

Molecular Structure for Complex 3a

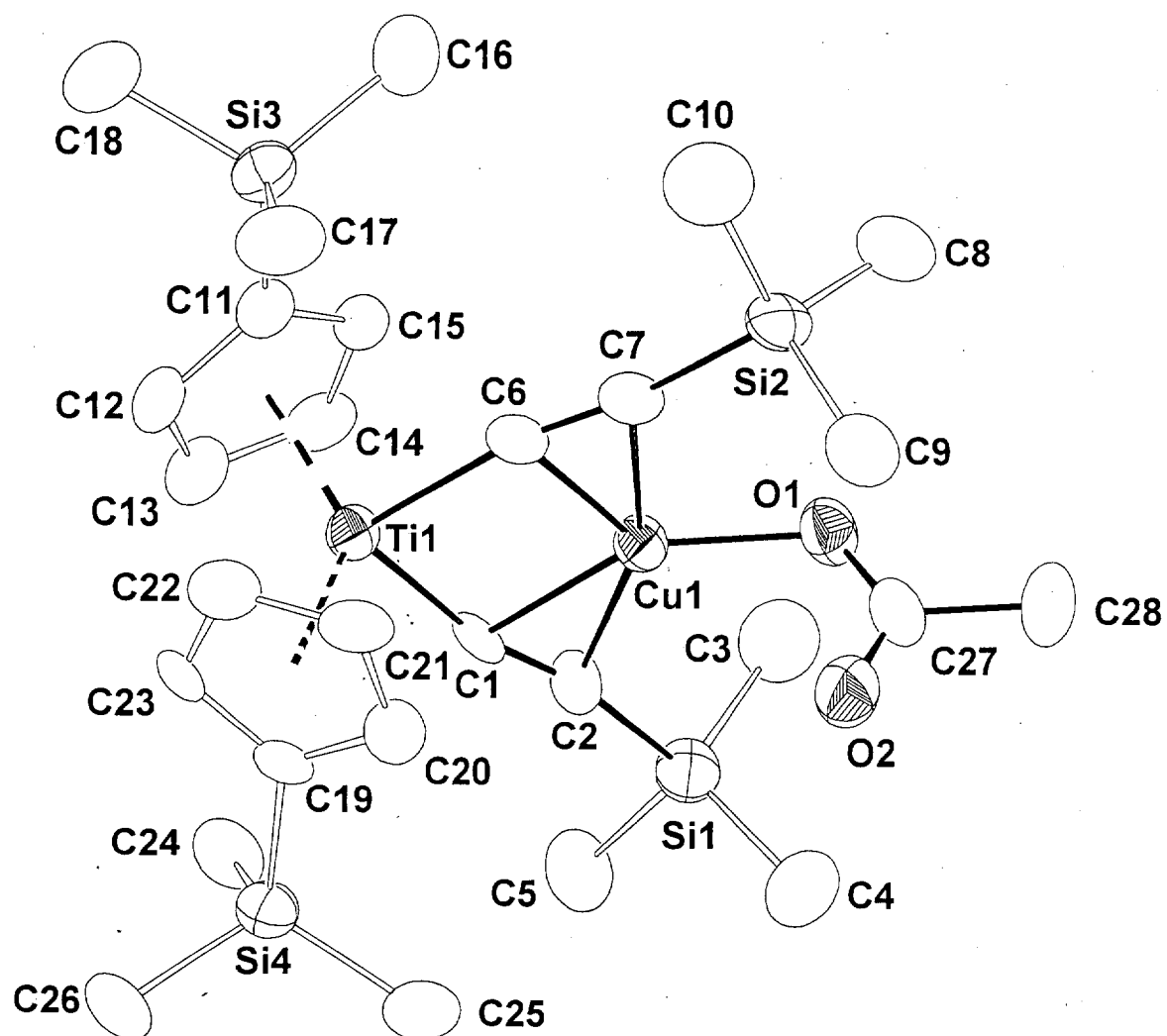


Table 1. Crystal data for 3a.

