Organometallics

Synthesis and Structure of 1,3,5-Tris(diorganohydroxysilyl)benzenes. Novel Building Blocks in Supramolecular Silanol Chemistry

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Supporting Information

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Table S1. Atomic coordinates and isotropic displacement parameters (in Å ^{2}) for TMSB.

Atom	Wyck.	x	y	z	U
Si1	2*i*	-0.12050(6)	-0.30822(6)	0.43631(5)	
Si2	2*i*	-0.31790(7)	-0.53881(6)	-0.15726(5)	
Si3	2*i*	0.27720(7)	0.06551(6)	0.21626(5)	
O1	2*i*	-0.26591(19)	-0.28316(18)	0.46420(15)	
H1	2*i*	-0.345(2)	-0.337(2)	0.408(2)	0.038(8)
O2	2*i*	-0.43040(18)	-0.49426(18)	-0.25298(15)	
H2	2*i*	-0.392(3)	-0.423(2)	-0.257(2)	0.031(7)
O3	2*i*	0.27367(18)	0.22389(17)	0.27917(16)	
H3	2*i*	0.270(3)	0.248(3)	0.343(2)	0.034(8)
C1	2*i*	-0.0894(2)	-0.2722(2)	0.28183(18)	
C2	2*i*	-0.1991(2)	-0.3880(2)	0.14404(19)	
H2A	2*i*	-0.2917(18)	-0.4786(18)	0.1306(15)	0.012(4)
C3	2*i*	-0.1765(2)	-0.3751(2)	0.02435(18)	
C4	2*i*	-0.0347(2)	-0.2354(2)	0.04883(19)	
H4A	2*i*	-0.0160(19)	-0.2236(18)	-0.0289(16)	0.018(5)
C5	2*i*	0.0802(2)	-0.1146(2)	0.18282(18)	
C6	2*i*	0.0484(2)	-0.1368(2)	0.29785(19)	
H6A	2*i*	0.1305(19)	-0.0542(19)	0.3908(16)	0.016(4)
C11	2*i*	0.0707(3)	-0.1667(3)	0.6019(2)	
H11A	2*i*	0.159(3)	-0.176(2)	0.5925(18)	0.040(6)
H11B	2*i*	0.099(2)	-0.070(2)	0.619(2)	0.043(7)
H11C	2*i*	0.057(2)	-0.184(2)	0.682(2)	0.061(7)
C21	2*i*	-0.1899(3)	-0.5154(3)	0.3945(3)	
H21A	2*i*	-0.293(3)	-0.581(2)	0.316(2)	0.049(7)
H21B	2*i*	-0.205(2)	-0.544(2)	0.467(2)	0.048(6)
H21C	2*i*	-0.110(3)	-0.532(2)	0.373(2)	0.050(7)
C31	2*i*	-0.4725(3)	-0.7173(3)	-0.1511(3)	
H31A	2*i*	-0.416(3)	-0.757(2)	-0.103(2)	0.053(7)
H31B	2*i*	-0.540(3)	-0.696(2)	-0.107(2)	0.050(7)
H31C	2*i*	-0.551(2)	-0.803(2)	-0.245(2)	0.048(6)
C41	2*i*	-0.1892(3)	-0.5757(3)	-0.2414(3)	
H41A	2*i*	-0.256(3)	-0.663(2)	-0.334(2)	0.050(7)
H41B	2*i*	-0.118(2)	-0.487(2)	-0.2486(19)	0.038(6)
H41C	2*i*	-0.126(3)	-0.602(2)	-0.185(2)	0.049(7)
C51	2*i*	0.3028(4)	0.0558(4)	0.0506(3)	
H51A	2*i*	0.310(3)	-0.028(3)	0.016(2)	0.054(8)
H51B	2*i*	0.217(3)	0.050(3)	-0.013(2)	0.059(8)
H51C	2*i*	0.402(3)	0.147(3)	0.072(2)	0.063(8)
C61	2*i*	0.4515(3)	0.0840(3)	0.3485(3)	
H61A	2*i*	0.440(3)	0.095(3)	0.433(2)	0.062(8)
H61B	2*i*	0.455(3)	-0.007(3)	0.317(3)	0.083(10)
H61C	2*i*	0.552(3)	0.167(3)	0.367(2)	0.069(8)

