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[Th(cot")2]

Identification code	JAN1997
Empirical formula	C40 H72 Si4 Th
Formula weight	897.4
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c (No.15)
Unit cell dimensions	a = 22.136(9) Å alpha = 90 deg. b = 10.412(5) Å beta = 112.64(4) deg. c = 20.807(10) Å gamma = 90 deg.
Volume	4426(4) $Å^3$
Z	4
Density (calculated)	1.35 Mg/m^3
Absorption coefficient	3.50 mm^{-1}
F(000)	1832
Crystal size	0.20 x 0.20 x 0.15 mm
Theta range for data collection	2 to 23 deg.
Index ranges	0<=h<=24, 0<=k<=11, -22<=l<=21
Reflections collected	3155
Independent reflections	3074 [R(int) = 0.0370]
Reflections with I>2sigma(I)	2506
Structure solution	Direct methods
Refinement method	Full-matrix least-squares on all F^2
Data / restraints / parameters	3073 / 0 / 204
Goodness-of-fit on F^2	1.009
Final R indices [I>2sigma(I)]	R1 = 0.039, wR2 = 0.071
R indices (all data)	R1 = 0.060, wR2 = 0.078
Largest diff. peak and hole	0.50 and -0.53 $e.Å^{-3}$
Abs.correction from psi scans	Tmax=1.00 ,Tmin=0.80
Maximum shift/e.s.d.	0.001

The molecule lies on a 2-fold rotation axis.

All non-H atoms were anisotropic. H's were included in riding

mode with $I/\sigma(I)$ equal to 1.2 eq(3) or 1.5 eq(3) for [illegible] groups.

Programs used were :
Data collection - Enraf-Nonius CAD4 software
Structure solution - SHELXS-86
Structure refinement - SHELXL-93
Interactive graphics and final drawings - CAMERON

References :

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Sheldrick,G.M.(1985) SHELXS-86. Program for the Solution of Crystal Structures. Univ. of Gottingen, Germany.

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Th	5000	1608.3(4)	7500	26(1)
Si(1)	6314(1)	-62(2)	9340(1)	33(1)
Si(2)	4040(1)	4877(2)	7917(1)	49(1)
C(1)	5504(3)	707(6)	8828(3)	26(2)
C(2)	5485(3)	2075(6)	8884(4)	29(2)
C(3)	5031(3)	3058(7)	8596(4)	33(2)
C(4)	4380(3)	3192(7)	8105(4)	31(2)
C(5)	3912(4)	2255(7)	7730(4)	32(2)
C(6)	3893(3)	909(7)	7689(4)	30(2)
C(7)	4342(3)	-97(7)	7993(3)	31(2)
C(8)	5001(3)	-148(7)	8453(3)	28(2)
C(9)	7001(3)	1053(7)	9413(4)	49(2)
C(10)	6422(3)	-1552(7)	8897(3)	39(2)
C(11)	6351(4)	-486(9)	10235(4)	47(2)
C(12)	5768(4)	-1316(8)	10189(4)	61(3)
C(13)	6995(4)	-1233(10)	10629(4)	73(3)
C(14)	6348(4)	732(9)	10653(4)	68(3)
C(15)	4709(4)	6100(7)	8244(5)	69(3)
C(16)	3607(4)	5069(8)	6951(4)	66(3)
C(17)	3445(4)	5185(8)	8353(6)	59(3)
C(18)	3810(5)	5161(10)	9139(5)	82(3)
C(19)	3140(4)	6524(8)	8134(5)	77(3)
C(20)	2884(4)	4208(8)	8131(6)	78(3)

Table 3. Bond lengths [Å] and angles [deg] for 1.

Th-C(1)	2.717(7)	Th-C(2)	2.702(7)
Th-C(3)	2.713(7)	Th-C(4)	2.742(7)
Th-C(5)	2.714(7)	Th-C(6)	2.726(7)
Th-C(7)	2.734(7)	Th-C(8)	2.696(7)
Th-M(1)	1.999(7)	Si(1)-C(10)	1.866(7)
Si(1)-C(9)	1.872(7)	Si(1)-C(1)	1.877(7)
Si(1)-C(11)	1.885(8)	Si(2)-C(15)	1.871(8)
Si(2)-C(16)	1.876(8)	Si(2)-C(4)	1.889(7)
Si(2)-C(17)	1.892(9)	C(1)-C(8)	1.404(9)
C(1)-C(2)	1.431(9)	C(2)-C(3)	1.396(9)
C(3)-C(4)	1.417(9)	C(4)-C(5)	1.418(10)
C(5)-C(6)	1.403(9)	C(6)-C(7)	1.415(9)
C(7)-C(8)	1.404(9)	C(11)-C(12)	1.526(11)
C(11)-C(14)	1.540(11)	C(11)-C(13)	1.552(10)
C(17)-C(18)	1.519(12)	C(17)-C(20)	1.534(11)
C(17)-C(19)	1.539(11)		

M(1)-Th-M(1)'	172.3(3)	C(10)-Si(1)-C(9)	107.5(3)
C(10)-Si(1)-C(1)	110.5(3)	C(9)-Si(1)-C(1)	110.5(3)
C(10)-Si(1)-C(11)	109.2(4)	C(9)-Si(1)-C(11)	109.9(4)
C(1)-Si(1)-C(11)	109.2(3)	C(15)-Si(2)-C(16)	108.9(4)
C(15)-Si(2)-C(4)	111.1(3)	C(16)-Si(2)-C(4)	108.6(4)
C(15)-Si(2)-C(17)	108.0(4)	C(16)-Si(2)-C(17)	109.5(4)
C(4)-Si(2)-C(17)	110.7(4)	C(8)-C(1)-C(2)	129.3(7)
C(8)-C(1)-Si(1)	115.1(5)	C(2)-C(1)-Si(1)	115.5(5)
C(3)-C(2)-C(1)	137.2(7)	C(2)-C(3)-C(4)	138.2(7)
C(3)-C(4)-C(5)	130.8(7)	C(3)-C(4)-Si(2)	117.0(5)
C(5)-C(4)-Si(2)	112.1(5)	C(6)-C(5)-C(4)	136.0(8)
C(5)-C(6)-C(7)	135.5(8)	C(8)-C(7)-C(6)	134.3(7)
C(7)-C(8)-C(1)	138.4(7)	C(12)-C(11)-C(14)	108.3(7)
C(12)-C(11)-C(13)	109.4(7)	C(14)-C(11)-C(13)	108.5(7)
C(12)-C(11)-Si(1)	111.0(5)	C(14)-C(11)-Si(1)	110.9(6)
C(13)-C(11)-Si(1)	108.7(5)	C(18)-C(17)-C(20)	110.2(8)
C(18)-C(17)-C(19)	108.9(8)	C(20)-C(17)-C(19)	107.4(7)
C(18)-C(17)-Si(2)	109.5(6)	C(20)-C(17)-Si(2)	112.0(6)

M(1) is the centroid of the C(1) to C(8) ring.
Symmetry element ' is 1-x,y,1.5-z

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Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for 1.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Th	19(1)	17(1)	39(1)	0	7(1)	0
Si(1)	21(1)	37(1)	32(1)	-7(1)	2(1)	5(1)
Si(2)	37(1)	18(1)	93(2)	5(1)	27(1)	8(1)
C(1)	22(4)	19(4)	33(4)	-7(3)	7(3)	-3(3)
C(2)	26(4)	24(4)	34(4)	-12(3)	8(3)	-4(3)
C(3)	27(4)	21(5)	51(5)	-6(4)	14(4)	-5(3)
C(4)	23(4)	16(4)	57(5)	-2(4)	17(4)	-2(4)
C(5)	25(4)	28(5)	45(5)	9(4)	15(4)	6(4)
C(6)	20(4)	33(5)	36(5)	3(4)	9(4)	-4(4)
C(7)	24(4)	25(4)	39(5)	3(4)	8(4)	-4(4)
C(8)	34(4)	18(4)	31(4)	9(3)	11(4)	4(4)
C(9)	22(4)	55(5)	56(5)	-19(4)	2(4)	-1(4)
C(10)	31(4)	36(4)	40(4)	-4(4)	4(3)	19(4)
C(11)	34(5)	68(6)	30(5)	3(4)	2(4)	16(5)
C(12)	51(5)	76(8)	50(5)	14(5)	12(4)	17(5)
C(13)	49(5)	116(10)	39(5)	3(5)	1(4)	22(6)
C(14)	68(7)	85(8)	51(6)	-15(6)	21(5)	-6(6)
C(15)	53(6)	21(5)	136(9)	-11(5)	41(6)	1(4)
C(16)	45(5)	43(6)	97(7)	35(5)	13(5)	3(5)
C(17)	47(5)	30(5)	112(8)	4(5)	44(6)	7(4)
C(18)	70(7)	70(8)	125(10)	-2(7)	58(7)	15(6)
C(19)	71(6)	26(5)	142(9)	-4(6)	49(6)	18(5)
C(20)	62(6)	33(5)	168(11)	-9(6)	77(7)	-2(5)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2)	5889(3)	2403(6)	9204(4)	35
H(3)	5211(3)	3868(7)	8782(4)	40
H(5)	3511(4)	2633(7)	7433(4)	39
H(6)	3478(3)	599(7)	7383(4)	36
H(7)	4156(3)	-924(7)	7855(3)	37
H(8)	5150(3)	-1011(7)	8533(3)	34
H(9C)	6958(3)	1847(7)	9644(4)	73
H(9B)	6985(3)	1254(7)	8946(4)	73
H(9A)	7420(3)	642(7)	9686(4)	73
H(10C)	6069(3)	-2157(7)	8851(3)	58
H(10B)	6845(3)	-1946(7)	9173(3)	58
H(10A)	6410(3)	-1335(7)	8434(3)	58
H(12C)	5762(4)	-2097(8)	9925(4)	92
H(12B)	5362(4)	-834(8)	9955(4)	92
H(12A)	5805(4)	-1548(8)	10660(4)	92
H(13C)	7370(4)	-700(10)	10659(4)	109
H(13B)	6998(4)	-2027(10)	10378(4)	109
H(13A)	7025(4)	-1442(10)	11099(4)	109
H(14C)	6721(4)	1277(9)	10688(4)	102
H(14B)	6382(4)	490(9)	11121(4)	102
H(14A)	5940(4)	1205(9)	10416(4)	102
H(15C)	4938(4)	6007(7)	8749(5)	103
H(15B)	4521(4)	6963(7)	8137(5)	103
H(15A)	5019(4)	5969(7)	8017(5)	103
H(16C)	3256(4)	4432(8)	6774(4)	99
H(16B)	3919(4)	4940(8)	6726(4)	99
H(16A)	3421(4)	5934(8)	6846(4)	99
H(18C)	4167(5)	5790(10)	9274(5)	123
H(18B)	3990(5)	4301(10)	9285(5)	123
H(18A)	3507(5)	5377(10)	9364(5)	123
H(19C)	2904(4)	6548(8)	7627(5)	116
H(19B)	3487(4)	7174(8)	8273(5)	116
H(19A)	2835(4)	6702(8)	8361(5)	116
H(20C)	2654(4)	4232(8)	7623(6)	117
H(20B)	2579(4)	4421(8)	8352(6)	117
H(20A)	3062(4)	3345(8)	8274(6)	117