Identification code	kosi	
Crystal shape	block	
Crystal colour	yellow	
Crystal size	0.2 x 0.2 x 0.2 mm ³	
Empirical formula	C ₆₄ H ₁₁₀ Cu ₂ O ₆ Si ₈ Ti ₂	
Chemical formula	C ₂₈ H ₄₇ Cu O ₂ Si ₄ Ti, C ₄ H ₈ O	
Formula weight	1423.12	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 21.686(9) Å	α = 90°.
	b = 16.678(6) Å	β = 116.48(3)°.
	c = 23.963(8) Å	γ = 90°.
Volume	7758(5) Å ³	
Z	4	
Density (calculated)	1.218 g/cm ³	
Radiation used	MoKα	
Wavelength	0.71073 Å	
Linear absorption coefficient	0.905mm ⁻¹	
Temperature	193(2) K	

Table 2. Data collection details for 3a.

Diffractometer	Siemens R3m/V-Diffraktometer
Scan method	ω scans
Absorption correction	Psi-scan
Number of measured reflections	8505
Number of independent reflections	8237
Number of observed reflections	5329
Criterion of recognition (σ-limit)	>2σ(I)
R(int) =	0.0689
Theta range for data collection	1.61 to 21.06°.
Completeness to theta = 21.06°	98.1 %
Index ranges	-7<=h<=21, -16<=k<=16, -24<=l<=21
F(000)	3024

Table 3. Refinement details for 3a.

Refinement method	Full-matrix least-squares on F^2
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0755$, $wR2 = 0.1819$
R indices (all data)	$R1 = 0.1240$, $wR2 = 0.2170$
$R1 = [\Sigma(F_o - F_c)] / \Sigma F_o $	
$wR2 = [\Sigma(w(F_o^2 - F_c^2)^2) / \Sigma(wF_o^4)]^{1/2}$	
H-locating and refining method	geom/mixed
Number of reflections used	8237
Number of L.S. restraints	10
Number of refined parameters	765
Goodness-of-fit on F^2	1.012
$S = [\Sigma w(F_o^2 - F_c^2)^2 / (n - p)]^{1/2}$,	n = number of reflections, p = parameters used.
Definition of w	
calc $w = 1 / [\sigma^2(F_o^2) + (0.1173P)^2 + 24.2255P]$ where $P = (F_o^2 + 2F_c^2) / 3$	
Maximum δ/σ	0.015
Maximum e-density	0.757 e.Å ⁻³
Minimum e-density	-1.690 e.Å ⁻³

Table 4. Computer Programs used for 3a.

Data collection program	XSCANS
Cell refinement program	XSCANS
Data reduction program	XPREP
Structure solving program	SHELXS-97 (Sheldrick, 1990)
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Pictures drawn with	ZORTEP
Tables made with	SHELX-97

Table 5. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3a.U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5244(1)	1843(1)	4103(1)	33(1)
Ti(1)	5967(1)	490(1)	3881(1)	30(1)
Si(1)	3900(2)	2328(2)	2627(1)	42(1)
Si(2)	6143(2)	2224(2)	5727(1)	42(1)
Si(3)	6637(2)	-868(2)	5324(1)	41(1)
Si(4)	5830(2)	1134(2)	2283(1)	41(1)
O(1)	4687(3)	2635(4)	4258(3)	41(2)
O(2)	5424(4)	3477(4)	4178(3)	53(2)
C(1)	5117(5)	1202(6)	3315(4)	30(2)
C(2)	4661(5)	1715(6)	3122(4)	36(2)
C(3)	3250(5)	2197(8)	2915(5)	66(4)
C(4)	4145(6)	3393(6)	2628(5)	63(3)
C(5)	3566(6)	1928(7)	1823(5)	56(3)
C(6)	6082(5)	1142(6)	4664(4)	33(2)
C(7)	6013(5)	1614(6)	5038(4)	35(2)
C(8)	5333(6)	2354(7)	5786(5)	62(3)
C(9)	6537(6)	3207(6)	5709(5)	54(3)
C(10)	6756(6)	1632(7)	6406(5)	71(4)
C(11)	6017(5)	-655(5)	4484(4)	34(2)
C(12)	6059(5)	-938(6)	3944(5)	40(3)
C(13)	5442(5)	-727(6)	3421(5)	44(3)
C(14)	4998(5)	-362(6)	3622(5)	41(3)
C(15)	5353(5)	-323(6)	4272(5)	35(2)
C(16)	6186(5)	-608(7)	5799(5)	55(3)
C(17)	7454(5)	-284(7)	5604(5)	58(3)
C(18)	6837(6)	-1959(6)	5390(5)	56(3)
C(19)	6345(5)	947(6)	3140(4)	31(2)
C(20)	6561(5)	1530(6)	3636(5)	39(3)
C(21)	7038(5)	1164(6)	4193(5)	38(3)
C(22)	7106(5)	360(7)	4052(5)	43(3)

