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Supporting Information

Molecular Tectonics. Hydrogen-Bonded Networks Built from Tetraphenols Derived from Tetraphenylmethane and Tetraphenylsilane

Jean-Hugues Fournier,[1] Thierry Maris, Michel Simard, and James D. Wuest*

Département de Chimie, Université de Montréal
Montréal, Québec H3C 3J7 Canada

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*Author to whom correspondence may be addressed: wuest@chimie.umontreal.ca

Université de Montréal

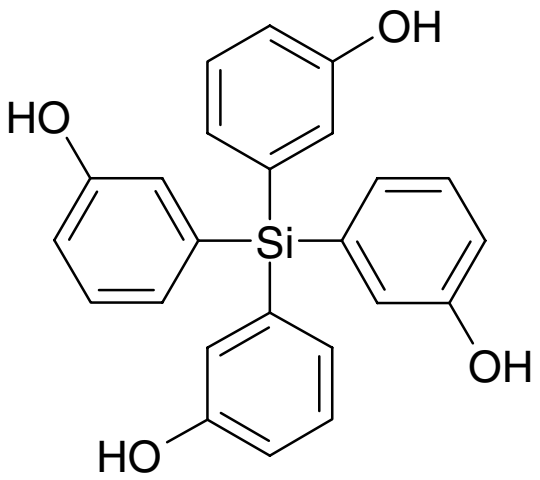
CRYSTAL AND MOLECULAR STRUCTURE OF

C24 H20 O4 Si COMPOUND (JIW376)

Equipe WUEST

Département de chimie, Université de Montréal,

C.P. 6128, Succ. Centre-Ville, Montréal, Québec, H3C 3J7 (Canada)



Structure solved and refined in the laboratory of X-ray diffraction, Université de Montréal by Dr. Thierry Maris.

Table 1. Crystal data and structure refinement for C24 H20 O4 Si.

Identification code	JIW376
Empirical formula	C24 H20 O4 Si
Formula weight	400.49
Temperature	226(2) K
Wavelength	1.54178 Å
Crystal system	Tetragonal
Space group	$I4_1/a$
Unit cell dimensions	a = 17.1641(2) Å α = 90° b = 17.1641(2) Å β = 90° c = 7.26760(10) Å γ = 90°
Volume	2141.08(5)Å^3
Z	4
Density (calculated)	1.242 Mg/m^3
Absorption coefficient	1.188 mm^{-1}
F(000)	840
Crystal size	0.50 x 0.50 x 0.30 mm
Theta range for data collection	5.15 to 72.81°
Index ranges	$-21 \le h \le 21$, $-20 \le k \le 17$, $-8 \le \ell \le 8$
Reflections collected	12866
Independent reflections	1062 [R_{int} = 0.064]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.4900
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1062 / 0 / 67
Goodness-of-fit on F^2	1.157
Final R indices [I>2sigma(I)]	R_1 = 0.0445, wR_2 = 0.1319
R indices (all data)	R_1 = 0.0446, wR_2 = 0.1321
Extinction coefficient	0.0016(5)
Largest diff. peak and hole	0.315 and -0.164 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for C24 H20 O4 Si.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U_{eq}
Si(1)	0	2500	6250	26(1)
O(12)	1688(1)	4785(1)	3539(2)	50(1)
C(10)	165(1)	3367(1)	4731(2)	29(1)
C(11)	862(1)	3777(1)	4764(2)	30(1)
C(12)	990(1)	4395(1)	3562(2)	34(1)
C(13)	415(1)	4626(1)	2353(2)	42(1)
C(14)	-286(1)	4226(1)	2328(3)	48(1)
C(15)	-407(1)	3596(1)	3474(2)	41(1)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for C24 H20 O4 Si.

	x	y	z	U_{eq}
H(12)	1984	4594	4322	74
H(11)	1252	3637	5587	39
H(13)	496	5043	1559	55
H(14)	-682	4383	1540	62
H(15)	-868	3313	3399	53

Table 4. Anisotropic parameters (Å^2 x 10^3) for C24 H20 O4 Si.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Si(1)	23(1)	23(1)	33(1)	0	0	0
O(12)	34(1)	43(1)	72(1)	25(1)	-9(1)	-11(1)
C(10)	28(1)	25(1)	34(1)	0(1)	0(1)	0(1)
C(11)	27(1)	26(1)	38(1)	3(1)	-1(1)	2(1)
C(12)	29(1)	27(1)	45(1)	4(1)	1(1)	-3(1)
C(13)	46(1)	38(1)	43(1)	14(1)	-6(1)	-5(1)
C(14)	42(1)	54(1)	46(1)	16(1)	-17(1)	-8(1)
C(15)	35(1)	44(1)	45(1)	8(1)	-10(1)	-10(1)

