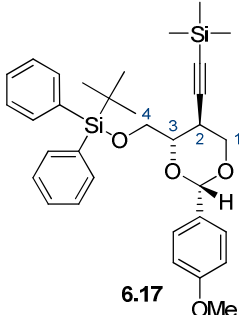


Appendix A: Crystallographic Data

X-ray Crystallographic Data for Acetal **6.17**.

Table 1. Crystal data and structure refinement for jb0603

Chemical formula	$C_{33}H_{42}O_4Si_2$	
M_r	558.85	
Cell setting, space group	Monoclinic, $P2(1)$	
Temperature (K)	180 (2)	
a, b, c (Å)	10.5083 (1), 49.9206 (5), 12.5186 (2)	
β (°)	99.784 (1)	
V (Å ³)	6471.50 (14)	
Z	8	
D_x (Mg m ⁻³)	1.147	
Radiation type	Mo $K\alpha$	
μ (mm ⁻¹)	0.14	
Crystal form, colour	Block, colourless	
Crystal size (mm)	0.28 × 0.12 × 0.12	
Data collection		
Diffractometer	Nonius Kappa CCD	
Data collection method	Thin slice ω and ϕ scans	
Absorption correction	Multi-scan (based on symmetry-related measurements)	
T_{\min}	0.872	
T_{\max}	0.986	
No. of measured, independent and observed reflections	37545, 15423, 13635	
Criterion for observed reflections	$I > 2\sigma(I)$	
R_{int}	0.029	
θ_{\max} (°)	25.3	
Refinement		
Refinement on	F^2	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.050, 0.115, 1.12	
No. of reflections	15423 reflections	

No. of parameters	1433
H-atom treatment	Constrained to parent site
Weighting scheme	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 5.5545P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$	0.014
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.27, -0.32
Absolute structure	Flack H D (1983), Acta Cryst. A39, 876-881
Flack parameter	0.08 (9)

Computer programs: *Collect* (Nonius B.V. 1998); *HKL Scalepack* (Otwinowski & Minor 1997); *HKL Denzo and Scalepack* (Otwinowski & Minor 1997); *SIR-92* (Altomare et al. 1994); *SHELXL-97* (Sheldrick 1997).

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for jb0603. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Si1_1	0.94841 (11)	-0.00067 (3)	0.18305 (8)	0.0322 (3)
Si2_1	0.67902 (13)	0.12941 (3)	0.34842 (11)	0.0471 (4)
O1_1	0.9157 (3)	0.01422 (6)	0.2930 (2)	0.0343 (7)
O2_1	1.0599 (3)	0.02460 (6)	0.5069 (2)	0.0321 (7)
O3_1	1.0881 (3)	0.05015 (6)	0.6645 (2)	0.0392 (8)
O4_1	1.4156 (3)	-0.04790 (7)	0.8556 (2)	0.0458 (8)
C1_1	0.9641 (4)	0.03966 (9)	0.3306 (3)	0.0352 (10)
H1A_1	0.9104	0.054	0.2911	0.042*
H1B_1	1.0537	0.0418	0.3173	0.042*
C2_1	0.9611 (4)	0.04176 (9)	0.4510 (3)	0.0319 (10)
H2_1	0.8753	0.0353	0.4649	0.038*
C3_1	0.9833 (4)	0.07036 (9)	0.4953 (3)	0.0369 (11)
H3_1	1.0672	0.0771	0.4782	0.044*
C4_1	0.9926 (5)	0.06918 (9)	0.6192 (3)	0.0396 (11)
H4A_1	1.0155	0.0871	0.6506	0.048*
H4B_1	0.9078	0.064	0.6373	0.048*
C5_1	0.8802 (5)	0.08878 (10)	0.4484 (3)	0.0381 (11)
C6_1	0.7973 (5)	0.10454 (10)	0.4118 (3)	0.0417 (11)
C7_1	0.8317 (4)	-0.02945 (10)	0.1632 (3)	0.0380 (11)
C8_1	0.8494 (5)	-0.04565 (11)	0.2696 (3)	0.0552 (14)
H8A_1	0.7886	-0.0607	0.2617	0.083*
H8B_1	0.833	-0.0341	0.3289	0.083*
H8C_1	0.938	-0.0525	0.2859	0.083*
C9_1	0.6905 (5)	-0.02041 (11)	0.1350 (5)	0.0594 (15)
H9A_1	0.6337	-0.0361	0.1305	0.089*
H9B_1	0.6769	-0.0111	0.065	0.089*
H9C_1	0.6705	-0.0083	0.1914	0.089*
C10_1	0.8620 (5)	-0.04781 (10)	0.0717 (4)	0.0465 (12)
H10A_1	0.7997	-0.0626	0.0609	0.070*
H10B_1	0.9495	-0.0551	0.0917	0.070*
H10C_1	0.856	-0.0375	0.0045	0.070*
C11_1	0.8124 (5)	0.03812 (11)	0.0424 (4)	0.0475 (13)
H11_1	0.7447	0.0344	0.0818	0.057*
C12_1	0.7910 (5)	0.05701 (11)	-0.0394 (4)	0.0529 (14)

H12_1	0.7103	0.066	-0.0558	0.063*
C13_1	0.8883 (6)	0.06262 (11)	-0.0965 (4)	0.0549 (15)
H13_1	0.8744	0.0755	-0.1531	0.066*
C14_1	1.0046 (6)	0.04997 (11)	-0.0732 (4)	0.0534 (14)
H14_1	1.0712	0.054	-0.1134	0.064*
C15_1	1.0255 (5)	0.03090 (10)	0.0109 (4)	0.0467 (12)
H15_1	1.1072	0.0223	0.0279	0.056*
C16_1	0.9285 (4)	0.02434 (9)	0.0698 (3)	0.0364 (11)
C17_1	1.1184 (4)	-0.01334 (9)	0.2096 (3)	0.0345 (10)
C18_1	1.1871 (4)	-0.01387 (9)	0.3155 (3)	0.0383 (11)
H18_1	1.1465	-0.0078	0.3733	0.046*
C19_1	1.3134 (5)	-0.02312 (10)	0.3379 (4)	0.0474 (12)
H19_1	1.3579	-0.0233	0.4106	0.057*
C20_1	1.3750 (5)	-0.03213 (11)	0.2557 (4)	0.0516 (13)
H20_1	1.4619	-0.0382	0.2711	0.062*
C21_1	1.3080 (5)	-0.03214 (11)	0.1502 (4)	0.0517 (13)
H21_1	1.3488	-0.0384	0.0929	0.062*
C22_1	1.1829 (5)	-0.02308 (10)	0.1281 (4)	0.0435 (12)
H22_1	1.1386	-0.0234	0.0553	0.052*
C23_1	0.5921 (8)	0.1131 (2)	0.2233 (6)	0.122 (3)
H23A_1	0.5276	0.1255	0.1852	0.183*
H23B_1	0.5491	0.0968	0.2428	0.183*
H23C_1	0.654	0.1084	0.1759	0.183*
C24_1	0.7645 (7)	0.15916 (16)	0.3136 (9)	0.135 (4)
H24A_1	0.7944	0.1696	0.3793	0.202*
H24B_1	0.7061	0.1701	0.2619	0.202*
H24C_1	0.8389	0.1537	0.281	0.202*
C25_1	0.5617 (9)	0.13754 (16)	0.4357 (7)	0.127 (4)
H25A_1	0.6073	0.1416	0.5089	0.191*
H25B_1	0.5041	0.1222	0.4387	0.191*
H25C_1	0.5109	0.1531	0.4065	0.191*
C26_1	1.0580 (4)	0.02434 (9)	0.6202 (3)	0.0321 (10)
H26_1	0.9699	0.0191	0.6327	0.038*
C27_1	1.1554 (4)	0.00466 (9)	0.6761 (3)	0.0316 (10)
C28_1	1.1263 (4)	-0.00974 (10)	0.7639 (3)	0.0364 (11)
H28_1	1.0443	-0.0075	0.7852	0.044*
C29_1	1.2144 (4)	-0.02708 (10)	0.8200 (3)	0.0394 (11)
H29_1	1.1924	-0.0368	0.8795	0.047*
C30_1	1.2751 (4)	0.00102 (9)	0.6477 (3)	0.0371 (11)
H30_1	1.2965	0.0107	0.5879	0.045*
C31_1	1.3652 (4)	-0.01636 (10)	0.7034 (3)	0.0400 (11)
H31_1	1.4471	-0.0186	0.6822	0.048*
C32_1	1.3340 (4)	-0.03064 (9)	0.7916 (3)	0.0366 (11)
C33_1	1.5424 (5)	-0.05069 (12)	0.8337 (4)	0.0585 (15)
H33A_1	1.5936	-0.0615	0.8907	0.088*
H33B_1	1.5819	-0.033	0.8318	0.088*
H33C_1	1.5396	-0.0595	0.7635	0.088*
Si1_2	0.49891 (12)	0.25199 (3)	0.42641 (9)	0.0363 (3)
Si2_2	0.21158 (14)	0.23459 (3)	-0.11180 (11)	0.0506 (4)
O1_2	0.4925 (3)	0.26703 (6)	0.3080 (2)	0.0384 (8)
O2_2	0.5164 (3)	0.31919 (6)	0.2450 (2)	0.0368 (7)
O3_2	0.6310 (3)	0.33020 (7)	0.1079 (2)	0.0454 (8)
O4_2	0.8651 (4)	0.40877 (8)	0.4894 (3)	0.0641 (11)
C1_2	0.3850 (4)	0.28129 (10)	0.2506 (3)	0.0382 (11)
H1A_2	0.3375	0.2901	0.3029	0.046*
H1B_2	0.3254	0.2686	0.2065	0.046*

