	18(4)	0(6)	-7(5)
C53	62(6)	46(5)	73(7)	5(5)	1(5)	-11(4)
C54	46(5)	43(4)	49(5)	8(4)	-4(4)	0(3)

Table 3: Bond Lengths in Å for **REM1017G**.

Atom	Atom	Length/Å
Si1	O1	1.612(7)
Si1	O2	1.622(6)
Si1	O3	1.620(6)
Si1	C1	1.847(9)
Si2	O2	1.612(6)
Si2	O4	1.615(6)
Si2	O10	1.610(6)
Si2	C7	1.850(7)
Si3	O4	1.628(6)
Si3	O5	1.618(6)
Si3	O6	1.621(6)
Si3	C13	1.854(8)
Si4	O3	1.608(6)
Si4	O6	1.628(6)
Si4	O7	1.619(6)
Si4	C19	1.855(7)
Si5	O5	1.675(6)
Si5	C25	1.854(11)
Si5	C26	1.855(10)
Si5	C27	1.858(10)
Si6	O8	1.624(7)
Si6	O9	1.608(6)
Si6	O11	1.620(6)
Si6	C34	1.860(8)
Si7	O7	1.602(6)
Si7	O11	1.599(7)
Si7	O13	1.633(6)
Si7	C28	1.857(8)
Si8	O12	1.621(6)
Si8	O13	1.609(6)
Si8	O14	1.610(7)
Si8	C40	1.867(8)
Si9	O9	1.618(6)
Si9	O10	1.608(6)
Si9	O12	1.627(6)
Si9	C49	1.844(7)
Si10	O14	1.684(6)
Si10	C46	1.844(12)
Si10	C47	1.837(13)
Si10	C48	1.890(15)
C1	C2	1.390(14)
C1	C6	1.358(15)
C2	C3	1.398(16)
C3	C4	1.392(19)

Atom	Atom	Length/Å
C4	C5	1.325(19)
C5	C6	1.431(16)
C7	C8	1.384(12)
C7	C12	1.384(12)
C8	C9	1.389(13)
C9	C10	1.377(16)
C10	C11	1.348(16)
C11	C12	1.395(13)
C13	C14	1.366(14)
C13	C18	1.412(14)
C14	C15	1.393(15)
C15	C16	1.36(2)
C16	C17	1.39(2)
C17	C18	1.373(16)
C19	C20	1.393(12)
C19	C24	1.390(12)
C20	C21	1.382(14)
C21	C22	1.357(17)
C22	C23	1.383(16)
C23	C24	1.392(13)
C28	C29	1.392(12)
C28	C33	1.382(12)
C29	C30	1.392(13)
C30	C31	1.346(15)
C31	C32	1.375(15)
C32	C33	1.389(13)
C34	C35	1.399(12)
C34	C39	1.379(13)
C35	C36	1.375(13)
C36	C37	1.355(16)
C37	C38	1.367(16)
C38	C39	1.385(15)
C40	C41	1.362(14)
C40	C45	1.400(14)
C41	C42	1.391(15)
C42	C43	1.36(2)
C43	C44	1.37(2)
C44	C45	1.352(16)
C49	C50	1.381(12)
C49	C54	1.391(12)
C50	C51	1.401(14)
C51	C52	1.354(16)
C52	C53	1.369(16)
C53	C54	1.395(13)

Table 4: Bond Angles in ° for **REM1017G**.

Atom	Atom	Atom	Angle/°
O1	Si1	O2	110.4(4)
O1	Si1	O3	111.3(3)
O1	Si1	C1	106.5(4)
O2	Si1	C1	108.3(4)
O3	Si1	O2	107.8(3)
O3	Si1	C1	112.5(4)
O2	Si2	O4	108.3(4)
O2	Si2	C7	109.1(4)
O4	Si2	C7	110.7(3)
O10	Si2	O2	110.9(3)
O10	Si2	O4	108.8(3)