Table 5. Bond lengths [Å] and angles [°] for C24 H20 O4 Si

Si(1)-C(10)#1	1.8740(14)	C(10)-Si(1)-C(10)#2	110.32(4)
Si(1)-C(10)	1.8740(14)	C(10)#1-Si(1)-C(10)#3	110.32(4)
Si(1)-C(10)#2	1.8740(14)	C(10)-Si(1)-C(10)#3	110.32(5)
Si(1)-C(10)#3	1.8740(14)	C(10)#2-Si(1)-C(10)#3	107.80(9)
O(12)-C(12)	1.374(2)	C(11)-C(10)-C(15)	118.30(13)
C(10)-C(11)	1.389(2)	C(11)-C(10)-Si(1)	121.45(11)
C(10)-C(15)	1.397(2)	C(15)-C(10)-Si(1)	120.20(11)
C(11)-C(12)	1.392(2)	C(10)-C(11)-C(12)	120.72(13)
C(12)-C(13)	1.379(2)	O(12)-C(12)-C(13)	118.43(14)
C(13)-C(14)	1.386(3)	O(12)-C(12)-C(11)	121.11(14)
C(14)-C(15)	1.380(2)	C(13)-C(12)-C(11)	120.46(14)
		C(12)-C(13)-C(14)	119.14(15)
C(10)#1-Si(1)-C(10)	107.80(9)	C(15)-C(14)-C(13)	120.70(15)
C(10)#1-Si(1)-C(10)#2	110.32(5)	C(14)-C(15)-C(10)	120.63(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1/2,z #2 -y+1/4,x+1/4,-z+5/4 #3 y-1/4,-x+1/4,-z+5/4

Table 6. Torsion angles [°] for C24 H20 O4 Si.

C(10)#1-Si(1)-C(10)-C(11	-118.12(13)	C(10)-C(11)-C(12)-O(12)	-177.58(15)
C(10)#2-Si(1)-C(10)-C(11)	121.37(15)	C(10)-C(11)-C(12)-C(13)	2.0(2)
C(10)#3-Si(1)-C(10)-C(11)	2.39(12)	O(12)-C(12)-C(13)-C(14)	178.43(18)
C(10)#1-Si(1)-C(10)-C(15)	59.25(12)	C(11)-C(12)-C(13)-C(14)	-1.1(3)
C(10)#2-Si(1)-C(10)-C(15)	-61.26(10)	C(12)-C(13)-C(14)-C(15)	-1.0(3)
C(10)#3-Si(1)-C(10)-C(15)	179.75(14)	C(13)-C(14)-C(15)-C(10)	2.3(3)
C(15)-C(10)-C(11)-C(12)	-0.7(2)	C(11)-C(10)-C(15)-C(14)	-1.4(3)
Si(1)-C(10)-C(11)-C(12)	176.75(12)	Si(1)-C(10)-C(15)-C(14)	-178.90(15)

Symmetry transformations used to generate equivalent atoms:

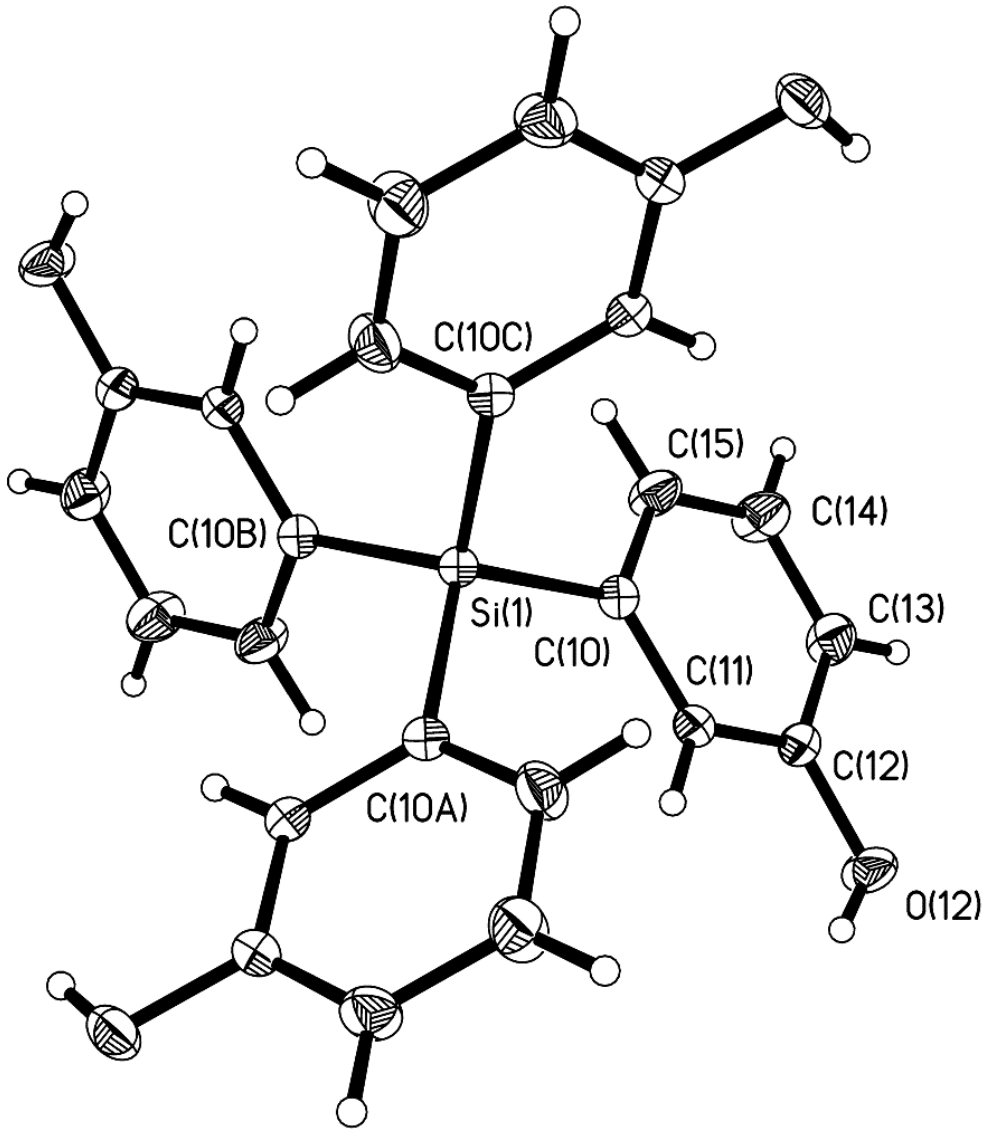
#1 -x,-y+1/2,z #2 -y+1/4,x+1/4,-z+5/4 #3 y-1/4,-x+1/4,-z+5/4

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C24 H20 O4 Si.

