SUPPORTING INFORMATION

Conformational Study of the Intramolecular Diels-Alder Reaction of a Pentadienyl Acrylate. Comparison of Theory with Experiment.

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18: mp 145-146 °C (colorless needles from hexane); $[\alpha]_D^{23}$ +69.9 (c 7.1, $CHCl_3$); IR (KBr) 1786, 1471, 1383, 1257, 1169, 1152, 1139, 1115, 1097, 988, 905, 836, 778 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.07 (3H, s), 0.09 (3H, s), 0.84 (3H, s), 0.89 (9H, s) 107 (3H, s), 1.27 (3H, d, J = 6 Hz), 1.38 (3H, s), 1.61-1.70 (1H, m), 2.53 (1H, d, J = 14 Hz), 2.57-2.62 (2H, m), 2.72 (1H, d, J = 9 Hz), 3.37-3.43 (2H, m), 3.59 (1H, d, J = 11 Hz), 3.61 (1H, d, J = 11 Hz), 3.93 (1H, dd, J = 10.5 Hz), 4.01 (1H, dq, J = 6, 6 Hz), 5.92 (1H, ddd (J = 10, 3, 1 Hz), 6.17 (1H, dq, J = 6, 6 Hz), 5.92 (1H, ddd (J = 10, 3, 1 Hz), 6.17 (1H, ddd, J = 10, 2, 1 Hz); ^{13}C NMR ($CDCl_3$) δ –4.6 (x2), 17.3, 18.0, 20.8, 21.7, 22.5, 23.0, 25.8, 29.9, 42.3, 42.5 (x2), 69.4, 70.2, 70.4, 85.5, 100.4, 128.2, 129.8, 176.0; MS (EI) *m/z* 424 (M^+), 409, 367, 159, 129, 75, 43; HRMS (EI) *m/z* 409.2408 $(M–CH_3)+$, calcd for $C_{22}H_{37}O_5Si$ 409.2410.

19: mp 111-112 °C (colorless needles from hexane); $[\alpha]_D^{23}$ + 20.8 (c 1.2, $CHCl_3$); IR (KBr) 1779, 1473, 1382, 1313, 1256, 1217, 1158, 1131, 1102, 1086, 1057, 996, 981, 907, 834, 778 cm^{-1}; 1H NMR ($CDCl_3$) δ 0.08 (3H, s), 0.09 (3H,s), 0.86 (3H, s), 088 (9H, s), 1.05 (3H, s), 1.22 (3H, d, J = 6 Hz), 1.34 (3H, s), 1.48 (1H, ddd, J = 13, 13, 11 Hz), 2.23 (1H, ddd, J = 13, 5, 5 Hz), 2.54-2.58 (1H, m), 2.77 (1H, ddd, J = 13, 9, 5 Hz), 3.03-3.11 (1H, m), 3.42 (1H, d, J = 12 Hz), 3.59 (1H, d, J = 12 Hz), 3.61 (1H, d, J = 12 Hz), 4.03-4.11 (2H, m), 5.76 (1H, ddd, J = 10, 3, 3 Hz), 6.01 (1H, d, J = 10 Hz); ^{13}C NMR ($CDCl_3$) δ –4.7, –4.6, 16.7, 18.0, 20.2, 22.5, 23.0, 23.6, 25.8, 30.0, 35.1, 40.0, 42.2, 69.0, 70.1, 70.4, 87.2, 99.6, 126.5, 129.8, 178.5; MS (EI) *m/z* 409 $(M–CH_3)^+$, 367, 159, 129, 75; HRMS (EI) *m/z* 409.2408 $(M–CH_3)^+$, calcd for $C_{22}H_{37}O_5Si$ 409.2410.

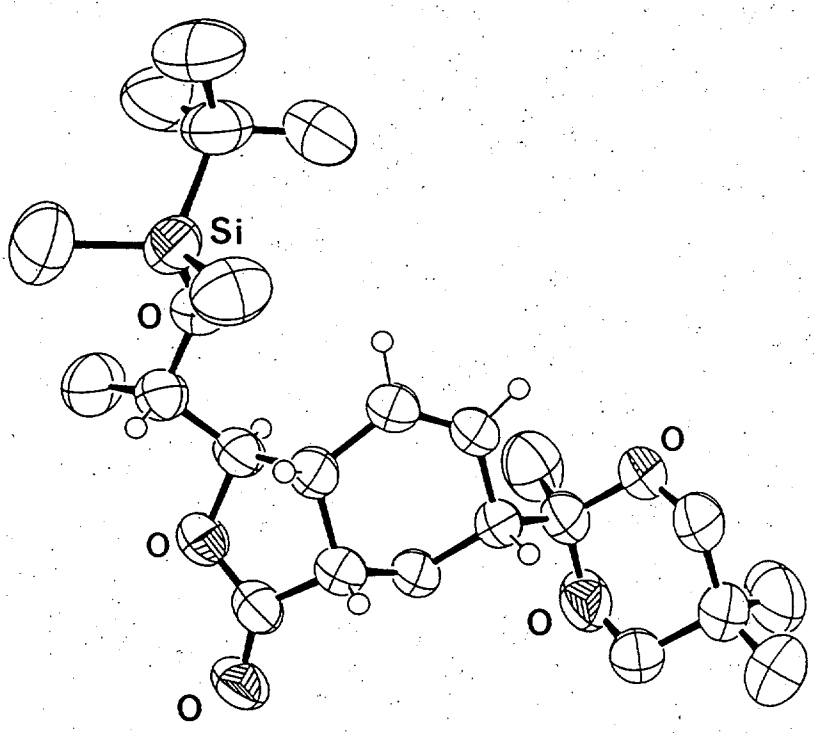
20: oil; $[\alpha]_D^{25}$ –6.8 (c 0.8, $CHCl_3$); IR (film) 1778, 1472, 1376, 1254, 1180, 1122, 1088, 998,