C2_2	0.4288 (4)	0.30206 (9)	0.1781 (3)	0.0354 (11)
H2_2	0.3522	0.3129	0.1445	0.042*
C3_2	0.4941 (4)	0.29072 (9)	0.0873 (3)	0.0369 (11)
H3_2	0.5676	0.2791	0.1212	0.044*
C4_2	0.5488 (5)	0.31369 (11)	0.0297 (3)	0.0474 (13)
H4A_2	0.5994	0.3065	-0.0238	0.057*
H4B_2	0.4774	0.3246	-0.0097	0.057*
C5_2	0.4023 (5)	0.27391 (10)	0.0136 (3)	0.0405 (11)
C6_2	0.3242 (5)	0.25999 (11)	-0.0419 (4)	0.0460 (13)
C7_2	0.3742 (4)	0.22420 (10)	0.4120 (3)	0.0424 (11)
C8_2	0.2380 (5)	0.23557 (12)	0.4036 (5)	0.0667 (16)
H8A_2	0.1757	0.2208	0.3983	0.100*
H8B_2	0.2185	0.2469	0.339	0.100*
H8C_2	0.2325	0.2463	0.4683	0.100*
C9_2	0.3854 (5)	0.20827 (11)	0.3085 (4)	0.0549 (14)
H9A_2	0.323	0.1935	0.3	0.082*
H9B_2	0.473	0.201	0.3143	0.082*
H9C_2	0.3674	0.2201	0.2454	0.082*
C10_2	0.3957 (6)	0.20425 (10)	0.5080 (4)	0.0582 (15)
H10A_2	0.3312	0.1899	0.4948	0.087*
H10B_2	0.3872	0.2137	0.5751	0.087*
H10C_2	0.4824	0.1965	0.5149	0.087*
C11_2	0.7494 (4)	0.24034 (10)	0.3789 (3)	0.0411 (11)
H11_2	0.7192	0.2487	0.3113	0.049*
C12_2	0.8736 (5)	0.23037 (11)	0.3993 (4)	0.0516 (13)
H12_2	0.9272	0.232	0.3457	0.062*
C13_2	0.9205 (5)	0.21815 (11)	0.4963 (5)	0.0597 (15)
H13_2	1.0059	0.2112	0.51	0.072*
C14_2	0.8419 (5)	0.21608 (12)	0.5734 (4)	0.0623 (16)
H14_2	0.8738	0.2078	0.6411	0.075*
C15_2	0.7172 (5)	0.22585 (11)	0.5534 (4)	0.0506 (13)
H15_2	0.6643	0.224	0.6075	0.061*
C16_2	0.6671 (4)	0.23837 (10)	0.4551 (3)	0.0396 (11)
C17_2	0.4780 (5)	0.27759 (10)	0.5327 (3)	0.0424 (12)
C18_2	0.4744 (5)	0.30454 (11)	0.5125 (4)	0.0533 (14)
H18_2	0.4805	0.3105	0.4414	0.064*
C19_2	0.4624 (6)	0.32354 (12)	0.5907 (4)	0.0678 (17)
H19_2	0.4605	0.342	0.5727	0.081*
C20_2	0.4534 (6)	0.31576 (13)	0.6929 (4)	0.0643 (16)
H20_2	0.4439	0.3287	0.7465	0.077*
C21_2	0.4580 (6)	0.28923 (13)	0.7180 (4)	0.0717 (18)
H21_2	0.4529	0.2837	0.7899	0.086*
C22_2	0.4703 (6)	0.26983 (12)	0.6390 (4)	0.0665 (17)
H22_2	0.4733	0.2514	0.6577	0.080*
C23_2	0.2186 (7)	0.20474 (15)	-0.0190 (5)	0.085 (2)
H23A_2	0.1841	0.2097	0.0462	0.128*
H23B_2	0.3084	0.1989	0.0015	0.128*
H23C_2	0.1669	0.1901	-0.0565	0.128*
C24_2	0.2659 (7)	0.22407 (15)	-0.2379 (5)	0.095 (2)
H24A_2	0.2561	0.239	-0.2894	0.142*
H24B_2	0.2136	0.2089	-0.2696	0.142*
H24C_2	0.3569	0.2187	-0.2216	0.142*
C25_2	0.0438 (5)	0.24696 (13)	-0.1399 (4)	0.0691 (16)
H25A_2	0.0386	0.2625	-0.1884	0.104*
H25B_2	0.0168	0.2522	-0.0717	0.104*
H25C_2	-0.0131	0.2327	-0.1744	0.104*

C26_2	0.5610 (4)	0.34035 (9)	0.1860 (3)	0.0393 (11)
H26_2	0.4853	0.3508	0.1485	0.047*
C27_2	0.6459 (4)	0.35835 (10)	0.2633 (3)	0.0380 (11)
C28_2	0.6757 (5)	0.38349 (11)	0.2327 (4)	0.0510 (13)
H28_2	0.6456	0.3892	0.1604	0.061*
C29_2	0.7501 (5)	0.40132 (11)	0.3056 (4)	0.0516 (13)
H29_2	0.7706	0.4187	0.2828	0.062*
C30_2	0.6930 (5)	0.35036 (11)	0.3708 (4)	0.0495 (13)
H30_2	0.6738	0.3329	0.3943	0.059*
C31_2	0.7662 (5)	0.36753 (12)	0.4417 (4)	0.0550 (14)
H31_2	0.7992	0.3617	0.5133	0.066*
C32_2	0.7923 (5)	0.39294 (11)	0.4106 (4)	0.0461 (12)
C33_2	0.8791 (6)	0.43594 (13)	0.4650 (5)	0.0740 (18)
H33A_2	0.9349	0.4447	0.5257	0.111*
H33B_2	0.7942	0.4446	0.4527	0.111*
H33C_2	0.9182	0.4375	0.3995	0.111*
Si1_3	0.39924 (12)	0.10786 (3)	0.77483 (9)	0.0349 (3)
Si2_3	0.13672 (13)	0.12264 (3)	0.22505 (9)	0.0425 (3)
O1_3	0.4353 (3)	0.09723 (6)	0.6593 (2)	0.0380 (7)
O2_3	0.5061 (3)	0.04611 (6)	0.5721 (2)	0.0324 (7)
O3_3	0.5221 (3)	0.02025 (6)	0.4195 (2)	0.0418 (8)
O4_3	0.8573 (3)	-0.04460 (7)	0.7970 (2)	0.0496 (9)
C1_3	0.3544 (4)	0.08106 (10)	0.5813 (3)	0.0390 (11)
H1A_3	0.2892	0.0924	0.5361	0.047*
H1B_3	0.3086	0.0676	0.6188	0.047*
C2_3	0.4372 (4)	0.06720 (9)	0.5110 (3)	0.0309 (10)
H2_3	0.5002	0.0803	0.4898	0.037*
C3_3	0.3567 (4)	0.05490 (9)	0.4072 (3)	0.0333 (10)
H3_3	0.2925	0.0421	0.4288	0.040*
C4_3	0.4503 (5)	0.03934 (10)	0.3479 (3)	0.0430 (12)
H4A_3	0.401	0.0299	0.2844	0.052*
H4B_3	0.5105	0.052	0.3214	0.052*
C5_3	0.2873 (4)	0.07576 (10)	0.3379 (3)	0.0367 (11)
C6_3	0.2296 (5)	0.09360 (10)	0.2864 (3)	0.0412 (12)
C7_3	0.5222 (4)	0.13479 (10)	0.8184 (3)	0.0428 (11)
C8_3	0.6568 (5)	0.12311 (14)	0.8307 (6)	0.089 (2)
H8A_3	0.7206	0.1373	0.8512	0.133*
H8B_3	0.6697	0.1152	0.7617	0.133*
H8C_3	0.6673	0.1093	0.887	0.133*
C9_3	0.5092 (7)	0.15735 (12)	0.7321 (4)	0.0731 (18)
H9A_3	0.5735	0.1713	0.7556	0.110*
H9B_3	0.4224	0.1651	0.7234	0.110*
H9C_3	0.5237	0.1499	0.6627	0.110*
C10_3	0.5023 (7)	0.14755 (14)	0.9257 (4)	0.084 (2)
H10A_3	0.5635	0.1623	0.9437	0.126*
H10B_3	0.5169	0.1341	0.9834	0.126*
H10C_3	0.4139	0.1544	0.9186	0.126*
C11_3	0.1867 (5)	0.13762 (11)	0.6580 (4)	0.0499 (13)
H11_3	0.2411	0.14	0.6054	0.060*
C12_3	0.0675 (5)	0.14907 (12)	0.6407 (4)	0.0602 (15)
H12_3	0.0408	0.1593	0.5769	0.072*
C13_3	-0.0161 (5)	0.14606 (12)	0.7149 (4)	0.0598 (15)
H13_3	-0.0993	0.1541	0.7022	0.072*
C14_3	0.0245 (5)	0.13123 (12)	0.8074 (4)	0.0546 (14)
H14_3	-0.0306	0.129	0.8595	0.066*
C15_3	0.1463 (4)	0.11950 (10)	0.8240 (4)	0.0455 (12)

H15_3	0.1721	0.1091	0.8876	0.055*
C16_3	0.2319 (4)	0.12237 (10)	0.7512 (3)	0.0383 (11)
C17_3	0.4107 (4)	0.07922 (9)	0.8731 (3)	0.0334 (10)
C18_3	0.4426 (5)	0.05390 (10)	0.8431 (4)	0.0439 (12)
H18_3	0.4606	0.051	0.7722	0.053*
C19_3	0.4487 (5)	0.03252 (11)	0.9153 (4)	0.0557 (14)
H19_3	0.4713	0.0152	0.8931	0.067*
C20_3	0.4227 (5)	0.03609 (12)	1.0181 (4)	0.0556 (14)
H20_3	0.4263	0.0214	1.0667	0.067*
C21_3	0.3913 (6)	0.06114 (12)	1.0498 (4)	0.0587 (15)
H21_3	0.3725	0.0638	1.1206	0.070*
C22_3	0.3869 (5)	0.08263 (11)	0.9792 (3)	0.0526 (14)
H22_3	0.3675	0.1	1.003	0.063*
C23_3	0.1121 (5)	0.14448 (11)	0.3402 (4)	0.0522 (13)
H23A_3	0.1962	0.1494	0.3822	0.078*
H23B_3	0.0617	0.1348	0.3868	0.078*
H23C_3	0.0655	0.1607	0.3121	0.078*
C24_3	-0.0161 (6)	0.11057 (13)	0.1464 (4)	0.0733 (18)
H24A_3	0.0019	0.0992	0.0868	0.110*
H24B_3	-0.0689	0.1259	0.1168	0.110*
H24C_3	-0.0628	0.1001	0.1936	0.110*
C25_3	0.2329 (6)	0.14150 (12)	0.1375 (4)	0.0661 (16)
H25A_3	0.2454	0.1303	0.0758	0.099*
H25B_3	0.3172	0.1462	0.1797	0.099*
H25C_3	0.1866	0.1579	0.1109	0.099*
C26_3	0.5913 (4)	0.03284 (9)	0.5134 (3)	0.0349 (10)
H26_3	0.6539	0.046	0.4918	0.042*
C27_3	0.6635 (4)	0.01167 (10)	0.5852 (3)	0.0341 (10)
C28_3	0.6880 (4)	-0.01321 (10)	0.5460 (3)	0.0408 (11)
H28_3	0.6593	-0.0171	0.4716	0.049*
C29_3	0.7538 (5)	-0.03280 (11)	0.6129 (3)	0.0459 (12)
H29_3	0.7705	-0.0499	0.5845	0.055*
C30_3	0.7070 (4)	0.01726 (10)	0.6942 (3)	0.0385 (11)
H30_3	0.6916	0.0344	0.7225	0.046*
C31_3	0.7725 (4)	-0.00205 (10)	0.7617 (3)	0.0419 (12)
H31_3	0.8024	0.0019	0.8359	0.050*
C32_3	0.7946 (4)	-0.02695 (11)	0.7216 (3)	0.0409 (12)
C33_3	0.8750 (6)	-0.07135 (12)	0.7638 (4)	0.0669 (16)
H33A_3	0.9133	-0.082	0.8268	0.100*
H33B_3	0.9327	-0.0715	0.71	0.100*
H33C_3	0.7913	-0.079	0.7318	0.100*
Si1_4	0.98584 (12)	0.35189 (3)	-0.12381 (9)	0.0387 (3)
Si2_4	0.74357 (13)	0.22463 (3)	0.02917 (10)	0.0456 (3)
O1_4	0.9714 (3)	0.33462 (6)	-0.0138 (2)	0.0408 (8)
O2_4	1.1088 (3)	0.32991 (6)	0.2003 (2)	0.0362 (7)
O3_4	0.9778 (3)	0.32785 (7)	0.3324 (2)	0.0473 (8)
O4_4	1.3895 (4)	0.41271 (7)	0.5444 (3)	0.0590 (10)
C1_4	1.0509 (5)	0.31214 (9)	0.0229 (3)	0.0389 (11)
H1A_4	1.1406	0.3156	0.0122	0.047*
H1B_4	1.0189	0.2961	-0.0197	0.047*
C2_4	1.0485 (4)	0.30720 (9)	0.1422 (3)	0.0373 (11)
H2_4	1.1009	0.2909	0.1657	0.045*
C3_4	0.9125 (4)	0.30309 (10)	0.1651 (3)	0.0393 (11)
H3_4	0.8569	0.3181	0.1311	0.047*
C4_4	0.9155 (5)	0.30385 (11)	0.2881 (4)	0.0504 (13)
H4A_4	0.8262	0.3032	0.3035	0.060*