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 14.330 (0.029) x - 0.641 (0.019) y + 19.774 (0.017) z = 9.560 (0.023)

*	-0.038 (0.006)	C1
*	0.015 (0.006)	C2
*	0.031 (0.006)	C3
*	-0.015 (0.005)	C4
*	-0.025 (0.006)	C5
*	0.007 (0.006)	C6
*	0.028 (0.005)	C7
*	-0.004 (0.005)	C8
	-1.998 (0.003)	Th
	-0.136 (0.007)	Si1
	-0.008 (0.008)	Si2

Rms deviation of fitted atoms = 0.023

- 14.330 (0.029) x + 0.641 (0.019) y + 19.774 (0.017) z = 5.771 (0.022)

Angle to previous plane (with approximate esd) = 7.06 (0.18)

*	0.038 (0.006)	C1_$1
*	-0.015 (0.006)	C2_$1
*	-0.031 (0.006)	C3_$1
*	0.015 (0.005)	C4_$1
*	0.025 (0.006)	C5_$1
*	-0.007 (0.006)	C6_$1
*	-0.028 (0.005)	C7_$1
*	0.004 (0.005)	C8_$1

Rms deviation of fitted atoms = 0.023

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Crystal data and structure refinement for 2

Identification code	97SRC054
Empirical formula	C48 H92 K O4 Si4 Th
Formula weight	1116.72
Temperature	120(2) K
Wavelength	0.71069 A
Crystal system	Orthorhombic
Space group	Pbcn
Unit cell dimensions	a = 19.0274(14) A b = 26.419(4) A c = 23.9502(12) A
Volume	12040(2) A^3
Z	8
Density (calculated)	1.232 Mg/m^3
Absorption coefficient	2.660 mm^-1
F(000)	4616
Crystal size	0.28 x 0.145 x 0.145 mm
Theta range for data collection	1.76 to 25.08 deg.
Index ranges	-21<=h<=21, -26<=k<=31, -28<=l<=25
Reflections collected	37757
Independent reflections	9384 [R(int) = 0.0811]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9367 / 0 / 547
Goodness-of-fit on F^2	0.725
Final R indices [I>2sigma(I)]	R1 = 0.0310, wR2 = 0.0733
R indices (all data)	R1 = 0.0777, wR2 = 0.1324
Largest diff. peak and hole	1.085 and -0.481 e.A^-3

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

	x	y	z	U(eq)
Th(1)	7014(1)	5380(1)	8578(1)	15(1)
Si(1)	8087(1)	5960(1)	7140(1)	22(1)
Si(2)	7271(1)	3807(1)	8720(1)	24(1)
Si(3)	8957(1)	5895(1)	9296(1)	21(1)
Si(4)	5453(1)	6484(1)	8741(1)	20(1)
O(1)	7402(3)	7086(2)	10570(2)	42(1)
O(2)	6128(3)	6835(2)	11133(2)	57(2)
O(3)	5831(2)	5670(2)	10974(2)	27(1)
O(4)	7275(2)	5779(2)	11266(2)	30(1)
K(1)	6800(1)	6180(1)	10322(1)	24(1)
C(1)	7548(3)	5457(3)	7494(2)	19(2)
C(2)	7908(3)	5040(3)	7741(2)	18(2)
C(3)	7746(3)	4627(3)	8045(2)	16(2)
C(4)	7126(3)	4375(2)	8255(2)	21(2)
C(5)	6395(3)	4509(2)	8181(2)	17(2)
C(6)	6014(3)	4881(3)	7926(2)	17(2)
C(7)	6165(3)	5324(3)	7635(2)	19(2)
C(8)	6800(3)	5570(2)	7464(2)	18(2)
C(9)	9054(3)	5873(3)	7304(3)	32(2)
C(10)	7819(3)	6601(3)	7383(3)	39(2)
C(11)	7998(3)	5929(2)	6354(3)	19(2)
C(12)	8183(3)	5403(3)	6139(3)	34(2)
C(13)	8480(4)	6308(3)	6075(3)	36(2)
C(14)	7250(3)	6061(3)	6148(3)	33(2)
C(15)	8130(3)	3851(3)	9099(3)	35(2)
C(16)	6578(4)	3750(3)	9261(3)	34(2)
C(17)	7263(4)	3208(3)	8287(3)	43(2)
C(18)	7261(4)	2730(3)	8679(3)	54(3)
C(19)	7940(4)	3193(3)	7914(3)	56(2)
C(20)	6580(5)	3184(3)	7919(3)	59(3)
C(21)	7972(3)	5838(2)	9336(2)	16(1)
C(22)	7586(3)	6234(3)	9104(2)	15(2)
C(23)	6872(3)	6362(2)	9000(2)	17(2)
C(24)	6200(3)	6124(3)	9087(2)	15(2)
C(25)	6016(3)	5675(3)	9358(2)	17(2)
C(26)	6387(3)	5269(3)	9608(2)	16(2)
C(27)	7067(3)	5149(2)	9706(2)	17(2)
C(28)	7737(3)	5387(3)	9588(2)	19(2)
C(29)	9226(3)	6438(3)	8842(3)	34(2)
C(30)	9338(3)	5311(3)	8981(3)	33(2)
C(31)	9346(3)	6009(3)	10009(3)	23(2)
C(32)	10140(3)	6074(3)	9969(3)	38(2)
C(33)	9198(3)	5568(3)	10416(3)	31(2)
C(34)	9022(3)	6489(3)	10259(3)	31(2)
C(35)	4736(3)	6032(2)	8540(3)	28(2)
C(36)	5768(3)	6806(3)	8092(3)	34(2)
C(37)	5064(3)	6982(3)	9234(3)	25(2)
C(38)	5607(4)	7388(3)	9356(4)	57(3)
C(39)	4433(4)	7230(3)	8935(3)	52(3)
C(40)	4839(4)	6749(3)	9775(3)	55(3)
C(41)	7540(4)	7460(4)	10156(3)	65(3)
C(42)	7208(4)	7282(3)	11092(3)	55(3)
C(43)	6437(4)	7310(3)	11191(4)	52(3)
C(44)	5427(4)	6816(3)	11311(4)	65(3)

C(46)	6174(3)	5330(3)	11341(3)	42(2)
C(47)	6741(4)	5625(3)	11654(3)	44(2)
C(48)	7875(4)	5964(3)	11564(3)	38(2)

Table 4. Bond lengths [A] and angles [deg] for 2 .

Th(1)-C(3)	2.746(7)	Th(1)-C(26)	2.755(6)
Th(1)-C(8)	2.747(6)	Th(1)-C(5)	2.756(6)
Th(1)-C(25)	2.775(6)	Th(1)-C(2)	2.780(6)
Th(1)-C(27)	2.771(6)	Th(1)-C(24)	2.783(6)
Th(1)-C(7)	2.781(6)	Th(1)-C(4)	2.773(6)
Th(1)-C(6)	2.792(6)	Th(1)-C(28)	2.782(6)
Si(1)-C(10)	1.860(7)	Si(1)-C(1)	1.881(7)
Si(1)-C(9)	1.896(6)	Si(1)-C(11)	1.893(6)
Si(2)-C(16)	1.853(7)	Si(2)-C(15)	1.874(6)
Si(2)-C(4)	1.890(7)	Si(2)-C(17)	1.891(8)
Si(3)-C(30)	1.866(7)	Si(3)-C(29)	1.871(7)
Si(3)-C(31)	1.885(7)	Si(3)-C(21)	1.883(7)
Si(4)-C(36)	1.871(7)	Si(4)-C(35)	1.876(6)
Si(4)-C(24)	1.901(6)	Si(4)-C(37)	1.915(7)
O(1)-C(41)	1.424(9)	O(1)-C(42)	1.404(8)
O(1)-K(1)	2.721(5)	O(2)-C(44)	1.402(8)
O(2)-C(43)	1.394(8)	O(2)-K(1)	2.898(5)
O(3)-C(46)	1.418(8)	O(3)-C(45)	1.436(7)
O(3)-K(1)	2.764(4)	O(4)-C(48)	1.433(7)
O(4)-C(47)	1.435(7)	O(4)-K(1)	2.655(5)
K(1)-C(26)	3.054(6)	K(1)-C(25)	3.054(6)
K(1)-C(27)	3.138(6)	K(1)-C(24)	3.174(6)
K(1)-C(23)	3.207(6)	K(1)-C(28)	3.265(7)
K(1)-C(22)	3.282(6)	K(1)-C(21)	3.371(6)
C(1)-C(2)	1.426(9)	C(1)-C(8)	1.456(8)
C(2)-C(3)	1.347(9)	C(3)-C(4)	1.446(8)
C(4)-C(5)	1.445(8)	C(5)-C(6)	1.366(8)
C(6)-C(7)	1.393(9)	C(7)-C(8)	1.433(8)
C(11)-C(13)	1.515(9)	C(11)-C(12)	1.522(9)
C(11)-C(14)	1.546(8)	C(17)-C(19)	1.568(10)
C(17)-C(20)	1.574(10)	C(17)-C(18)	1.573(10)
C(21)-C(22)	1.392(8)	C(21)-C(28)	1.409(9)
C(22)-C(23)	1.423(8)	C(23)-C(24)	1.439(8)
C(24)-C(25)	1.397(9)	C(25)-C(26)	1.416(9)
C(26)-C(27)	1.354(8)	C(27)-C(28)	1.449(8)
C(31)-C(32)	1.523(8)	C(31)-C(34)	1.532(9)
C(31)-C(33)	1.545(9)	C(37)-C(40)	1.498(9)
C(37)-C(38)	1.520(9)	C(37)-C(39)	1.544(9)
C(42)-C(43)	1.488(10)	C(46)-C(47)	1.527(10)
C(3)-Th(1)-C(26)	124.0(2)	C(3)-Th(1)-C(8)	75.8(2)
C(26)-Th(1)-C(8)	145.6(2)	C(3)-Th(1)-C(5)	56.7(2)
C(26)-Th(1)-C(5)	92.0(2)	C(8)-Th(1)-C(5)	75.8(2)
C(3)-Th(1)-C(25)	149.8(2)	C(26)-Th(1)-C(25)	29.7(2)
C(8)-Th(1)-C(25)	120.1(2)	C(5)-Th(1)-C(25)	100.1(2)
C(3)-Th(1)-C(2)	28.2(2)	C(26)-Th(1)-C(2)	151.2(2)
C(8)-Th(1)-C(2)	56.5(2)	C(5)-Th(1)-C(2)	75.0(2)
C(25)-Th(1)-C(2)	174.4(2)	C(3)-Th(1)-C(27)	106.0(2)
C(26)-Th(1)-C(27)	28.4(2)	C(8)-Th(1)-C(27)	173.3(2)
C(5)-Th(1)-C(27)	99.7(2)	C(25)-Th(1)-C(27)	55.3(2)
C(2)-Th(1)-C(27)	127.5(2)	C(3)-Th(1)-C(24)	176.6(2)
C(26)-Th(1)-C(24)	56.1(2)	C(8)-Th(1)-C(24)	102.4(2)
C(5)-Th(1)-C(24)	120.2(2)	C(25)-Th(1)-C(24)	29.1(2)
C(2)-Th(1)-C(24)	152.2(2)	C(27)-Th(1)-C(24)	75.5(2)
C(3)-Th(1)-C(7)	83.0(2)	C(26)-Th(1)-C(7)	118.0(2)
C(8)-Th(1)-C(7)	30.0(2)	C(5)-Th(1)-C(7)	55.1(2)
C(25)-Th(1)-C(7)	99.4(2)	C(2)-Th(1)-C(7)	75.7(2)
C(27)-Th(1)-C(7)	143.3(2)	C(24)-Th(1)-C(7)	94.0(2)
C(3)-Th(1)-C(4)	30.4(2)	C(26)-Th(1)-C(4)	