834, 777 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.08 (3H, s), 0.09 (3H, s), 0.85 (3H, s), 0.88 (9H, s), 1.06 (3H, s), 1.26 (3H, d, J = 6 Hz), 1.33 (3H, s), 1.61 (1H, ddd, J = 13, 10, 10 Hz), 2.18 (1H, ddd, J = 13, 7, 7 Hz), 2.53-2.58 (1H, m), 2.75 (1H, ddd, J = 10, 9, 7 Hz), 3.19-3.25 (1H, m), 3.36-3.43 (2H, m), 3.57 (1H, d, J = 12 Hz), 3.63 (1H, d, J = 12 Hz), 3.99 (1H, dq, J = 8,6 Hz), 4.24 (1H, dd, J = 8, 8 Hz), 5.91 (1H, ddd, J = 10, 3, 3 Hz), 6.07 (1H, ddd, J = 10, 2, 2 Hz); ^{13}C NMR ($CDCl_3$) δ –4.3, –3.5, 16.5, 18.0, 21.2, 22.5, 23.0, 23.1, 26.0, 29.9, 36.2, 38.1, 41.6, 68.2, 70.0, 70.3, 84.4, 99.7, 124.0, 130,1, 178.8; MS (EI) *m/z* 409 $(M–CH_3)^+$, 367, 159, 129, 75; HRMS (EI) *m/z* 409.2410 $(M–CH_3)^+$, calcd for $C_{22}H_{37}O_5Si$ 409.2410.

21: oil; $[\alpha]_D^{23}$ +24.6 (c 4.8, $CHCl_3$); IR (film) 3620-3100, 1780, 1470, 1395, 1379, 1255, 1133, 1099, 1022, 902, 869,834, 779, 734 cm^{-1}; ^1H NMR (CDC_{l3}) δ 0.15 (6H, s), 0.71 (3H, s), 0.92 (9H, s), 1.11 (3H, s), 1.37 (3H, d, J = 6 Hz), 1.46 (3H, s), 1.67 (1H, ddd, J = 13, 13, 7 Hz), 2.19 (1H, d, J = 7 Hz), 2.28 (1H, ddd, J = 14, 9, 9 Hz), 2.36 (1H, dd, J = 13, 3 Hz), 2.66 (1H, br s), 2.92 (1H, ddd, J = 14, 3, 3 Hz), 3.27-3.33 (2H, m), 3.63 (1H, d, J = 12 Hz), 3.67 (1H, d, J = 12 Hz), 3.85 (1H, m), 3.98 (1H, dd, J = 9, 8 Hz), 4.01 (1H, dd, J = 9, 3 Hz), 4.27 (1H, br s), 4.44 (1H, br s); ^{13}C NMR (CDCl3) δ –4.3, –3.6, 16.7, 18.3, 1995, 21.8, 22.2, 23.5, 26.0, 29.7, 41.1, 46.4, 49.7, 68.7, 70.2, 70.3, 71.4, 72.0, 86.8, 100.3, 175.8; MS (EI) *m/z* 458 (M^+), 443, 401,159, 129, 75; HRMS (EI) *m/z* 443.2466 $(M–CH_3)^+$, calcd for $C_{22}H_{39}O_7Si$ 443.2465.

22: mp 122-123 °C (colorless prisms from hexane); $[\alpha]_D^{23}$ +19.2 (c 2.4, $CHCl_3$); IR (KBr) 1776, 1470, 1461, 1380, 1257, 1244, 1218, 1182, 1127, 1123, 1097, 1050, 979, 838, 778 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.63 (3H, s), 0.72 (3H, s), 0.76 (3H, s), 0.86 (9H, s), 1.13 (3H, s), 1.32 (3H, d, J = 7 Hz), 1.38 (3H, s), 1.49 (3H, s), 1.52 (3H, s), 1.62 (1H, ddd, J = 14, 12, 7 Hz), 2.38-2.46 (3H, m), 2.69 (1H, ddd, J = 14, 12, 3 Hz), 3.33 (1H, dd, J = 11, 2 Hz), 3.39 (1H, dd, J = 11, 2 Hz), 3.63 (1H, d, J = 11 Hz), 3.72 (1H, d, J = 11 Hz), 4.10 (1H, d, J = 10 Hz), 4.11 (1H, dd, J = 10,5