H4B_4	0.9627	0.288	0.3222	0.060*
C5_4	0.8574 (4)	0.27776 (11)	0.1203 (3)	0.0415 (11)
C6_4	0.8150 (5)	0.25603 (10)	0.0864 (4)	0.0434 (12)
C7_4	0.8569 (5)	0.37818 (10)	-0.1341 (4)	0.0455 (12)
C8_4	0.8792 (5)	0.39492 (12)	-0.0288 (4)	0.0605 (15)
H8A_4	0.8124	0.4088	-0.0329	0.091*
H8B_4	0.9644	0.4034	-0.0199	0.091*
H8C_4	0.8748	0.3832	0.0333	0.091*
C9_4	0.7195 (5)	0.36692 (14)	-0.1487 (6)	0.080 (2)
H9A_4	0.6584	0.3815	-0.1436	0.120*
H9B_4	0.7138	0.3537	-0.0919	0.120*
H9C_4	0.6982	0.3583	-0.2199	0.120*
C10_4	0.8671 (6)	0.39731 (12)	-0.2297 (4)	0.0680 (17)
H10A_4	0.8058	0.4121	-0.2297	0.102*
H10B_4	0.8469	0.3875	-0.2982	0.102*
H10C_4	0.9551	0.4045	-0.2216	0.102*
C11_4	0.8559 (7)	0.31498 (16)	-0.2756 (8)	0.120 (3)
H11_4	0.7843	0.3186	-0.2405	0.144*
C12_4	0.8417 (11)	0.2964 (2)	-0.3611 (11)	0.168 (6)
H12_4	0.7612	0.2877	-0.3831	0.201*
C13_4	0.9391 (16)	0.29112 (18)	-0.4106 (6)	0.146 (5)
H13_4	0.9267	0.2791	-0.4704	0.176*
C14_4	1.0597 (14)	0.30253 (18)	-0.3781 (7)	0.166 (6)
H14_4	1.1311	0.298	-0.4119	0.199*
C15_4	1.0714 (10)	0.32103 (16)	-0.2935 (6)	0.123 (4)
H15_4	1.1529	0.3293	-0.2702	0.148*
C16_4	0.9691 (6)	0.32794 (10)	-0.2417 (4)	0.0517 (14)
C17_4	1.1501 (4)	0.36779 (10)	-0.0995 (3)	0.0402 (11)
C18_4	1.2098 (4)	0.37316 (9)	0.0073 (3)	0.0387 (11)
H18_4	1.1675	0.368	0.0654	0.046*
C19_4	1.3276 (5)	0.38562 (10)	0.0300 (4)	0.0461 (12)
H19_4	1.3651	0.3891	0.1032	0.055*
C20_4	1.3917 (5)	0.39312 (11)	-0.0516 (5)	0.0553 (14)
H20_4	1.4738	0.4015	-0.0351	0.066*
C21_4	1.3360 (5)	0.38835 (11)	-0.1588 (4)	0.0564 (14)
H21_4	1.3805	0.3933	-0.2159	0.068*
C22_4	1.2152 (5)	0.37639 (11)	-0.1822 (4)	0.0480 (13)
H22_4	1.1759	0.374	-0.2557	0.058*
C23_4	0.6816 (6)	0.23039 (14)	-0.1170 (4)	0.0757 (19)
H23A_4	0.7497	0.2384	-0.1512	0.114*
H23B_4	0.6072	0.2425	-0.1248	0.114*
H23C_4	0.6552	0.2133	-0.1523	0.114*
C24_4	0.6092 (5)	0.21507 (10)	0.1000 (4)	0.0508 (13)
H24A_4	0.6415	0.2135	0.178	0.076*
H24B_4	0.5733	0.1978	0.0721	0.076*
H24C_4	0.5416	0.2288	0.0875	0.076*
C25_4	0.8690 (6)	0.19798 (13)	0.0491 (6)	0.084 (2)
H25A_4	0.8979	0.1951	0.1269	0.126*
H25B_4	0.9425	0.2035	0.0156	0.126*
H25C_4	0.8326	0.1813	0.0155	0.126*
C26_4	1.1049 (4)	0.32841 (10)	0.3134 (3)	0.0378 (11)
H26_4	1.1496	0.3117	0.3432	0.045*
C27_4	1.1758 (4)	0.35215 (10)	0.3685 (3)	0.0381 (11)
C28_4	1.1280 (5)	0.36674 (10)	0.4484 (4)	0.0458 (12)
H28_4	1.0453	0.3626	0.465	0.055*
C29_4	1.2010 (5)	0.38720 (10)	0.5035 (4)	0.0470 (13)

H29_4	1.1668	0.3973	0.5565	0.056*
C30_4	1.2955 (4)	0.35904 (10)	0.3451 (3)	0.0426 (12)
H30_4	1.3281	0.3497	0.2894	0.051*
C31_4	1.3695 (5)	0.37931 (11)	0.4009 (4)	0.0469 (12)
H31_4	1.4515	0.3838	0.3836	0.056*
C32_4	1.3214 (5)	0.39298 (9)	0.4824 (3)	0.0424 (12)
C33_4	1.5201 (6)	0.41668 (15)	0.5310 (6)	0.091 (2)
H33A_4	1.5631	0.4287	0.5879	0.136*
H33B_4	1.522	0.4247	0.4598	0.136*
H33C_4	1.565	0.3994	0.5359	0.136*

Table 3. Bond lengths [Å] and angles [°] for jb0603.

Si1_1—O1_1	1.651 (3)	Si1_3—O1_3	1.644 (3)
Si1_1—C17_1	1.871 (4)	Si1_3—C17_3	1.877 (4)
Si1_1—C16_1	1.874 (4)	Si1_3—C16_3	1.878 (5)
Si1_1—C7_1	1.878 (5)	Si1_3—C7_3	1.880 (5)
Si2_1—C25_1	1.827 (7)	Si2_3—C24_3	1.837 (5)
Si2_1—C24_1	1.826 (7)	Si2_3—C6_3	1.841 (5)
Si2_1—C6_1	1.839 (5)	Si2_3—C23_3	1.859 (5)
Si2_1—C23_1	1.862 (7)	Si2_3—C25_3	1.867 (5)
O1_1—C1_1	1.418 (5)	O1_3—C1_3	1.430 (5)
O2_1—C26_1	1.421 (4)	O2_3—C26_3	1.416 (5)
O2_1—C2_1	1.434 (5)	O2_3—C2_3	1.425 (5)
O3_1—C26_1	1.417 (5)	O3_3—C26_3	1.420 (5)
O3_1—C4_1	1.427 (5)	O3_3—C4_3	1.432 (5)
O4_1—C32_1	1.373 (5)	O4_3—C32_3	1.375 (6)
O4_1—C33_1	1.411 (5)	O4_3—C33_3	1.420 (6)
C1_1—C2_1	1.516 (5)	C1_3—C2_3	1.506 (6)
C1_1—H1A_1	0.99	C1_3—H1A_3	0.99
C1_1—H1B_1	0.99	C1_3—H1B_3	0.99
C2_1—C3_1	1.535 (6)	C2_3—C3_3	1.552 (5)
C2_1—H2_1	1	C2_3—H2_3	1
C3_1—C5_1	1.465 (6)	C3_3—C5_3	1.467 (6)
C3_1—C4_1	1.538 (5)	C3_3—C4_3	1.540 (6)
C3_1—H3_1	1	C3_3—H3_3	1
C4_1—H4A_1	0.99	C4_3—H4A_3	0.99
C4_1—H4B_1	0.99	C4_3—H4B_3	0.99
C5_1—C6_1	1.205 (6)	C5_3—C6_3	1.202 (6)
C7_1—C9_1	1.534 (7)	C7_3—C8_3	1.514 (7)
C7_1—C10_1	1.541 (6)	C7_3—C10_3	1.532 (7)
C7_1—C8_1	1.543 (6)	C7_3—C9_3	1.551 (7)
C8_1—H8A_1	0.98	C8_3—H8A_3	0.98
C8_1—H8B_1	0.98	C8_3—H8B_3	0.98
C8_1—H8C_1	0.98	C8_3—H8C_3	0.98
C9_1—H9A_1	0.98	C9_3—H9A_3	0.98
C9_1—H9B_1	0.98	C9_3—H9B_3	0.98
C9_1—H9C_1	0.98	C9_3—H9C_3	0.98
C10_1—H10A_1	0.98	C10_3—H10A_3	0.98
C10_1—H10B_1	0.98	C10_3—H10B_3	0.98
C10_1—H10C_1	0.98	C10_3—H10C_3	0.98
C11_1—C12_1	1.382 (7)	C11_3—C12_3	1.360 (7)
C11_1—C16_1	1.392 (6)	C11_3—C16_3	1.406 (6)
C11_1—H11_1	0.95	C11_3—H11_3	0.95

C12_1—C13_1	1.372 (7)	C12_3—C13_3	1.390 (7)
C12_1—H12_1	0.95	C12_3—H12_3	0.95
C13_1—C14_1	1.362 (7)	C13_3—C14_3	1.379 (7)
C13_1—H13_1	0.95	C13_3—H13_3	0.95
C14_1—C15_1	1.409 (7)	C14_3—C15_3	1.390 (7)
C14_1—H14_1	0.95	C14_3—H14_3	0.95
C15_1—C16_1	1.395 (6)	C15_3—C16_3	1.393 (6)
C15_1—H15_1	0.95	C15_3—H15_3	0.95
C17_1—C18_1	1.399 (6)	C17_3—C18_3	1.377 (6)
C17_1—C22_1	1.404 (6)	C17_3—C22_3	1.402 (6)
C18_1—C19_1	1.388 (6)	C18_3—C19_3	1.393 (7)
C18_1—H18_1	0.95	C18_3—H18_3	0.95
C19_1—C20_1	1.382 (7)	C19_3—C20_3	1.372 (7)
C19_1—H19_1	0.95	C19_3—H19_3	0.95
C20_1—C21_1	1.387 (7)	C20_3—C21_3	1.369 (8)
C20_1—H20_1	0.95	C20_3—H20_3	0.95
C21_1—C22_1	1.373 (7)	C21_3—C22_3	1.386 (7)
C21_1—H21_1	0.95	C21_3—H21_3	0.95
C22_1—H22_1	0.95	C22_3—H22_3	0.95
C23_1—H23A_1	0.98	C23_3—H23A_3	0.98
C23_1—H23B_1	0.98	C23_3—H23B_3	0.98
C23_1—H23C_1	0.98	C23_3—H23C_3	0.98
C24_1—H24A_1	0.98	C24_3—H24A_3	0.98
C24_1—H24B_1	0.98	C24_3—H24B_3	0.98
C24_1—H24C_1	0.98	C24_3—H24C_3	0.98
C25_1—H25A_1	0.98	C25_3—H25A_3	0.98
C25_1—H25B_1	0.98	C25_3—H25B_3	0.98
C25_1—H25C_1	0.98	C25_3—H25C_3	0.98
C26_1—C27_1	1.503 (6)	C26_3—C27_3	1.506 (6)
C26_1—H26_1	1	C26_3—H26_3	1
C27_1—C30_1	1.377 (6)	C27_3—C28_3	1.375 (6)
C27_1—C28_1	1.390 (6)	C27_3—C30_3	1.392 (6)
C28_1—C29_1	1.371 (6)	C28_3—C29_3	1.392 (6)
C28_1—H28_1	0.95	C28_3—H28_3	0.95
C29_1—C32_1	1.375 (6)	C29_3—C32_3	1.387 (6)
C29_1—H29_1	0.95	C29_3—H29_3	0.95
C30_1—C31_1	1.382 (6)	C30_3—C31_3	1.386 (6)
C30_1—H30_1	0.95	C30_3—H30_3	0.95
C31_1—C32_1	1.399 (6)	C31_3—C32_3	1.375 (7)
C31_1—H31_1	0.95	C31_3—H31_3	0.95
C33_1—H33A_1	0.98	C33_3—H33A_3	0.98
C33_1—H33B_1	0.98	C33_3—H33B_3	0.98
C33_1—H33C_1	0.98	C33_3—H33C_3	0.98
Si1_2—O1_2	1.652 (3)	Si1_4—O1_4	1.654 (3)
Si1_2—C16_2	1.871 (5)	Si1_4—C7_4	1.875 (5)
Si1_2—C17_2	1.885 (5)	Si1_4—C17_4	1.877 (5)
Si1_2—C7_2	1.896 (5)	Si1_4—C16_4	1.884 (5)
Si2_2—C24_2	1.843 (6)	Si2_4—C6_4	1.831 (5)
Si2_2—C25_2	1.844 (6)	Si2_4—C24_4	1.853 (5)
Si2_2—C6_2	1.850 (5)	Si2_4—C23_4	1.858 (5)
Si2_2—C23_2	1.883 (7)	Si2_4—C25_4	1.859 (6)
O1_2—C1_2	1.423 (5)	O1_4—C1_4	1.427 (5)
O2_2—C26_2	1.414 (5)	O2_4—C26_4	1.426 (5)
O2_2—C2_2	1.421 (5)	O2_4—C2_4	1.435 (5)