C(25)-Th(1)-C(4)	120.6(2)	C(2)-Th(1)-C(4)	56.1(2)
C(27)-Th(1)-C(4)	93.3(2)	C(24)-Th(1)-C(4)	147.2(2)
C(7)-Th(1)-C(4)	76.5(2)	C(3)-Th(1)-C(6)	75.1(2)
C(26)-Th(1)-C(6)	98.9(2)	C(8)-Th(1)-C(6)	56.1(2)
C(5)-Th(1)-C(6)	28.5(2)	C(25)-Th(1)-C(6)	92.5(2)
C(2)-Th(1)-C(6)	82.0(2)	C(27)-Th(1)-C(6)	117.8(2)
C(24)-Th(1)-C(6)	101.5(2)	C(7)-Th(1)-C(6)	28.9(2)
C(4)-Th(1)-C(6)	56.2(2)	C(3)-Th(1)-C(28)	99.1(2)
C(26)-Th(1)-C(28)	55.7(2)	C(8)-Th(1)-C(28)	156.5(2)
C(5)-Th(1)-C(28)	121.1(2)	C(25)-Th(1)-C(28)	75.6(2)
C(2)-Th(1)-C(28)	109.0(2)	C(27)-Th(1)-C(28)	30.3(2)
C(24)-Th(1)-C(28)	83.7(2)	C(7)-Th(1)-C(28)	173.5(2)
C(4)-Th(1)-C(28)	102.1(2)	C(6)-Th(1)-C(28)	145.7(2)
C(10)-Si(1)-C(1)	110.7(3)	C(10)-Si(1)-C(9)	108.1(3)
C(1)-Si(1)-C(9)	110.4(3)	C(10)-Si(1)-C(11)	109.1(3)
C(1)-Si(1)-C(11)	111.6(3)	C(9)-Si(1)-C(11)	106.7(3)
C(16)-Si(2)-C(15)	106.7(3)	C(16)-Si(2)-C(4)	111.8(3)
C(15)-Si(2)-C(4)	111.3(3)	C(16)-Si(2)-C(17)	108.1(3)
C(15)-Si(2)-C(17)	108.9(3)	C(4)-Si(2)-C(17)	109.9(3)
C(30)-Si(3)-C(29)	107.0(3)	C(30)-Si(3)-C(31)	110.2(3)
C(29)-Si(3)-C(31)	107.2(3)	C(30)-Si(3)-C(21)	110.0(3)
C(29)-Si(3)-C(21)	111.3(3)	C(31)-Si(3)-C(21)	111.0(3)
C(36)-Si(4)-C(35)	108.0(3)	C(36)-Si(4)-C(24)	110.5(3)
C(35)-Si(4)-C(24)	109.7(3)	C(36)-Si(4)-C(37)	108.9(3)
C(35)-Si(4)-C(37)	108.3(3)	C(24)-Si(4)-C(37)	111.4(3)
C(41)-O(1)-C(42)	114.4(7)	C(41)-O(1)-K(1)	122.4(5)
C(42)-O(1)-K(1)	114.1(4)	C(44)-O(2)-C(43)	113.7(6)
C(44)-O(2)-K(1)	127.0(4)	C(43)-O(2)-K(1)	114.8(4)
C(46)-O(3)-C(45)	110.0(5)	C(46)-O(3)-K(1)	110.6(4)
C(45)-O(3)-K(1)	122.4(4)	C(48)-O(4)-C(47)	109.8(5)
C(48)-O(4)-K(1)	124.0(4)	C(47)-O(4)-K(1)	115.0(4)
O(4)-K(1)-O(1)	91.2(2)	O(4)-K(1)-O(3)	63.39(13)
O(1)-K(1)-O(3)	125.9(2)	O(4)-K(1)-O(2)	79.5(2)
O(1)-K(1)-O(2)	60.9(2)	O(3)-K(1)-O(2)	67.6(2)
O(4)-K(1)-C(26)	104.5(2)	O(1)-K(1)-C(26)	157.5(2)
O(3)-K(1)-C(26)	76.2(2)	O(2)-K(1)-C(26)	137.1(2)
O(4)-K(1)-C(25)	129.5(2)	O(1)-K(1)-C(25)	139.0(2)
O(3)-K(1)-C(25)	83.6(2)	O(2)-K(1)-C(25)	123.5(2)
C(26)-K(1)-C(25)	26.8(2)	O(4)-K(1)-C(27)	90.0(2)
O(1)-K(1)-C(27)	142.9(2)	O(3)-K(1)-C(27)	87.2(2)
O(2)-K(1)-C(27)	154.8(2)	C(26)-K(1)-C(27)	25.21(14)
C(25)-K(1)-C(27)	49.1(2)	O(4)-K(1)-C(24)	153.9(2)
O(1)-K(1)-C(24)	113.3(2)	O(3)-K(1)-C(24)	105.3(2)
O(2)-K(1)-C(24)	119.6(2)	C(26)-K(1)-C(24)	49.4(2)
C(25)-K(1)-C(24)	25.8(2)	C(27)-K(1)-C(24)	65.2(2)
O(4)-K(1)-C(23)	152.5(2)	O(1)-K(1)-C(23)	93.7(2)
O(3)-K(1)-C(23)	131.2(2)	O(2)-K(1)-C(23)	126.2(2)
C(26)-K(1)-C(23)	64.9(2)	C(25)-K(1)-C(23)	48.7(2)
C(27)-K(1)-C(23)	70.1(2)	C(24)-K(1)-C(23)	26.06(14)
O(4)-K(1)-C(28)	91.0(2)	O(1)-K(1)-C(28)	116.9(2)
O(3)-K(1)-C(28)	110.9(2)	O(2)-K(1)-C(28)	170.0(2)
C(26)-K(1)-C(28)	48.2(2)	C(25)-K(1)-C(28)	65.1(2)
C(27)-K(1)-C(28)	26.1(2)	C(24)-K(1)-C(28)	70.4(2)
C(23)-K(1)-C(28)	62.7(2)	O(4)-K(1)-C(22)	128.3(2)
O(1)-K(1)-C(22)	87.9(2)	O(3)-K(1)-C(22)	145.8(2)
O(2)-K(1)-C(22)	140.4(2)	C(26)-K(1)-C(22)	69.7(2)
C(25)-K(1)-C(22)	64.5(2)	C(27)-K(1)-C(22)	63.0(2)
C(24)-K(1)-C(22)	48.5(2)	C(23)-K(1)-C(22)	25.30(14)
C(28)-K(1)-C(22)	45.6(2)	O(4)-K(1)-C(21)	105.37(14)
O(1)-K(1)-C(21)	96.3(2)	O(3)-K(1)-C(21)	134.9(2)
O(2)-K(1)-C(21)	157.1(2)	C(26)-K(1)-C(21)	64.3(2)
C(25)-K(1)-C(21)	71.1(2)	C(27)-K(1)-C(21)	48.0(2)
C(24)-K(1)-C(21)	64.7(2)	C(23)-K(1)-C(21)	47.2(2)