hz), 4.24 (1H, dq, J = 6, 1 Hz), 4.71 (1H, d, J = 5 Hz); ^{13}C NMR ($CDCl_3$) δ –4.8 (x2), 16.7, 18.0, 18.2, 21.4, 22.3, 23.4, 25.8, 26.5, 28.2, 29.8, 39.8, 42.9, 46.5, 67.1, 70.1, 70.4, 74.5, 76.8, 88.3, 100.4, 107.2, 176.0; MS (EI) *m/z* 483 $(M–CH_3)^+$, 441. 159, 129, 75; HRMS (EI) *m/z* 483.2778 $(M–CH_3)^+$, calcd for $C_{25}H_{43}O_7Si$ 483.2777. Anal. Calcd for $C_{26}H_{46}O_7Si$: C, 62.62; H, 9.30. Found: C, 62.53; H, 8.76.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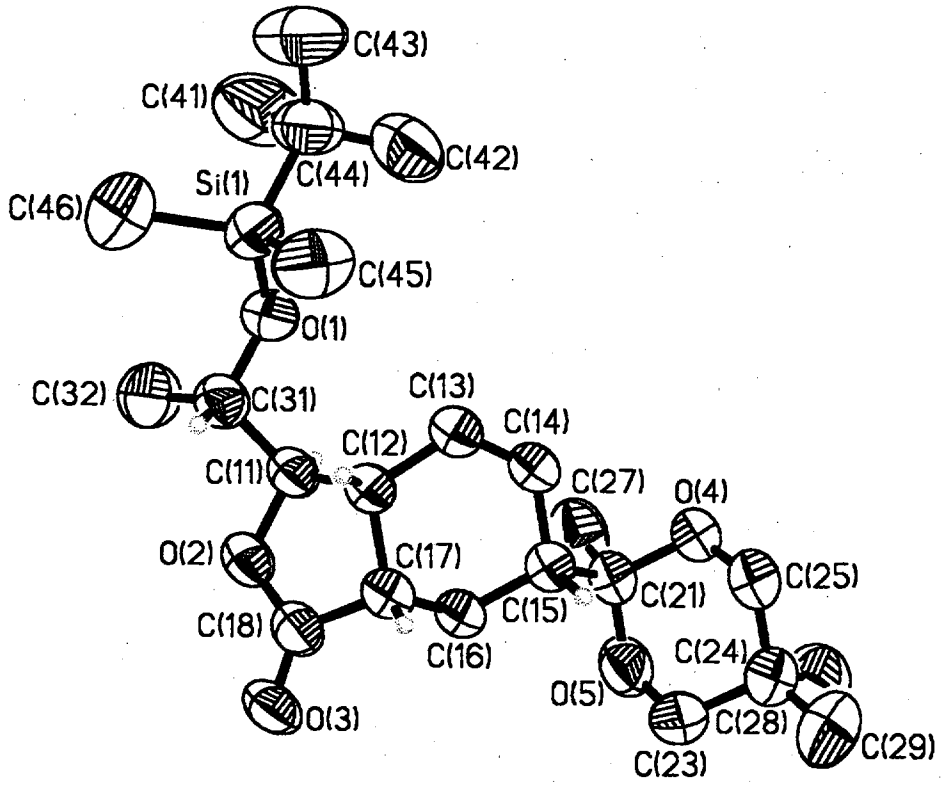
C(43)
C(41)
C(42)
Si(1)
C(44)
C(46)
C(45)
O(1)
C(32)
C(31)
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C(11)
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O(4)
O(2)
C(17)
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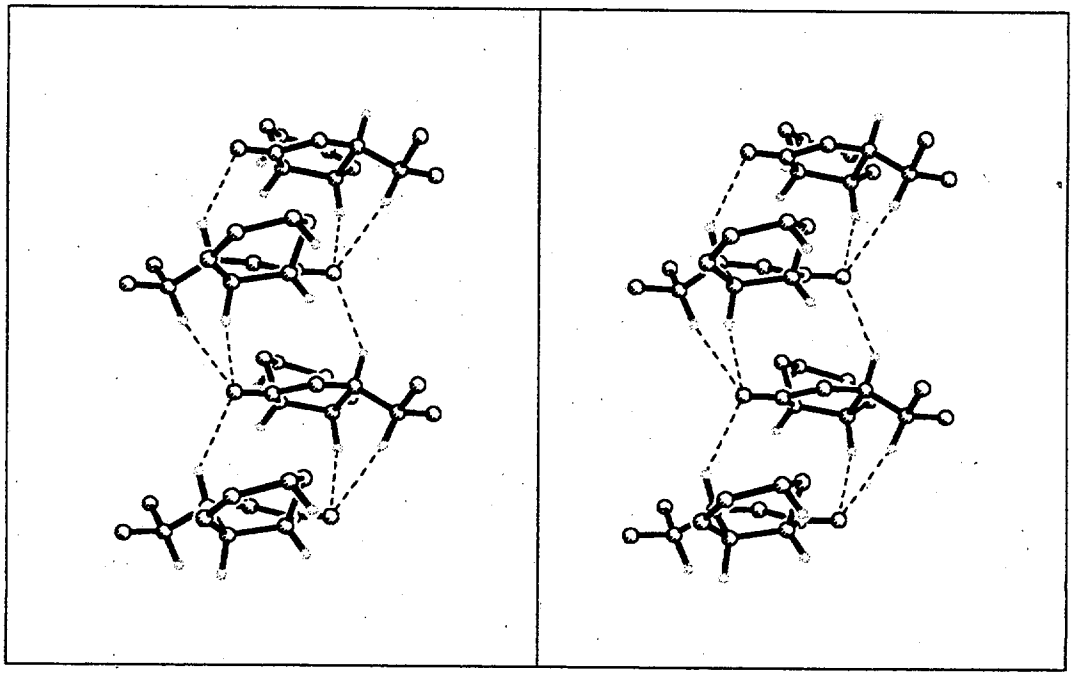

Experimental details for the structural characterization of "CH 4b" (STR8)

The crystals examined were obtained from the vapor diffusion of water into an acetonitrile solution of the compound, and over the course of a few days clusters of long needle-shaped crystals grew. From these, a well shaped specimen of approximate dimensions 0.6 x 0.25 x 0.2 mm^3 was chosen, and was mounted on the end of a pyrex fiber using a drop of epoxy glue. The crystal was indexed and data collected as previously described elsewhere[1] with the following specific details.

The automated search procedure yielded a list of 18 reflections with $11.4 < 2\theta < 28.2$ from which the crystal was indexed, revealing a primitive orthorhombic lattice. Using these parameters, the list was expanded to 86 reflections with $11.4 < 2\theta < 69.0°$, and the lattice parameters refined using this list. Two unique octants of data in the range $2 < 2\theta < 115°$ and where $-7 < h < 0$, $-14 < k < 0$, $-31 < l < 0$ or $-1 < h < 6$, $-1 < k < 14$, $-1 < l < 31$ were collected. An empirical correction for the effects of absorption anisotropy was done by performing psi-scans on 12 reflections.[2]

The structure was solved using direct methods as programmed in SHELXS-90,[3] which yielded the positions of most non-H atoms. The remaining non-H atoms were subsequently found from successive iterations of least squares refinements followed by Fourier synthesis using SHELXL-93.[4] During the refinement all H atoms could be found in the electron density maps but to preserve a favorable data-to-parameter ratio all H atoms, with the exception of those on C(11), C(12), C(15), C(17) and C(31), were placed in idealized positions. The refinement of both absolute configurations was performed, and, thanks to the presence of an Si atom in the molecule, the structure presented yielding a value of 0.00(4) for the Flack parameter,[5] indicating this is the correct absolute structure. This conclusion is confirmed by the fact that the absolute configurations of C(31) and C(11) are known, since these remain unchanged from the starting material for this synthesis.