O3_2—C26_2	1.413 (5)	O3_4—C26_4	1.395 (5)
O3_2—C4_2	1.448 (5)	O3_4—C4_4	1.432 (6)
O4_2—C32_2	1.387 (6)	O4_4—C32_4	1.377 (5)
O4_2—C33_2	1.404 (7)	O4_4—C33_4	1.425 (7)
C1_2—C2_2	1.502 (6)	C1_4—C2_4	1.518 (6)
C1_2—H1A_2	0.99	C1_4—H1A_4	0.99
C1_2—H1B_2	0.99	C1_4—H1B_4	0.99
C2_2—C3_2	1.532 (6)	C2_4—C3_4	1.519 (6)
C2_2—H2_2	1	C2_4—H2_4	1
C3_2—C5_2	1.478 (6)	C3_4—C5_4	1.463 (6)
C3_2—C4_2	1.519 (6)	C3_4—C4_4	1.535 (6)
C3_2—H3_2	1	C3_4—H3_4	1
C4_2—H4A_2	0.99	C4_4—H4A_4	0.99
C4_2—H4B_2	0.99	C4_4—H4B_4	0.99
C5_2—C6_2	1.202 (6)	C5_4—C6_4	1.221 (7)
C7_2—C8_2	1.526 (7)	C7_4—C9_4	1.531 (7)
C7_2—C9_2	1.542 (6)	C7_4—C8_4	1.546 (7)
C7_2—C10_2	1.548 (6)	C7_4—C10_4	1.549 (7)
C8_2—H8A_2	0.98	C8_4—H8A_4	0.98
C8_2—H8B_2	0.98	C8_4—H8B_4	0.98
C8_2—H8C_2	0.98	C8_4—H8C_4	0.98
C9_2—H9A_2	0.98	C9_4—H9A_4	0.98
C9_2—H9B_2	0.98	C9_4—H9B_4	0.98
C9_2—H9C_2	0.98	C9_4—H9C_4	0.98
C10_2—H10A_2	0.98	C10_4—H10A_4	0.98
C10_2—H10B_2	0.98	C10_4—H10B_4	0.98
C10_2—H10C_2	0.98	C10_4—H10C_4	0.98
C11_2—C12_2	1.379 (6)	C11_4—C16_4	1.357 (8)
C11_2—C16_2	1.396 (6)	C11_4—C12_4	1.404 (12)
C11_2—H11_2	0.95	C11_4—H11_4	0.95
C12_2—C13_2	1.373 (7)	C12_4—C13_4	1.312 (15)
C12_2—H12_2	0.95	C12_4—H12_4	0.95
C13_2—C14_2	1.377 (7)	C13_4—C14_4	1.386 (15)
C13_2—H13_2	0.95	C13_4—H13_4	0.95
C14_2—C15_2	1.380 (7)	C14_4—C15_4	1.395 (10)
C14_2—H14_2	0.95	C14_4—H14_4	0.95
C15_2—C16_2	1.402 (6)	C15_4—C16_4	1.390 (9)
C15_2—H15_2	0.95	C15_4—H15_4	0.95
C17_2—C18_2	1.368 (7)	C17_4—C22_4	1.402 (6)
C17_2—C22_2	1.401 (6)	C17_4—C18_4	1.403 (6)
C18_2—C19_2	1.384 (7)	C18_4—C19_4	1.372 (6)
C18_2—H18_2	0.95	C18_4—H18_4	0.95
C19_2—C20_2	1.356 (7)	C19_4—C20_4	1.368 (7)
C19_2—H19_2	0.95	C19_4—H19_4	0.95
C20_2—C21_2	1.360 (8)	C20_4—C21_4	1.391 (7)
C20_2—H20_2	0.95	C20_4—H20_4	0.95
C21_2—C22_2	1.406 (8)	C21_4—C22_4	1.388 (7)
C21_2—H21_2	0.95	C21_4—H21_4	0.95
C22_2—H22_2	0.95	C22_4—H22_4	0.95
C23_2—H23A_2	0.98	C23_4—H23A_4	0.98
C23_2—H23B_2	0.98	C23_4—H23B_4	0.98
C23_2—H23C_2	0.98	C23_4—H23C_4	0.98
C24_2—H24A_2	0.98	C24_4—H24A_4	0.98
C24_2—H24B_2	0.98	C24_4—H24B_4	0.98

C24_2—H24C_2	0.98	C24_4—H24C_4	0.98
C25_2—H25A_2	0.98	C25_4—H25A_4	0.98
C25_2—H25B_2	0.98	C25_4—H25B_4	0.98
C25_2—H25C_2	0.98	C25_4—H25C_4	0.98
C26_2—C27_2	1.499 (6)	C26_4—C27_4	1.503 (6)
C26_2—H26_2	1	C26_4—H26_4	1
C27_2—C28_2	1.364 (7)	C27_4—C30_4	1.383 (6)
C27_2—C30_2	1.410 (6)	C27_4—C28_4	1.397 (6)
C28_2—C29_2	1.411 (7)	C28_4—C29_4	1.389 (7)
C28_2—H28_2	0.95	C28_4—H28_4	0.95
C29_2—C32_2	1.379 (6)	C29_4—C32_4	1.367 (7)
C29_2—H29_2	0.95	C29_4—H29_4	0.95
C30_2—C31_2	1.373 (7)	C30_4—C31_4	1.390 (6)
C30_2—H30_2	0.95	C30_4—H30_4	0.95
C31_2—C32_2	1.368 (7)	C31_4—C32_4	1.393 (7)
C31_2—H31_2	0.95	C31_4—H31_4	0.95
C33_2—H33A_2	0.98	C33_4—H33A_4	0.98
C33_2—H33B_2	0.98	C33_4—H33B_4	0.98
C33_2—H33C_2	0.98	C33_4—H33C_4	0.98
O1_1—Si1_1—C17_1	109.38 (17)	O1_3—Si1_3—C17_3	109.40 (18)
O1_1—Si1_1—C16_1	108.58 (18)	O1_3—Si1_3—C16_3	109.60 (17)
C17_1—Si1_1—C16_1	109.9 (2)	C17_3—Si1_3—C16_3	110.5 (2)
O1_1—Si1_1—C7_1	103.36 (17)	O1_3—Si1_3—C7_3	103.66 (19)
C17_1—Si1_1—C7_1	110.3 (2)	C17_3—Si1_3—C7_3	112.97 (19)
C16_1—Si1_1—C7_1	115.05 (19)	C16_3—Si1_3—C7_3	110.4 (2)
C25_1—Si2_1—C24_1	111.8 (4)	C24_3—Si2_3—C6_3	108.6 (3)
C25_1—Si2_1—C6_1	111.5 (3)	C24_3—Si2_3—C23_3	112.6 (3)
C24_1—Si2_1—C6_1	109.2 (3)	C6_3—Si2_3—C23_3	105.8 (2)
C25_1—Si2_1—C23_1	108.5 (4)	C24_3—Si2_3—C25_3	111.2 (3)
C24_1—Si2_1—C23_1	110.2 (5)	C6_3—Si2_3—C25_3	109.9 (2)
C6_1—Si2_1—C23_1	105.4 (3)	C23_3—Si2_3—C25_3	108.7 (3)
C1_1—O1_1—Si1_1	124.5 (2)	C1_3—O1_3—Si1_3	125.7 (3)
C26_1—O2_1—C2_1	111.2 (3)	C26_3—O2_3—C2_3	112.1 (3)
C26_1—O3_1—C4_1	110.7 (3)	C26_3—O3_3—C4_3	111.4 (3)
C32_1—O4_1—C33_1	117.7 (3)	C32_3—O4_3—C33_3	118.2 (4)
O1_1—C1_1—C2_1	109.0 (3)	O1_3—C1_3—C2_3	108.8 (3)
O1_1—C1_1—H1A_1	109.9	O1_3—C1_3—H1A_3	109.9
C2_1—C1_1—H1A_1	109.9	C2_3—C1_3—H1A_3	109.9
O1_1—C1_1—H1B_1	109.9	O1_3—C1_3—H1B_3	109.9
C2_1—C1_1—H1B_1	109.9	C2_3—C1_3—H1B_3	109.9
H1A_1—C1_1—H1B_1	108.3	H1A_3—C1_3—H1B_3	108.3
O2_1—C2_1—C1_1	108.0 (3)	O2_3—C2_3—C1_3	108.5 (3)
O2_1—C2_1—C3_1	109.0 (3)	O2_3—C2_3—C3_3	108.2 (3)
C1_1—C2_1—C3_1	113.3 (3)	C1_3—C2_3—C3_3	112.6 (3)
O2_1—C2_1—H2_1	108.8	O2_3—C2_3—H2_3	109.2
C1_1—C2_1—H2_1	108.8	C1_3—C2_3—H2_3	109.2
C3_1—C2_1—H2_1	108.8	C3_3—C2_3—H2_3	109.2
C5_1—C3_1—C2_1	112.5 (4)	C5_3—C3_3—C4_3	111.6 (3)
C5_1—C3_1—C4_1	110.1 (4)	C5_3—C3_3—C2_3	111.1 (4)
C2_1—C3_1—C4_1	108.0 (3)	C4_3—C3_3—C2_3	107.6 (3)
C5_1—C3_1—H3_1	108.7	C5_3—C3_3—H3_3	108.9
C2_1—C3_1—H3_1	108.7	C4_3—C3_3—H3_3	108.9
C4_1—C3_1—H3_1	108.7	C2_3—C3_3—H3_3	108.9