[illegible]	24.4(2)	C(22)-K(1)-C(21)	24.12(14)
C(2)-C(1)-C(8)	130.5(6)	C(2)-C(1)-Si(1)	118.2(5)
C(8)-C(1)-Si(1)	111.3(5)	C(2)-C(1)-Th(1)	74.6(3)
C(8)-C(1)-Th(1)	72.9(3)	Si(1)-C(1)-Th(1)	131.9(3)
C(3)-C(2)-C(1)	137.7(6)	C(3)-C(2)-Th(1)	74.5(4)
C(1)-C(2)-Th(1)	75.8(3)	C(2)-C(3)-C(4)	138.4(6)
C(2)-C(3)-Th(1)	77.3(4)	C(4)-C(3)-Th(1)	75.9(4)
C(5)-C(4)-C(3)	129.1(6)	C(5)-C(4)-Si(2)	114.0(5)
C(3)-C(4)-Si(2)	116.8(5)	C(5)-C(4)-Th(1)	74.2(4)
C(3)-C(4)-Th(1)	73.8(4)	Si(2)-C(4)-Th(1)	127.4(3)
C(6)-C(5)-C(4)	137.8(6)	C(6)-C(5)-Th(1)	77.2(4)
C(4)-C(5)-Th(1)	75.5(3)	C(5)-C(6)-C(7)	136.1(6)
C(5)-C(6)-Th(1)	74.3(4)	C(7)-C(6)-Th(1)	75.1(4)
C(6)-C(7)-C(8)	134.3(6)	C(6)-C(7)-Th(1)	76.0(4)
C(8)-C(7)-Th(1)	73.7(3)	C(7)-C(8)-C(1)	135.8(6)
C(7)-C(8)-Th(1)	76.3(3)	C(1)-C(8)-Th(1)	76.6(3)
C(13)-C(11)-C(12)	108.4(5)	C(13)-C(11)-C(14)	105.6(5)
C(12)-C(11)-C(14)	108.2(5)	C(13)-C(11)-Si(1)	110.8(5)
C(12)-C(11)-Si(1)	110.9(4)	C(14)-C(11)-Si(1)	112.9(4)
C(19)-C(17)-C(20)	110.9(7)	C(19)-C(17)-C(18)	108.8(6)
C(20)-C(17)-C(18)	107.5(6)	C(19)-C(17)-Si(2)	109.2(5)
C(20)-C(17)-Si(2)	110.3(5)	C(18)-C(17)-Si(2)	110.1(5)
C(22)-C(21)-C(28)	129.8(6)	C(22)-C(21)-Si(3)	116.4(5)
C(28)-C(21)-Si(3)	113.9(5)	C(22)-C(21)-Th(1)	74.2(4)
C(28)-C(21)-Th(1)	73.1(3)	Si(3)-C(21)-Th(1)	129.8(3)
C(22)-C(21)-K(1)	74.4(4)	C(28)-C(21)-K(1)	73.6(4)
Si(3)-C(21)-K(1)	132.3(3)	Th(1)-C(21)-K(1)	97.9(2)
C(21)-C(22)-C(23)	138.8(6)	C(21)-C(22)-Th(1)	77.3(4)
C(23)-C(22)-Th(1)	75.0(3)	C(21)-C(22)-K(1)	81.5(4)
C(23)-C(22)-K(1)	74.4(3)	Th(1)-C(22)-K(1)	100.8(2)
C(22)-C(23)-C(24)	135.9(6)	C(22)-C(23)-Th(1)	75.5(4)
C(24)-C(23)-Th(1)	74.5(4)	C(22)-C(23)-K(1)	80.3(3)
C(24)-C(23)-K(1)	75.7(3)	Th(1)-C(23)-K(1)	102.7(2)
C(25)-C(24)-C(23)	131.4(6)	C(25)-C(24)-Si(4)	116.1(4)
C(23)-C(24)-Si(4)	112.5(5)	C(25)-C(24)-Th(1)	75.1(4)
C(23)-C(24)-Th(1)	75.6(3)	Si(4)-C(24)-Th(1)	125.4(3)
C(25)-C(24)-K(1)	72.3(3)	C(23)-C(24)-K(1)	78.3(3)
Si(4)-C(24)-K(1)	130.7(3)	Th(1)-C(24)-K(1)	103.9(2)
C(24)-C(25)-C(26)	135.6(6)	C(24)-C(25)-Th(1)	75.8(4)
C(26)-C(25)-Th(1)	74.4(3)	C(24)-C(25)-K(1)	81.9(4)
C(26)-C(25)-K(1)	76.6(4)	Th(1)-C(25)-K(1)	107.3(2)
C(27)-C(26)-C(25)	136.7(6)	C(27)-C(26)-Th(1)	76.5(3)
C(25)-C(26)-Th(1)	75.9(3)	C(27)-C(26)-K(1)	80.9(4)
C(25)-C(26)-K(1)	76.6(4)	Th(1)-C(26)-K(1)	107.8(2)
C(26)-C(27)-C(28)	134.8(6)	C(26)-C(27)-Th(1)	75.1(3)
C(28)-C(27)-Th(1)	75.3(3)	C(26)-C(27)-K(1)	73.9(4)
C(28)-C(27)-K(1)	81.9(4)	Th(1)-C(27)-K(1)	105.1(2)
C(21)-C(28)-C(27)	136.8(6)	C(21)-C(28)-Th(1)	77.9(3)
C(27)-C(28)-Th(1)	74.5(3)	C(21)-C(28)-K(1)	82.0(4)
C(27)-C(28)-K(1)	72.1(3)	Th(1)-C(28)-K(1)	101.6(2)
C(32)-C(31)-C(34)	109.3(6)	C(32)-C(31)-C(33)	107.7(5)
C(34)-C(31)-C(33)	107.7(6)	C(32)-C(31)-Si(3)	110.5(4)
C(34)-C(31)-Si(3)	109.2(5)	C(33)-C(31)-Si(3)	112.3(5)
C(40)-C(37)-C(38)	108.5(6)	C(40)-C(37)-C(39)	110.7(6)
C(38)-C(37)-C(39)	108.5(6)	C(40)-C(37)-Si(4)	111.3(5)
C(38)-C(37)-Si(4)	109.9(5)	C(39)-C(37)-Si(4)	107.9(5)
O(1)-C(42)-C(43)	114.8(7)	O(2)-C(43)-C(42)	110.8(7)
O(3)-C(46)-C(47)	107.7(6)	O(4)-C(47)-C(46)	109.1(6)
O(4)-C(47)-K(1)	43.2(3)	C(46)-C(47)-K(1)	77.9(4)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for 2
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Th(1)	17(1)	17(1)	12(1)	-1(1)	0(1)	0(1)
Si(1)	22(1)	24(1)	19(1)	0(1)	4(1)	-4(1)
Si(2)	30(1)	19(1)	22(1)	1(1)	2(1)	-1(1)
Si(3)	16(1)	28(1)	19(1)	1(1)	-2(1)	-1(1)
Si(4)	18(1)	21(1)	23(1)	-4(1)	-3(1)	1(1)
O(1)	53(3)	26(4)	46(3)	-2(3)	11(3)	-13(3)
O(2)	60(4)	31(4)	81(4)	-29(3)	26(3)	-11(3)
O(3)	31(3)	26(3)	23(3)	7(2)	-3(2)	-3(2)
O(4)	31(3)	37(4)	23(3)	1(2)	3(2)	-3(2)
K(1)	31(1)	24(1)	18(1)	-1(1)	0(1)	-7(1)
C(1)	23(4)	23(5)	11(3)	-2(3)	3(3)	-5(4)
C(2)	17(4)	23(5)	13(3)	0(3)	1(3)	-1(4)
C(3)	15(4)	18(4)	15(3)	-3(4)	2(2)	3(4)
C(4)	32(5)	17(4)	14(4)	-4(3)	-6(3)	-1(4)
C(5)	20(4)	14(5)	16(4)	-1(3)	3(3)	-8(3)
C(6)	15(4)	23(5)	13(4)	7(3)	-2(3)	-5(4)
C(7)	12(4)	33(5)	13(3)	-4(4)	-1(3)	15(4)
C(8)	29(4)	12(4)	13(4)	1(3)	0(3)	-1(3)
C(9)	26(4)	33(6)	38(5)	7(4)	1(3)	-9(4)
C(10)	37(5)	39(6)	43(5)	-1(4)	16(4)	-9(4)
C(11)	15(3)	13(4)	29(4)	2(3)	10(4)	-4(3)
C(12)	38(5)	40(5)	23(4)	-4(4)	3(3)	-6(4)
C(13)	35(5)	48(6)	24(4)	5(4)	9(3)	1(4)
C(14)	35(5)	41(6)	22(4)	9(4)	3(3)	10(4)
C(15)	35(5)	42(6)	28(4)	11(4)	-5(3)	4(4)
C(16)	49(5)	22(5)	32(5)	5(4)	-7(4)	-2(4)
C(17)	75(6)	18(5)	36(5)	3(4)	-3(4)	11(4)
C(18)	101(7)	26(6)	36(5)	0(4)	-6(5)	11(5)
C(19)	89(7)	43(6)	36(5)	-11(4)	17(5)	21(6)
C(20)	112(8)	20(6)	45(6)	-6(4)	-33(5)	12(5)
C(21)	21(3)	14(4)	12(3)	1(3)	-3(3)	-4(4)
C(22)	13(4)	17(5)	14(4)	-4(3)	-4(3)	-3(3)
C(23)	17(4)	16(4)	18(4)	-6(3)	4(3)	1(3)
C(24)	14(4)	14(4)	19(4)	-5(3)	3(3)	2(3)
C(25)	13(4)	23(5)	15(4)	-6(3)	5(3)	-6(3)
C(26)	18(4)	14(5)	16(4)	2(3)	0(3)	-11(3)
C(27)	21(4)	18(4)	13(3)	5(3)	-1(3)	-1(4)
C(28)	22(4)	27(5)	10(3)	2(4)	-7(3)	8(4)
C(29)	22(4)	44(6)	37(5)	10(4)	-3(3)	-4(4)
C(30)	28(4)	43(6)	27(4)	-5(4)	2(3)	7(4)
C(31)	22(4)	26(5)	23(4)	-2(3)	0(3)	-2(3)
C(32)	16(4)	64(7)	33(5)	-9(4)	-5(3)	-4(4)
C(33)	29(4)	33(6)	31(4)	1(4)	-9(3)	-3(4)
C(34)	30(4)	30(5)	32(4)	-2(4)	1(3)	-16(4)
C(35)	18(4)	28(5)	37(4)	-11(4)	-7(3)	2(3)
C(36)	33(5)	41(6)	27(4)	2(4)	-8(3)	16(4)
C(37)	15(4)	16(5)	45(5)	-7(4)	-6(3)	1(3)
C(38)	39(5)	53(7)	80(7)	-39(5)	-10(5)	10(5)
C(39)	37(5)	35(6)	83(7)	-32(5)	-2(5)	9(4)
C(40)	64(6)	56(7)	45(6)	-7(5)	23(5)	16(5)
C(41)	66(7)	73(8)	55(7)	23(6)	-16(5)	-19(5)
C(42)	82(8)	36(6)	48(6)	-22(5)	3(5)	-9(5)
C(43)	58(6)	36(7)	62(6)	-17(5)	11(5)	-10(5)
C(44)	59(6)	52(7)	85(8)	-29(6)	36(5)	-12(5)