Table 1. Crystal data and structure refinement for 'CH 4b'.

Identification code	STR 8	
Empirical formula	C23 H40 O5 Si	
Formula weight	424.64	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1) 2(1) 2(1)	
Unit cell dimensions	a = 6.7150(10)Å	α= 90°.
	b = 13.6630(10)Å	β= 90°.
	c = 28.397(2)Å	γ = 90°.
Volume	2605.3(5)Å^3	
Z	4	
Density (calculated)	1.083 Mg/m^3	
Absorption coefficient	1.011 mm^{-1}	
F(000)	928	
Crystal size	0.60 x 0.25 x 0.20 mm^3	
Theta range for data collection	3.11 to 57.51 °.	
Index ranges	-7<=h<=6, -14<=k<=14, -31<=l<=31	
Reflections collected	3908	
Independent reflections	3331 [R(int) = 0.0409]	
Absorption correction	Empirical (psi-scans)	
Max. and min. transmission	0.8234 and 0.5822	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3331 / 0 / 309	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0432, wR2 = 0.1149	
R indices (all data)	R1 = 0.0493, wR2 = 0.1233	
Absolute structure parameter	-0.07(4)	
Extinction coefficient	0.0043(5)	
Largest diff. peak and hole	0.176 and -0.145 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 'CH 4b'.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Si(1)	1252(2)	1025(1)	9182(1)	79(1)
O(2)	-1740(3)	-1841(1)	10006(1)	70(1)
O(1)	-661(3)	379(1)	9359(1)	75(1)
O(4)	-4718(4)	-3412(2)	7854(1)	83(1)
C(17)	-1088(5)	-2819(2)	9347(1)	63(1)
C(12)	-707(5)	-1754(2)	9209(1)	64(1)
O(5)	-5422(4)	-4418(2)	8494(1)	94(1)
C(15)	-2891(5)	-3159(2)	8585(1)	63(1)
C(18)	-1372(4)	-2771(2)	9869(1)	66(1)
C(31)	-690(6)	-252(2)	9759(1)	68(1)
C(16)	-2982(5)	-3239(2)	9123(1)	66(1)
C(13)	-1405(5)	-1518(2)	8720(1)	75(1)
C(14)	-2307(5)	-2145(2)	8443(1)	73(1)
C(21)	-4853(5)	-3467(2)	8356(1)	74(1)
C(44)	154(7)	1945(2)	8772(1)	98(1)
C(11)	-1726(6)	-1179(2)	9604(1)	65(1)
C(24)	-4197(9)	-5153(3)	7771(1)	110(2)
C(42)	-904(9)	1435(4)	8369(2)	124(2)
C(27)	-6563(7)	-2814(4)	8483(1)	110(1)
C(32)	-1759(8)	243(3)	10166(1)	105(1)
C(23)	-4273(9)	-5179(2)	8310(1)	108(2)
C(25)	-3556(8)	-4128(2)	7644(1)	96(1)
C(29)	-2640(14)	-5882(3)	7592(2)	178(3)
C(45)	3090(6)	234(3)	8887(2)	107(1)
C(43)	1812(11)	2598(3)	8570(2)	156(2)
C(28)	-6216(11)	-5363(4)	7570(2)	160(3)
C(41)	-1344(10)	2578(4)	9037(2)	160(3)
O(3)	-1391(3)	-3428(2)	10152(1)	79(1)
C(46)	2503(8)	1621(3)	9690(2)	130(2)

Table 3. Bond lengths [Å] and angles [°] for 'CH 4b'.

Si(1)-O(1)	1.638(2)
Si(1)-C(45)	1.843(4)
Si(1)-C(46)	1.857(4)
Si(1)-C(44)	1.866(4)
O(2)-C(18)	1.351(3)
O(2)-C(11)	1.457(3)
O(1)-C(31)	1.427(3)
O(4)-C(25)	1.387(4)
O(4)-C(21)	1.429(3)
C(17)-C(18)	1.496(4)
C(17)-C(12)	1.528(4)
C(17)-C(16)	1.534(4)
C(12)-C(13)	1.502(4)
C(12)-C(11)	1.531(4)
O(5)-C(23)	1.396(5)
O(5)-C(21)	1.410(4)
C(15)-C(14)	1.495(4)
C(15)-C(21)	1.528(5)
C(15)-C(16)	1.534(3)
C(18)-O(3)	1.204(3)
C(31)-C(11)	1.511(4)
C(31)-C(32)	1.519(4)
C(13)-C(14)	1.310(4)
C(21)-C(27)	1.498(5)
C(44)-C(42)	1.516(6)
C(44)-C(41)	1.526(6)
C(44)-C(43)	1.539(7)
C(24)-C(28)	1.500(8)
C(24)-C(25)	1.509(5)
C(24)-C(23)	1.532(5)
C(24)-C(29)	1.532(8)
O(1)-Si(1)-C(45)	110.37(16)
O(1)-Si(1)-C(46)	110.70(19)