C(23)	6702(5)	250(6)	3412(4)	36(3)
C(24)	5057(5)	483(7)	1932(5)	51(3)
C(25)	5607(5)	2207(7)	2157(5)	53(3)
C(26)	6408(6)	831(7)	1931(5)	53(3)
C(27)	4933(6)	3337(7)	4285(4)	41(3)
C(28)	4579(6)	4013(6)	4462(5)	58(3)
Ti(2)	8435(1)	476(1)	1298(1)	34(1)
Cu(2)	7620(1)	1798(1)	1436(1)	34(1)
Si(5)	6172(2)	1985(2)	-33(1)	42(1)
Si(6)	8513(2)	2370(2)	3022(1)	47(1)
Si(7)	6976(2)	-890(2)	221(1)	55(1)
Si(8)	10258(2)	1266(2)	2321(2)	52(1)
O(3)	7051(3)	2616(4)	1545(3)	42(2)
O(4)	7670(4)	3436(5)	1262(4)	63(2)
C(29)	7502(5)	1028(6)	714(4)	35(2)
C(30)	6995(5)	1471(6)	489(4)	31(2)
C(31)	5584(5)	1983(8)	337(6)	70(4)
C(32)	6348(6)	3011(7)	-214(6)	66(4)
C(33)	5779(7)	1388(8)	-763(5)	79(4)
C(34)	8517(5)	1239(6)	2024(4)	35(2)
C(35)	8428(5)	1748(7)	2354(5)	44(3)
C(36)	7718(6)	2365(8)	3105(5)	70(4)
C(37)	8742(6)	3410(6)	2912(6)	67(4)
C(38)	9211(7)	1894(8)	3720(5)	80(4)
C(39)	7714(5)	-694(5)	1005(4)	35(2)
C(40)	7692(5)	-353(6)	1531(5)	40(3)
C(41)	8357(6)	-395(7)	2037(5)	51(3)
C(42)	8771(6)	-746(6)	1825(6)	56(3)
C(43)	8400(6)	-933(6)	1195(6)	51(3)
C(44)	6966(10)	-1990(7)	83(6)	112(6)
C(45)	6174(6)	-596(8)	267(5)	79(4)
C(46)	7061(6)	-373(6)	-428(4)	57(3)
C(47)	9547(5)	1020(6)	1534(5)	38(3)
C(48)	9458(5)	303(7)	1203(5)	46(3)
C(49)	8930(6)	370(7)	612(5)	45(3)
C(50)	8669(6)	1134(7)	536(5)	48(3)

C(51)	9035(5)	1549(7)	1113(5)	41(3)
C(52)	10195(6)	2333(7)	2501(6)	63(3)
C(53)	11083(6)	1086(8)	2279(6)	77(4)
C(54)	10245(6)	599(7)	2936(5)	67(4)
C(55)	7218(5)	3314(7)	1424(5)	44(3)
C(56)	6809(6)	3998(7)	1507(6)	67(4)
O(5)	3334(6)	-147(8)	2363(6)	129(4)
C(57)	3494(7)	-796(9)	2077(7)	91(5)
C(58)	2849(10)	-1181(12)	1634(8)	141(9)
C(59)	2298(10)	-643(15)	1636(11)	192(15)
C(60)	2636(9)	-102(13)	2172(11)	153(9)
O(6)	8800(12)	926(17)	5291(16)	340(20)
C(61)	9102(19)	1200(20)	5894(13)	270(20)
C(62)	9815(15)	1115(16)	6023(11)	185(12)
C(63)	9813(14)	650(20)	5518(15)	280(20)
C(64)	9129(18)	295(19)	5190(20)	290(20)

Table 6. Bond lengths [Å] and angles [°] for 3a.