Atom	Atom	Atom	Angle/°
O10	Si2	C7	109.1(3)
O4	Si3	C13	109.7(4)
O5	Si3	O4	110.3(3)
O5	Si3	O6	106.2(3)
O5	Si3	C13	112.3(4)
O6	Si3	O4	108.2(3)
O6	Si3	C13	110.0(3)
O3	Si4	O6	110.9(3)
O3	Si4	O7	108.9(3)
O3	Si4	C19	108.8(3)
O6	Si4	C19	112.5(3)

Atom	Atom	Atom	Angle/°
O7	Si4	O6	106.9(3)
O7	Si4	C19	108.8(3)
O5	Si5	C25	105.6(4)
O5	Si5	C26	107.7(5)
O5	Si5	C27	109.3(4)
C25	Si5	C26	111.2(6)
C25	Si5	C27	112.7(6)
C26	Si5	C27	110.2(5)
O8	Si6	C34	106.1(4)
O9	Si6	O8	112.1(4)
O9	Si6	O11	108.0(3)
O9	Si6	C34	108.6(3)
O11	Si6	O8	110.7(4)
O11	Si6	C34	111.4(3)
O7	Si7	O13	109.0(3)
O7	Si7	C28	109.2(3)
O11	Si7	O7	111.0(3)
O11	Si7	O13	108.7(4)
O11	Si7	C28	107.9(3)
O13	Si7	C28	111.1(3)
O12	Si8	C40	113.1(3)
O13	Si8	O12	108.7(3)
O13	Si8	O14	112.0(4)
O13	Si8	C40	107.6(4)
O14	Si8	O12	104.4(3)
O14	Si8	C40	111.1(4)
O9	Si9	O12	109.8(3)
O9	Si9	C49	109.3(4)
O10	Si9	O9	109.4(4)
O10	Si9	O12	107.5(3)
O10	Si9	C49	109.9(3)
O12	Si9	C49	110.9(3)
O14	Si10	C46	107.2(5)
O14	Si10	C47	108.3(5)
O14	Si10	C48	107.3(6)
C46	Si10	C48	111.4(6)
C47	Si10	C46	110.7(8)
C47	Si10	C48	111.7(9)
Si2	O2	Si1	144.1(4)
Si4	O3	Si1	159.6(4)
Si2	O4	Si3	137.4(4)
Si3	O5	Si5	138.2(4)
Si3	O6	Si4	144.0(4)
Si7	O7	Si4	154.0(4)
Si6	O9	Si9	151.3(4)
Si9	O10	Si2	162.8(4)
Si7	O11	Si6	155.7(5)
Si8	O12	Si9	146.3(4)
Si8	O13	Si7	137.8(4)
Si8	O14	Si10	142.1(5)
C2	C1	Si1	121.6(7)
C6	C1	Si1	121.3(7)
C6	C1	C2	117.1(9)
C1	C2	C3	122.0(11)
C4	C3	C2	118.1(11)
C5	C4	C3	121.9(11)
C4	C5	C6	118.7(12)
C1	C6	C5	122.1(11)

Atom	Atom	Atom	Angle/°
C8	C7	Si2	120.8(7)
C12	C7	Si2	120.6(6)
C12	C7	C8	118.6(8)
C7	C8	C9	120.7(9)
C10	C9	C8	119.4(10)
C11	C10	C9	120.6(9)
C10	C11	C12	120.4(10)
C7	C12	C11	120.2(9)
C14	C13	Si3	120.7(7)
C14	C13	C18	118.9(9)
C18	C13	Si3	120.1(8)
C13	C14	C15	120.7(11)
C16	C15	C14	119.9(11)
C15	C16	C17	120.7(10)
C18	C17	C16	119.4(12)
C17	C18	C13	120.4(12)
C20	C19	Si4	119.5(7)
C24	C19	Si4	121.6(7)
C24	C19	C20	118.9(8)
C21	C20	C19	119.8(10)
C22	C21	C20	121.6(11)
C21	C22	C23	119.0(9)
C22	C23	C24	120.8(9)
C19	C24	C23	119.7(9)
C29	C28	Si7	121.6(6)
C33	C28	Si7	120.2(7)
C33	C28	C29	118.2(8)
C30	C29	C28	120.0(9)
C31	C30	C29	120.4(9)
C30	C31	C32	121.4(9)
C31	C32	C33	118.5(9)
C28	C33	C32	121.6(9)
C35	C34	Si6	122.1(7)
C39	C34	Si6	120.5(7)
C39	C34	C35	117.4(8)
C36	C35	C34	120.1(9)
C37	C36	C35	122.4(9)
C36	C37	C38	117.8(9)
C37	C38	C39	121.6(10)
C34	C39	C38	120.7(9)
C41	C40	Si8	122.0(7)
C41	C40	C45	117.9(9)
C45	C40	Si8	120.1(8)
C40	C41	C42	121.2(11)
C43	C42	C41	118.9(12)
C42	C43	C44	121.0(10)
C45	C44	C43	119.8(12)
C44	C45	C40	121.2(12)
C50	C49	Si9	121.6(7)
C50	C49	C54	117.7(8)
C54	C49	Si9	120.6(6)
C49	C50	C51	121.5(9)
C52	C51	C50	119.0(10)
C51	C52	C53	121.5(9)
C52	C53	C54	119.3(10)
C49	C54	C53	120.9(9)

