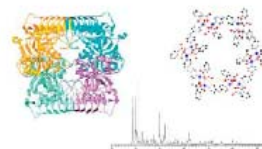


# REM617A



Submitted by: **Badru-Deen Barry**  
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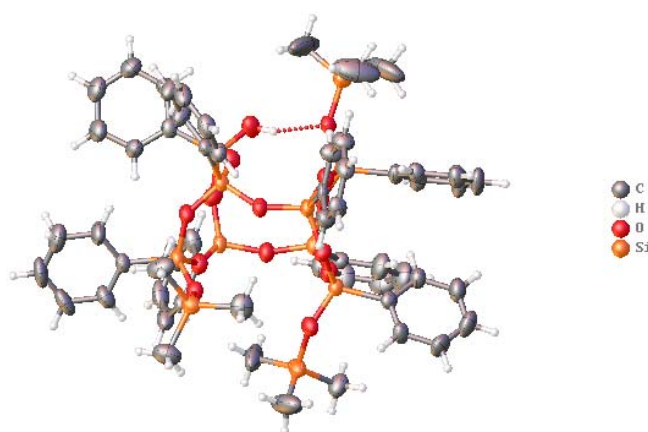
Solved by: **Richard J Staples**

Sample ID: **BDB 31-17 SiH S1R**

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Crystal structure from crystal chosen of the crystals provided. The crystal is rotationally twinned where the second domain is rotated by 180.0 degrees about reciprocal axis -0.099 0.000 1.000 and real axis 0.001 0.000 1.000 of the first domain.

## Crystal Data and Experimental



**Experimental.** Single colourless block-shaped crystals of (REM617A) were used as received. A suitable crystal (0.26×0.24×0.07) mm<sup>3</sup> 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 **XL** (Sheldrick, 2008) using Least Squares minimisation.

**Crystal Data.** C<sub>57</sub>H<sub>69</sub>O<sub>14</sub>Si<sub>11</sub>,  $M_r = 1287.11$ , monoclinic, P2<sub>1</sub>/c (No. 14),  $a = 21.347(3)$  Å,  $b = 14.0292(19)$  Å,  $c = 22.671(3)$  Å,  $\beta = 96.019(2)^\circ$ ,  $\alpha = \gamma = 90^\circ$ ,  $V = 6752.0(16)$  Å<sup>3</sup>,  $T = 173(2)$  K,  $Z = 4$ ,  $Z' = 1$ ,  $\mu(\text{MoK}\alpha) = 0.270$ , 12519 reflections measured, 12519 unique ( $R_{\text{int}} = .$ ) which were used in all calculations. The final  $wR_2$  was 0.1616 (all data) and  $R_1$  was 0.0688 ( $I > 2(I)$ ).

Compound	REM617A
Formula	C <sub>57</sub> H <sub>69</sub> O <sub>14</sub> Si <sub>11</sub>
$D_{\text{calc.}} / \text{g cm}^{-3}$	1.266
$\mu / \text{mm}^{-1}$	0.270
Formula Weight	1287.11
Colour	colourless
Shape	block
Size/mm <sup>3</sup>	0.26×0.24×0.07
$T/\text{K}$	173(2)
Crystal System	monoclinic
Space Group	P2 <sub>1</sub> /c
$a/\text{\AA}$	21.347(3)
$b/\text{\AA}$	14.0292(19)
$c/\text{\AA}$	22.671(3)
$\alpha^\circ$	90
$\beta^\circ$	96.019(2)
$\gamma^\circ$	90
$V/\text{\AA}^3$	6752.0(16)
$Z$	4
$Z'$	1
Wavelength/Å	0.710730
Radiation type	MoK $\alpha$
$\theta_{\text{min}}^\circ$	1.710
$\theta_{\text{max}}^\circ$	25.452
Measured Refl.	12519
Independent Refl.	12519
Reflections Used	8312
$R_{\text{int}}$	.
Parameters	750
Restraints	0
Largest Peak	0.463
Deepest Hole	-0.311
GooF	1.019
$wR_2$ (all data)	0.1616
$wR_2$	0.1410
$R_1$ (all data)	0.1155
$R_1$	0.0688

## Structure Quality Indicators

Reflections:	d min (Mo) 0.83	I/ $\sigma$ 7.8	R <sub>int</sub> Merged!	complete 100%
Refinement:	Shift 0.000	Max Peak 0.5	Min Peak -0.3	GooF 1.019

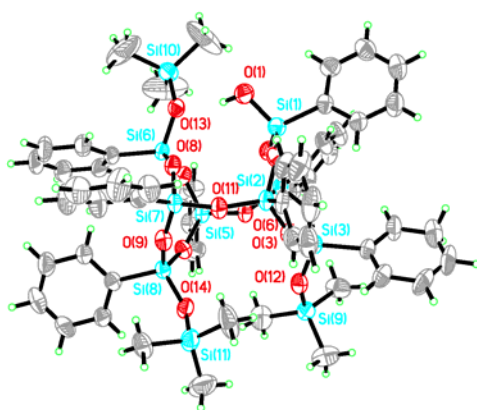
A colourless block-shaped crystal with dimensions 0.26×0.24×0.07 mm<sup>3</sup> was mounted on a nylon loop with paratone oil. Data were collected using a Bruker APEX-II CCD diffractometer equipped with a Oxford Cryosystems low-temperature device, operating at  $T = 173(2)$  K.