D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(12)-H(12)	O(12)#4	0.83	1.90	2.7304(13)	176.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1/2,z #2 -y+1/4,x+1/4,-z+5/4
#3 y-1/4,-x+1/4,-z+5/4 #4 -y+3/4,x+1/4,z+1/4



ORTEP view of the C24 H20 O4 Si compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogens represented by sphere of arbitrary size.

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Université de Montréal

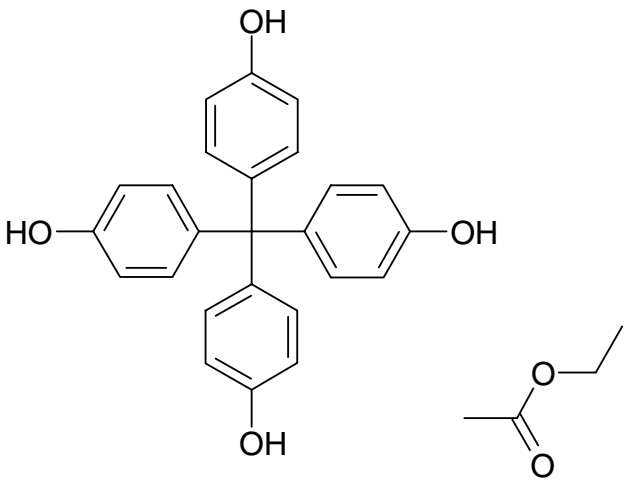
CRYSTAL AND MOLECULAR STRUCTURE OF

C29 H28 O6 COMPOUND (JIW226)

Equipe WUEST

Département de chimie, Université de Montréal,

C.P. 6128, Succ. Centre-Ville, Montréal, Québec, H3C 3J7 (Canada)



Structure solved and refined in the laboratory of X-ray diffraction, Université de Montréal by Dr. Thierry Maris.

Table 1. Crystal data and structure refinement for C29 H28 O6.

Identification code	JIW226
Empirical formula	C29 H28 O6
Formula weight	472.51
Temperature	223(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 10.243(4) Å α = 90° b = 15.673(6) Å β = 100.86(4)° c = 15.412(8) Å γ = 90°
Volume	2429.9(18)Å^3
Z	4
Density (calculated)	1.292 Mg/m^3
Absorption coefficient	0.732 mm^{-1}
F(000)	1000
Crystal size	0.24 x 0.22 x 0.20 mm
Theta range for data collection	4.06 to 70.02°
Index ranges	$0 \le h \le 12$, $0 \le k \le 19$, $-18 \le \ell \le 18$
Reflections collected	4603
Independent reflections	4603 [R_{int} = 0.040]
Absorption correction	None
Max. and min. transmission	0.8700 and 0.8400
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4603 / 0 / 317
Goodness-of-fit on F^2	1.117
Final R indices [I>2sigma(I)]	R_1 = 0.0584, wR_2 = 0.1740
R indices (all data)	R_1 = 0.0715, wR_2 = 0.1835
Extinction coefficient	0.0034(5)
Largest diff. peak and hole	0.470 and -0.452 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for C29 H28 O6.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U_{eq}
C(1)	2620(2)	2742(1)	-59(1)	32(1)
O(14)	3353(2)	5148(1)	-2715(1)	47(1)
C(11)	2748(2)	3358(1)	-823(1)	34(1)
C(12)	3869(2)	3889(1)	-714(1)	39(1)
C(13)	4057(2)	4473(1)	-1349(2)	40(1)
C(14)	3111(2)	4556(1)	-2115(1)	38(1)
C(15)	1985(2)	4052(1)	-2227(1)	42(1)
C(16)	1809(2)	3462(1)	-1586(1)	39(1)
O(24)	-1585(1)	292(1)	-737(1)	40(1)
C(21)	1395(2)	2149(1)	-258(1)	33(1)
C(22)	1223(2)	1615(1)	-996(1)	37(1)
C(23)	224(2)	1012(1)	-1152(1)	37(1)
C(24)	-628(2)	915(1)	-557(1)	34(1)
C(25)	-470(2)	1419(1)	185(1)	38(1)
C(26)	538(2)	2027(1)	332(1)	36(1)
O(34)	6841(1)	293(1)	496(1)	40(1)
C(31)	3807(2)	2116(1)	114(1)	33(1)
C(32)	4620(2)	1981(1)	-501(1)	36(1)
C(33)	5622(2)	1369(1)	-368(1)	37(1)
C(34)	5834(2)	887(1)	388(1)	33(1)
C(35)	5016(2)	990(1)	1008(1)	37(1)
C(36)	4007(2)	1587(1)	858(1)	37(1)
O(44)	2273(2)	5046(1)	2768(1)	53(1)
C(41)	2549(2)	3337(1)	729(1)	34(1)
C(42)	3514(2)	3390(1)	1486(1)	40(1)
C(43)	3419(2)	3966(2)	2156(2)	44(1)
C(44)	2342(2)	4507(1)	2074(1)	40(1)
C(45)	1368(2)	4483(1)	1320(2)	43(1)
C(46)	1483(2)	3908(1)	658(2)	41(1)
O(50)	8541(2)	1662(1)	2365(1)	62(1)
O(51)	7587(3)	2910(2)	2501(2)	105(1)
C(50)	7308(5)	1880(3)	3499(3)	127(2)
C(52)	7867(3)	2124(2)	2729(2)	62(1)
C(53)	8327(4)	3308(3)	1776(3)	102(1)
C(54)	7365(5)	3245(3)	1077(4)	167(3)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for C29 H28 O6.