C(45)-Si(1)-C(46)	107.9(2)
O(1)-Si(1)-C(44)	104.15(16)
C(45)-Si(1)-C(44)	112.02(18)
C(46)-Si(1)-C(44)	111.7(2)
C(18)-O(2)-C(11)	110.96(19)
C(31)-O(1)-Si(1)	125.5(2)
C(25)-O(4)-C(21)	115.3(2)
C(18)-C(17)-C(12)	103.5(2)
C(18)-C(17)-C(16)	108.8(3)
C(12)-C(17)-C(16)	112.8(3)
C(13)-C(12)-C(17)	112.9(2)
C(13)-C(12)-C(11)	115.4(3)
C(17)-C(12)-C(11)	103.1(2)
C(23)-O(5)-C(21)	115.7(3)
C(14)-C(15)-C(21)	111.5(3)
C(14)-C(15)-C(16)	110.1(2)
C(21)-C(15)-C(16)	111.7(2)
O(3)-C(18)-O(2)	120.5(2)
O(3)-C(18)-C(17)	129.0(3)
O(2)-C(18)-C(17)	110.4(2)
O(1)-C(31)-C(11)	106.2(2)
O(1)-C(31)-C(32)	110.1(3)
C(11)-C(31)-C(32)	112.2(3)
C(17)-C(16)-C(15)	110.7(2)
C(14)-C(13)-C(12)	123.9(3)
C(13)-C(14)-C(15)	124.5(3)
O(5)-C(21)-O(4)	110.0(2)
O(5)-C(21)-C(27)	105.9(3)
O(4)-C(21)-C(27)	104.9(3)
O(5)-C(21)-C(15)	111.6(3)
O(4)-C(21)-C(15)	110.7(3)
C(27)-C(21)-C(15)	113.3(3)
C(42)-C(44)-C(41)	109.0(4)
C(42)-C(44)-C(43)	108.9(4)
C(41)-C(44)-C(43)	109.4(4)
C(42)-C(44)-Si(1)	110.3(2)

C(41)-C(44)-Si(1)	109.5(3)
C(43)-C(44)-Si(1)	109.8(4)
O(2)-C(11)-C(31)	107.2(2)
O(2)-C(11)-C(12)	104.9(2)
C(31)-C(11)-C(12)	116.0(3)
C(28)-C(24)-C(25)	110.1(4)
C(28)-C(24)-C(23)	110.3(5)
C(25)-C(24)-C(23)	105.8(3)
C(28)-C(24)-C(29)	111.4(4)
C(25)-C(24)-C(29)	109.2(4)
C(23)-C(24)-C(29)	109.9(4)
O(5)-C(23)-C(24)	111.9(3)
O(4)-C(25)-C(24)	113.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 'CH 4b'.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U11 + ... + 2\ h\ k\ a^*\ b^*\ U12]$

	U11	U22	U33	U23	U13	U12
Si(1)	99(1)	64(1)	74(1)	-5(1)	5(1)	-11(1)
O(2)	88(1)	75(1)	48(1)	8(1)	6(1)	0(1)
O(1)	92(2)	64(1)	68(1)	8(1)	1(1)	-4(1)
O(4)	122(2)	72(1)	54(1)	3(1)	-5(1)	-2(1)
C(17)	77(2)	59(2)	54(1)	7(1)	0(1)	-1(2)
C(12)	81(2)	61(2)	50(1)	4(1)	6(1)	-9(1)
O(5)	125(2)	94(2)	63(1)	5(1)	1(1)	-35(2)
C(15)	84(2)	56(1)	50(1)	0(1)	3(1)	0(2)
C(18)	66(2)	76(2)	56(1)	10(1)	-6(1)	-10(2)
C(31)	85(2)	63(2)	57(1)	1(1)	6(1)	6(2)
C(16)	88(2)	59(1)	50(1)	9(1)	-1(1)	-9(2)
C(13)	111(2)	60(2)	54(1)	9(1)	5(2)	-12(2)
C(14)	107(2)	64(2)	49(1)	8(1)	0(2)	-10(2)
C(21)	97(2)	73(2)	52(1)	3(1)	-1(2)	-9(2)
C(44)	130(3)	70(2)	94(2)	12(2)	21(2)	1(2)
C(11)	78(2)	67(2)	52(1)	8(1)	1(1)	3(2)
C(24)	192(5)	71(2)	69(2)	-6(2)	-18(2)	-18(3)
C(42)	160(4)	117(3)	95(2)	24(2)	-13(3)	12(3)
C(27)	101(3)	137(3)	92(2)	-10(2)	0(2)	26(3)
C(32)	148(4)	87(2)	80(2)	-15(2)	28(2)	9(2)
C(23)	181(4)	68(2)	76(2)	9(2)	-14(2)	-27(3)
C(25)	149(4)	82(2)	56(2)	-2(1)	8(2)	-10(2)
C(29)	322(10)	100(3)	111(3)	-28(3)	-13(5)	48(5)
C(45)	104(3)	93(2)	124(3)	7(2)	23(2)	2(2)
C(43)	213(6)	100(3)	155(4)	41(3)	18(4)	-42(4)
C(28)	260(8)	121(3)	98(3)	11(3)	-53(4)	-78(5)
C(41)	224(7)	104(3)	152(4)	25(3)	46(4)	67(4)
O(3)	91(1)	85(1)	60(1)	24(1)	-7(1)	-11(1)
C(46)	149(4)	122(3)	120(3)	-22(3)	-22(3)	-41(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 'CH 4b'.