Data were measured using  $\omega$  of  $-0.50^\circ$  per frame for 200.84 s using MoK $\alpha$  radiation (sealed tube, 50 kV, 40 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  $\Theta = 25.452$ .

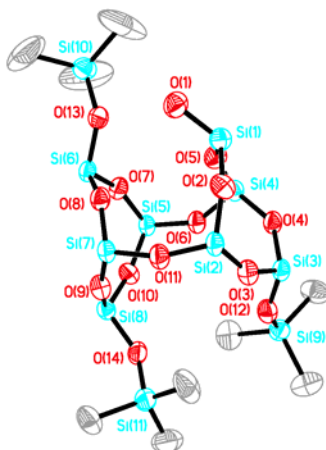
Cell parameters were retrieved using the SAINT (Bruker, V8.34A, after 2013) software and refined using SAINT (Bruker, V8.34A, after 2013) on 5941 reflections, 47 % of the observed reflections. Data reduction was performed using the SAINT (Bruker, V8.34A, after 2013) software which corrects for Lorentz polarisation. The final completeness is 100.00 out to 25.452 in  $\Theta$ . A multi-scan absorption correction was performed using TWINABS-2012/1 (Bruker, 2012) was used for absorption correction. For component 1:  $wR_2(\text{int})$  was 0.0641 before and 0.0585 after correction. The Ratio of minimum to maximum transmission not present. The  $\lambda/2$  correction factor is Not present For component 2:  $wR_2(\text{int})$  was 0.0739 before and 0.0661 after correction. The Ratio of minimum to maximum transmission is 0.89. The  $\lambda/2$  correction factor is Not present Final HKLF 4 output contains 122687 reflections,  $R_{\text{int}} = 0.1267$  (15615 with  $I > 3\text{sig}(I)$ ,  $R_{\text{int}} = 0.0468$ ) The absorption coefficient  $\mu$  of this material is 0.270 mm<sup>-1</sup> at this wavelength ( $\lambda = 0.71073\text{\AA}$ ) and the minimum and maximum transmissions are 0.6772 and 0.7452. TWINABS-2012/1 (Bruker, 2012) was used for absorption correction. For component 1:  $wR_2(\text{int})$  was 0.0641 before and 0.0585 after correction. The Ratio of minimum to maximum transmission not present. The  $\lambda/2$  correction factor is Not present For component 2:  $wR_2(\text{int})$  was 0.0739 before and 0.0661 after correction. The Ratio of minimum to maximum transmission is 0.89. The  $\lambda/2$  correction factor is Not present Final HKLF 4 output contains 122687 reflections,  $R_{\text{int}} = 0.1267$  (15615 with  $I > 3\text{sig}(I)$ ,  $R_{\text{int}} = 0.0468$ )

The structure was solved in the space group P2<sub>1</sub>/c (# 14) 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. The crystal is rotationally twined where the second domain is rotated by 180.0 degrees about reciprocal axis -0.099 0.000 1.000 and real axis 0.001 0.000 1.000 of the first domain. Final refinement was performed with both domains using a HKLF 5 format file, and results in a BASF parameter of 0.2638(1)

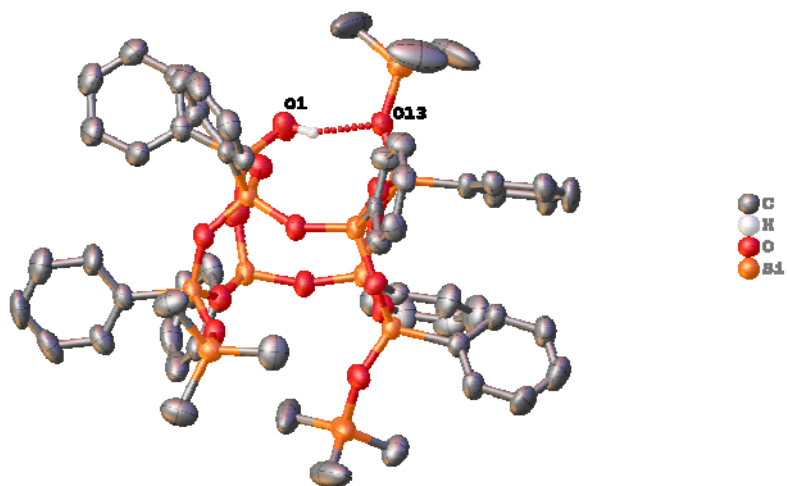
There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1.