	x	y	z	U_{eq}
H(14)	2711	5168	-3133	71
H(12)	4511	3845	-193	47
H(13)	4826	4814	-1262	48
H(15)	1332	4109	-2742	50
H(16)	1034	3127	-1674	46
H(24)	-1982	249	-317	60
H(22)	1803	1668	-1398	45
H(23)	121	668	-1660	45
H(25)	-1041	1354	591	45
H(26)	642	2365	844	44
H(34)	7074	180	1029	59
H(32)	4488	2311	-1019	43
H(33)	6153	1287	-797	44
H(35)	5150	657	1524	44
H(36)	3438	1639	1267	44
H(44)	1843	5479	2581	79
H(42)	4256	3027	1549	48
H(43)	4088	3986	2665	53
H(45)	634	4853	1259	51
H(46)	825	3900	143	49
H(51A)	7874	1455	3840	191
H(51B)	6425	1644	3305	191
H(51C)	7252	2378	3864	191
H(53A)	8586	3903	1909	123
H(53B)	9110	2974	1709	123
H(54A)	7671	3469	564	250
H(54B)	6600	3568	1176	250
H(54C)	7119	2650	978	250

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C29 H28 O6.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	30(1)	33(1)	33(1)	0(1)	5(1)	-1(1)
O(14)	49(1)	46(1)	48(1)	13(1)	11(1)	2(1)
C(11)	32(1)	32(1)	36(1)	0(1)	6(1)	2(1)
C(12)	36(1)	38(1)	40(1)	4(1)	1(1)	-2(1)
C(13)	36(1)	35(1)	48(1)	4(1)	5(1)	-3(1)
C(14)	40(1)	32(1)	43(1)	5(1)	10(1)	6(1)
C(15)	39(1)	43(1)	40(1)	4(1)	2(1)	4(1)
C(16)	31(1)	40(1)	43(1)	2(1)	4(1)	-1(1)
O(24)	37(1)	37(1)	46(1)	-4(1)	9(1)	-6(1)
C(21)	29(1)	31(1)	37(1)	0(1)	5(1)	0(1)
C(22)	35(1)	40(1)	39(1)	-4(1)	11(1)	-2(1)
C(23)	38(1)	37(1)	38(1)	-7(1)	9(1)	-2(1)
C(24)	28(1)	30(1)	42(1)	-1(1)	4(1)	1(1)
C(25)	36(1)	40(1)	39(1)	-5(1)	12(1)	-2(1)
C(26)	38(1)	35(1)	37(1)	-6(1)	9(1)	-3(1)
O(34)	36(1)	37(1)	46(1)	6(1)	8(1)	5(1)
C(31)	29(1)	32(1)	36(1)	1(1)	5(1)	-3(1)
C(32)	36(1)	35(1)	36(1)	5(1)	8(1)	1(1)
C(33)	36(1)	37(1)	38(1)	3(1)	11(1)	1(1)
C(34)	28(1)	29(1)	42(1)	1(1)	6(1)	-3(1)
C(35)	38(1)	35(1)	39(1)	8(1)	9(1)	-1(1)
C(36)	34(1)	37(1)	42(1)	5(1)	12(1)	0(1)
O(44)	75(1)	41(1)	44(1)	-9(1)	12(1)	-6(1)
C(41)	33(1)	32(1)	37(1)	1(1)	6(1)	-5(1)
C(42)	34(1)	41(1)	43(1)	0(1)	3(1)	-1(1)
C(43)	46(1)	45(1)	39(1)	-1(1)	1(1)	-8(1)
C(44)	53(1)	32(1)	38(1)	-4(1)	13(1)	-12(1)
C(45)	43(1)	36(1)	49(1)	-5(1)	9(1)	0(1)
C(46)	39(1)	38(1)	43(1)	-6(1)	0(1)	1(1)
O(50)	63(1)	48(1)	79(1)	-7(1)	25(1)	4(1)
O(51)	154(3)	56(1)	125(2)	12(1)	73(2)	32(2)
C(50)	208(6)	66(2)	144(4)	2(2)	126(4)	18(3)
C(52)	63(2)	44(1)	82(2)	-12(1)	24(2)	-2(1)
C(53)	70(2)	80(2)	151(4)	-35(3)	6(2)	7(2)
C(54)	118(4)	143(5)	206(6)	-94(5)	-54(4)	32(3)