Table S2. Anisotropic displacement parameters (in Å ^{2}) for TMSB.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	0.0238(3)	0.0260(4)	0.0208(3)	0.0101(3)	0.0093(2)	0.0110(3)
Si2	0.0249(3)	0.0236(3)	0.0221(3)	0.0105(3)	0.0084(2)	0.0104(3)
Si3	0.0286(3)	0.0215(4)	0.0265(3)	0.0087(3)	0.0140(3)	0.0107(3)
O1	0.0229(9)	0.0345(10)	0.0225(8)	0.0116(8)	0.0081(7)	0.0082(8)
O2	0.0268(8)	0.0238(9)	0.0324(8)	0.0083(7)	0.0061(6)	0.0153(8)
O3	0.0432(10)	0.0271(9)	0.0272(9)	0.0162(7)	0.0215(8)	0.0148(8)
C1	0.0219(11)	0.0212(12)	0.0226(10)	0.011(1)	0.0098(9)	0.0087(10)
C2	0.0205(11)	0.0214(12)	0.0298(11)	0.0093(10)	0.0127(10)	0.0141(11)
C3	0.0218(11)	0.0227(12)	0.024(1)	0.0126(10)	0.0105(9)	0.0114(10)
C4	0.0294(12)	0.0305(13)	0.0236(11)	0.017(1)	0.0146(10)	0.0159(11)
C5	0.0250(11)	0.0209(12)	0.0244(10)	0.0121(10)	0.0117(9)	0.0111(10)
C6	0.0252(12)	0.0201(12)	0.0223(11)	0.0106(10)	0.0091(10)	0.0062(10)
C11	0.0287(13)	0.0377(17)	0.0289(13)	0.0142(12)	0.011(1)	0.0140(13)
C21	0.0448(17)	0.0369(16)	0.0369(14)	0.0208(14)	0.0184(14)	0.0226(13)
C31	0.0378(14)	0.0262(14)	0.0352(14)	0.0122(12)	0.0140(12)	0.0148(13)
C41	0.0412(15)	0.0425(17)	0.0319(14)	0.0219(14)	0.0151(12)	0.0123(14)
C51	0.0496(18)	0.0365(17)	0.0368(15)	0.0134(15)	0.0268(14)	0.0147(14)
C61	0.0313(15)	0.0375(17)	0.0537(17)	0.0129(14)	0.0157(13)	0.0200(14)

Table S3. Selected geometric parameters (Å, °) for TMSB.

Si1—O1	1.653(2)	C3—C2	1.397(3)
Si1—C11	1.849(4)	C3—C4	1.403(3)
Si1—C21	1.851(3)	C3—Si2	1.867(4)
Si1—C1	1.875(2)	C4—C5	1.390(3)
Si2—O2	1.647(2)	C4—C3	1.403(3)
Si2—C41	1.846(4)	C5—C4	1.390(3)
Si2—C31	1.851(3)	C5—C6	1.407(3)
Si2—C3	1.867(4)	C5—Si3	1.874(3)
Si3—O3	1.645(2)	C6—C1	1.392(3)
Si3—C61	1.850(4)	C6—C5	1.407(3)
Si3—C51	1.851(4)	C11—Si1	1.849(4)
Si3—C5	1.874(3)	C21—Si1	1.851(3)
O1—Si1	1.653(2)	C31—Si2	1.851(3)
O2—Si2	1.647(2)	C41—Si2	1.846(4)
O3—Si3	1.645(2)	C51—Si3	1.851(4)
C1—C6	1.392(3)	C61—Si3	1.850(4)
C1—C2	1.395(3)	O1—H1	0.701(14)
C1—Si1	1.875(2)	O2—H2	0.694(21)
C2—C1	1.395(3)	O3—H3	0.684(25)
C2—C3	1.397(3)		