Table 5: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters

($\text{\AA}^2 \times 10^3$) for **REM1017G**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Atom	x	y	z	U_{eq}
H1	6422	5077	4052	83
H8	8615	4878	3262	84
H2	5597	5268	2499	75
H3	5088	5512	1326	93
H4	5373	5785	-118	92
H5	6126	5775	-432	93
H6	6635	5528	767	84
H8A	6653	4006	764	58
H9	6486	3283	193	70
H10	6855	2659	835	70
H11	7375	2749	2027	74
H12	7589	3473	2520	60
H14	7322	5290	166	68
H15	7289	5811	-1085	93
H16	7927	6213	-1512	96
H17	8613	6091	-726	101
H18	8644	5584	536	80
H20	6785	6368	2443	63
H21	6775	7067	1694	89
H22	7414	7359	992	74
H23	8085	6944	1031	70
H24	8116	6249	1819	59
H25A	9429	5020	1082	106
H25B	9646	4534	1291	106
H25C	9456	4834	2150	106
H26A	8922	3994	2665	112
H26B	8993	3716	1700	112
H26C	8495	3848	2041	112
H27A	8386	4276	33	100
H27B	8902	4165	-204	100
H27C	8721	4673	-279	100
H29	8025	6612	4353	50
H30	8372	7247	5023	66
H31	8596	7241	6579	68
H32	8535	6589	7496	70
H33	8182	5954	6845	62
H35	9441	4722	5001	58
H36	9884	4488	6259	69
H37	9574	4282	7699	69
H38	8799	4346	7900	79
H39	8337	4585	6664	60
H41	7680	5029	7329	66
H42	7682	4651	8793	93
H43	7097	4165	9159	95
H44	6505	4062	8110	96
H45	6497	4438	6681	77
H46A	6294	6101	4603	111
H46B	5846	6235	5173	111
H46C	5837	5823	4436	111
H47A	5635	5018	5722	180
H47B	5429	5432	6309	180
H47C	5765	5084	6819	180
H48A	6479	5692	7448	162
H48B	6215	6140	7132	162
H48C	6713	6044	6739	162
H50	7861	3819	5966	66
H51	7671	3123	6657	86
H52	7097	2699	6007	77
H53	6747	2919	4609	72

Atom	x	y	z	U_{eq}
H54	6917	3624	3942	55

Table 6: Hydrogen Bond information for **REM1017G**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1	O14	0.84	2.08	2.887(9)	162.1
O8	H8	O5	0.84	2.06	2.846(9)	155.2

Citations

COSMO-V1.61 - Software for the CCD Detector Systems for Determining Data Collection Parameters, Bruker axs, Madison, WI (2000).

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

Sheldrick, G.M., A short history of ShelX, *Acta Cryst.*, (2008), **A64**, 339-341.

Sheldrick, G.M., Crystal structure refinement with ShelXL, *Acta Cryst.*, (2015), **C27**, 3-8.

Software for the Integration of CCD Detector System Bruker Analytical X-ray Systems, Bruker axs, Madison, WI (after 2013).