Table 5. Bond lengths [Å] and angles [°] for C29 H28 O6

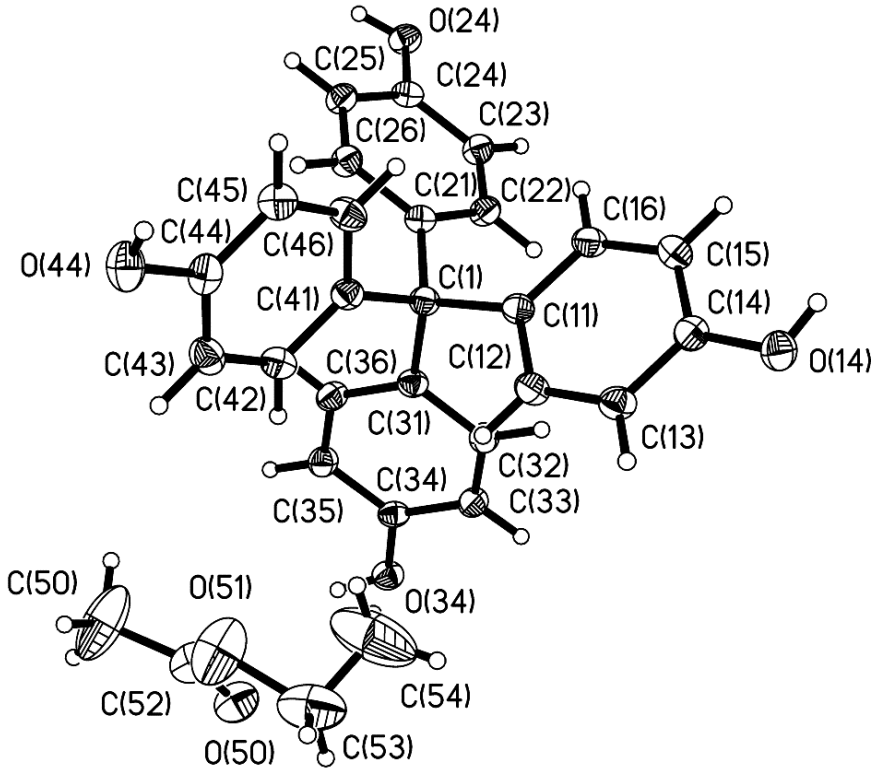
C(1)-C(41)	1.544(3)	C(16)-C(11)-C(12)	117.07(19)
C(1)-C(21)	1.545(3)	C(16)-C(11)-C(1)	125.17(18)
C(1)-C(31)	1.546(3)	C(12)-C(11)-C(1)	117.66(17)
C(1)-C(11)	1.548(3)	C(13)-C(12)-C(11)	121.98(19)
O(14)-C(14)	1.364(3)	C(12)-C(13)-C(14)	119.9(2)
C(11)-C(16)	1.382(3)	O(14)-C(14)-C(15)	123.9(2)
C(11)-C(12)	1.402(3)	O(14)-C(14)-C(13)	117.00(19)
C(12)-C(13)	1.379(3)	C(15)-C(14)-C(13)	119.1(2)
C(13)-C(14)	1.386(3)	C(14)-C(15)-C(16)	120.6(2)
C(14)-C(15)	1.381(3)	C(11)-C(16)-C(15)	121.37(19)
C(15)-C(16)	1.390(3)	C(26)-C(21)-C(22)	116.88(18)
O(24)-C(24)	1.376(2)	C(26)-C(21)-C(1)	122.78(18)
C(21)-C(26)	1.392(3)	C(22)-C(21)-C(1)	119.71(18)
C(21)-C(22)	1.396(3)	C(23)-C(22)-C(21)	121.89(19)
C(22)-C(23)	1.380(3)	C(22)-C(23)-C(24)	119.78(19)
C(23)-C(24)	1.389(3)	C(25)-C(24)-O(24)	123.01(19)
C(24)-C(25)	1.373(3)	C(25)-C(24)-C(23)	119.81(18)
C(25)-C(26)	1.392(3)	O(24)-C(24)-C(23)	117.16(18)
O(34)-C(34)	1.376(2)	C(24)-C(25)-C(26)	119.79(19)
C(31)-C(32)	1.390(3)	C(25)-C(26)-C(21)	121.81(19)
C(31)-C(36)	1.398(3)	C(32)-C(31)-C(36)	117.05(19)
C(32)-C(33)	1.391(3)	C(32)-C(31)-C(1)	122.10(18)
C(33)-C(34)	1.372(3)	C(36)-C(31)-C(1)	120.43(18)
C(34)-C(35)	1.395(3)	C(31)-C(32)-C(33)	121.65(19)
C(35)-C(36)	1.380(3)	C(34)-C(33)-C(32)	119.94(19)
O(44)-C(44)	1.376(3)	C(33)-C(34)-O(34)	118.10(18)
C(41)-C(42)	1.382(3)	C(33)-C(34)-C(35)	119.92(18)
C(41)-C(46)	1.399(3)	O(34)-C(34)-C(35)	121.96(18)
C(42)-C(43)	1.388(3)	C(36)-C(35)-C(34)	119.41(19)
C(43)-C(44)	1.379(3)	C(35)-C(36)-C(31)	121.91(19)
C(44)-C(45)	1.381(3)	C(42)-C(41)-C(46)	116.82(19)
C(45)-C(46)	1.384(3)	C(42)-C(41)-C(1)	124.61(18)
O(50)-C(52)	1.208(3)	C(46)-C(41)-C(1)	118.42(17)
O(51)-C(52)	1.299(4)	C(41)-C(42)-C(43)	121.8(2)
O(51)-C(53)	1.590(5)	C(44)-C(43)-C(42)	119.9(2)
C(50)-C(52)	1.463(5)	O(44)-C(44)-C(43)	117.6(2)
C(53)-C(54)	1.319(6)	O(44)-C(44)-C(45)	122.4(2)
		C(43)-C(44)-C(45)	119.9(2)
		C(44)-C(45)-C(46)	119.3(2)
C(41)-C(1)-C(21)	111.26(16)	C(45)-C(46)-C(41)	122.1(2)
C(41)-C(1)-C(31)	113.58(16)	C(52)-O(51)-C(53)	116.8(3)
C(21)-C(1)-C(31)	103.61(17)	O(50)-C(52)-O(51)	124.0(3)
C(41)-C(1)-C(11)	104.15(17)	O(50)-C(52)-C(50)	124.5(3)
C(21)-C(1)-C(11)	113.98(16)	O(51)-C(52)-C(50)	111.5(3)
C(31)-C(1)-C(11)	110.55(16)	C(54)-C(53)-O(51)	99.4(4)

Table 6. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C29 H28 O6.