O3_1—C4_1—C3_1	110.3 (3)	O3_3—C4_3—C3_3	110.2 (3)
O3_1—C4_1—H4A_1	109.6	O3_3—C4_3—H4A_3	109.6
C3_1—C4_1—H4A_1	109.6	C3_3—C4_3—H4A_3	109.6
O3_1—C4_1—H4B_1	109.6	O3_3—C4_3—H4B_3	109.6
C3_1—C4_1—H4B_1	109.6	C3_3—C4_3—H4B_3	109.6
H4A_1—C4_1—H4B_1	108.1	H4A_3—C4_3—H4B_3	108.1
C6_1—C5_1—C3_1	178.0 (5)	C6_3—C5_3—C3_3	176.3 (5)
C5_1—C6_1—Si2_1	175.5 (4)	C5_3—C6_3—Si2_3	172.3 (4)
C9_1—C7_1—C10_1	108.5 (4)	C8_3—C7_3—C10_3	109.6 (5)
C9_1—C7_1—C8_1	108.9 (4)	C8_3—C7_3—C9_3	108.7 (5)
C10_1—C7_1—C8_1	108.7 (4)	C10_3—C7_3—C9_3	107.5 (5)
C9_1—C7_1—Si1_1	112.9 (3)	C8_3—C7_3—Si1_3	109.8 (4)
C10_1—C7_1—Si1_1	109.9 (3)	C10_3—C7_3—Si1_3	111.2 (4)
C8_1—C7_1—Si1_1	107.9 (3)	C9_3—C7_3—Si1_3	110.0 (3)
C7_1—C8_1—H8A_1	109.5	C7_3—C8_3—H8A_3	109.5
C7_1—C8_1—H8B_1	109.5	C7_3—C8_3—H8B_3	109.5
H8A_1—C8_1—H8B_1	109.5	H8A_3—C8_3—H8B_3	109.5
C7_1—C8_1—H8C_1	109.5	C7_3—C8_3—H8C_3	109.5
H8A_1—C8_1—H8C_1	109.5	H8A_3—C8_3—H8C_3	109.5
H8B_1—C8_1—H8C_1	109.5	H8B_3—C8_3—H8C_3	109.5
C7_1—C9_1—H9A_1	109.5	C7_3—C9_3—H9A_3	109.5
C7_1—C9_1—H9B_1	109.5	C7_3—C9_3—H9B_3	109.5
H9A_1—C9_1—H9B_1	109.5	H9A_3—C9_3—H9B_3	109.5
C7_1—C9_1—H9C_1	109.5	C7_3—C9_3—H9C_3	109.5
H9A_1—C9_1—H9C_1	109.5	H9A_3—C9_3—H9C_3	109.5
H9B_1—C9_1—H9C_1	109.5	H9B_3—C9_3—H9C_3	109.5
C7_1—C10_1—H10A_1	109.5	C7_3—C10_3—H10A_3	109.5
C7_1—C10_1—H10B_1	109.5	C7_3—C10_3—H10B_3	109.5
H10A_1—C10_1—H10B_1	109.5	H10A_3—C10_3—H10B_3	109.5
C7_1—C10_1—H10C_1	109.5	C7_3—C10_3—H10C_3	109.5
H10A_1—C10_1—H10C_1	109.5	H10A_3—C10_3—H10C_3	109.5
H10B_1—C10_1—H10C_1	109.5	H10B_3—C10_3—H10C_3	109.5
C12_1—C11_1—C16_1	123.0 (5)	C12_3—C11_3—C16_3	122.1 (5)
C12_1—C11_1—H11_1	118.5	C12_3—C11_3—H11_3	118.9
C16_1—C11_1—H11_1	118.5	C16_3—C11_3—H11_3	118.9
C13_1—C12_1—C11_1	118.9 (5)	C11_3—C12_3—C13_3	121.1 (5)
C13_1—C12_1—H12_1	120.5	C11_3—C12_3—H12_3	119.4
C11_1—C12_1—H12_1	120.5	C13_3—C12_3—H12_3	119.4
C14_1—C13_1—C12_1	121.0 (5)	C14_3—C13_3—C12_3	118.6 (5)
C14_1—C13_1—H13_1	119.5	C14_3—C13_3—H13_3	120.7
C12_1—C13_1—H13_1	119.5	C12_3—C13_3—H13_3	120.7
C13_1—C14_1—C15_1	119.6 (5)	C13_3—C14_3—C15_3	119.8 (5)
C13_1—C14_1—H14_1	120.2	C13_3—C14_3—H14_3	120.1
C15_1—C14_1—H14_1	120.2	C15_3—C14_3—H14_3	120.1
C16_1—C15_1—C14_1	121.2 (5)	C14_3—C15_3—C16_3	122.6 (4)
C16_1—C15_1—H15_1	119.4	C14_3—C15_3—H15_3	118.7
C14_1—C15_1—H15_1	119.4	C16_3—C15_3—H15_3	118.7
C11_1—C16_1—C15_1	116.3 (4)	C15_3—C16_3—C11_3	115.7 (4)
C11_1—C16_1—Si1_1	119.7 (4)	C15_3—C16_3—Si1_3	123.3 (3)
C15_1—C16_1—Si1_1	124.0 (4)	C11_3—C16_3—Si1_3	121.0 (3)
C18_1—C17_1—C22_1	116.6 (4)	C18_3—C17_3—C22_3	117.5 (4)
C18_1—C17_1—Si1_1	119.9 (3)	C18_3—C17_3—Si1_3	120.8 (3)
C22_1—C17_1—Si1_1	123.5 (3)	C22_3—C17_3—Si1_3	121.8 (4)
C19_1—C18_1—C17_1	121.3 (4)	C17_3—C18_3—C19_3	120.8 (4)

C19_1—C18_1—H18_1	119.3	C17_3—C18_3—H18_3	119.6
C17_1—C18_1—H18_1	119.3	C19_3—C18_3—H18_3	119.6
C20_1—C19_1—C18_1	120.7 (4)	C20_3—C19_3—C18_3	121.0 (5)
C20_1—C19_1—H19_1	119.6	C20_3—C19_3—H19_3	119.5
C18_1—C19_1—H19_1	119.6	C18_3—C19_3—H19_3	119.5
C19_1—C20_1—C21_1	118.9 (4)	C21_3—C20_3—C19_3	119.1 (5)
C19_1—C20_1—H20_1	120.6	C21_3—C20_3—H20_3	120.5
C21_1—C20_1—H20_1	120.6	C19_3—C20_3—H20_3	120.5
C22_1—C21_1—C20_1	120.4 (5)	C20_3—C21_3—C22_3	120.4 (5)
C22_1—C21_1—H21_1	119.8	C20_3—C21_3—H21_3	119.8
C20_1—C21_1—H21_1	119.8	C22_3—C21_3—H21_3	119.8
C21_1—C22_1—C17_1	122.1 (4)	C21_3—C22_3—C17_3	121.2 (5)
C21_1—C22_1—H22_1	119	C21_3—C22_3—H22_3	119.4
C17_1—C22_1—H22_1	119	C17_3—C22_3—H22_3	119.4
Si2_1—C23_1—H23A_1	109.5	Si2_3—C23_3—H23A_3	109.5
Si2_1—C23_1—H23B_1	109.5	Si2_3—C23_3—H23B_3	109.5
H23A_1—C23_1—H23B_1	109.5	H23A_3—C23_3—H23B_3	109.5
Si2_1—C23_1—H23C_1	109.5	Si2_3—C23_3—H23C_3	109.5
H23A_1—C23_1—H23C_1	109.5	H23A_3—C23_3—H23C_3	109.5
H23B_1—C23_1—H23C_1	109.5	H23B_3—C23_3—H23C_3	109.5
Si2_1—C24_1—H24A_1	109.5	Si2_3—C24_3—H24A_3	109.5
Si2_1—C24_1—H24B_1	109.5	Si2_3—C24_3—H24B_3	109.5
H24A_1—C24_1—H24B_1	109.5	H24A_3—C24_3—H24B_3	109.5
Si2_1—C24_1—H24C_1	109.5	Si2_3—C24_3—H24C_3	109.5
H24A_1—C24_1—H24C_1	109.5	H24A_3—C24_3—H24C_3	109.5
H24B_1—C24_1—H24C_1	109.5	H24B_3—C24_3—H24C_3	109.5
Si2_1—C25_1—H25A_1	109.5	Si2_3—C25_3—H25A_3	109.5
Si2_1—C25_1—H25B_1	109.5	Si2_3—C25_3—H25B_3	109.5
H25A_1—C25_1—H25B_1	109.5	H25A_3—C25_3—H25B_3	109.5
Si2_1—C25_1—H25C_1	109.5	Si2_3—C25_3—H25C_3	109.5
H25A_1—C25_1—H25C_1	109.5	H25A_3—C25_3—H25C_3	109.5
H25B_1—C25_1—H25C_1	109.5	H25B_3—C25_3—H25C_3	109.5
O3_1—C26_1—O2_1	110.0 (3)	O2_3—C26_3—O3_3	110.9 (3)
O3_1—C26_1—C27_1	108.8 (3)	O2_3—C26_3—C27_3	108.5 (3)
O2_1—C26_1—C27_1	110.3 (3)	O3_3—C26_3—C27_3	108.6 (4)
O3_1—C26_1—H26_1	109.2	O2_3—C26_3—H26_3	109.6
O2_1—C26_1—H26_1	109.2	O3_3—C26_3—H26_3	109.6
C27_1—C26_1—H26_1	109.2	C27_3—C26_3—H26_3	109.6
C30_1—C27_1—C28_1	118.0 (4)	C28_3—C27_3—C30_3	118.7 (4)
C30_1—C27_1—C26_1	123.1 (4)	C28_3—C27_3—C26_3	121.8 (4)
C28_1—C27_1—C26_1	118.8 (4)	C30_3—C27_3—C26_3	119.5 (4)
C29_1—C28_1—C27_1	120.7 (4)	C27_3—C28_3—C29_3	121.6 (4)
C29_1—C28_1—H28_1	119.6	C27_3—C28_3—H28_3	119.2
C27_1—C28_1—H28_1	119.6	C29_3—C28_3—H28_3	119.2
C28_1—C29_1—C32_1	121.1 (4)	C32_3—C29_3—C28_3	118.8 (5)
C28_1—C29_1—H29_1	119.4	C32_3—C29_3—H29_3	120.6
C32_1—C29_1—H29_1	119.4	C28_3—C29_3—H29_3	120.6
C27_1—C30_1—C31_1	122.0 (4)	C31_3—C30_3—C27_3	120.3 (4)
C27_1—C30_1—H30_1	119	C31_3—C30_3—H30_3	119.8
C31_1—C30_1—H30_1	119	C27_3—C30_3—H30_3	119.8
C30_1—C31_1—C32_1	119.1 (4)	C32_3—C31_3—C30_3	120.2 (4)
C30_1—C31_1—H31_1	120.4	C32_3—C31_3—H31_3	119.9
C32_1—C31_1—H31_1	120.4	C30_3—C31_3—H31_3	119.9
O4_1—C32_1—C29_1	116.0 (4)	O4_3—C32_3—C31_3	114.8 (4)