C(46)	38(4)	37(6)	50(5)	17(5)	-10(4)	-7(4)
C(47)	38(5)	69(7)	26(4)	17(4)	0(4)	3(4)
C(48)	45(5)	34(5)	34(5)	-2(3)	-6(4)	-14(4)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2 .

	x	y	z	U(eq)
H(2)	8389(3)	5057(3)	7673(2)	21
H(3)	8151(3)	4453(3)	8149(2)	19
H(5)	6102(3)	4276(2)	8356(2)	20
H(6)	5533(3)	4824(3)	7954(2)	21
H(7)	5763(3)	5500(3)	7529(2)	23
H(8)	6714(3)	5879(2)	7290(2)	22
H(9A)	9214(6)	5559(8)	7147(15)	48
H(9B)	9119(4)	5867(16)	7702(3)	48
H(9C)	9317(4)	6148(8)	7147(15)	48
H(10A)	7828(21)	6611(5)	7783(3)	59
H(10B)	7353(9)	6674(7)	7253(15)	59
H(10C)	8140(13)	6849(3)	7237(15)	59
H(12A)	7867(13)	5159(3)	6298(12)	51
H(12B)	8656(7)	5322(6)	6244(13)	51
H(12C)	8142(19)	5397(5)	5740(3)	51
H(13A)	8368(14)	6643(3)	6204(13)	54
H(13B)	8419(16)	6292(11)	5678(3)	54
H(13C)	8959(4)	6231(10)	6168(14)	54
H(14A)	7134(9)	6400(6)	6259(15)	49
H(14B)	6918(4)	5829(10)	6310(14)	49
H(14C)	7232(7)	6035(16)	5749(3)	49
H(15A)	8194(11)	3555(8)	9326(14)	53
H(15B)	8130(9)	4146(9)	9333(14)	53
H(15C)	8506(4)	3875(17)	8834(3)	53
H(16A)	6714(11)	3500(11)	9531(10)	52
H(16B)	6144(6)	3650(16)	9088(4)	52
H(16C)	6515(16)	4071(5)	9443(12)	52
H(18A)	6877(16)	2755(9)	8938(13)	81
H(18B)	7696(11)	2714(10)	8881(15)	81
H(18C)	7207(26)	2430(3)	8457(4)	81
H(19A)	7947(15)	3484(10)	7674(16)	84
H(19B)	7937(15)	2891(10)	7691(17)	84
H(19C)	8350(4)	3195(21)	8148(3)	84
H(20A)	6173(5)	3211(22)	8154(4)	89
H(20B)	6566(16)	2868(9)	7721(18)	89
H(20C)	6582(15)	3459(12)	7656(16)	89
H(22)	7884(3)	6490(3)	8981(2)	18
H(23)	6828(3)	6679(2)	8833(2)	21
H(25)	5532(3)	5632(3)	9380(2)	20
H(26)	6083(3)	5020(3)	9738(2)	19
H(27)	7116(3)	4842(2)	9893(2)	21
H(28)	8111(3)	5189(3)	9710(2)	23
H(29A)	9714(6)	6406(8)	8748(14)	51
H(29B)	9152(19)	6750(3)	9039(7)	51
H(29C)	8949(15)	6437(9)	8507(8)	51
H(30A)	9838(4)	5350(6)	8945(15)	49
H(30B)	9135(15)	5255(8)	8620(7)	49
H(30C)	9239(18)	5026(4)	9218(8)	49
H(32A)	10348(4)	5762(5)	9847(18)	57
H(32B)	10324(4)	6162(17)	10329(5)	57
H(32C)	10247(3)	6337(11)	9707(14)	57
H(33A)	9366(17)	5257(3)	10257(7)	47
H(33B)	8701(4)	5543(9)	10481(13)	47
H(33C)	9434(16)	5630(7)	10764(6)	47
H(34A)	8520(4)	6456(6)	10269(15)	46

H(34C)	9196(16)	6537(8)	10632(6)	46
H(35A)	4493(13)	5921(11)	8869(3)	42
H(35B)	4937(3)	5745(7)	8352(14)	42
H(35C)	4411(11)	6199(5)	8294(12)	42
H(36A)	6007(19)	6566(4)	7859(8)	50
H(36B)	6085(17)	7075(10)	8190(3)	50
H(36C)	5374(4)	6944(14)	7894(9)	50
H(38A)	5759(20)	7540(13)	9012(4)	86
H(38B)	6003(12)	7239(5)	9542(19)	86
H(38C)	5403(9)	7643(11)	9591(18)	86
H(39A)	4600(4)	7440(15)	8636(13)	78
H(39B)	4175(15)	7434(15)	9197(6)	78
H(39C)	4131(14)	6972(3)	8788(18)	78
H(40A)	4519(21)	6476(12)	9703(3)	83
H(40B)	4610(24)	7000(5)	10001(9)	83
H(40C)	5244(5)	6622(18)	9969(10)	83
H(41A)	7673(27)	7297(4)	9813(7)	97
H(41B)	7915(20)	7675(13)	10279(10)	97
H(41C)	7125(10)	7658(14)	10095(17)	97
H(42A)	7403(4)	7620(3)	11129(3)	66
H(42B)	7417(4)	7074(3)	11381(3)	66
H(43A)	6349(4)	7438(3)	11564(4)	62
H(43B)	6227(4)	7543(3)	10926(4)	62
H(44A)	5407(5)	6862(22)	11708(5)	98
H(44B)	5228(10)	6494(9)	11215(22)	98
H(44C)	5165(8)	7080(14)	11130(18)	98
H(45A)	4992(13)	5667(6)	10488(14)	54
H(45B)	4895(10)	5353(15)	11038(3)	54
H(45C)	5347(4)	5134(9)	10547(15)	54
H(46A)	6385(3)	5055(3)	11132(3)	50
H(46B)	5839(3)	5188(3)	11603(3)	50
H(47A)	6535(4)	5921(3)	11830(3)	53
H(47B)	6946(4)	5414(3)	11943(3)	53
H(48A)	8224(10)	6077(16)	11303(3)	57
H(48B)	8066(14)	5697(5)	11791(14)	57
H(48C)	7737(6)	6241(11)	11799(14)	57

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Crystal data and structure refinement for 4

Identification code	97SRC053
Empirical formula	C48 H92 K O4 Si4 U
Formula weight	1122.71
Temperature	120(2) K
Wavelength	0.71069 A
Crystal system	Orthorhombic
Space group	Pbcn
Unit cell dimensions	a = 19.1026(5) A b = 26.493(5) A c = 23.701(4) A
Volume	11995(3) A^3
Z	8
Density (calculated)	1.243 Mg/m^3
Absorption coefficient	2.890 mm^-1
F(000)	4632
Crystal size	0.35 x 0.18 x 0.18 mm
Theta range for data collection	1.76 to 25.01 deg.
Index ranges	-20<=h<=14, -28<=k<=28, -18<=l<=26
Reflections collected	36777
Independent reflections	9000 [R(int) = 0.0699]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8974 / 0 / 547
Goodness-of-fit on F^2	0.882
Final R indices [I>2sigma(I)]	R1 = 0.0302, wR2 = 0.0747
R indices (all data)	R1 = 0.0553, wR2 = 0.1212
Largest diff. peak and hole	1.240 and -0.918 e.A^-3

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

	x	y	z	U(eq)
U(1)	7038(1)	5394(1)	8572(1)	13(1)
Si(1)	8095(1)	5970(1)	7135(1)	18(1)
Si(2)	7278(1)	3823(1)	8736(1)	20(1)
Si(3)	8963(1)	5900(1)	9300(1)	17(1)
Si(4)	5470(1)	6489(1)	8735(1)	17(1)
O(1)	7386(2)	7069(2)	10576(2)	37(1)
O(2)	6134(2)	6815(2)	11153(2)	47(1)
O(3)	5833(2)	5645(2)	10963(2)	25(1)
O(4)	7267(2)	5757(2)	11278(1)	24(1)
K(1)	6802(1)	6168(1)	10318(1)	21(1)
C(1)	7548(2)	5477(2)	7499(2)	15(1)
C(2)	7907(3)	5061(2)	7749(2)	18(1)
C(3)	7742(2)	4635(2)	8065(2)	15(1)
C(4)	7136(2)	4393(2)	8287(2)	17(1)
C(5)	6419(3)	4529(2)	8211(2)	18(1)
C(6)	6031(3)	4911(2)	7947(2)	15(1)
C(7)	6200(2)	5354(2)	7647(2)	14(1)
C(8)	6811(3)	5590(2)	7471(2)	17(1)
C(9)	9047(2)	5882(2)	7299(2)	30(2)
C(10)	7851(3)	6614(2)	7385(2)	31(2)
C(11)	7997(2)	5945(2)	6336(2)	18(1)
C(12)	8173(3)	5420(2)	6120(2)	26(1)
C(13)	8490(3)	6324(2)	6064(2)	31(2)
C(14)	7248(3)	6076(2)	6143(2)	35(2)
C(15)	8127(3)	3859(2)	9135(3)	35(2)
C(16)	6576(3)	3760(2)	9289(2)	26(1)
C(17)	7279(3)	3226(2)	8296(2)	31(2)
C(18)	7270(3)	2758(2)	8675(3)	44(2)
C(19)	7936(4)	3203(3)	7934(3)	58(2)
C(20)	6631(3)	3208(2)	7913(3)	49(2)
C(21)	7972(2)	5833(2)	9328(2)	15(1)
C(22)	7585(3)	6243(2)	9093(2)	15(1)
C(23)	6878(2)	6357(2)	8991(2)	14(1)
C(24)	6214(2)	6127(2)	9065(2)	14(1)
C(25)	6029(3)	5668(2)	9329(2)	15(1)
C(26)	6392(2)	5269(2)	9591(2)	14(1)
C(27)	7094(3)	5141(2)	9699(2)	16(1)
C(28)	7748(2)	5376(2)	9577(2)	14(1)
C(29)	9222(3)	6449(2)	8848(2)	26(2)
C(30)	9351(3)	5324(2)	8978(2)	27(2)
C(31)	9339(2)	6007(2)	10031(2)	19(1)
C(32)	10137(2)	6080(2)	10007(2)	35(2)
C(33)	9183(3)	5564(2)	10435(2)	29(2)
C(34)	9021(3)	6484(2)	10286(2)	30(2)
C(35)	4744(2)	6046(2)	8538(3)	26(1)
C(36)	5767(3)	6809(2)	8069(2)	30(2)
C(37)	5097(3)	6988(2)	9230(3)	26(1)
C(38)	5629(3)	7403(2)	9351(3)	47(2)
C(39)	4457(3)	7237(2)	8948(3)	49(2)
C(40)	4880(3)	6747(3)	9789(3)	49(2)
C(41)	7538(4)	7445(3)	10169(3)	51(2)
C(42)	7196(3)	7259(3)	11117(3)	47(2)
C(43)	6423(3)	7295(3)	11200(3)	47(2)
C(44)	5438(3)	6793(3)	11352(3)	56(2)