D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(14)-H(14)	O(24)#1	0.83	1.91	2.719(3)	165.1
O(24)-H(24)	O(34)#2	0.83	1.90	2.714(2)	168.1
O(34)-H(34)	O(44)#3	0.83	1.86	2.687(3)	173.0
O(44)-H(44)	O(50)#4	0.83	1.90	2.662(3)	152.0

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z-1/2 #2 x-1,y,z
#3 -x+1,y-1/2,-z+1/2 #4 -x+1,y+1/2,-z+1/2



ORTEP view of the C29 H28 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogens represented by sphere of arbitrary size.

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Université de Montréal

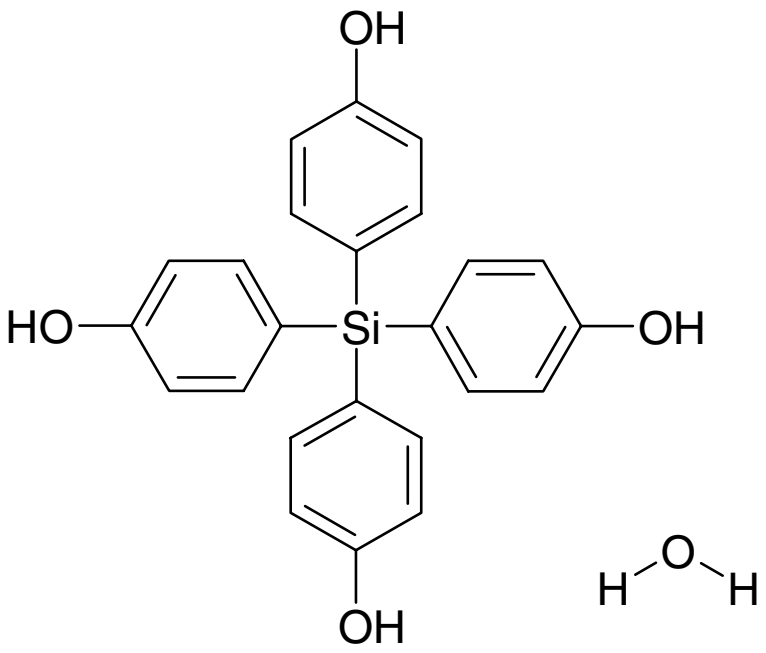
CRYSTAL AND MOLECULAR STRUCTURE OF

C24 H22 O5 Si COMPOUND (JIW262)

Equipe WUEST

Département de chimie, Université de Montréal,

C.P. 6128, Succ. Centre-Ville, Montréal, Québec, H3C 3J7 (Canada)



Structure solved and refined in the laboratory of X-ray diffraction, Université de Montréal by Dr. Thierry Maris.

Table 1. Crystal data and structure refinement for C24 H22 O5 Si.

Identification code	JIW262
Empirical formula	C24 H22 O5 Si
Formula weight	418.51
Temperature	210(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 14.962(9) Å α = 90° b = 15.855(11) Å β = 111.49(5)° c = 19.697(13) Å γ = 90°
Volume	4348(5)Å^3
Z	8
Density (calculated)	1.279 Mg/m^3
Absorption coefficient	1.226 mm^{-1}
F(000)	1760
Crystal size	0.30 x 0.20 x 0.10 mm
Theta range for data collection	4.23 to 69.93°
Index ranges	$0 \leq h \leq 18$, $0 \leq k \leq 19$, $-23 \leq \ell \leq 22$
Reflections collected	4117
Independent reflections	4117 [R_{int} = 0.070]
Absorption correction	None
Max. and min. transmission	0.8900 and 0.7100
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4117 / 2 / 279
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R_1 = 0.0784, wR_2 = 0.1879
R indices (all data)	R_1 = 0.1210, wR_2 = 0.2049
Largest diff. peak and hole	0.524 and -0.658 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for C24 H22 O5 Si.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U_{eq}
Si(1)	2420(1)	768(1)	2489(1)	43(1)
C(1)	1847(3)	1297(3)	3074(2)	42(1)
C(2)	1067(3)	961(3)	3228(2)	44(1)
C(3)	707(3)	1371(3)	3693(2)	46(1)
C(4)	1102(3)	2105(3)	4020(2)	43(1)
C(5)	1871(3)	2467(3)	3888(2)	50(1)
C(6)	2219(3)	2054(3)	3412(3)	54(1)
O(7)	732(2)	2489(2)	4489(2)	55(1)
C(11)	3571(3)	262(3)	3097(2)	41(1)
C(12)	3855(3)	-516(3)	2933(3)	56(1)
C(13)	4719(3)	-889(3)	3378(3)	58(1)
C(14)	5299(3)	-464(3)	3991(2)	48(1)
C(15)	5051(3)	316(3)	4172(2)	48(1)
C(16)	4186(3)	668(3)	3716(2)	50(1)
O(17)	6127(2)	-867(2)	4435(2)	62(1)
C(21)	2681(3)	1585(3)	1917(2)	43(1)
C(22)	2075(3)	2262(3)	1611(2)	53(1)
C(23)	2242(3)	2845(3)	1148(2)	54(1)
C(24)	3069(3)	2749(3)	980(2)	46(1)
C(25)	3677(3)	2094(3)	1265(2)	51(1)
C(26)	3506(3)	1520(3)	1727(2)	48(1)
O(27)	3229(2)	3325(2)	519(2)	61(1)
C(31)	1653(3)	-67(3)	1882(2)	42(1)
C(32)	1284(3)	-762(3)	2144(2)	52(1)
C(33)	764(3)	-1386(3)	1695(2)	54(1)
C(34)	604(3)	-1362(3)	961(2)	47(1)
C(35)	969(3)	-711(3)	679(2)	56(1)
C(36)	1475(3)	-72(3)	1135(2)	54(1)
O(37)	61(2)	-1992(2)	520(2)	65(1)
O(100)	7415(3)	78(3)	5386(3)	94(1)