O1—Si1—C11	105.47(12)	C61—Si3—C51	112.38(13)
O1—Si1—C21	108.10(13)	C61—Si3—C5	107.43(12)
O1—Si1—C1	111.69(9)	C51—Si3—C5	111.42(14)
C11—Si1—C21	112.72(13)	C6—C1—C2	116.90(18)
C11—Si1—C1	111.29(8)	C6—C1—Si1	122.51(15)
C21—Si1—C1	107.59(12)	C2—C1—Si1	120.40(13)
O2—Si2—C41	109.99(13)	C1—C2—C3	123.69(16)
O2—Si2—C31	104.57(12)	C2—C3—C4	116.15(18)
O2—Si2—C3	111.13(8)	C2—C3—Si2	122.32(13)
C41—Si2—C31	111.91(15)	C4—C3—Si2	121.41(14)
C41—Si2—C3	108.35(11)	C5—C4—C3	123.56(18)
C31—Si2—C3	110.89(11)	C4—C5—C6	116.76(16)
O3—Si3—C61	109.15(12)	C4—C5—Si3	123.50(15)
O3—Si3—C51	105.60(13)	C6—C5—Si3	119.62(15)
O3—Si3—C5	110.88(9)	C1—C6—C5	122.93(19)

Table S4. Atomic coordinates and isotropic displacement parameters (in Å ^{2}) for TPSB·H_2O.

Atom	Wyck.	x	y	z	U
C1	4*e*	0.3403(2)	0.10066(11)	0.56015(14)	
C2	4*e*	0.4372(2)	0.13295(12)	0.53231(15)	
H2A	4*e*	0.52050	0.11880	0.55030	0.0330
C3	4*e*	0.4142(2)	0.18532(12)	0.47885(15)	
C4	4*e*	0.28781(19)	0.20575(11)	0.45394(14)	
H4A	4*e*	0.27040	0.24030	0.41800	0.0310
C5	4*e*	0.18599(19)	0.17706(12)	0.48009(15)	
C6	4*e*	0.2154(2)	0.12505(12)	0.53280(15)	
H6A	4*e*	0.14960	0.10520	0.55110	0.0330
C11	4*e*	0.2770(2)	0.02734(14)	0.69793(15)	
C12	4*e*	0.2725(2)	0.08556(15)	0.73960(18)	
H12A	4*e*	0.31120	0.12410	0.72590	0.0580
C13	4*e*	0.2126(3)	0.08856(17)	0.8010(2)	
H13A	4*e*	0.21220	0.12850	0.82810	0.0760
C14	4*e*	0.1535(2)	0.03216(18)	0.82162(18)	
H14A	4*e*	0.11320	0.03360	0.86280	0.0650
C15	4*e*	0.1548(2)	-0.02630(17)	0.78073(19)	
H15A	4*e*	0.11440	-0.06440	0.79410	0.0600
C16	4*e*	0.2158(2)	-0.02885(14)	0.71966(17)	
H16A	4*e*	0.21590	-0.06890	0.69270	0.0530
C21	4*e*	0.5428(2)	0.01436(13)	0.66452(17)	
C22	4*e*	0.6234(2)	-0.01651(14)	0.62688(18)	
H22A	4*e*	0.59170	-0.03330	0.57790	0.0750
C23	4*e*	0.7529(3)	-0.02394(16)	0.6593(2)	
H23A	4*e*	0.80560	-0.04630	0.63250	0.0940
C24	4*e*	0.8005(3)	0.0013(2)	0.7292(2)	
H24A	4*e*	0.88620	-0.00390	0.75150	0.1010
C25	4*e*	0.7231(3)	0.0344(2)	0.7671(2)	
H25A	4*e*	0.75630	0.05360	0.81470	0.1580
C26	4*e*	0.5937(3)	0.03982(19)	0.7349(2)	
H26A	4*e*	0.54100	0.06140	0.76230	0.1150
C31	4*e*	0.5847(2)	0.30879(12)	0.48345(15)	
C32	4*e*	0.7070(2)	0.33523(14)	0.49239(16)	
H32A	4*e*	0.76940	0.30980	0.47680	0.0470
C33	4*e*	0.7381(3)	0.39804(15)	0.52372(18)	
H33A	4*e*	0.82070	0.41400	0.52960	0.0630
C34	4*e*	0.6478(3)	0.43673(15)	0.54612(19)	
H34A	4*e*	0.66830	0.47930	0.56670	0.0800
C35	4*e*	0.5256(3)	0.41213(15)	0.5380(2)	
H35A	4*e*	0.46380	0.43810	0.55340	0.0800
C36	4*e*	0.4953(2)	0.34964(14)	0.50724(17)	
H36A	4*e*	0.41250	0.33400	0.50210	0.0570
C41	4*e*	0.4743(2)	0.23775(15)	0.33357(16)	
C42	4*e*	0.4450(3)	0.29880(16)	0.3002(2)	
H42A	4*e*	0.46410	0.33720	0.33030	0.0840
C43	4*e*	0.3877(4)	0.3063(2)	0.2230(2)	
H43A	4*e*	0.37030	0.34910	0.20250	0.1180
C44	4*e*	0.3568(3)	0.2514(2)	0.1770(2)	
H44A	4*e*	0.31800	0.25600	0.12540	0.0860
C45	4*e*	0.3842(3)	0.1901(2)	0.2087(2)	
H45A	4*e*	0.36420	0.15180	0.17850	0.0880
C46	4*e*	0.4412(3)	0.18327(16)	0.2850(2)	
H46A	4*e*	0.45830	0.14020	0.30480	0.0740
C51	4*e*	0.04602(19)	0.30539(13)	0.47618(17)	
C52	4*e*	0.0688(2)	0.32106(14)	0.55343(17)	
H52A	4*e*	0.06180	0.28730	0.58830	0.0440
C53	4*e*	0.1015(2)	0.38521(16)	0.58083(18)	
H53A	4*e*	0.11630	0.39420	0.63320	0.0580
C54	4*e*	0.1119(2)	0.43556(15)	0.5296(2)	
H54A	4*e*	0.13570	0.47870	0.54720	0.0580
C55	4*e*	0.0870(3)	0.42195(15)	0.4522(2)	
H55A	4*e*	0.09150	0.45630	0.41750	0.0640
C56	4*e*	0.0550(2)	0.35710(15)	0.42550(18)	
H56A	4*e*	0.03950	0.34840	0.37310	0.0510