C(46)	6183(3)	5315(2)	11334(2)	34(2)
C(47)	6736(3)	5594(3)	11655(2)	35(2)
C(48)	7852(3)	5944(2)	11578(2)	32(2)

Table 4. Bond lengths [A] and angles [deg] for 4

U(1)-C(8)	2.696(5)	U(1)-C(3)	2.702(5)
U(1)-C(2)	2.709(5)	U(1)-C(7)	2.717(5)
U(1)-C(5)	2.717(5)	U(1)-C(25)	2.732(5)
U(1)-C(1)	2.732(5)	U(1)-C(26)	2.731(5)
U(1)-C(28)	2.742(5)	U(1)-C(4)	2.742(5)
U(1)-C(6)	2.745(5)	U(1)-C(23)	2.753(5)
Si(1)-C(10)	1.864(6)	Si(1)-C(9)	1.874(5)
Si(1)-C(1)	1.883(5)	Si(1)-C(11)	1.905(5)
Si(2)-C(4)	1.868(6)	Si(2)-C(16)	1.883(5)
Si(2)-C(15)	1.880(5)	Si(2)-C(17)	1.894(6)
Si(3)-C(30)	1.861(6)	Si(3)-C(29)	1.873(6)
Si(3)-C(21)	1.901(5)	Si(3)-C(31)	1.898(5)
Si(4)-C(36)	1.880(6)	Si(4)-C(24)	1.886(5)
Si(4)-C(35)	1.875(5)	Si(4)-C(37)	1.905(6)
O(1)-C(42)	1.424(7)	O(1)-C(41)	1.417(7)
O(1)-K(1)	2.707(4)	O(2)-C(43)	1.392(7)
O(2)-C(44)	1.413(7)	O(2)-K(1)	2.913(4)
O(3)-C(46)	1.409(6)	O(3)-C(45)	1.429(6)
O(3)-K(1)	2.770(4)	O(4)-C(48)	1.414(6)
O(4)-C(47)	1.419(6)	O(4)-K(1)	2.674(4)
K(1)-C(26)	3.041(5)	K(1)-C(25)	3.069(5)
K(1)-C(27)	3.139(6)	K(1)-C(24)	3.175(5)
K(1)-C(23)	3.188(5)	K(1)-C(28)	3.278(5)
K(1)-C(22)	3.273(5)	K(1)-C(21)	3.359(5)
C(1)-C(2)	1.427(7)	C(1)-C(8)	1.440(7)
C(2)-C(3)	1.391(7)	C(3)-C(4)	1.424(7)
C(4)-C(5)	1.426(7)	C(5)-C(6)	1.404(7)
C(6)-C(7)	1.410(7)	C(7)-C(8)	1.390(7)
C(11)-C(13)	1.518(7)	C(11)-C(12)	1.519(7)
C(11)-C(14)	1.541(7)	C(17)-C(19)	1.522(8)
C(17)-C(20)	1.536(8)	C(17)-C(18)	1.531(8)
C(21)-C(28)	1.412(7)	C(21)-C(22)	1.428(7)
C(22)-C(23)	1.405(7)	C(23)-C(24)	1.419(7)
C(24)-C(25)	1.412(7)	C(25)-C(26)	1.407(7)
C(26)-C(27)	1.406(6)	C(27)-C(28)	1.426(6)
C(31)-C(34)	1.526(7)	C(31)-C(33)	1.545(7)
C(31)-C(32)	1.538(7)	C(37)-C(38)	1.525(7)
C(37)-C(40)	1.527(8)	C(37)-C(39)	1.541(7)
C(42)-C(43)	1.491(8)	C(46)-C(47)	1.496(8)

C(8)-U(1)-C(3)	78.0(2)	C(8)-U(1)-C(2)	57.6(2)
C(3)-U(1)-C(2)	29.8(2)	C(8)-U(1)-C(7)	29.75(14)
C(3)-U(1)-C(7)	84.6(2)	C(2)-U(1)-C(7)	76.6(2)
C(8)-U(1)-C(5)	77.8(2)	C(3)-U(1)-C(5)	56.5(2)
C(2)-U(1)-C(5)	76.4(2)	C(7)-U(1)-C(5)	57.1(2)
C(8)-U(1)-C(25)	118.1(2)	C(3)-U(1)-C(25)	147.3(2)
C(2)-U(1)-C(25)	172.7(2)	C(7)-U(1)-C(25)	97.2(2)
C(5)-U(1)-C(25)	97.1(2)	C(8)-U(1)-C(1)	30.8(2)
C(3)-U(1)-C(1)	57.9(2)	C(2)-U(1)-C(1)	30.41(14)
C(7)-U(1)-C(1)	57.5(2)	C(5)-U(1)-C(1)	86.0(2)
C(25)-U(1)-C(1)	147.3(2)	C(8)-U(1)-C(26)	143.8(2)
C(3)-U(1)-C(26)	121.9(2)	C(2)-U(1)-C(26)	150.9(2)
C(7)-U(1)-C(26)	116.3(2)	C(5)-U(1)-C(26)	88.8(2)
C(25)-U(1)-C(26)	29.86(14)	C(1)-U(1)-C(26)	173.50(14)
C(8)-U(1)-C(28)	157.5(2)	C(3)-U(1)-C(28)	97.3(2)
C(2)-U(1)-C(28)	108.45(14)	C(7)-U(1)-C(28)	172.76(14)
C(5)-U(1)-C(28)	118.3(2)	C(25)-U(1)-C(28)	77.47(14)
C(1)-U(1)-C(28)	129.32(14)	C(26)-U(1)-C(28)	56.86(14)
C(8)-U(1)-C(4)	87.7(2)	C(3)-U(1)-C(4)	

C(5)-U(1)-C(4)	30.28(14)	C(25)-U(1)-C(4)	117.8(2)
C(1)-U(1)-C(4)	79.9(2)	C(26)-U(1)-C(4)	97.5(2)
C(28)-U(1)-C(4)	99.4(2)	C(8)-U(1)-C(6)	57.0(2)
C(3)-U(1)-C(6)	76.2(2)	C(2)-U(1)-C(6)	83.6(2)
C(7)-U(1)-C(6)	29.9(2)	C(5)-U(1)-C(6)	29.8(2)
C(25)-U(1)-C(6)	89.1(2)	C(1)-U(1)-C(6)	77.6(2)
C(26)-U(1)-C(6)	96.0(2)	C(28)-U(1)-C(6)	143.9(2)
C(4)-U(1)-C(6)	57.6(2)	C(8)-U(1)-C(23)	98.8(2)
C(3)-U(1)-C(23)	154.83(14)	C(2)-U(1)-C(23)	129.0(2)
C(7)-U(1)-C(23)	105.2(2)	C(5)-U(1)-C(23)	147.85(14)
C(25)-U(1)-C(23)	55.9(2)	C(1)-U(1)-C(23)	107.5(2)
C(26)-U(1)-C(23)	75.2(2)	C(28)-U(1)-C(23)	76.0(2)
C(4)-U(1)-C(23)	172.6(2)	C(6)-U(1)-C(23)	123.28(14)
C(10)-Si(1)-C(9)	106.9(3)	C(10)-Si(1)-C(1)	110.4(2)
C(9)-Si(1)-C(1)	110.9(2)	C(10)-Si(1)-C(11)	108.9(3)
C(9)-Si(1)-C(11)	107.4(2)	C(1)-Si(1)-C(11)	112.2(2)
C(4)-Si(2)-C(16)	111.4(2)	C(4)-Si(2)-C(15)	111.8(3)
C(16)-Si(2)-C(15)	105.6(2)	C(4)-Si(2)-C(17)	111.3(2)
C(16)-Si(2)-C(17)	108.1(3)	C(15)-Si(2)-C(17)	108.5(3)
C(30)-Si(3)-C(29)	107.3(3)	C(30)-Si(3)-C(21)	109.5(2)
C(29)-Si(3)-C(21)	110.8(2)	C(30)-Si(3)-C(31)	110.2(2)
C(29)-Si(3)-C(31)	107.8(3)	C(21)-Si(3)-C(31)	111.0(2)
C(36)-Si(4)-C(24)	110.5(2)	C(36)-Si(4)-C(35)	107.3(3)
C(24)-Si(4)-C(35)	109.9(2)	C(36)-Si(4)-C(37)	108.5(3)
C(24)-Si(4)-C(37)	112.3(2)	C(35)-Si(4)-C(37)	108.1(2)
C(42)-O(1)-C(41)	114.6(5)	C(42)-O(1)-K(1)	114.2(3)
C(41)-O(1)-K(1)	123.4(4)	C(43)-O(2)-C(44)	112.6(5)
C(43)-O(2)-K(1)	114.8(4)	C(44)-O(2)-K(1)	127.9(4)
C(46)-O(3)-C(45)	111.9(4)	C(46)-O(3)-K(1)	109.8(3)
C(45)-O(3)-K(1)	122.3(3)	C(48)-O(4)-C(47)	110.8(4)
C(48)-O(4)-K(1)	123.2(3)	C(47)-O(4)-K(1)	115.0(3)
O(4)-K(1)-O(1)	91.68(13)	O(4)-K(1)-O(3)	63.17(11)
O(1)-K(1)-O(3)	126.23(12)	O(4)-K(1)-O(2)	78.82(13)
O(1)-K(1)-O(2)	60.48(12)	O(3)-K(1)-O(2)	68.06(12)
O(4)-K(1)-C(26)	104.42(14)	O(1)-K(1)-C(26)	157.69(13)
O(3)-K(1)-C(26)	75.53(13)	O(2)-K(1)-C(26)	137.16(13)
O(4)-K(1)-C(25)	129.31(14)	O(1)-K(1)-C(25)	138.77(14)
O(3)-K(1)-C(25)	83.36(12)	O(2)-K(1)-C(25)	124.20(13)
C(26)-K(1)-C(25)	26.63(13)	O(4)-K(1)-C(27)	89.20(13)
O(1)-K(1)-C(27)	142.83(13)	O(3)-K(1)-C(27)	86.78(13)
O(2)-K(1)-C(27)	154.82(13)	C(26)-K(1)-C(27)	26.23(12)
C(25)-K(1)-C(27)	49.85(13)	O(4)-K(1)-C(24)	154.02(14)
O(1)-K(1)-C(24)	112.82(14)	O(3)-K(1)-C(24)	105.22(12)
O(2)-K(1)-C(24)	120.05(13)	C(26)-K(1)-C(24)	49.65(14)
C(25)-K(1)-C(24)	26.07(13)	C(27)-K(1)-C(24)	66.21(13)
O(4)-K(1)-C(23)	152.65(12)	O(1)-K(1)-C(23)	93.78(13)
O(3)-K(1)-C(23)	130.81(12)	O(2)-K(1)-C(23)	126.75(14)
C(26)-K(1)-C(23)	64.90(13)	C(25)-K(1)-C(23)	48.48(13)
C(27)-K(1)-C(23)	70.56(13)	C(24)-K(1)-C(23)	25.78(12)
O(4)-K(1)-C(28)	90.70(12)	O(1)-K(1)-C(28)	117.29(12)
O(3)-K(1)-C(28)	110.13(13)	O(2)-K(1)-C(28)	169.04(13)
C(26)-K(1)-C(28)	48.52(12)	C(25)-K(1)-C(28)	65.21(13)
C(27)-K(1)-C(28)	25.55(12)	C(24)-K(1)-C(28)	70.90(12)
C(23)-K(1)-C(28)	63.07(13)	O(4)-K(1)-C(22)	128.89(12)
O(1)-K(1)-C(22)	87.64(13)	O(3)-K(1)-C(22)	145.64(13)
O(2)-K(1)-C(22)	140.14(14)	C(26)-K(1)-C(22)	70.27(13)
C(25)-K(1)-C(22)	64.49(13)	C(27)-K(1)-C(22)	63.70(13)
C(24)-K(1)-C(22)	48.30(13)	C(23)-K(1)-C(22)	25.08(12)
C(28)-K(1)-C(22)	46.50(13)	O(4)-K(1)-C(21)	105.39(12)
O(1)-K(1)-C(21)	96.70(12)	O(3)-K(1)-C(21)	134.25(13)
O(2)-K(1)-C(21)	157.11(13)	C(26)-K(1)-C(21)	64.47(12)
C(25)-K(1)-C(21)	70.96(12)	C(27)-K(1)-C(21)	47.69(13)
C(24)-K(1)-C(21)	64.80(12)	C(23)-K(1)-C(21)	47.35(12)