O4_1—C32_1—C31_1	125.0 (4)	O4_3—C32_3—C29_3	124.8 (5)
C29_1—C32_1—C31_1	119.0 (4)	C31_3—C32_3—C29_3	120.4 (4)
O4_1—C33_1—H33A_1	109.5	O4_3—C33_3—H33A_3	109.5
O4_1—C33_1—H33B_1	109.5	O4_3—C33_3—H33B_3	109.5
H33A_1—C33_1—H33B_1	109.5	H33A_3—C33_3—H33B_3	109.5
O4_1—C33_1—H33C_1	109.5	O4_3—C33_3—H33C_3	109.5
H33A_1—C33_1—H33C_1	109.5	H33A_3—C33_3—H33C_3	109.5
H33B_1—C33_1—H33C_1	109.5	H33B_3—C33_3—H33C_3	109.5
O1_2—Si1_2—C16_2	103.31 (18)	O1_4—Si1_4—C7_4	104.76 (19)
O1_2—Si1_2—C17_2	109.46 (19)	O1_4—Si1_4—C17_4	107.30 (18)
C16_2—Si1_2—C17_2	109.3 (2)	C7_4—Si1_4—C17_4	110.4 (2)
O1_2—Si1_2—C7_2	108.96 (18)	O1_4—Si1_4—C16_4	108.2 (2)
C16_2—Si1_2—C7_2	111.6 (2)	C7_4—Si1_4—C16_4	114.8 (2)
C17_2—Si1_2—C7_2	113.7 (2)	C17_4—Si1_4—C16_4	110.9 (2)
C24_2—Si2_2—C25_2	110.9 (3)	C6_4—Si2_4—C24_4	109.1 (2)
C24_2—Si2_2—C6_2	109.5 (3)	C6_4—Si2_4—C23_4	107.8 (3)
C25_2—Si2_2—C6_2	112.0 (3)	C24_4—Si2_4—C23_4	110.1 (3)
C24_2—Si2_2—C23_2	108.5 (4)	C6_4—Si2_4—C25_4	109.0 (3)
C25_2—Si2_2—C23_2	108.6 (3)	C24_4—Si2_4—C25_4	109.4 (3)
C6_2—Si2_2—C23_2	107.2 (3)	C23_4—Si2_4—C25_4	111.4 (3)
C1_2—O1_2—Si1_2	126.0 (3)	C1_4—O1_4—Si1_4	123.1 (3)
C26_2—O2_2—C2_2	112.4 (3)	C26_4—O2_4—C2_4	112.2 (3)
C26_2—O3_2—C4_2	110.6 (3)	C26_4—O3_4—C4_4	109.8 (4)
C32_2—O4_2—C33_2	117.5 (4)	C32_4—O4_4—C33_4	116.9 (4)
O1_2—C1_2—C2_2	110.6 (3)	O1_4—C1_4—C2_4	109.7 (3)
O1_2—C1_2—H1A_2	109.5	O1_4—C1_4—H1A_4	109.7
C2_2—C1_2—H1A_2	109.5	C2_4—C1_4—H1A_4	109.7
O1_2—C1_2—H1B_2	109.5	O1_4—C1_4—H1B_4	109.7
C2_2—C1_2—H1B_2	109.5	C2_4—C1_4—H1B_4	109.7
H1A_2—C1_2—H1B_2	108.1	H1A_4—C1_4—H1B_4	108.2
O2_2—C2_2—C1_2	107.0 (3)	O2_4—C2_4—C1_4	106.9 (3)
O2_2—C2_2—C3_2	109.4 (3)	O2_4—C2_4—C3_4	111.1 (4)
C1_2—C2_2—C3_2	114.5 (4)	C1_4—C2_4—C3_4	112.4 (4)
O2_2—C2_2—H2_2	108.6	O2_4—C2_4—H2_4	108.8
C1_2—C2_2—H2_2	108.6	C1_4—C2_4—H2_4	108.8
C3_2—C2_2—H2_2	108.6	C3_4—C2_4—H2_4	108.8
C5_2—C3_2—C4_2	113.1 (3)	C5_4—C3_4—C2_4	111.6 (4)
C5_2—C3_2—C2_2	110.2 (4)	C5_4—C3_4—C4_4	110.2 (4)
C4_2—C3_2—C2_2	109.1 (4)	C2_4—C3_4—C4_4	109.1 (4)
C5_2—C3_2—H3_2	108.1	C5_4—C3_4—H3_4	108.6
C4_2—C3_2—H3_2	108.1	C2_4—C3_4—H3_4	108.6
C2_2—C3_2—H3_2	108.1	C4_4—C3_4—H3_4	108.6
O3_2—C4_2—C3_2	109.8 (3)	O3_4—C4_4—C3_4	109.9 (4)
O3_2—C4_2—H4A_2	109.7	O3_4—C4_4—H4A_4	109.7
C3_2—C4_2—H4A_2	109.7	C3_4—C4_4—H4A_4	109.7
O3_2—C4_2—H4B_2	109.7	O3_4—C4_4—H4B_4	109.7
C3_2—C4_2—H4B_2	109.7	C3_4—C4_4—H4B_4	109.7
H4A_2—C4_2—H4B_2	108.2	H4A_4—C4_4—H4B_4	108.2
C6_2—C5_2—C3_2	176.6 (5)	C6_4—C5_4—C3_4	177.1 (5)
C5_2—C6_2—Si2_2	171.3 (5)	C5_4—C6_4—Si2_4	176.2 (5)
C8_2—C7_2—C9_2	109.8 (4)	C9_4—C7_4—C8_4	107.6 (4)
C8_2—C7_2—C10_2	107.7 (4)	C9_4—C7_4—C10_4	108.8 (4)
C9_2—C7_2—C10_2	107.4 (4)	C8_4—C7_4—C10_4	107.8 (5)
C8_2—C7_2—Si1_2	111.0 (4)	C9_4—C7_4—Si1_4	114.0 (4)

C9_2—C7_2—Si1_2	107.9 (3)	C8_4—C7_4—Si1_4	108.5 (3)
C10_2—C7_2—Si1_2	112.9 (3)	C10_4—C7_4—Si1_4	109.9 (4)
C7_2—C8_2—H8A_2	109.5	C7_4—C8_4—H8A_4	109.5
C7_2—C8_2—H8B_2	109.5	C7_4—C8_4—H8B_4	109.5
H8A_2—C8_2—H8B_2	109.5	H8A_4—C8_4—H8B_4	109.5
C7_2—C8_2—H8C_2	109.5	C7_4—C8_4—H8C_4	109.5
H8A_2—C8_2—H8C_2	109.5	H8A_4—C8_4—H8C_4	109.5
H8B_2—C8_2—H8C_2	109.5	H8B_4—C8_4—H8C_4	109.5
C7_2—C9_2—H9A_2	109.5	C7_4—C9_4—H9A_4	109.5
C7_2—C9_2—H9B_2	109.5	C7_4—C9_4—H9B_4	109.5
H9A_2—C9_2—H9B_2	109.5	H9A_4—C9_4—H9B_4	109.5
C7_2—C9_2—H9C_2	109.5	C7_4—C9_4—H9C_4	109.5
H9A_2—C9_2—H9C_2	109.5	H9A_4—C9_4—H9C_4	109.5
H9B_2—C9_2—H9C_2	109.5	H9B_4—C9_4—H9C_4	109.5
C7_2—C10_2—H10A_2	109.5	C7_4—C10_4—H10A_4	109.5
C7_2—C10_2—H10B_2	109.5	C7_4—C10_4—H10B_4	109.5
H10A_2—C10_2—H10B_2	109.5	H10A_4—C10_4—H10B_4	109.5
C7_2—C10_2—H10C_2	109.5	C7_4—C10_4—H10C_4	109.5
H10A_2—C10_2—H10C_2	109.5	H10A_4—C10_4—H10C_4	109.5
H10B_2—C10_2—H10C_2	109.5	H10B_4—C10_4—H10C_4	109.5
C12_2—C11_2—C16_2	121.6 (4)	C16_4—C11_4—C12_4	121.8 (9)
C12_2—C11_2—H11_2	119.2	C16_4—C11_4—H11_4	119.1
C16_2—C11_2—H11_2	119.2	C12_4—C11_4—H11_4	119.1
C13_2—C12_2—C11_2	120.7 (5)	C13_4—C12_4—C11_4	120.2 (10)
C13_2—C12_2—H12_2	119.7	C13_4—C12_4—H12_4	119.9
C11_2—C12_2—H12_2	119.7	C11_4—C12_4—H12_4	119.9
C12_2—C13_2—C14_2	119.0 (5)	C12_4—C13_4—C14_4	121.7 (8)
C12_2—C13_2—H13_2	120.5	C12_4—C13_4—H13_4	119.1
C14_2—C13_2—H13_2	120.5	C14_4—C13_4—H13_4	119.1
C13_2—C14_2—C15_2	120.7 (5)	C13_4—C14_4—C15_4	117.0 (10)
C13_2—C14_2—H14_2	119.7	C13_4—C14_4—H14_4	121.5
C15_2—C14_2—H14_2	119.7	C15_4—C14_4—H14_4	121.5
C14_2—C15_2—C16_2	121.3 (5)	C16_4—C15_4—C14_4	122.9 (8)
C14_2—C15_2—H15_2	119.3	C16_4—C15_4—H15_4	118.5
C16_2—C15_2—H15_2	119.3	C14_4—C15_4—H15_4	118.5
C11_2—C16_2—C15_2	116.6 (4)	C11_4—C16_4—C15_4	116.2 (6)
C11_2—C16_2—Si1_2	121.2 (3)	C11_4—C16_4—Si1_4	120.5 (5)
C15_2—C16_2—Si1_2	122.2 (4)	C15_4—C16_4—Si1_4	123.1 (4)
C18_2—C17_2—C22_2	116.3 (5)	C22_4—C17_4—C18_4	116.7 (4)
C18_2—C17_2—Si1_2	122.6 (3)	C22_4—C17_4—Si1_4	124.1 (3)
C22_2—C17_2—Si1_2	121.0 (4)	C18_4—C17_4—Si1_4	119.0 (3)
C17_2—C18_2—C19_2	123.1 (5)	C19_4—C18_4—C17_4	121.7 (4)
C17_2—C18_2—H18_2	118.5	C19_4—C18_4—H18_4	119.1
C19_2—C18_2—H18_2	118.5	C17_4—C18_4—H18_4	119.1
C20_2—C19_2—C18_2	120.1 (6)	C20_4—C19_4—C18_4	120.7 (4)
C20_2—C19_2—H19_2	120	C20_4—C19_4—H19_4	119.6
C18_2—C19_2—H19_2	120	C18_4—C19_4—H19_4	119.6
C19_2—C20_2—C21_2	119.4 (5)	C19_4—C20_4—C21_4	119.6 (5)
C19_2—C20_2—H20_2	120.3	C19_4—C20_4—H20_4	120.2
C21_2—C20_2—H20_2	120.3	C21_4—C20_4—H20_4	120.2
C20_2—C21_2—C22_2	120.8 (5)	C22_4—C21_4—C20_4	119.8 (5)
C20_2—C21_2—H21_2	119.6	C22_4—C21_4—H21_4	120.1
C22_2—C21_2—H21_2	119.6	C20_4—C21_4—H21_4	120.1
C17_2—C22_2—C21_2	120.3 (6)	C21_4—C22_4—C17_4	121.3 (5)

C17_2—C22_2—H22_2	119.8	C21_4—C22_4—H22_4	119.3
C21_2—C22_2—H22_2	119.8	C17_4—C22_4—H22_4	119.3
Si2_2—C23_2—H23A_2	109.5	Si2_4—C23_4—H23A_4	109.5
Si2_2—C23_2—H23B_2	109.5	Si2_4—C23_4—H23B_4	109.5
H23A_2—C23_2—H23B_2	109.5	H23A_4—C23_4—H23B_4	109.5
Si2_2—C23_2—H23C_2	109.5	Si2_4—C23_4—H23C_4	109.5
H23A_2—C23_2—H23C_2	109.5	H23A_4—C23_4—H23C_4	109.5
H23B_2—C23_2—H23C_2	109.5	H23B_4—C23_4—H23C_4	109.5
Si2_2—C24_2—H24A_2	109.5	Si2_4—C24_4—H24A_4	109.5
Si2_2—C24_2—H24B_2	109.5	Si2_4—C24_4—H24B_4	109.5
H24A_2—C24_2—H24B_2	109.5	H24A_4—C24_4—H24B_4	109.5
Si2_2—C24_2—H24C_2	109.5	Si2_4—C24_4—H24C_4	109.5
H24A_2—C24_2—H24C_2	109.5	H24A_4—C24_4—H24C_4	109.5
H24B_2—C24_2—H24C_2	109.5	H24B_4—C24_4—H24C_4	109.5
Si2_2—C25_2—H25A_2	109.5	Si2_4—C25_4—H25A_4	109.5
Si2_2—C25_2—H25B_2	109.5	Si2_4—C25_4—H25B_4	109.5
H25A_2—C25_2—H25B_2	109.5	H25A_4—C25_4—H25B_4	109.5
Si2_2—C25_2—H25C_2	109.5	Si2_4—C25_4—H25C_4	109.5
H25A_2—C25_2—H25C_2	109.5	H25A_4—C25_4—H25C_4	109.5
H25B_2—C25_2—H25C_2	109.5	H25B_4—C25_4—H25C_4	109.5
O3_2—C26_2—O2_2	110.5 (4)	O3_4—C26_4—O2_4	111.1 (3)
O3_2—C26_2—C27_2	109.8 (4)	O3_4—C26_4—C27_4	110.6 (4)
O2_2—C26_2—C27_2	108.9 (3)	O2_4—C26_4—C27_4	108.6 (3)
O3_2—C26_2—H26_2	109.2	O3_4—C26_4—H26_4	108.8
O2_2—C26_2—H26_2	109.2	O2_4—C26_4—H26_4	108.8
C27_2—C26_2—H26_2	109.2	C27_4—C26_4—H26_4	108.8
C28_2—C27_2—C30_2	117.9 (4)	C30_4—C27_4—C28_4	118.2 (4)
C28_2—C27_2—C26_2	120.7 (4)	C30_4—C27_4—C26_4	119.8 (4)
C30_2—C27_2—C26_2	121.3 (4)	C28_4—C27_4—C26_4	121.9 (4)
C27_2—C28_2—C29_2	121.8 (4)	C29_4—C28_4—C27_4	120.3 (5)
C27_2—C28_2—H28_2	119.1	C29_4—C28_4—H28_4	119.9
C29_2—C28_2—H28_2	119.1	C27_4—C28_4—H28_4	119.9
C32_2—C29_2—C28_2	118.5 (5)	C32_4—C29_4—C28_4	120.7 (4)
C32_2—C29_2—H29_2	120.7	C32_4—C29_4—H29_4	119.7
C28_2—C29_2—H29_2	120.7	C28_4—C29_4—H29_4	119.7
C31_2—C30_2—C27_2	120.5 (5)	C27_4—C30_4—C31_4	121.8 (4)
C31_2—C30_2—H30_2	119.7	C27_4—C30_4—H30_4	119.1
C27_2—C30_2—H30_2	119.7	C31_4—C30_4—H30_4	119.1
C32_2—C31_2—C30_2	120.8 (5)	C30_4—C31_4—C32_4	118.9 (5)
C32_2—C31_2—H31_2	119.6	C30_4—C31_4—H31_4	120.5
C30_2—C31_2—H31_2	119.6	C32_4—C31_4—H31_4	120.5
C31_2—C32_2—C29_2	120.3 (5)	C29_4—C32_4—O4_4	116.8 (4)
C31_2—C32_2—O4_2	116.0 (4)	C29_4—C32_4—C31_4	120.1 (4)
C29_2—C32_2—O4_2	123.6 (5)	O4_4—C32_4—C31_4	123.0 (5)
O4_2—C33_2—H33A_2	109.5	O4_4—C33_4—H33A_4	109.5
O4_2—C33_2—H33B_2	109.5	O4_4—C33_4—H33B_4	109.5
H33A_2—C33_2—H33B_2	109.5	H33A_4—C33_4—H33B_4	109.5
O4_2—C33_2—H33C_2	109.5	O4_4—C33_4—H33C_4	109.5
H33A_2—C33_2—H33C_2	109.5	H33A_4—C33_4—H33C_4	109.5
H33B_2—C33_2—H33C_2	109.5	H33B_4—C33_4—H33C_4	109.5