C61	4*e*	-0.0308(2)	0.21270(12)	0.33998(15)	
C62	4*e*	0.0468(2)	0.20529(14)	0.28723(18)	
H62A	4*e*	0.13260	0.19600	0.30540	0.0580
C63	4*e*	0.0011(2)	0.21119(15)	0.20881(18)	
H63A	4*e*	0.05610	0.20670	0.17540	0.0680
C64	4*e*	-0.1259(3)	0.22372(14)	0.18027(17)	
H64A	4*e*	-0.15710	0.22820	0.12770	0.0580
C65	4*e*	-0.2062(2)	0.22950(14)	0.23031(18)	
H65A	4*e*	-0.29240	0.23700	0.21150	0.0560
C66	4*e*	-0.1592(2)	0.22425(13)	0.30844(17)	
H66A	4*e*	-0.21510	0.22860	0.34130	0.0450
O1	4*e*	0.32768(13)	-0.04330(8)	0.56685(10)	
H1	4*e*	0.26790	-0.03380	0.53160	0.0490
O2	4*e*	0.66915(12)	0.17892(8)	0.45261(10)	
H2	4*e*	0.65190	0.14120	0.46590	0.0430
O3	4*e*	-0.07025(12)	0.17570(8)	0.49108(9)	
H3	4*e*	-0.14230	0.19100	0.47760	0.0410
O4	4*e*	-0.0937(3)	0.04293(17)	0.5299(3)	
Si1	4*e*	0.36958(6)	0.02409(4)	0.62155(5)	
Si2	4*e*	0.53979(6)	0.22634(4)	0.43747(5)	
Si3	4*e*	0.02620(6)	0.21553(4)	0.44558(5)	
H4	4*e*	-0.078(3)	0.0895(17)	0.526(2)	0.150(18)
H5	4*e*	-0.063(3)	0.0232(19)	0.503(3)	0.09(2)