	x	y	z	U(eq)
H(17)	-80(5)	-3200(2)	9266(9)	66(9)
H(12)	730(6)	-1610(2)	9243(10)	81(9)
H(15)	-1900(4)	-3580(2)	8454(9)	57(7)
H(31)	630(5)	-470(2)	9853(11)	77(9)
H(16A)	-4140(3)	-2883(9)	9239(3)	94(4)
H(16B)	-3129(7)	-3922(18)	9213(3)	94(4)
H(13)	-1162(9)	-830(2)	8595(4)	74(6)
H(14)	-2599(12)	-1949(7)	8143(11)	74(6)
H(11)	-3050(5)	-1040(2)	9535(9)	56(8)
H(42A)	-1990(4)	990(2)	8500(3)	167(4)
H(42B)	100(3)	1020(2)	8183(9)	167(4)
H(42C)	-1530(5)	1946(13)	8152(9)	167(4)
H(27A)	-7720(4)	-3004(17)	8307(11)	167(4)
H(27B)	-6230(2)	-2150(2)	8410(11)	167(4)
H(27C)	-6840(4)	-2871(19)	8813(10)	167(4)
H(32A)	-1140(4)	840(2)	10233(9)	167(4)
H(32B)	-1710(5)	-159(17)	10430(8)	167(4)
H(32C)	-3080(4)	350(2)	10084(5)	167(4)
H(23A)	-4888(14)	-5869(16)	8423(3)	94(4)
H(23B)	-2780(4)	-5127(2)	8448(3)	94(4)
H(25A)	-2090(4)	-4030(3)	7745(2)	94(4)
H(25B)	-3628(8)	-4046(3)	7282(8)	94(4)
H(29A)	-3070(3)	-6580(2)	7677(11)	167(4)
H(29B)	-1290(4)	-5733(16)	7745(10)	167(4)
H(29C)	-2520(4)	-5820(17)	7233(10)	167(4)
H(45A)	3510(4)	-250(2)	9094(7)	167(4)
H(45B)	4170(4)	607(12)	8792(12)	167(4)
H(45C)	2510(2)	-60(2)	8626(10)	167(4)
H(43A)	2910(4)	2164(12)	8426(11)	167(4)
H(43B)	2410(4)	3020(2)	8836(8)	167(4)

H(43C)	1230(2)	3050(2)	8312(11)	167(4)
H(28A)	-6560(3)	-5980(2)	7634(11)	167(4)
H(28B)	-6187(17)	-5270(2)	7256(10)	167(4)
H(28C)	-7110(3)	-4960(2)	7698(10)	167(4)
H(41A)	-2030(4)	3050(2)	8803(7)	167(4)
H(41B)	-610(2)	2980(2)	9295(10)	167(4)
H(41C)	-2410(4)	2133(12)	9194(11)	167(4)
H(46A)	1580(3)	1980(2)	9859(9)	167(4)
H(46B)	3500(5)	2030(2)	9582(3)	167(4)
H(46C)	3050(5)	1147(15)	9883(9)	167(4)

[1] There's no such reference yet.
[2]North, A. C. T., Phillips, D. C., Mathews, F. S., *Acta Crystallogr.* **1968**, *A24*, 351.
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[4]Sheldrick, G. M. In *Crystallographic Computing 6*, Flack, H. D., Parkanyi, L., Simon, K., Eds., Oxford University Press, Oxford, 1993.
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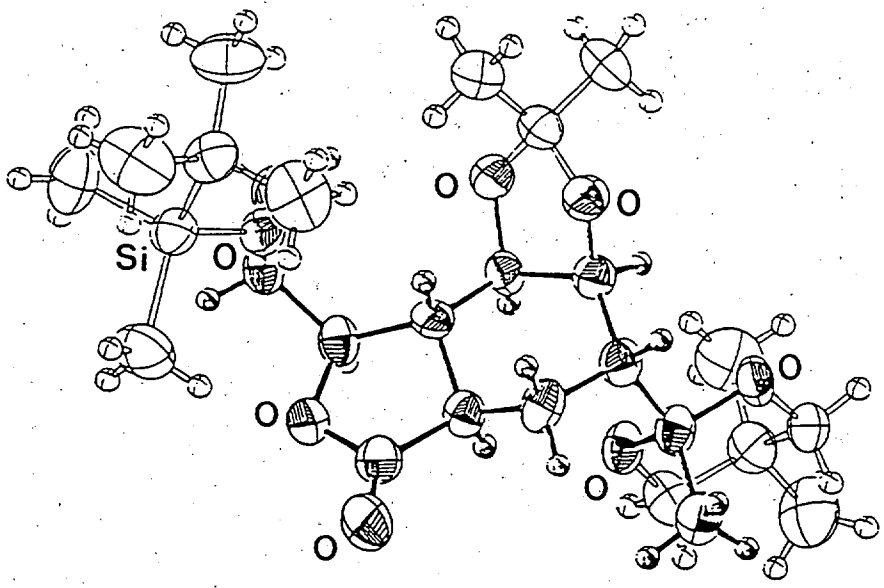
Si
O
O
O
O
O
O
O

Empirical Formula	C(26)H(46)O(7)Si(1)
Formula Weight	498.73
Crystal System	Orthorhombic
Lattice Parameters:	a = 10.803 (3) angstroms b = 29.102 (4) angstroms c = 9.175 (5) angstroms V = 2884 (2) angstroms**3
Space Group	P212121 (#19)
Z value	4
Dcalc	1.15 g/cm**3
F000	1088
mu(Mo K-alpha)	1.14 cm**-1
Diffractometer	Rigaku AFC6
Radiation	Mo K-alpha (lambda= 0.71069) Graphite-monochromated
Temperature	23 degrees Cent.
2-theta(max)	50.0 degrees
No. Observations (I>3.50(sig(I)))	1803
No. Variables	307
Residuals: R; Rw	0.048; 0.065
Goodness of Fit Indicator	1.71
Maximum Shift in Final Cycle	0.00
Largest Peak in Final Diff. Map	0.20 e/angstrom**3