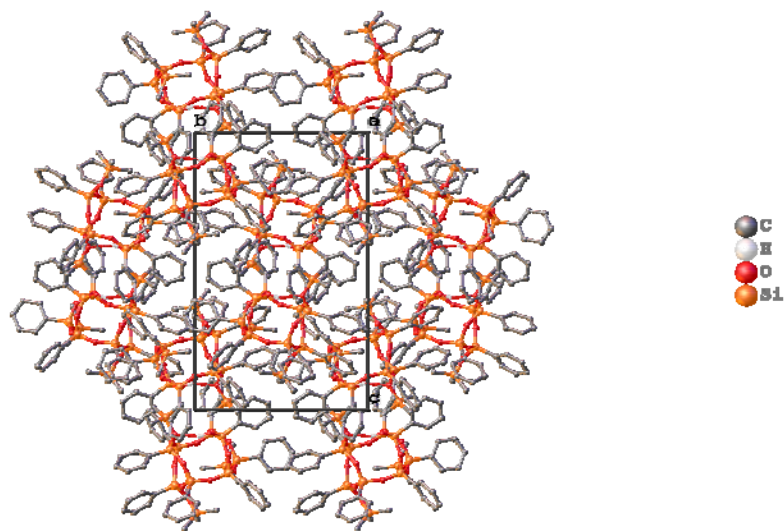
**Figure 1:**



**Figure 2:** Drawing of the cage and substituted groups. Hydrogen atoms and carbon atoms of the phenyl groups removed for clarity.

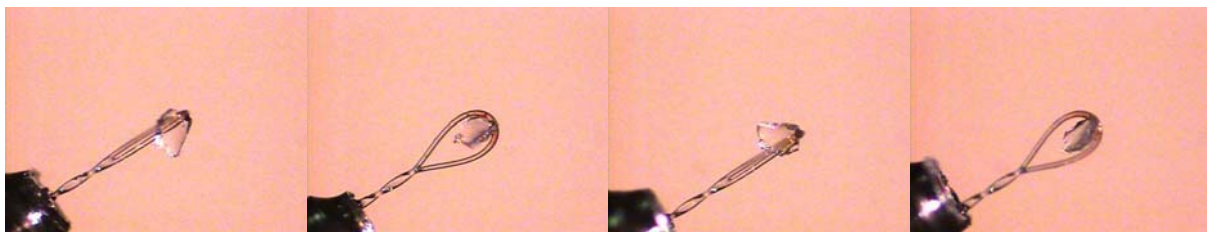


**Figure 3:** The following hydrogen bonding interactions with a maximum D-D distance of 3.1 Å and a minimum angle of 110 ° are present in **REM617A**: O1–O13: %( O1 O13 )s Å.



**Figure 4:** Packing diagram of REM617A.

### 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 **REM617A**.  $U_{eq}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$ .