Table S5. Anisotropic displacement parameters (in Å ^{2}) for TPSB·H_2O.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0235(15)	0.0230(17)	0.030(2)	0.0017(13)	0.0072(13)	-0.0016(14)
C2	0.0166(15)	0.0276(18)	0.038(2)	0.0057(13)	0.0033(13)	-0.0053(16)
C3	0.0175(14)	0.0248(18)	0.035(2)	0.0019(12)	0.0057(13)	-0.0014(15)
C4	0.0244(14)	0.0244(17)	0.0281(19)	0.0032(13)	0.0047(12)	0.0031(14)
C5	0.0211(14)	0.0233(17)	0.0288(19)	0.0003(13)	0.0078(13)	-0.0006(15)
C6	0.0223(15)	0.0295(18)	0.032(2)	-0.0049(13)	0.0101(13)	-0.0025(15)
C11	0.0285(15)	0.0245(18)	0.040(2)	0.0001(14)	0.0094(14)	0.0031(17)
C12	0.0511(19)	0.049(2)	0.052(3)	-0.0087(16)	0.0280(19)	-0.001(2)
C13	0.072(2)	0.062(3)	0.065(3)	-0.011(2)	0.035(2)	-0.009(2)
C14	0.0405(18)	0.071(3)	0.054(3)	0.0020(19)	0.0191(17)	0.014(2)
C15	0.0372(18)	0.054(3)	0.060(3)	-0.0004(17)	0.0159(18)	0.023(2)
C16	0.0406(18)	0.032(2)	0.060(3)	0.0036(15)	0.0116(17)	0.0080(19)
C21	0.0291(16)	0.0312(19)	0.037(2)	0.0045(14)	0.0087(15)	0.0058(16)
C22	0.0367(19)	0.070(3)	0.080(3)	0.0007(17)	0.0144(19)	-0.037(2)
C23	0.037(2)	0.078(3)	0.125(4)	0.014(2)	0.028(2)	-0.019(3)
C24	0.031(2)	0.144(4)	0.071(3)	0.014(2)	-0.002(2)	0.021(3)
C25	0.046(2)	0.286(6)	0.055(3)	0.022(3)	-0.007(2)	-0.036(4)
C26	0.041(2)	0.187(4)	0.056(3)	0.027(2)	0.0010(19)	-0.035(3)
C31	0.0276(15)	0.0233(18)	0.035(2)	0.0028(13)	0.0059(14)	0.0024(15)
C32	0.0361(18)	0.025(2)	0.054(2)	-0.0015(14)	0.0043(15)	-0.0006(17)
C33	0.046(2)	0.039(2)	0.066(3)	-0.0083(17)	-0.0026(18)	0.004(2)
C34	0.094(3)	0.033(2)	0.072(3)	-0.017(2)	0.017(2)	-0.018(2)
C35	0.082(3)	0.037(2)	0.095(3)	-0.0010(19)	0.048(2)	-0.019(2)
C36	0.0483(19)	0.029(2)	0.071(3)	-0.0056(16)	0.0254(18)	-0.0076(18)
C41	0.0258(16)	0.033(2)	0.038(2)	-0.0050(14)	0.0147(14)	0.0019(18)
C42	0.110(3)	0.050(3)	0.039(3)	-0.017(2)	-0.005(2)	0.002(2)
C43	0.160(4)	0.068(3)	0.050(3)	-0.015(3)	-0.012(3)	0.014(3)
C44	0.075(3)	0.098(4)	0.039(3)	-0.009(2)	0.005(2)	0.010(3)
C45	0.097(3)	0.077(3)	0.043(3)	-0.018(2)	0.011(2)	-0.019(2)
C46	0.086(2)	0.050(3)	0.046(3)	0.002(2)	0.009(2)	-0.002(2)
C51	0.0165(14)	0.0288(19)	0.031(2)	0.0024(12)	0.0045(13)	0.0057(16)
C52	0.0388(17)	0.028(2)	0.039(2)	-0.0017(14)	-0.0019(15)	0.0044(17)
C53	0.0475(19)	0.046(2)	0.044(2)	-0.0027(16)	-0.0047(17)	-0.004(2)
C54	0.0511(19)	0.030(2)	0.062(3)	-0.0034(15)	0.009(2)	-0.003(2)
C55	0.071(2)	0.031(2)	0.060(3)	-0.0044(17)	0.018(2)	0.012(2)
C56	0.0496(19)	0.033(2)	0.046(2)	0.0010(15)	0.0109(16)	-0.0011(19)
C61	0.0237(15)	0.0299(18)	0.040(2)	-0.0003(13)	0.0081(14)	0.0010(16)
C62	0.0300(16)	0.071(3)	0.042(2)	-0.0002(15)	0.0052(17)	-0.0072(19)
C63	0.0409(19)	0.093(3)	0.040(3)	-0.0116(18)	0.0145(17)	-0.009(2)
C64	0.054(2)	0.059(2)	0.029(2)	-0.0091(18)	0.0005(17)	-0.0031(18)
C65	0.0400(18)	0.050(2)	0.043(3)	0.0017(16)	-0.0026(18)	-0.0032(19)
C66	0.0320(17)	0.043(2)	0.038(2)	0.0011(14)	0.0076(15)	-0.0014(17)
O1	0.0382(10)	0.0292(13)	0.0501(15)	0.0033(9)	-0.0016(9)	-0.004(1)
O2	0.0226(9)	0.0211(11)	0.0653(15)	-0.0005(8)	0.0143(9)	0.0085(10)
O3	0.0177(9)	0.0334(12)	0.0516(14)	0.0017(8)	0.0089(9)	0.0068(10)
O4	0.0459(15)	0.040(2)	0.182(4)	-0.0102(15)	-0.015(2)	0.023(2)
Si1	0.0283(4)	0.0285(5)	0.0404(6)	0.0009(4)	0.0065(4)	0.0009(5)
Si2	0.0211(4)	0.0285(5)	0.0417(6)	-0.0002(4)	0.0087(4)	0.0002(5)
Si3	0.0198(4)	0.0306(5)	0.0375(6)	0.0000(4)	0.0051(4)	0.0013(5)