Table 3. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2\ x\ 10^3$) for C24 H22 O5 Si.

	x	y	z	U_{eq}
H(2)	784	445	3008	53
H(3)	178	1136	3784	55
H(5)	2149	2982	4115	60
H(6)	2737	2303	3315	65
H(71)	926	2990	4561	74
H(12)	3454	-806	2509	67
H(13)	4902	-1426	3259	69
H(15)	5457	606	4594	57
H(16)	4010	1209	3833	60
H(171)	6495	-514	4722	50
H(22)	1516	2327	1727	63
H(23)	1808	3298	951	64
H(25)	4232	2032	1144	61
H(26)	3947	1072	1922	58
H(27)	2948	3778	536	91
H(32)	1402	-797	2651	63
H(33)	513	-1837	1889	65
H(35)	873	-701	175	68
H(36)	1710	382	933	64
H(371)	173	-2012	132	122
H(101)	7210(80)	520(40)	5080(40)	260(60)
H(102)	7830(50)	-230(50)	5750(30)	180(40)

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C24 H22 O5 Si.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Si(1)	32(1)	57(1)	49(1)	-1(1)	26(1)	0(1)
C(1)	29(2)	58(3)	45(2)	0(2)	23(2)	1(2)
C(2)	28(2)	61(3)	47(2)	-2(2)	18(2)	-7(2)
C(3)	29(2)	66(3)	51(3)	1(2)	23(2)	-3(2)
C(4)	32(2)	61(3)	45(2)	1(2)	23(2)	3(2)
C(5)	41(2)	58(3)	64(3)	-7(2)	36(2)	-8(2)
C(6)	42(2)	67(3)	70(3)	-13(3)	40(2)	-10(2)
O(7)	54(2)	69(2)	64(2)	0(2)	47(2)	6(2)
C(11)	34(2)	51(3)	50(3)	-1(2)	28(2)	1(2)
C(12)	44(2)	65(3)	59(3)	-9(3)	19(2)	0(2)
C(13)	47(2)	62(3)	66(3)	-10(3)	22(2)	8(2)
C(14)	36(2)	59(3)	54(3)	3(2)	23(2)	2(2)
C(15)	40(2)	55(3)	50(3)	-3(2)	18(2)	-1(2)
C(16)	40(2)	58(3)	56(3)	-6(2)	24(2)	1(2)
O(17)	38(2)	66(2)	73(2)	-6(2)	10(2)	5(2)
C(21)	35(2)	53(3)	50(3)	-2(2)	27(2)	-1(2)
C(22)	36(2)	67(3)	66(3)	12(3)	32(2)	11(2)
C(23)	41(2)	67(3)	63(3)	11(3)	32(2)	12(2)
C(24)	39(2)	58(3)	49(3)	4(2)	24(2)	-2(2)
C(25)	36(2)	61(3)	68(3)	5(2)	34(2)	3(2)
C(26)	35(2)	60(3)	60(3)	5(2)	31(2)	8(2)
O(27)	58(2)	65(2)	75(2)	18(2)	43(2)	7(2)
C(31)	35(2)	54(3)	46(2)	2(2)	24(2)	5(2)
C(32)	55(3)	63(3)	50(3)	0(2)	33(2)	-5(2)
C(33)	54(3)	64(3)	60(3)	-7(3)	40(2)	-13(2)
C(34)	41(2)	63(3)	50(3)	-10(2)	31(2)	-9(2)
C(35)	62(3)	71(3)	49(3)	-7(3)	36(2)	-12(3)
C(36)	48(2)	73(3)	53(3)	-1(2)	34(2)	-10(2)
O(37)	61(2)	87(3)	68(2)	-27(2)	50(2)	-30(2)
O(100)	76(3)	89(3)	89(3)	14(3)	-4(3)	-11(3)