Atom	x	y	z	$U_{eq}$
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Atom	x	y	z	$U_{eq}$
Si1	6584.4(7)	3493.8(10)	4051.0(7)	39.1(4)
Si2	6801.0(7)	3110.6(9)	2726.4(7)	35.9(3)
Si3	8188.0(7)	2613.2(9)	3176.2(6)	35.4(3)
Si4	7991.7(7)	4044(1)	4172.0(6)	34.6(3)
Si5	8140.3(7)	6062.3(9)	3646.7(6)	34.1(3)
Si6	6696.2(7)	6484.7(10)	3571.1(6)	34.8(3)
Si7	6620.6(7)	5306.0(9)	2410.1(6)	35.1(3)
Si8	7958.2(7)	6216.7(10)	2266.5(6)	35.7(3)
Si9	9509.1(7)	3266.3(11)	2967.9(7)	43.7(4)
Si10	6087.1(8)	6763.4(11)	4724.9(7)	48.5(4)
Si11	8348.2(10)	4975.3(13)	1265.1(7)	58.5(5)
O1	5999.3(18)	4194(3)	4144(2)	53.4(10)
O2	6560.0(17)	3106(2)	3373.4(16)	45.6(9)
O3	7532.7(16)	2819(2)	2763.4(16)	43.6(9)
O4	8149.2(17)	3078(2)	3827.5(15)	40.1(9)
O5	7240.8(17)	4081(2)	4204.7(16)	44.3(9)
O6	8221.3(16)	4936(2)	3794.3(15)	39.0(8)
O7	7440.9(16)	6372(2)	3783.4(15)	41.4(9)
O8	6479.0(16)	5714(2)	3054.6(15)	39.2(9)
O9	7245.7(17)	5811(2)	2224.9(16)	44.5(9)
O10	8242.2(17)	6224(2)	2957.7(15)	41.3(9)
O11	6721.5(17)	4169(2)	2452.1(16)	43.1(9)
O12	8741.0(17)	3088(2)	2854.3(16)	43.9(9)
O13	6288.5(16)	6224(2)	4118.0(16)	41.5(9)
O14	8390.3(17)	5544(3)	1902.0(16)	45.1(9)
C1	6536(2)	2433(4)	4524(2)	39.5(13)
C2	6276(3)	2476(4)	5068(3)	50.1(15)
C3	6230(3)	1699(5)	5423(3)	63.0(18)
C4	6430(3)	833(5)	5245(3)	63.6(18)
C5	6692(3)	741(5)	4711(3)	61.6(18)
C6	6741(3)	1542(4)	4368(3)	50.1(15)
C7	6329(3)	2228(3)	2260(2)	39.7(13)
C8	5720(3)	1971(4)	2372(3)	54.3(16)
C9	5378(3)	1279(4)	2030(3)	65.5(19)
C10	5640(4)	848(4)	1576(3)	69(2)
C11	6235(4)	1093(4)	1446(3)	69(2)
C12	6587(3)	1766(4)	1793(3)	55.6(16)
C13	8344(2)	1319(4)	3287(3)	40.3(13)
C14	8458(3)	937(4)	3850(3)	59.9(18)
C15	8632(4)	-16(5)	3939(4)	78(2)
C16	8676(4)	-595(5)	3459(4)	78(2)
C17	8560(3)	-235(5)	2901(4)	73(2)
C18	8389(3)	717(4)	2813(3)	54.4(16)
C19	8414(3)	4055(4)	4930(2)	38.2(13)
C20	8970(3)	4577(4)	5052(3)	44.4(14)
C21	9289(3)	4587(4)	5620(3)	55.1(16)
C22	9056(3)	4076(4)	6063(3)	61.4(18)
C23	8511(3)	3556(4)	5949(3)	60.6(18)
C24	8198(3)	3548(4)	5392(3)	52.3(15)
C25	8727(3)	6795(3)	4107(2)	36.7(13)
C26	8595(3)	7175(4)	4638(3)	50.8(16)
C27	9036(3)	7724(4)	4976(3)	56.3(16)
C28	9610(3)	7889(4)	4789(3)	50.2(15)
C29	9757(3)	7526(4)	4263(3)	50.1(15)
C30	9311(3)	6970(4)	3925(3)	47.7(15)
C31	6576(3)	7723(4)	3320(3)	41.1(13)
C32	6026(3)	7995(4)	2962(3)	55.7(16)
C33	5947(3)	8944(4)	2776(3)	70(2)
C34	6395(4)	9603(4)	2946(3)	70(2)
C35	6928(3)	9365(4)	3294(3)	59.2(17)
C36	7013(3)	8433(4)	3477(3)	46.7(14)

Atom	x	y	z	$U_{eq}$
C37	5958(2)	5571(4)	1842(2)	40.1(13)
C38	5525(3)	4917(5)	1627(3)	62.6(18)
C39	5028(3)	5141(6)	1198(3)	79(2)
C40	4965(3)	6051(6)	997(3)	73(2)
C41	5372(4)	6742(6)	1214(3)	80(2)
C42	5876(3)	6495(5)	1623(3)	66.3(19)
C43	7928(2)	7426(3)	1933(2)	39.0(13)
C44	7420(3)	8034(4)	1998(3)	47.3(15)
C45	7375(3)	8911(4)	1707(3)	62.8(18)
C46	7825(4)	9173(5)	1349(3)	74(2)
C47	8334(3)	8598(5)	1289(3)	64.0(18)
C48	8381(3)	7727(4)	1587(3)	49.7(15)
C49	9790(3)	2866(6)	3727(3)	70(2)
C50	9881(3)	2557(6)	2407(3)	79(2)
C51	9662(3)	4560(5)	2885(3)	71(2)
C52	6747(5)	7435(9)	5091(5)	152(5)
C53	5775(8)	5856(7)	5181(5)	189(7)
C54	5439(5)	7581(8)	4489(4)	145(5)
C55	7971(5)	3801(4)	1363(3)	103(3)
C56	7857(3)	5665(4)	697(3)	61.3(18)
C57	9155(4)	4879(7)	1060(3)	119(4)