Intramolecular distances involving the nonhydrogen atoms

atom	atom	distance	atom	atom	distance
SI	O3	1.653(4)	C3	C4	1.522(8)
SI	C18	1.864(7)	C3	C5	1.525(8)
SI	C19	1.866(8)	C4	C9	1.517(9)
SI	C20	1.866(8)	C5	C6	1.522(8)
O1	C1	1.376(8)	C6	C7	1.549(8)
O1	C4	1.472(7)	C7	C8	1.525(8)
O2	C1	1.186(7)	C7	C11	1.54(1)
O3	C9	1.431(8)	C9	C10	1.508(9)
O4	C13	1.416(8)	C11	C12	1.515(8)
O4	C11	1.432(7)	C13	C15	1.520(8)
O5	C11	1.432(7)	C14	C15	1.51(1)
O5	C14	1.438(8)	C15	C17	1.51(1)
O6	C5	1.414(7)	C15	C16	1.55(1)
O6	C24	1.444(8)	C20	C21	1.53(1)
O7	C24	1.433(7)	C20	C23	1.53(1)
O7	C6	1.438(8)	C20	C22	1.55(1)
C1	C2	1.482(8)	C24	C25	1.50(1)
C2	C3	1.516(8)	C24	C26	1.507(9)
C2	C8	1.520(9)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving Hydrogen Atoms

atom	atom	distance	atom	atom	distance
C2	H2	0.950	C17	H26	0.950
C3	H1	0.950	C17	H27	0.950
C4	H9	0.950	C18	H8	0.950
C5	H3	0.950	C18	H28	0.950
C6	H4	0.950	C18	H29	0.950
C7	H10	0.950	C19	H30	0.950
C8	H13	0.950	C19	H31	0.950
C8	H14	0.950	C19	H32	0.950
C9	H15	0.950	C21	H33	0.950
C10	H12	0.950	C21	H34	0.950
C10	H16	0.950	C21	H35	0.950
C10	H17	0.950	C22	H36	0.950
C12	H7	0.950	C22	H37	0.950
C12	H18	0.950	C22	H38	0.950
C12	H19	0.950	C23	H39	0.950
C13	H20	0.950	C23	H40	0.950
C13	H21	0.950	C23	H41	0.950
C14	H22	0.950	C25	H42	0.950
C14	H23	0.950	C25	H43	0.950
C16	H11	0.950	C25	H44	0.950
C16	H24	0.950	C26	H6	0.950
C16	H25	0.950	C26	H45	0.950
C17	H5	0.950	C26	H46	0.950

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
O3	SI	C18	110.8(3)	C6	C5	C3	110.8(5)
O3	SI	C19	108.6(3)	O7	C6	C5	99.9(5)
O3	SI	C20	103.5(3)	O7	C6	C7	109.1(5)
C18	SI	C19	109.5(4)	C5	C6	C7	120.1(5)
C18	SI	C20	112.4(4)	C8	C7	C11	115.0(5)
C19	SI	C20	111.3(4)	C8	C7	C6	112.7(5)
C1	O1	C4	110.6(5)	C11	C7	C6	109.6(5)
C9	O3	SI	125.1(4)	C2	C8	C7	109.5(5)
C13	O4	C11	114.6(5)	O3	C9	C10	110.1(5)
C11	O5	C14	113.8(4)	O3	C9	C4	108.1(5)
C5	O6	C24	108.3(4)	C10	C9	C4	112.1(5)
C24	O7	C6	106.3(5)	O5	C11	O4	109.1(5)
O2	C1	O1	120.7(6)	O5	C11	C12	110.7(5)
O2	C1	C2	131.4(7)	O5	C11	C7	105.9(5)
O1	C1	C2	107.8(5)	O4	C11	C12	111.4(5)
C1	C2	C3	103.9(5)	O4	C11	C7	106.9(4)
C1	C2	C8	120.0(5)	C12	C11	C7	112.6(5)
C3	C2	C8	110.7(5)	O4	C13	C15	111.0(5)
C2	C3	C4	101.5(4)	O5	C14	C15	112.5(5)
C2	C3	C5	110.2(5)	C17	C15	C14	110.1(6)
C4	C3	C5	120.8(5)	C17	C15	C13	111.4(6)
O1	C4	C9	106.1(5)	C17	C15	C16	111.1(6)
O1	C4	C3	104.0(5)	C14	C15	C13	107.1(5)
C9	C4	C3	119.9(5)	C14	C15	C16	108.2(6)
O6	C5	C6	102.5(4)	C13	C15	C16	108.8(6)
O6	C5	C3	114.2(5)	C21	C20	C23	108.3(7)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Bond angles involving the nonhydrogen atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C21	C20	C22	107.5(7)				
C21	C20	SI	109.8(6)				
C23	C20	C22	111.2(6)				
C23	C20	SI	110.6(5)				
C22	C20	SI	108.9(5)				
O7	C24	O6	105.2(5)				
O7	C24	C25	109.4(6)				
O7	C24	C26	110.8(5)				
O6	C24	C25	110.8(5)				
O6	C24	C26	107.7(6)				
C25	C24	C26	112.7(6)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular bond angles involving the hydrogen atoms

atom	atom	atom	angle	atom	atom	atom	angle
H2	C2	C1	107.19	H12	C10	H16	109.47
H2	C2	C3	107.19	H12	C10	H17	109.47
H2	C2	C8	107.19	H12	C10	C9	109.47
H1	C3	C2	107.88	H16	C10	H17	109.47
H1	C3	C4	107.88	H16	C10	C9	109.47
H1	C3	C5	107.88	H17	C10	C9	109.47
H9	C4	O1	108.75	H7	C12	H18	109.47
H9	C4	C9	108.75	H7	C12	H19	109.47
H9	C4	C3	108.75	H7	C12	C11	109.47
H3	C5	O6	109.70	H18	C12	H19	109.47
H3	C5	C6	109.70	H18	C12	C11	109.47
H3	C5	C8	109.70	H19	C12	C11	109.47
H4	C6	C7	109.03	H20	C13	H21	109.46
H4	C6	C5	109.03	H20	C13	O4	109.09
H4	C6	C7	109.04	H20	C13	C15	109.09
H10	C7	C8	106.33	H21	C13	O4	109.09
H10	C7	C11	106.33	H21	C13	C15	109.09
H10	C7	C6	106.33	H22	C14	H23	109.46
H13	C8	H14	109.46	H22	C14	O5	108.72
H13	C8	C2	109.46	H22	C14	C15	108.72
H13	C8	C7	109.46	H23	C14	O5	108.72
H14	C8	C2	109.46	H23	C14	C15	108.72
H14	C8	C7	109.46	H11	C16	H24	109.47
H15	C9	O3	108.78	H11	C16	H25	109.47
H15	C9	C10	108.79	H11	C16	C15	109.47
H15	C9	C4	108.79	H24	C16	H25	109.47