Table S6. Selected geometric parameters (Å, °) for TPSB·H_2O.

C1—C2	1.404(5)	C42—C41	1.359(4)
C1—C6	1.415(5)	C42—C43	1.391(7)
C1—Si1	1.863(3)	C43—C44	1.364(6)
C2—C3	1.398(4)	C43—C42	1.391(7)
C2—C1	1.404(5)	C44—C45	1.350(6)
C3—C2	1.398(4)	C44—C43	1.364(6)
C3—C4	1.399(4)	C45—C44	1.350(6)
C3—Si2	1.862(5)	C45—C46	1.374(7)
C4—C3	1.399(4)	C46—C45	1.374(7)
C4—C5	1.402(4)	C46—C41	1.385(5)
C5—C6	1.388(4)	C51—C52	1.382(5)
C5—C4	1.402(4)	C51—C56	1.386(4)
C5—Si3	1.864(5)	C51—Si3	1.868(3)
C6—C5	1.388(4)	C52—C51	1.382(5)
C6—C1	1.415(5)	C52—C53	1.385(4)
C11—C12	1.382(4)	C53—C54	1.376(5)
C11—C16	1.394(4)	C53—C52	1.385(4)
C11—Si1	1.853(6)	C54—C55	1.375(5)
C12—C11	1.382(4)	C54—C53	1.376(5)
C12—C13	1.386(6)	C55—C54	1.375(5)
C13—C14	1.378(5)	C55—C56	1.393(4)
C13—C12	1.386(6)	C56—C51	1.386(4)
C14—C15	1.374(5)	C56—C55	1.393(4)
C14—C13	1.378(5)	C61—C62	1.393(6)
C15—C14	1.374(5)	C61—C66	1.396(5)
C15—C16	1.388(6)	C61—Si3	1.852(6)
C16—C15	1.388(6)	C62—C63	1.384(6)
C16—C11	1.394(4)	C62—C61	1.393(6)
C21—C22	1.353(5)	C63—C64	1.377(5)
C21—C26	1.355(6)	C63—C62	1.384(6)
C21—Si1	1.870(6)	C64—C65	1.374(6)
C22—C21	1.353(5)	C64—C63	1.377(5)
C22—C23	1.399(6)	C65—C64	1.374(6)
C23—C24	1.340(6)	C65—C66	1.380(6)
C23—C22	1.399(6)	C66—C65	1.380(6)
C24—C23	1.340(6)	C66—C61	1.396(5)
C24—C25	1.351(6)	O1—Si1	1.662(3)
C25—C24	1.351(6)	O2—Si2	1.657(2)
C25—C26	1.394(6)	O3—Si3	1.651(4)
C26—C21	1.355(6)	Si1—O1	1.662(3)
C26—C25	1.394(6)	Si1—C11	1.853(6)
C31—C36	1.394(4)	Si1—C1	1.863(3)
C31—C32	1.396(3)	Si1—C21	1.870(6)
C31—Si2	1.851(3)	Si2—O2	1.657(2)
C32—C33	1.380(4)	Si2—C41	1.850(6)
C32—C31	1.396(3)	Si2—C31	1.851(3)
C33—C34	1.365(5)	Si2—C3	1.862(5)
C33—C32	1.380(4)	Si3—O3	1.651(4)
C34—C33	1.365(5)	Si3—C61	1.852(6)
C34—C35	1.383(5)	Si3—C5	1.864(5)
C35—C36	1.370(4)	Si3—C51	1.868(3)
C35—C34	1.383(5)	O1—H1	0.820(4)
C36—C35	1.370(4)	O2—H2	0.820(2)
C36—C31	1.394(4)	O3—H3	0.820(2)
C41—C42	1.359(4)	O4—H4	0.947(34)
C41—C46	1.385(5)	O4—H5	0.749(48)
C41—Si2	1.850(6)		