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jb0603. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ¹²	U ¹³	U ²³
Si1_1	0.0360 (7)	0.0346 (7)	0.0259 (6)	0.0016 (6)	0.0053 (5)	-0.0018 (5)
Si2_1	0.0439 (8)	0.0454 (9)	0.0508 (7)	0.0066 (7)	0.0044 (6)	0.0141 (6)
O1_1	0.0412 (17)	0.0354 (19)	0.0276 (14)	-0.0009 (15)	0.0094 (13)	-0.0056 (12)
O2_1	0.0333 (16)	0.0354 (18)	0.0273 (14)	0.0066 (14)	0.0042 (12)	0.0007 (12)
O3_1	0.0492 (19)	0.038 (2)	0.0287 (15)	0.0073 (16)	0.0005 (14)	-0.0036 (13)
O4_1	0.0419 (18)	0.050 (2)	0.0447 (17)	0.0086 (17)	0.0052 (15)	0.0156 (15)
C1_1	0.043 (3)	0.032 (3)	0.032 (2)	0.002 (2)	0.0079 (19)	0.0002 (19)
C2_1	0.031 (2)	0.036 (3)	0.029 (2)	0.006 (2)	0.0068 (18)	-0.0012 (18)
C3_1	0.037 (2)	0.040 (3)	0.032 (2)	0.003 (2)	0.002 (2)	0.0012 (19)
C4_1	0.052 (3)	0.032 (3)	0.033 (2)	0.010 (2)	0.003 (2)	-0.0071 (19)
C5_1	0.048 (3)	0.035 (3)	0.031 (2)	0.002 (2)	0.003 (2)	-0.0007 (19)
C6_1	0.057 (3)	0.034 (3)	0.032 (2)	0.003 (3)	0.003 (2)	-0.003 (2)
C7_1	0.043 (3)	0.039 (3)	0.030 (2)	-0.001 (2)	0.003 (2)	-0.0030 (19)
C8_1	0.079 (4)	0.051 (3)	0.036 (3)	-0.023 (3)	0.013 (3)	-0.001 (2)
C9_1	0.043 (3)	0.052 (4)	0.083 (4)	-0.008 (3)	0.010 (3)	-0.011 (3)
C10_1	0.058 (3)	0.039 (3)	0.042 (3)	-0.002 (3)	0.010 (2)	-0.010 (2)
C11_1	0.049 (3)	0.047 (3)	0.044 (3)	-0.009 (3)	0.002 (2)	0.004 (2)
C12_1	0.055 (3)	0.041 (3)	0.055 (3)	0.003 (3)	-0.011 (3)	0.011 (2)
C13_1	0.087 (4)	0.040 (3)	0.032 (2)	-0.003 (3)	-0.006 (3)	0.007 (2)
C14_1	0.078 (4)	0.047 (4)	0.039 (3)	-0.005 (3)	0.022 (3)	0.004 (2)
C15_1	0.053 (3)	0.048 (3)	0.040 (3)	0.002 (3)	0.011 (2)	-0.001 (2)
C16_1	0.040 (3)	0.037 (3)	0.030 (2)	0.000 (2)	-0.002 (2)	-0.0026 (19)
C17_1	0.037 (2)	0.035 (3)	0.032 (2)	-0.002 (2)	0.006 (2)	0.0003 (18)
C18_1	0.043 (3)	0.032 (3)	0.041 (3)	0.003 (2)	0.012 (2)	0.001 (2)
C19_1	0.046 (3)	0.045 (3)	0.049 (3)	0.002 (3)	0.004 (2)	0.008 (2)
C20_1	0.038 (3)	0.052 (4)	0.064 (3)	0.010 (3)	0.006 (3)	0.012 (3)
C21_1	0.051 (3)	0.052 (4)	0.059 (3)	0.007 (3)	0.027 (3)	0.005 (2)
C22_1	0.048 (3)	0.048 (3)	0.037 (2)	0.008 (3)	0.011 (2)	-0.001 (2)
C23_1	0.103 (6)	0.168 (9)	0.079 (5)	0.034 (6)	-0.031 (4)	-0.013 (5)
C24_1	0.078 (5)	0.067 (6)	0.262 (11)	0.020 (4)	0.035 (6)	0.069 (6)
C25_1	0.172 (8)	0.081 (6)	0.159 (7)	0.070 (6)	0.116 (6)	0.059 (5)
C26_1	0.038 (2)	0.034 (3)	0.025 (2)	0.002 (2)	0.0062 (19)	-0.0009 (18)
C27_1	0.034 (2)	0.033 (3)	0.027 (2)	0.002 (2)	0.0024 (18)	-0.0001 (18)
C28_1	0.031 (2)	0.048 (3)	0.031 (2)	0.000 (2)	0.0067 (19)	0.007 (2)
C29_1	0.043 (3)	0.049 (3)	0.026 (2)	0.001 (2)	0.007 (2)	0.010 (2)
C30_1	0.043 (3)	0.036 (3)	0.032 (2)	0.002 (2)	0.007 (2)	0.0048 (19)
C31_1	0.039 (3)	0.047 (3)	0.037 (2)	0.006 (2)	0.011 (2)	0.004 (2)
C32_1	0.041 (3)	0.038 (3)	0.029 (2)	0.004 (2)	0.000 (2)	0.0025 (19)
C33_1	0.048 (3)	0.063 (4)	0.064 (3)	0.015 (3)	0.007 (3)	0.024 (3)
Si1_2	0.0457 (7)	0.0355 (8)	0.0296 (6)	0.0034 (6)	0.0120 (6)	0.0048 (5)
Si2_2	0.0560 (9)	0.0525 (10)	0.0431 (7)	-0.0007 (8)	0.0079 (7)	-0.0106 (6)
O1_2	0.0406 (17)	0.045 (2)	0.0309 (15)	0.0082 (15)	0.0091 (13)	0.0073 (13)
O2_2	0.0428 (17)	0.038 (2)	0.0302 (15)	-0.0029 (15)	0.0091 (13)	0.0040 (13)
O3_2	0.053 (2)	0.049 (2)	0.0380 (17)	-0.0063 (18)	0.0179 (15)	-0.0011 (15)
O4_2	0.084 (3)	0.054 (3)	0.048 (2)	0.000 (2)	-0.0067 (19)	-0.0091 (17)
C1_2	0.042 (3)	0.043 (3)	0.030 (2)	0.001 (2)	0.007 (2)	0.003 (2)
C2_2	0.037 (3)	0.039 (3)	0.029 (2)	-0.002 (2)	0.004 (2)	0.0011 (19)
C3_2	0.046 (3)	0.038 (3)	0.029 (2)	0.000 (2)	0.011 (2)	-0.0010 (19)
C4_2	0.057 (3)	0.056 (3)	0.031 (2)	-0.008 (3)	0.014 (2)	0.002 (2)
C5_2	0.051 (3)	0.043 (3)	0.030 (2)	0.005 (3)	0.014 (2)	0.004 (2)
C6_2	0.055 (3)	0.053 (3)	0.031 (2)	0.000 (3)	0.008 (2)	-0.001 (2)
C7_2	0.052 (3)	0.034 (3)	0.045 (3)	0.002 (2)	0.019 (2)	0.007 (2)