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Bond Angles (cont.)

atom	atom	atom	angle	atom	atom	atom	angle
H24	C16	C15	109.47	H36	C22	H37	109.47
H25	C16	C15	109.47	H36	C22	H38	109.47
H5	C17	H26	109.47	H36	C22	C20	109.47
H5	C17	H27	109.47	H37	C22	H38	109.47
H5	C17	C15	109.47	H37	C22	C20	109.47
H26	C17	H27	109.47	H38	C22	C20	109.47
H26	C17	C15	109.47	H39	C23	H40	109.47
H27	C17	C15	109.47	H39	C23	H41	109.47
H8	C18	H28	109.47	H39	C23	C20	109.47
H8	C18	H29	109.47	H40	C23	H41	109.47
H8	C18	SI	109.47	H40	C23	C20	109.47
H28	C18	H29	109.47	H41	C23	C20	109.47
H28	C18	SI	109.47	H42	C25	H43	109.47
H29	C18	SI	109.47	H42	C25	H44	109.47
H30	C19	H31	109.47	H42	C25	C24	109.47
H30	C19	H32	109.47	H43	C25	H44	109.47
H30	C19	SI	109.47	H43	C25	C24	109.47
H31	C19	H32	109.47	H44	C25	C24	109.47
H31	C19	SI	109.47	H6	C26	H45	109.47
H32	C19	SI	109.47	H6	C26	H46	109.47
H33	C21	H34	109.47	H6	C26	C24	109.47
H33	C21	H35	109.47	H45	C26	H46	109.47
H33	C21	C20	109.47	H45	C26	C24	109.47
H34	C21	H35	109.47	H46	C26	C24	109.47
H34	C21	C20	109.47				
H35	C21	C20	109.47				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Torsion Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
SI	O3	C9	C10	113.7(5)	O5	C14	C15	C16	-169.3(5)
SI	O3	C9	C4	-123.4(5)	O6	C5	C6	O7	40.1(5)
O1	C1	C2	C3	26.3(7)	O6	C5	C6	C7	159.0(5)
O1	C1	C2	C8	150.6(5)	O6	C5	C3	C2	-165.5(5)
O1	C4	C9	O3	71.4(6)	O6	C5	C3	C4	76.7(7)
O1	C4	C9	C10	-166.9(5)	O6	C24	O7	C6	24.0(6)
O1	C4	C8	C2	30.2(6)	O7	C24	O6	C5	3.0(6)
O1	C4	C8	C5	152.4(5)	O7	C6	C5	C3	-82.2(5)
O2	C1	O1	C4	176.3(6)	O7	C6	C7	C8	79.0(6)
O2	C1	C2	C3	-157.2(8)	O7	C6	C7	C11	-151.7(5)
O2	C1	C2	C8	-33(1)	C1	O1	C4	C9	-142.9(5)
O3	C9	C4	C3	-45.8(7)	C1	O1	C4	C3	-15.5(7)
O3	SI	C20	C21	-55.3(6)	C1	C2	C3	C4	-34.2(6)
O3	SI	C20	C25	64.3(6)	C1	C2	C3	C5	-163.4(5)
O3	SI	C20	C22	-173.2(6)	C1	C2	C8	C7	175.5(6)
O4	C13	C15	C17	-67.4(8)	C2	C1	O1	C4	-6.7(7)
O4	C13	C15	C14	53.1(7)	C2	C3	C4	C9	148.5(5)
O4	C13	C15	C16	169.8(6)	C2	C3	C5	C6	-50.3(7)
O4	C11	O5	C14	-54.5(6)	C2	C8	C7	C11	-80.6(6)
O4	C11	C7	C8	74.5(6)	C2	C8	C7	C6	46.0(7)
O4	C11	C7	C6	-53.6(6)	C3	C2	C8	C7	-63.5(7)
O5	C11	O4	C13	56.9(6)	C3	C4	C9	C10	75.9(7)
O5	C11	C7	C8	-169.2(5)	C3	C5	O6	C24	93.1(6)
O5	C11	C7	C6	62.7(6)	C3	C5	C6	C7	36.8(8)
O5	C14	C15	C17	69.2(7)	C4	C3	C2	C8	-164.3(5)
O5	C14	C15	C13	-52.2(7)	C4	C3	C5	C6	-168.2(5)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion Angles (cont.)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
C5	O6	C24	C25	-115.2(5)	C19	SI	C20	C23	-52.5(6)
C5	O6	C24	C26	121.2(6)	C19	SI	C20	C22	70.0(6)
C5	C6	O7	C24	-39.2(5)					
C5	C6	C7	C8	-35.3(8)					
C5	C6	C7	C11	94.1(7)					
C5	C8	C2	C3	66.5(6)					
C5	C8	C4	C9	-39.4(7)					
C6	O7	C24	C25	148.0(5)					
C6	O7	C24	C26	-92.2(6)					
C6	C5	O6	C24	-26.9(6)					
C6	C7	C11	C12	-176.2(5)					
C7	C11	O5	C14	-169.3(5)					
C7	C11	O4	C13	171.0(5)					
C7	C8	O7	C24	-166.0(4)					
C8	C7	C11	C12	-48.1(7)					
C9	O3	SI	C18	67.4(6)					
C9	O3	SI	C19	-53.0(6)					
C9	O3	SI	C20	-171.9(5)					
C11	O5	C14	C15	55.4(6)					
C11	O4	C13	C15	-58.3(7)					
C12	C11	O5	C14	68.5(7)					
C12	C11	O4	C13	-65.7(6)					
C18	SI	C20	C21	63.3(6)					
C18	SI	C20	C23	-176.1(6)					
C18	SI	C20	C22	-53.6(7)					
C19	SI	C20	C21	-172.5(5)					

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.