Table 5. Bond lengths [Å] and angles [°] for C24 H22 O5 Si

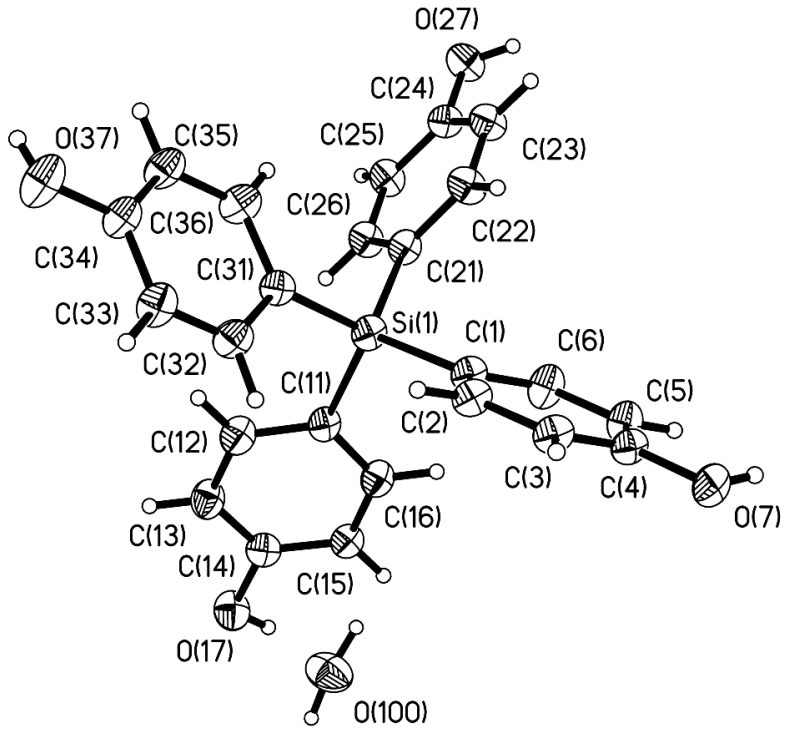
Si(1)-C(21)	1.850(4)	C(6)-C(1)-SI1	119.4(3)
Si(1)-C(31)	1.868(5)	C(2)-C(1)-SI1	124.4(3)
Si(1)-C(1)	1.869(4)	C(3)-C(2)-C(1)	121.1(4)
Si(1)-C(11)	1.879(4)	C(4)-C(3)-C(2)	120.8(4)
C(1)-C(6)	1.387(6)	C(3)-C(4)-O(7)	119.1(3)
C(1)-C(2)	1.413(5)	C(3)-C(4)-C(5)	120.7(4)
C(2)-C(3)	1.383(5)	O(7)-C(4)-C(5)	120.3(4)
C(3)-C(4)	1.356(6)	C(6)-C(5)-C(4)	118.1(4)
C(4)-O(7)	1.379(4)	C(1)-C(6)-C(5)	123.2(4)
C(4)-C(5)	1.393(5)		
C(5)-C(6)	1.391(6)	C(12)-C(11)-C(16)	117.3(4)
C(11)-C(12)	1.381(6)	C(12)-C(11)-SI1	121.4(3)
C(11)-C(16)	1.388(6)	C(16)-C(11)-SI1	121.3(3)
C(12)-C(13)	1.399(6)	C(11)-C(12)-C(13)	121.6(5)
C(13)-C(14)	1.377(6)	C(14)-C(13)-C(12)	119.0(5)
C(14)-C(15)	1.376(6)	C(15)-C(14)-C(13)	121.5(4)
C(14)-O(17)	1.383(5)	C(15)-C(14)-O(17)	121.0(4)
C(15)-C(16)	1.394(6)	C(13)-C(14)-O(17)	117.4(4)
C(21)-C(22)	1.392(6)	C(14)-C(15)-C(16)	118.0(4)
C(21)-C(26)	1.417(5)	C(11)-C(16)-C(15)	122.7(4)
C(22)-C(23)	1.384(6)	C(22)-C(21)-C(26)	115.8(4)
C(23)-C(24)	1.403(5)	C(22)-C(21)-SI1	123.6(3)
C(24)-C(25)	1.359(6)	C(26)-C(21)-SI1	120.5(3)
C(24)-O(27)	1.368(5)	C(23)-C(22)-C(21)	123.6(4)
C(25)-C(26)	1.376(6)	C(22)-C(23)-C(24)	118.1(4)
C(31)-C(36)	1.396(6)	C(25)-C(24)-O(27)	122.1(4)
C(31)-C(32)	1.412(6)	C(25)-C(24)-C(23)	120.0(4)
C(32)-C(33)	1.364(6)	O(27)-C(24)-C(23)	117.9(4)
C(33)-C(34)	1.377(6)	C(24)-C(25)-C(26)	121.4(4)
C(34)-C(35)	1.377(6)	C(25)-C(26)-C(21)	121.1(4)
C(34)-O(37)	1.378(5)	C(36)-C(31)-C(32)	115.5(4)
C(35)-C(36)	1.382(6)	C(36)-C(31)-SI1	120.9(3)
		C(32)-C(31)-SI1	123.4(3)
C(21)-SI1-C(31)	108.90(19)	C(33)-C(32)-C(31)	122.4(4)
C(21)-SI1-C(1)	108.0(2)	C(32)-C(33)-C(34)	119.9(4)
C(31)-SI1-C(1)	113.53(18)	C(33)-C(34)-C(35)	120.2(4)
C(21)-SI1-C(11)	109.77(18)	C(33)-C(34)-O(37)	118.6(4)
C(31)-SI1-C(11)	108.1(2)	C(35)-C(34)-O(37)	121.2(4)
C(1)-SI1-C(11)	108.57(19)	C(34)-C(35)-C(36)	119.4(4)
C(6)-C(1)-C(2)	116.2(4)	C(35)-C(36)-C(31)	122.5(4)

Table 6. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C24 H22 O5 Si.

D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(7)-H(71)	O(17)#1	0.84	1.87	2.683(5)	163.2
O(17)-H(171)	O(100)	0.84	1.78	2.611(6)	169.9
O(27)-H(27)	O(100)#2	0.84	1.96	2.781(6)	165.6
O(37)-H(371)	O(7)#3	0.84	1.91	2.692(4)	153.9

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,y+1/2,z #2 x-1/2,-y+1/2,z-1/2
#3 x,-y,z-1/2 #4 x+1/2,-y+1/2,z+1/2



ORTEP view of the C24 H22 O5 Si compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogens represented by sphere of arbitrary size.

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