C8_2	0.056 (3)	0.059 (4)	0.090 (4)	-0.006 (3)	0.027 (3)	0.009 (3)
C9_2	0.058 (3)	0.064 (4)	0.043 (3)	-0.012 (3)	0.007 (2)	-0.004 (2)
C10_2	0.101 (5)	0.035 (3)	0.042 (3)	-0.009 (3)	0.024 (3)	0.003 (2)
C11_2	0.048 (3)	0.038 (3)	0.037 (2)	-0.006 (2)	0.006 (2)	0.001 (2)
C12_2	0.038 (3)	0.058 (4)	0.060 (3)	0.000 (3)	0.010 (2)	0.001 (3)
C13_2	0.047 (3)	0.055 (4)	0.074 (4)	0.010 (3)	0.003 (3)	0.016 (3)
C14_2	0.063 (4)	0.065 (4)	0.055 (3)	0.008 (3)	-0.002 (3)	0.019 (3)
C15_2	0.062 (3)	0.054 (4)	0.037 (3)	0.001 (3)	0.011 (2)	0.010 (2)
C16_2	0.051 (3)	0.035 (3)	0.033 (2)	0.000 (2)	0.008 (2)	0.000 (2)
C17_2	0.055 (3)	0.040 (3)	0.035 (2)	0.000 (3)	0.014 (2)	0.002 (2)
C18_2	0.072 (4)	0.048 (4)	0.041 (3)	0.002 (3)	0.012 (3)	-0.002 (2)
C19_2	0.111 (5)	0.047 (4)	0.044 (3)	0.004 (3)	0.009 (3)	-0.008 (2)
C20_2	0.092 (4)	0.056 (4)	0.048 (3)	0.001 (3)	0.020 (3)	-0.017 (3)
C21_2	0.122 (5)	0.058 (4)	0.042 (3)	-0.007 (4)	0.034 (3)	-0.004 (3)
C22_2	0.105 (5)	0.053 (4)	0.046 (3)	0.002 (4)	0.024 (3)	0.001 (3)
C23_2	0.078 (4)	0.082 (5)	0.092 (5)	-0.015 (4)	0.003 (4)	0.013 (4)
C24_2	0.110 (5)	0.093 (6)	0.091 (5)	-0.030 (5)	0.045 (4)	-0.046 (4)
C25_2	0.077 (4)	0.063 (4)	0.067 (3)	-0.004 (3)	0.009 (3)	-0.017 (3)
C26_2	0.042 (3)	0.036 (3)	0.041 (2)	0.005 (2)	0.011 (2)	0.003 (2)
C27_2	0.037 (3)	0.038 (3)	0.038 (2)	0.003 (2)	0.005 (2)	0.001 (2)
C28_2	0.054 (3)	0.055 (4)	0.041 (3)	0.004 (3)	-0.002 (2)	0.004 (2)
C29_2	0.059 (3)	0.041 (3)	0.054 (3)	-0.003 (3)	0.008 (3)	0.005 (2)
C30_2	0.064 (3)	0.043 (3)	0.040 (3)	-0.004 (3)	0.006 (2)	-0.001 (2)
C31_2	0.071 (4)	0.056 (4)	0.036 (3)	-0.004 (3)	0.002 (3)	0.002 (2)
C32_2	0.050 (3)	0.048 (3)	0.039 (3)	0.002 (3)	0.004 (2)	-0.010 (2)
C33_2	0.087 (5)	0.061 (4)	0.068 (4)	-0.010 (4)	-0.004 (3)	-0.019 (3)
Si1_3	0.0427 (7)	0.0344 (7)	0.0273 (6)	0.0037 (6)	0.0053 (5)	-0.0030 (5)
Si2_3	0.0555 (8)	0.0396 (8)	0.0312 (6)	0.0055 (7)	0.0043 (6)	0.0028 (5)
O1_3	0.0471 (18)	0.0394 (19)	0.0278 (14)	0.0004 (15)	0.0070 (14)	-0.0075 (12)
O2_3	0.0349 (16)	0.0363 (18)	0.0267 (14)	0.0054 (14)	0.0068 (12)	0.0002 (12)
O3_3	0.059 (2)	0.039 (2)	0.0260 (15)	0.0079 (16)	0.0014 (14)	-0.0026 (13)
O4_3	0.062 (2)	0.044 (2)	0.0386 (17)	0.0048 (18)	-0.0016 (16)	0.0069 (15)
C1_3	0.043 (3)	0.050 (3)	0.025 (2)	0.006 (2)	0.007 (2)	-0.0080 (19)
C2_3	0.037 (2)	0.028 (3)	0.028 (2)	-0.002 (2)	0.0076 (19)	-0.0005 (17)
C3_3	0.035 (2)	0.033 (3)	0.031 (2)	0.001 (2)	0.0042 (19)	0.0020 (18)
C4_3	0.059 (3)	0.045 (3)	0.023 (2)	0.013 (3)	0.001 (2)	0.003 (2)
C5_3	0.045 (3)	0.044 (3)	0.021 (2)	-0.002 (2)	0.007 (2)	0.000 (2)
C6_3	0.054 (3)	0.043 (3)	0.026 (2)	0.000 (3)	0.004 (2)	-0.001 (2)
C7_3	0.047 (3)	0.040 (3)	0.039 (2)	0.002 (2)	0.003 (2)	-0.003 (2)
C8_3	0.047 (3)	0.060 (5)	0.156 (7)	-0.002 (3)	0.007 (4)	-0.004 (4)
C9_3	0.104 (5)	0.049 (4)	0.064 (3)	-0.023 (4)	0.009 (3)	0.006 (3)
C10_3	0.117 (5)	0.082 (5)	0.055 (3)	-0.036 (4)	0.022 (3)	-0.035 (3)
C11_3	0.062 (3)	0.048 (3)	0.042 (3)	0.014 (3)	0.015 (2)	0.002 (2)
C12_3	0.066 (4)	0.060 (4)	0.051 (3)	0.023 (3)	0.000 (3)	0.013 (3)
C13_3	0.049 (3)	0.061 (4)	0.068 (4)	0.017 (3)	0.006 (3)	-0.005 (3)
C14_3	0.048 (3)	0.068 (4)	0.049 (3)	0.014 (3)	0.012 (2)	-0.006 (3)
C15_3	0.047 (3)	0.050 (3)	0.038 (2)	0.003 (3)	0.006 (2)	-0.003 (2)
C16_3	0.050 (3)	0.037 (3)	0.028 (2)	0.004 (2)	0.007 (2)	-0.0069 (19)
C17_3	0.030 (2)	0.040 (3)	0.028 (2)	0.000 (2)	0.0004 (18)	-0.0026 (19)
C18_3	0.052 (3)	0.042 (3)	0.037 (2)	0.004 (3)	0.006 (2)	-0.002 (2)
C19_3	0.077 (4)	0.032 (3)	0.054 (3)	0.002 (3)	-0.001 (3)	-0.005 (2)
C20_3	0.063 (3)	0.062 (4)	0.039 (3)	-0.002 (3)	0.004 (2)	0.021 (3)
C21_3	0.078 (4)	0.062 (4)	0.038 (3)	0.016 (3)	0.014 (3)	0.010 (3)
C22_3	0.074 (4)	0.048 (3)	0.036 (3)	0.016 (3)	0.010 (2)	0.002 (2)

C23_3	0.062 (3)	0.050 (4)	0.048 (3)	-0.003 (3)	0.020 (2)	-0.009 (2)
C24_3	0.078 (4)	0.065 (4)	0.066 (3)	0.010 (3)	-0.020 (3)	-0.009 (3)
C25_3	0.095 (4)	0.061 (4)	0.050 (3)	0.012 (3)	0.034 (3)	0.011 (3)
C26_3	0.039 (3)	0.035 (3)	0.031 (2)	-0.002 (2)	0.009 (2)	-0.0065 (19)
C27_3	0.035 (2)	0.043 (3)	0.025 (2)	0.000 (2)	0.0073 (18)	0.0006 (19)
C28_3	0.049 (3)	0.043 (3)	0.031 (2)	0.009 (2)	0.008 (2)	-0.005 (2)
C29_3	0.049 (3)	0.046 (3)	0.044 (3)	0.013 (3)	0.011 (2)	-0.003 (2)
C30_3	0.040 (3)	0.040 (3)	0.036 (2)	-0.003 (2)	0.006 (2)	-0.006 (2)
C31_3	0.041 (3)	0.048 (3)	0.033 (2)	-0.006 (3)	-0.001 (2)	-0.004 (2)
C32_3	0.038 (3)	0.048 (3)	0.037 (2)	-0.003 (2)	0.008 (2)	0.003 (2)
C33_3	0.086 (4)	0.059 (4)	0.053 (3)	0.016 (3)	0.004 (3)	0.006 (3)
Si1_4	0.0425 (7)	0.0416 (8)	0.0305 (6)	-0.0066 (6)	0.0023 (5)	0.0007 (5)
Si2_4	0.0500 (8)	0.0407 (9)	0.0478 (7)	-0.0089 (7)	0.0135 (6)	-0.0063 (6)
O1_4	0.0467 (19)	0.044 (2)	0.0314 (15)	-0.0026 (16)	0.0062 (14)	0.0051 (13)
O2_4	0.0440 (18)	0.0382 (19)	0.0269 (15)	-0.0080 (15)	0.0075 (13)	-0.0031 (13)
O3_4	0.050 (2)	0.051 (2)	0.0447 (18)	-0.0118 (17)	0.0175 (16)	-0.0105 (15)
O4_4	0.071 (2)	0.050 (2)	0.056 (2)	-0.010 (2)	0.0100 (18)	-0.0209 (17)
C1_4	0.051 (3)	0.032 (3)	0.034 (2)	-0.002 (2)	0.007 (2)	-0.0042 (19)
C2_4	0.046 (3)	0.030 (3)	0.035 (2)	-0.005 (2)	0.005 (2)	-0.0026 (19)
C3_4	0.039 (3)	0.041 (3)	0.037 (2)	-0.005 (2)	0.006 (2)	-0.001 (2)
C4_4	0.055 (3)	0.055 (4)	0.045 (3)	-0.016 (3)	0.020 (2)	-0.007 (2)
C5_4	0.040 (3)	0.048 (3)	0.040 (2)	-0.009 (2)	0.015 (2)	0.003 (2)
C6_4	0.050 (3)	0.043 (3)	0.040 (3)	-0.005 (3)	0.015 (2)	0.004 (2)
C7_4	0.046 (3)	0.046 (3)	0.044 (3)	-0.009 (2)	0.006 (2)	0.002 (2)
C8_4	0.068 (4)	0.063 (4)	0.052 (3)	0.005 (3)	0.015 (3)	0.000 (3)
C9_4	0.042 (3)	0.081 (5)	0.116 (5)	0.001 (3)	0.008 (3)	-0.004 (4)
C10_4	0.089 (4)	0.064 (4)	0.047 (3)	0.015 (4)	0.001 (3)	0.009 (3)
C11_4	0.075 (5)	0.080 (6)	0.187 (8)	0.005 (4)	-0.032 (5)	-0.075 (6)
C12_4	0.131 (9)	0.084 (7)	0.242 (14)	0.030 (6)	-0.102 (9)	-0.081 (9)
C13_4	0.309 (16)	0.054 (6)	0.051 (4)	-0.039 (8)	-0.042 (7)	-0.004 (4)
C14_4	0.335 (16)	0.096 (7)	0.102 (6)	-0.096 (9)	0.135 (9)	-0.055 (5)
C15_4	0.196 (9)	0.095 (7)	0.101 (5)	-0.087 (6)	0.088 (6)	-0.057 (5)
C16_4	0.079 (4)	0.041 (3)	0.031 (2)	-0.009 (3)	-0.003 (3)	0.003 (2)
C17_4	0.044 (3)	0.036 (3)	0.040 (2)	-0.001 (2)	0.005 (2)	-0.001 (2)
C18_4	0.046 (3)	0.031 (3)	0.037 (2)	-0.002 (2)	0.000 (2)	0.0021 (19)
C19_4	0.046 (3)	0.033 (3)	0.053 (3)	0.001 (2)	-0.009 (3)	0.002 (2)
C20_4	0.036 (3)	0.040 (3)	0.088 (4)	0.004 (2)	0.004 (3)	-0.006 (3)
C21_4	0.054 (3)	0.055 (4)	0.067 (4)	0.003 (3)	0.028 (3)	0.002 (3)
C22_4	0.049 (3)	0.051 (3)	0.045 (3)	-0.006 (3)	0.011 (2)	0.001 (2)
C23_4	0.094 (4)	0.089 (5)	0.045 (3)	-0.031 (4)	0.014 (3)	-0.012 (3)
C24_4	0.052 (3)	0.040 (3)	0.062 (3)	-0.010 (3)	0.017 (3)	-0.007 (2)
C25_4	0.074 (4)	0.052 (4)	0.132 (6)	0.001 (4)	0.036 (4)	0.001 (4)
C26_4	0.039 (3)	0.042 (3)	0.033 (2)	-0.002 (2)	0.007 (2)	-0.003 (2)
C27_4	0.044 (3)	0.043 (3)	0.028 (2)	0.002 (2)	0.006 (2)	-0.005 (2)
C28_4	0.050 (3)	0.047 (3)	0.043 (3)	-0.004 (3)	0.016 (2)	-0.008 (2)
C29_4	0.066 (3)	0.044 (3)	0.035 (2)	0.003 (3)	0.018 (2)	-0.008 (2)
C30_4	0.045 (3)	0.048 (3)	0.035 (2)	0.009 (2)	0.006 (2)	-0.010 (2)
C31_4	0.043 (3)	0.052 (3)	0.044 (3)	0.004 (3)	0.003 (2)	-0.004 (2)
C32_4	0.060 (3)	0.031 (3)	0.035 (2)	-0.002 (2)	0.003 (2)	-0.006 (2)
C33_4	0.084 (5)	0.088 (6)	0.100 (5)	-0.041 (4)	0.016 (4)	-0.042 (4)