**Table 2:** Anisotropic Displacement Parameters ( $\times 10^4$ ) **REM617A**. 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	41.9(9)	32.4(8)	43.0(9)	-3.7(7)	5.0(7)	-5.7(7)
Si2	43.6(9)	24.6(7)	37.8(8)	0.5(6)	-3.7(7)	1.6(6)
Si3	43.1(8)	25.6(7)	36.2(8)	-1.2(6)	-1.6(7)	2.9(6)
Si4	42.5(9)	25.0(7)	35.4(8)	-3.1(6)	0.1(7)	-0.6(6)
Si5	39.2(8)	26.1(7)	35.8(8)	2.3(6)	-1.1(7)	1.2(6)
Si6	39.0(8)	25.7(7)	39.4(8)	0.2(6)	3.4(7)	4.4(6)
Si7	41.6(8)	26.3(7)	36.0(8)	2.5(6)	-3.1(7)	1.6(7)
Si8	41.9(9)	29.7(7)	34.9(8)	1.6(6)	1.6(7)	-0.6(6)
Si9	45.0(9)	45.7(9)	39.7(9)	-2.4(7)	1.6(8)	2.6(7)
Si10	59.6(11)	42.7(9)	44.5(9)	-2.6(8)	11.2(8)	-3.7(8)
Si11	89.0(14)	47.3(10)	38.6(9)	-1.2(8)	4.6(9)	20.2(9)
O1	53(2)	37(2)	72(3)	0(2)	17(2)	-2.8(19)
O2	47(2)	44(2)	44(2)	3.0(17)	0.7(18)	-10.0(18)
O3	49(2)	36(2)	45(2)	2.0(17)	-2.3(19)	0.6(17)
O4	53(2)	29.8(19)	37(2)	-2.1(15)	-1.6(18)	3.9(17)
O5	48(2)	38(2)	47(2)	-7.4(18)	4.1(18)	-2.6(17)
O6	44(2)	29.0(18)	43(2)	0.8(16)	-1.1(17)	0.6(16)
O7	44(2)	35(2)	44(2)	-3.1(17)	0.7(18)	6.5(16)
O8	47(2)	30.1(19)	39(2)	-1.9(16)	-1.5(17)	2.3(16)
O9	46(2)	39(2)	47(2)	6.5(18)	-2.6(18)	0.0(17)
O10	48(2)	40(2)	35(2)	3.8(16)	0.5(17)	-2.8(17)
O11	52(2)	31.4(19)	45(2)	2.7(17)	0.5(18)	1.9(17)
O12	49(2)	38(2)	42(2)	2.8(17)	-4.1(18)	2.7(17)
O13	50(2)	30(2)	45(2)	-1.9(16)	7.6(18)	1.8(16)
O14	51(2)	41(2)	42(2)	0.2(18)	-1.4(18)	12.3(18)
C1	38(3)	33(3)	46(3)	-1(2)	-3(3)	-4(2)
C2	58(4)	49(4)	44(4)	-7(3)	11(3)	-2(3)
C3	76(5)	65(5)	48(4)	12(3)	9(3)	3(4)
C4	71(5)	52(4)	65(5)	17(3)	-6(4)	3(3)
C5	79(5)	49(4)	54(4)	8(3)	-1(4)	16(3)
C6	56(4)	47(4)	48(3)	8(3)	11(3)	10(3)
C7	51(4)	22(3)	42(3)	0(2)	-12(3)	9(2)
C8	43(4)	42(3)	74(4)	-6(3)	-11(3)	5(3)
C9	49(4)	44(4)	99(6)	-14(4)	-13(4)	2(3)
C10	90(6)	30(3)	78(5)	-10(3)	-36(4)	1(4)