C(2)-C(1)-C(8)	130.5(5)	C(2)-C(1)-Si(1)	117.3(3)
C(8)-C(1)-Si(1)	112.2(4)	C(2)-C(1)-U(1)	73.9(3)
C(8)-C(1)-U(1)	73.3(3)	Si(1)-C(1)-U(1)	132.9(2)
C(3)-C(2)-C(1)	137.8(5)	C(3)-C(2)-U(1)	74.8(3)
C(1)-C(2)-U(1)	75.7(3)	C(2)-C(3)-C(4)	138.5(5)
C(2)-C(3)-U(1)	75.4(3)	C(4)-C(3)-U(1)	76.4(3)
C(5)-C(4)-C(3)	128.4(5)	C(5)-C(4)-Si(2)	114.5(4)
C(3)-C(4)-Si(2)	117.1(4)	C(5)-C(4)-U(1)	73.9(3)
C(3)-C(4)-U(1)	73.3(3)	Si(2)-C(4)-U(1)	130.7(2)
C(6)-C(5)-C(4)	138.1(5)	C(6)-C(5)-U(1)	76.2(3)
C(4)-C(5)-U(1)	75.8(3)	C(5)-C(6)-C(7)	134.9(5)
C(5)-C(6)-U(1)	74.0(3)	C(7)-C(6)-U(1)	74.0(3)
C(8)-C(7)-C(6)	136.0(5)	C(8)-C(7)-U(1)	74.3(3)
C(6)-C(7)-U(1)	76.1(3)	C(7)-C(8)-C(1)	135.5(5)
C(7)-C(8)-U(1)	76.0(3)	C(1)-C(8)-U(1)	76.0(3)
C(13)-C(11)-C(12)	109.0(4)	C(13)-C(11)-C(14)	107.6(5)
C(12)-C(11)-C(14)	108.2(4)	C(13)-C(11)-Si(1)	109.7(4)
C(12)-C(11)-Si(1)	110.1(4)	C(14)-C(11)-Si(1)	112.2(3)
C(19)-C(17)-C(20)	109.2(5)	C(19)-C(17)-C(18)	108.0(5)
C(20)-C(17)-C(18)	108.1(5)	C(19)-C(17)-Si(2)	110.2(4)
C(20)-C(17)-Si(2)	110.6(4)	C(18)-C(17)-Si(2)	110.7(4)
C(28)-C(21)-C(22)	131.2(5)	C(28)-C(21)-Si(3)	113.4(4)
C(22)-C(21)-Si(3)	115.5(4)	C(28)-C(21)-U(1)	73.5(3)
C(22)-C(21)-U(1)	74.5(3)	Si(3)-C(21)-U(1)	130.9(2)
C(28)-C(21)-K(1)	74.5(3)	C(22)-C(21)-K(1)	74.2(3)
Si(3)-C(21)-K(1)	131.5(2)	U(1)-C(21)-K(1)	97.64(13)
C(23)-C(22)-C(21)	136.8(5)	C(23)-C(22)-U(1)	74.6(3)
C(21)-C(22)-U(1)	75.7(3)	C(23)-C(22)-K(1)	74.1(3)
C(21)-C(22)-K(1)	81.0(3)	U(1)-C(22)-K(1)	100.0(2)
C(22)-C(23)-C(24)	138.3(5)	C(22)-C(23)-U(1)	75.9(3)
C(24)-C(23)-U(1)	75.3(3)	C(22)-C(23)-K(1)	80.8(3)
C(24)-C(23)-K(1)	76.6(3)	U(1)-C(23)-K(1)	102.4(2)
C(25)-C(24)-C(23)	130.4(5)	C(25)-C(24)-Si(4)	115.7(4)
C(23)-C(24)-Si(4)	113.8(4)	C(25)-C(24)-U(1)	74.0(3)
C(23)-C(24)-U(1)	74.9(3)	Si(4)-C(24)-U(1)	127.8(2)
C(25)-C(24)-K(1)	72.8(3)	C(23)-C(24)-K(1)	77.6(3)
Si(4)-C(24)-K(1)	129.6(2)	U(1)-C(24)-K(1)	102.6(2)
C(26)-C(25)-C(24)	135.8(5)	C(26)-C(25)-U(1)	75.0(3)
C(24)-C(25)-U(1)	76.1(3)	C(26)-C(25)-K(1)	75.6(3)
C(24)-C(25)-K(1)	81.2(3)	U(1)-C(25)-K(1)	106.0(2)
C(27)-C(26)-C(25)	137.0(5)	C(27)-C(26)-U(1)	76.1(3)
C(25)-C(26)-U(1)	75.1(3)	C(27)-C(26)-K(1)	80.8(3)
C(25)-C(26)-K(1)	77.8(3)	U(1)-C(26)-K(1)	106.8(2)
C(26)-C(27)-C(28)	133.9(5)	C(26)-C(27)-U(1)	74.2(3)
C(28)-C(27)-U(1)	74.4(3)	C(26)-C(27)-K(1)	73.0(3)
C(28)-C(27)-K(1)	82.7(3)	U(1)-C(27)-K(1)	103.6(2)
C(21)-C(28)-C(27)	136.4(5)	C(21)-C(28)-U(1)	76.9(3)
C(27)-C(28)-U(1)	75.5(3)	C(21)-C(28)-K(1)	80.9(3)
C(27)-C(28)-K(1)	71.8(3)	U(1)-C(28)-K(1)	100.4(2)
C(34)-C(31)-C(33)	107.9(5)	C(34)-C(31)-C(32)	107.8(5)
C(33)-C(31)-C(32)	108.0(4)	C(34)-C(31)-Si(3)	109.5(4)
C(33)-C(31)-Si(3)	112.3(4)	C(32)-C(31)-Si(3)	111.1(4)
C(38)-C(37)-C(40)	108.5(5)	C(38)-C(37)-C(39)	107.6(5)
C(40)-C(37)-C(39)	109.9(5)	C(38)-C(37)-Si(4)	111.5(4)
C(40)-C(37)-Si(4)	110.2(4)	C(39)-C(37)-Si(4)	109.1(4)
O(1)-C(42)-C(43)	113.2(5)	O(1)-C(42)-K(1)	44.2(3)
C(43)-C(42)-K(1)	85.0(4)	O(2)-C(43)-C(42)	108.9(6)
O(3)-C(46)-C(47)	110.2(5)	O(3)-C(46)-K(1)	48.0(2)
C(47)-C(46)-K(1)	78.1(3)	O(4)-C(47)-C(46)	109.6(5)
O(4)-C(47)-K(1)	43.6(2)	C(46)-C(47)-K(1)	77.3(3)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for 4
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
U(1)	13(1)	16(1)	9(1)	-1(1)	0(1)	0(1)
Si(1)	19(1)	20(1)	15(1)	-1(1)	4(1)	-3(1)
Si(2)	25(1)	17(1)	17(1)	2(1)	2(1)	1(1)
Si(3)	11(1)	25(1)	15(1)	1(1)	-1(1)	0(1)
Si(4)	12(1)	20(1)	20(1)	-3(1)	-2(1)	2(1)
O(1)	47(3)	26(3)	38(3)	-3(2)	9(2)	-10(2)
O(2)	44(3)	33(3)	63(3)	-21(2)	17(2)	-8(2)
O(3)	25(2)	32(3)	20(2)	5(2)	-2(2)	-7(2)
O(4)	22(2)	37(3)	14(2)	0(2)	0(2)	-4(2)
K(1)	27(1)	23(1)	13(1)	-2(1)	0(1)	-5(1)
C(1)	9(3)	21(4)	16(3)	-2(3)	2(2)	3(2)
C(2)	16(3)	24(4)	13(3)	-2(2)	2(2)	-2(3)
C(3)	16(3)	11(3)	17(3)	-3(3)	-2(2)	6(2)
C(4)	14(3)	27(3)	11(3)	-8(2)	2(2)	1(2)
C(5)	20(3)	20(4)	14(3)	-3(3)	2(2)	-7(2)
C(6)	13(3)	21(4)	11(3)	-6(3)	0(2)	-4(2)
C(7)	11(3)	20(3)	10(3)	-1(3)	-4(2)	8(2)
C(8)	21(3)	21(3)	9(3)	5(2)	-1(2)	1(2)
C(9)	20(3)	41(4)	28(4)	9(3)	4(2)	-9(3)
C(10)	40(4)	25(4)	28(4)	-5(3)	13(3)	-10(3)
C(11)	11(3)	22(3)	20(3)	2(2)	1(2)	2(2)
C(12)	29(3)	34(4)	17(3)	-5(3)	3(2)	0(3)
C(13)	37(4)	37(4)	21(4)	7(3)	9(3)	-4(3)
C(14)	39(4)	47(5)	17(3)	10(3)	-2(3)	8(3)
C(15)	35(4)	36(4)	34(4)	13(3)	-9(3)	3(3)
C(16)	29(3)	23(4)	25(3)	8(3)	-2(3)	-2(3)
C(17)	47(4)	29(4)	17(3)	1(3)	1(3)	10(3)
C(18)	85(5)	18(4)	29(4)	-4(3)	-2(3)	8(3)
C(19)	111(6)	32(5)	30(4)	-2(3)	1(4)	18(4)
C(20)	89(5)	24(4)	36(4)	-7(3)	-26(4)	6(4)
C(21)	11(3)	20(3)	13(3)	-4(2)	0(2)	-4(2)
C(22)	15(3)	17(3)	12(3)	0(2)	3(2)	-3(2)
C(23)	17(4)	15(3)	9(3)	1(2)	-2(2)	-4(2)
C(24)	15(3)	18(3)	7(3)	-6(2)	1(2)	2(2)
C(25)	12(3)	23(3)	11(3)	-5(3)	6(2)	-5(2)
C(26)	9(3)	18(4)	14(3)	-3(2)	3(2)	-4(2)
C(27)	25(4)	17(3)	6(3)	7(2)	-4(2)	-2(3)
C(28)	10(3)	19(3)	13(3)	2(3)	-4(2)	1(2)
C(29)	10(3)	41(4)	27(3)	7(3)	2(2)	-4(3)
C(30)	15(3)	38(4)	29(4)	0(3)	-4(2)	3(3)
C(31)	9(3)	28(4)	20(3)	0(3)	-2(2)	-3(2)
C(32)	26(4)	53(5)	25(4)	2(3)	-9(3)	-6(3)
C(33)	27(4)	36(4)	25(4)	1(3)	-11(3)	-1(3)
C(34)	32(4)	34(4)	23(4)	-2(3)	-2(3)	-6(3)
C(35)	17(3)	26(4)	36(4)	-2(3)	-7(3)	2(2)
C(36)	23(3)	35(4)	32(4)	3(3)	-4(3)	9(3)
C(37)	19(3)	25(4)	34(4)	-12(3)	-2(3)	6(2)
C(38)	30(4)	38(5)	72(5)	-23(4)	-5(3)	3(3)
C(39)	39(4)	41(5)	68(5)	-27(4)	-11(4)	22(3)
C(40)	52(4)	54(5)	41(5)	-11(4)	25(3)	10(4)
C(41)	62(5)	45(5)	46(5)	13(4)	-12(4)	-15(4)
C(42)	66(5)	36(5)	37(4)	-18(4)	0(3)	-7(3)
C(43)	55(5)	42(5)	44(5)	-12(4)	12(3)	-15(4)
C(44)	49(5)	52(5)	68(6)	-26(4)	28(4)	9(4)