C2—C1—C6	116.46(20)	C41—C42—C43	122.77(31)
C2—C1—Si1	122.45(18)	C44—C43—C42	120.59(33)
C6—C1—Si1	120.78(17)	C45—C44—C43	117.93(37)
C3—C2—C1	123.04(22)	C44—C45—C46	121.01(33)
C2—C3—C4	116.83(21)	C45—C46—C41	122.83(31)
C2—C3—Si2	123.97(18)	C52—C51—C56	117.38(27)
C4—C3—Si2	119.16(17)	C52—C51—Si3	119.46(21)

C3—C4—C5	123.63(20)	C56—C51—Si3	122.64(21)
C6—C5—C4	116.55(21)	C51—C52—C53	122.48(27)
C6—C5—Si3	126.19(18)	C54—C53—C52	119.16(28)
C4—C5—Si3	117.15(16)	C55—C54—C53	119.77(31)
C5—C6—C1	123.46(22)	C54—C55—C56	120.42(30)
C12—C11—C16	116.70(25)	C51—C56—C55	120.75(27)
C12—C11—Si1	120.69(20)	C62—C61—C66	115.56(21)
C16—C11—Si1	122.49(19)	C62—C61—Si3	124.95(21)
C11—C12—C13	122.43(27)	C66—C61—Si3	119.27(19)
C14—C13—C12	119.70(29)	C63—C62—C61	122.51(27)
C15—C14—C13	119.32(31)	C64—C63—C62	119.95(25)
C14—C15—C16	120.49(27)	C65—C64—C63	119.29(27)
C15—C16—C11	121.35(24)	C64—C65—C66	120.18(27)
C22—C21—C26	116.94(28)	C65—C66—C61	122.46(24)
C22—C21—Si1	122.28(18)	O1—Si1—C11	109.74(11)
C26—C21—Si1	120.76(22)	O1—Si1—C1	108.91(10)
C21—C22—C23	122.15(24)	O1—Si1—C21	106.2(1)
C24—C23—C22	119.62(31)	C11—Si1—C1	110.68(12)
C23—C24—C25	119.55(34)	C11—Si1—C21	110.46(11)
C24—C25—C26	120.11(32)	C1—Si1—C21	110.74(11)
C21—C26—C25	121.56(31)	O2—Si2—C41	111.13(10)
C36—C31—C32	116.26(20)	O2—Si2—C31	107.53(10)
C36—C31—Si2	121.27(19)	O2—Si2—C3	110.08(9)
C32—C31—Si2	122.37(18)	C41—Si2—C31	110.02(13)
C33—C32—C31	121.92(25)	C41—Si2—C3	107.25(12)
C34—C33—C32	120.13(28)	C31—Si2—C3	110.86(11)
C33—C34—C35	119.47(31)	O3—Si3—C61	112.21(10)
C36—C35—C34	120.21(28)	O3—Si3—C5	105.95(9)
C35—C36—C31	122.00(26)	O3—Si3—C51	111.13(10)
C42—C41—C46	114.88(28)	C61—Si3—C5	113.90(11)
C42—C41—Si2	123.44(23)	C61—Si3—C51	108.56(12)
C46—C41—Si2	121.46(23)	C5—Si3—C51	104.87(11)