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C11	120(7)	37(4)	45(4)	-4(3)	-10(4)	7(4)
C12	79(5)	38(3)	50(4)	-3(3)	3(3)	-7(3)
C13	44(3)	28(3)	48(3)	-3(3)	0(3)	2(2)
C14	85(5)	36(3)	56(4)	9(3)	-3(4)	14(3)
C15	88(6)	53(4)	90(6)	24(4)	-4(5)	8(4)
C16	90(6)	26(3)	114(7)	4(4)	2(5)	11(3)
C17	75(5)	40(4)	105(6)	-25(4)	13(5)	13(3)
C18	59(4)	36(3)	67(4)	-13(3)	2(3)	4(3)
C19	47(3)	28(3)	40(3)	-4(2)	5(3)	0(2)
C20	50(4)	39(3)	43(3)	3(3)	-3(3)	4(3)
C21	53(4)	41(3)	67(4)	-6(3)	-10(3)	3(3)
C22	92(5)	44(4)	43(4)	-6(3)	-17(4)	13(4)
C23	92(5)	46(4)	41(4)	6(3)	-5(4)	-12(4)
C24	73(4)	38(3)	44(3)	2(3)	-5(3)	-16(3)
C25	45(3)	20(3)	44(3)	5(2)	-3(3)	4(2)
C26	50(4)	57(4)	45(4)	-13(3)	4(3)	-9(3)
C27	63(4)	61(4)	44(4)	-11(3)	1(3)	0(3)
C28	62(4)	42(3)	43(3)	-7(3)	-11(3)	-2(3)
C29	45(3)	39(3)	66(4)	-2(3)	4(3)	-9(3)
C30	54(4)	42(3)	49(4)	-6(3)	9(3)	-2(3)
C31	43(3)	29(3)	52(3)	5(3)	10(3)	0(3)
C32	51(4)	46(4)	70(4)	15(3)	5(3)	4(3)
C33	60(4)	47(4)	103(6)	29(4)	3(4)	11(3)
C34	80(5)	31(3)	102(6)	21(4)	16(4)	7(3)
C35	67(4)	35(3)	76(5)	2(3)	13(4)	1(3)
C36	47(3)	36(3)	58(4)	-2(3)	9(3)	0(3)
C37	40(3)	46(3)	34(3)	1(3)	0(2)	4(3)
C38	62(4)	58(4)	64(4)	4(3)	-11(4)	-5(3)
C39	62(5)	74(5)	92(6)	-5(4)	-34(4)	0(4)
C40	55(4)	106(6)	53(4)	5(4)	-19(3)	5(4)
C41	84(5)	73(5)	76(5)	21(4)	-22(4)	16(4)
C42	67(4)	57(4)	71(5)	18(4)	-15(4)	3(3)
C43	46(3)	29(3)	41(3)	-2(2)	2(3)	-7(2)
C44	53(4)	36(3)	53(4)	6(3)	8(3)	2(3)
C45	78(5)	38(3)	72(5)	8(3)	6(4)	8(3)
C46	95(6)	49(4)	76(5)	27(4)	6(4)	-7(4)
C47	77(5)	50(4)	69(5)	17(3)	23(4)	-11(4)
C48	52(4)	33(3)	65(4)	4(3)	14(3)	-2(3)
C49	53(4)	108(6)	47(4)	12(4)	-1(3)	4(4)
C50	72(5)	97(6)	70(5)	-19(4)	18(4)	4(4)
C51	60(4)	66(4)	84(5)	1(4)	-5(4)	-10(3)
C52	120(8)	223(13)	119(9)	-104(9)	41(7)	-68(9)
C53	410(20)	72(6)	116(8)	-14(6)	163(12)	-53(9)
C54	144(9)	199(12)	92(7)	-47(7)	16(6)	99(8)
C55	214(10)	34(4)	58(5)	0(3)	0(6)	-2(5)
C56	82(5)	52(4)	47(4)	6(3)	-11(3)	-8(3)
C57	133(8)	167(10)	60(5)	12(6)	28(5)	86(7)

**Table 3:** Bond Lengths in Å for **REM617A**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Si1	O1	1.620(4)	Si3	O12	1.597(4)
Si1	O2	1.625(4)	Si3	C13	1.859(5)
Si1	O5	1.631(4)	Si4	O4	1.617(3)
Si1	C1	1.844(5)	Si4	O5	1.613(4)
Si2	O2	1.605(4)	Si4	O6	1.621(4)
Si2	O3	1.608(4)	Si4	C19	1.854(5)
Si2	O11	1.612(4)	Si5	O6	1.621(3)
Si2	C7	1.856(5)	Si5	O7	1.616(4)
Si3	O3	1.625(4)	Si5	O10	1.616(4)
Si3	O4	1.624(4)	Si5	C25	1.855(5)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Si6	O7	1.620(4)	C13	C14	1.383(8)
Si6	O8	1.625(4)	C13	C18	1.378(8)
Si6	O13	1.629(4)	C14	C15	1.396(8)
Si6	C31	1.838(5)	C15	C16	1.369(10)
Si7	O8	1.627(4)	C16	C17	1.361(10)
Si7	O9	1.605(4)	C17	C18	1.394(8)
Si7	O11	1.611(4)	C19	C20	1.398(7)
Si7	C37	1.848(5)	C19	C24	1.384(8)
Si8	O9	1.618(4)	C20	C21	1.392(8)
Si8	O10	1.620(4)	C21	C22	1.370(9)
Si8	O14	1.607(4)	C22	C23	1.375(9)
Si8	C43	1.857(5)	C23	C24	1.366(8)
Si9	O12	1.652(4)	C25	C26	1.372(8)
Si9	C49	1.850(6)	C25	C30	1.375(7)
Si9	C50	1.856(7)	C26	C27	1.383(8)
Si9	C51	1.857(7)	C27	C28	1.360(8)
Si10	O13	1.666(4)	C28	C29	1.362(8)
Si10	C52	1.822(9)	C29	C30	1.396(8)
Si10	C53	1.811(8)	C31	C32	1.408(8)
Si10	C54	1.832(9)	C31	C36	1.385(7)
Si11	O14	1.644(4)	C32	C33	1.401(8)
Si11	C55	1.857(7)	C33	C34	1.357(9)
Si11	C56	1.846(6)	C34	C35	1.357(9)
Si11	C57	1.836(9)	C35	C36	1.378(8)
C1	C2	1.406(8)	C37	C38	1.356(8)
C1	C6	1.382(8)	C37	C42	1.393(8)
C2	C3	1.363(8)	C38	C39	1.397(9)
C3	C4	1.362(9)	C39	C40	1.357(10)
C4	C5	1.392(9)	C40	C41	1.360(10)
C5	C6	1.377(8)	C41	C42	1.389(9)
C7	C8	1.397(8)	C43	C44	1.401(7)
C7	C12	1.402(8)	C43	C48	1.372(7)
C8	C9	1.399(8)	C44	C45	1.395(8)
C9	C10	1.363(10)	C45	C46	1.370(9)
C10	C11	1.379(10)	C46	C47	1.370(9)
C11	C12	1.397(8)	C47	C48	1.395(8)