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C(46)	31(4)	34(4)	37(4)	16(3)	-4(3)	-5(3)
C(47)	30(4)	53(5)	21(3)	18(3)	1(3)	-1(3)
C(48)	32(4)	40(4)	24(4)	4(3)	-6(3)	-5(3)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 4 .

	x	y	z	U(eq)
H(2)	8386(3)	5081(2)	7682(2)	21
H(3)	8144(2)	4456(2)	8158(2)	18
H(5)	6125(3)	4298(2)	8388(2)	22
H(6)	5551(3)	4860(2)	7976(2)	18
H(7)	5802(2)	5533(2)	7540(2)	16
H(8)	6724(3)	5896(2)	7291(2)	20
H(9A)	9222(5)	5594(8)	7098(12)	44
H(9B)	9104(3)	5829(14)	7697(3)	44
H(9C)	9302(4)	6178(6)	7187(14)	44
H(10A)	7862(17)	6622(4)	7790(2)	47
H(10B)	7387(8)	6694(5)	7256(12)	47
H(10C)	8176(11)	6856(3)	7237(12)	47
H(12A)	7845(10)	5182(3)	6272(11)	40
H(12B)	8638(7)	5331(5)	6237(11)	40
H(12C)	8147(16)	5417(4)	5716(2)	40
H(13A)	8383(12)	6656(3)	6199(11)	47
H(13B)	8434(13)	6313(9)	5662(2)	47
H(13C)	8964(3)	6240(8)	6160(12)	47
H(14A)	7117(8)	6399(7)	6294(13)	52
H(14B)	6929(4)	5823(8)	6278(14)	52
H(14C)	7231(5)	6088(14)	5739(2)	52
H(15A)	8511(3)	3857(15)	8873(3)	52
H(15B)	8166(10)	3573(8)	9382(12)	52
H(15C)	8139(9)	4164(7)	9353(13)	52
H(16A)	6698(9)	3495(8)	9546(8)	39
H(16B)	6138(4)	3682(13)	9111(3)	39
H(16C)	6534(12)	4072(4)	9492(9)	39
H(18A)	6844(10)	2752(8)	8889(12)	66
H(18B)	7663(12)	2768(7)	8927(11)	66
H(18C)	7297(20)	2460(2)	8445(3)	66
H(19A)	7978(14)	3510(8)	7720(15)	86
H(19B)	7905(12)	2922(11)	7680(14)	86
H(19C)	8339(4)	3164(18)	8172(3)	86
H(20A)	6217(4)	3191(17)	8141(3)	74
H(20B)	6656(12)	2915(9)	7675(13)	74
H(20C)	6617(13)	3506(8)	7683(13)	74
H(22)	7879(3)	6503(2)	8976(2)	18
H(23)	6832(2)	6674(2)	8827(2)	16
H(25)	5547(3)	5616(2)	9331(2)	18
H(26)	6087(2)	5025(2)	9728(2)	16
H(27)	7141(3)	4838(2)	9892(2)	19
H(28)	8124(2)	5177(2)	9690(2)	17
H(29A)	9114(15)	6758(2)	9041(6)	39
H(29B)	8968(12)	6437(7)	8499(5)	39
H(29C)	9715(4)	6434(7)	8773(11)	39
H(30A)	9122(12)	5254(7)	8626(7)	41
H(30B)	9290(14)	5043(3)	9229(6)	41
H(30C)	9842(4)	5377(5)	8913(13)	41
H(32A)	10349(3)	5789(6)	9836(15)	52
H(32B)	10317(4)	6121(15)	10382(3)	52
H(32C)	10245(3)	6374(8)	9787(14)	52
H(33A)	9346(15)	5254(3)	10270(6)	44
H(33B)	8688(3)	5542(8)	10500(11)	44
H(33C)	9420(14)	5619(6)	10788(5)	44
H(34A)	9119(14)	6767(3)	10045(7)	45

H(34C)	8524(4)	6443(5)	10321(13)	45
H(35A)	4498(11)	5944(10)	8873(3)	39
H(35B)	4937(3)	5755(6)	8355(13)	39
H(35C)	4426(10)	6214(5)	8287(11)	39
H(36A)	5368(3)	6941(11)	7871(8)	45
H(36B)	6006(15)	6570(3)	7834(6)	45
H(36C)	6079(14)	7081(8)	8162(2)	45
H(38A)	5774(16)	7555(10)	9003(3)	70
H(38B)	6029(10)	7260(4)	9538(16)	70
H(38C)	5420(8)	7655(8)	9589(14)	70
H(39A)	4597(5)	7392(14)	8600(9)	74
H(39B)	4267(14)	7490(11)	9196(8)	74
H(39C)	4107(10)	6985(4)	8874(17)	74
H(40A)	4541(16)	6487(10)	9719(3)	73
H(40B)	4680(19)	7000(4)	10030(7)	73
H(40C)	5284(5)	6603(14)	9968(9)	73
H(41A)	7650(20)	7288(3)	9816(5)	77
H(41B)	7928(14)	7644(10)	10295(8)	77
H(41C)	7137(9)	7659(10)	10121(13)	77
H(42A)	7400(3)	7592(3)	11165(3)	56
H(42B)	7391(3)	7041(3)	11405(3)	56
H(43A)	6323(3)	7434(3)	11570(3)	57
H(43B)	6222(3)	7517(3)	10918(3)	57
H(44A)	5265(9)	6454(5)	11317(19)	85
H(44B)	5150(6)	7016(14)	11132(13)	85
H(44C)	5424(5)	6893(18)	11741(6)	85
H(45A)	5010(10)	5649(5)	10463(11)	44
H(45B)	4898(8)	5336(12)	11017(3)	44
H(45C)	5355(4)	5115(7)	10527(13)	44
H(46A)	6395(3)	5043(2)	11121(2)	41
H(46B)	5849(3)	5170(2)	11596(2)	41
H(47A)	6530(3)	5883(3)	11843(2)	41
H(47B)	6937(3)	5374(3)	11940(2)	41
H(48A)	7713(5)	6232(8)	11798(12)	48
H(48B)	8210(8)	6042(13)	11316(2)	48
H(48C)	8028(12)	5686(5)	11824(11)	48