**Table 4:** Bond Angles in ° for **REM617A**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Si1	O2	112.2(2)	O5	Si4	O4	107.87(19)
O1	Si1	O5	108.8(2)	O5	Si4	O6	110.9(2)
O1	Si1	C1	108.8(2)	O5	Si4	C19	110.2(2)
O2	Si1	O5	108.2(2)	O6	Si4	C19	109.8(2)
O2	Si1	C1	106.4(2)	O6	Si5	C25	111.9(2)
O5	Si1	C1	112.5(2)	O7	Si5	O6	107.68(19)
O2	Si2	O3	110.7(2)	O7	Si5	C25	109.0(2)
O2	Si2	O11	109.0(2)	O10	Si5	O6	108.31(19)
O2	Si2	C7	108.1(2)	O10	Si5	O7	111.62(19)
O3	Si2	O11	108.5(2)	O10	Si5	C25	108.3(2)
O3	Si2	C7	109.1(2)	O7	Si6	O8	110.27(19)
O11	Si2	C7	111.5(2)	O7	Si6	O13	109.76(19)
O3	Si3	C13	112.5(2)	O7	Si6	C31	106.5(2)
O4	Si3	O3	109.2(2)	O8	Si6	O13	105.31(19)
O4	Si3	C13	107.2(2)	O8	Si6	C31	112.7(2)
O12	Si3	O3	107.18(19)	O13	Si6	C31	112.3(2)
O12	Si3	O4	111.0(2)	O8	Si7	C37	110.8(2)
O12	Si3	C13	109.8(2)	O9	Si7	O8	108.51(19)
O4	Si4	O6	107.59(19)	O9	Si7	O11	110.0(2)
O4	Si4	C19	110.4(2)	O9	Si7	C37	109.0(2)



Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O11	Si7	O8	109.37(19)	C9	C10	C11	120.8(6)
O11	Si7	C37	109.2(2)	C10	C11	C12	120.0(7)
O9	Si8	O10	108.2(2)	C11	C12	C7	120.5(7)
O9	Si8	C43	107.8(2)	C14	C13	Si3	121.0(4)
O10	Si8	C43	112.5(2)	C18	C13	Si3	121.3(5)
O14	Si8	O9	110.5(2)	C18	C13	C14	117.6(5)
O14	Si8	O10	108.9(2)	C13	C14	C15	121.5(6)
O14	Si8	C43	108.9(2)	C16	C15	C14	119.6(7)
O12	Si9	C49	108.6(3)	C17	C16	C15	119.9(6)
O12	Si9	C50	107.5(3)	C16	C17	C18	120.5(7)
O12	Si9	C51	108.3(2)	C13	C18	C17	120.9(6)
C49	Si9	C50	110.7(3)	C20	C19	Si4	120.6(4)
C49	Si9	C51	110.4(3)	C24	C19	Si4	121.9(4)
C50	Si9	C51	111.2(4)	C24	C19	C20	117.5(5)
O13	Si10	C52	110.9(3)	C21	C20	C19	120.8(6)
O13	Si10	C53	107.1(3)	C22	C21	C20	119.5(6)
O13	Si10	C54	107.2(3)	C21	C22	C23	120.4(6)
C52	Si10	C54	109.5(6)	C24	C23	C22	120.0(6)
C53	Si10	C52	114.6(6)	C23	C24	C19	121.8(6)
C53	Si10	C54	107.2(6)	C26	C25	Si5	121.3(4)
O14	Si11	C55	108.1(3)	C26	C25	C30	118.0(5)
O14	Si11	C56	109.4(3)	C30	C25	Si5	120.7(4)
O14	Si11	C57	107.0(3)	C25	C26	C27	120.9(6)
C56	Si11	C55	109.0(4)	C28	C27	C26	120.3(6)
C57	Si11	C55	113.3(4)	C27	C28	C29	120.5(6)
C57	Si11	C56	109.9(3)	C28	C29	C30	118.9(6)
Si2	O2	Si1	151.8(2)	C25	C30	C29	121.5(6)
Si2	O3	Si3	148.0(3)	C32	C31	Si6	121.0(4)
Si4	O4	Si3	144.0(2)	C36	C31	Si6	122.1(4)
Si4	O5	Si1	144.1(2)	C36	C31	C32	116.9(5)
Si5	O6	Si4	146.1(2)	C33	C32	C31	119.9(6)
Si5	O7	Si6	150.1(2)	C34	C33	C32	120.2(6)
Si6	O8	Si7	144.6(2)	C33	C34	C35	121.4(6)
Si7	O9	Si8	160.5(3)	C34	C35	C36	118.9(6)
Si5	O10	Si8	149.3(3)	C35	C36	C31	122.8(6)
Si7	O11	Si2	160.5(3)	C38	C37	Si7	123.9(5)
Si3	O12	Si9	139.6(2)	C38	C37	C42	116.5(5)
Si6	O13	Si10	137.0(2)	C42	C37	Si7	119.6(4)
Si8	O14	Si11	139.0(2)	C37	C38	C39	122.4(6)
C2	C1	Si1	121.8(4)	C40	C39	C38	119.2(7)
C6	C1	Si1	122.9(4)	C39	C40	C41	120.7(6)
C6	C1	C2	115.3(5)	C40	C41	C42	119.1(7)
C3	C2	C1	122.8(6)	C41	C42	C37	122.0(7)
C4	C3	C2	119.6(6)	C44	C43	Si8	120.5(4)
C3	C4	C5	120.5(6)	C48	C43	Si8	121.2(4)
C6	C5	C4	118.4(6)	C48	C43	C44	118.3(5)
C5	C6	C1	123.3(6)	C45	C44	C43	120.1(6)
C8	C7	Si2	121.9(4)	C46	C45	C44	120.0(6)
C8	C7	C12	117.7(5)	C45	C46	C47	120.9(6)
C12	C7	Si2	120.3(5)	C46	C47	C48	118.9(6)
C7	C8	C9	121.3(6)	C43	C48	C47	121.8(6)
C10	C9	C8	119.6(7)				

**Table 5:** Hydrogen Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **REM617A**.  $U_{eq}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$ .

Atom	x	y	z	$U_{eq}$
H1	6090	4754	4052	80
H2	6125	3071	5194	60
H3	6061	1762	5792	76

Atom	x	y	z	$U_{eq}$
H4	6390	289	5487	76
H5	6834	139	4586	74
H6	6924	1480	4006	60
H8	5534	2273	2686	65
H9	4965	1111	2114	79
H10	5409	373	1347	83
H11	6407	805	1119	83
H12	7005	1911	1713	67
H14	8418	1332	4185	72
H15A	9046	-25	4180	94
H15B	8325	-311	4182	94
H16	8788	-1247	3516	93
H17	8595	-637	2568	88
H18	8303	955	2420	65
H20	9131	4931	4745	53
H21	9666	4945	5700	66
H22	9272	4081	6452	74
H23	8352	3202	6258	73
H24	7822	3185	5319	63
H26	8197	7059	4775	61
H27	8936	7986	5341	68
H28	9912	8261	5026	60
H29	10156	7650	4129	60
H30	9413	6706	3561	57
H32	5710	7536	2846	67
H33	5578	9126	2530	84
H34	6333	10245	2820	84
H35	7239	9833	3409	71
H36	7386	8271	3722	56
H38	5560	4283	1774	75
H39	4738	4663	1050	95
H40	4632	6206	700	87
H41	5312	7384	1088	96
H42	6175	6970	1757	80
H44	7105	7850	2242	57
H45	7033	9326	1755	75
H46	7784	9760	1141	88
H47	8649	8790	1048	77
H48	8735	7331	1550	60
H49A	9538	3171	4012	105
H49B	10234	3041	3820	105
H49C	9746	2172	3753	105
H50A	9844	1877	2496	118
H50B	10326	2730	2418	118
H50C	9667	2690	2012	118
H51A	9455	4783	2503	106
H51B	10117	4668	2898	106
H51C	9496	4911	3208	106
H52A	7046	6996	5307	228
H52B	6592	7891	5369	228
H52C	6959	7781	4793	228
H53A	5428	5522	4950	283
H53B	5619	6155	5528	283
H53C	6108	5399	5312	283
H54A	5504	7855	4103	217
H54B	5427	8092	4782	217
H54C	5040	7231	4456	217
H55A	8212	3451	1685	154
H55B	7962	3435	994	154
H55C	7540	3898	1462	154
H56A	7425	5698	804	92

Atom	x	y	z	$U_{eq}$
H56B	7858	5351	311	92
H56C	8028	6310	675	92
H57A	9361	5504	1101	178
H57B	9143	4663	647	178
H57C	9392	4419	1321	178

**Table 6:** Hydrogen Bond information for **REM617A**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1	O13	0.84	2.11	2.916(5)	161.2

## Citations

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