Cu(1)-O(1)	1.934(7)	Ti(1)-C(20)	2.385(10)
Cu(1)-C(6)	2.072(9)	Ti(1)-C(12)	2.388(10)
Cu(1)-C(1)	2.080(8)	Ti(1)-C(19)	2.388(9)
Cu(1)-C(2)	2.125(9)	Si(1)-C(3)	1.838(12)
Cu(1)-C(7)	2.149(9)	Si(1)-C(2)	1.851(10)
Cu(1)-O(2)	2.747(7)	Si(1)-C(5)	1.854(10)
Cu(1)-Ti(1)	2.929(2)	Si(1)-C(4)	1.854(11)
Ti(1)-C(6)	2.085(10)	Si(2)-C(8)	1.837(12)
Ti(1)-C(1)	2.102(10)	Si(2)-C(7)	1.851(10)
Ti(1)-C(22)	2.327(10)	Si(2)-C(9)	1.857(10)
Ti(1)-C(13)	2.349(10)	Si(2)-C(10)	1.859(11)
Ti(1)-C(23)	2.358(9)	Si(3)-C(16)	1.852(11)
Ti(1)-C(15)	2.366(9)	Si(3)-C(18)	1.862(11)
Ti(1)-C(11)	2.367(9)	Si(3)-C(17)	1.865(10)
Ti(1)-C(14)	2.379(10)	Si(3)-C(11)	1.890(10)
Ti(1)-C(21)	2.381(9)	Si(4)-C(25)	1.843(11)

Si(4)-C(24)	1.854(10)	Si(5)-C(32)	1.847(11)
Si(4)-C(26)	1.865(10)	Si(5)-C(31)	1.848(11)
Si(4)-C(19)	1.877(9)	Si(5)-C(33)	1.857(11)
O(1)-C(27)	1.276(13)	Si(5)-C(30)	1.869(10)
O(2)-C(27)	1.224(12)	Si(6)-C(36)	1.822(12)
C(1)-C(2)	1.233(12)	Si(6)-C(35)	1.847(12)
C(6)-C(7)	1.252(13)	Si(6)-C(37)	1.855(11)
C(11)-C(15)	1.409(13)	Si(6)-C(38)	1.860(11)
C(11)-C(12)	1.418(13)	Si(7)-C(45)	1.857(13)
C(12)-C(13)	1.412(13)	Si(7)-C(46)	1.858(10)
C(13)-C(14)	1.395(14)	Si(7)-C(44)	1.863(13)
C(14)-C(15)	1.397(13)	Si(7)-C(39)	1.875(10)
C(19)-C(23)	1.387(13)	Si(8)-C(52)	1.850(12)
C(19)-C(20)	1.444(13)	Si(8)-C(54)	1.857(11)
C(20)-C(21)	1.411(13)	Si(8)-C(53)	1.860(12)
C(21)-C(22)	1.407(14)	Si(8)-C(47)	1.872(10)
C(22)-C(23)	1.397(13)	O(3)-C(55)	1.291(13)
C(27)-C(28)	1.526(14)	O(4)-C(55)	1.222(13)
Ti(2)-C(29)	2.093(11)	C(29)-C(30)	1.231(12)
Ti(2)-C(34)	2.098(11)	C(34)-C(35)	1.234(14)
Ti(2)-C(49)	2.335(10)	C(39)-C(40)	1.402(13)
Ti(2)-C(42)	2.337(10)	C(39)-C(43)	1.407(14)
Ti(2)-C(48)	2.345(9)	C(40)-C(41)	1.413(14)
Ti(2)-C(41)	2.356(10)	C(41)-C(42)	1.348(16)
Ti(2)-C(43)	2.361(10)	C(42)-C(43)	1.393(15)
Ti(2)-C(51)	2.367(10)	C(47)-C(48)	1.402(14)
Ti(2)-C(50)	2.371(10)	C(47)-C(51)	1.424(13)
Ti(2)-C(40)	2.373(10)	C(48)-C(49)	1.373(14)
Ti(2)-C(47)	2.396(9)	C(49)-C(50)	1.373(15)
Ti(2)-C(39)	2.401(9)	C(50)-C(51)	1.429(14)
Cu(2)-O(3)	1.933(7)	C(55)-C(56)	1.510(14)
Cu(2)-C(34)	2.048(9)	O(5)-C(60)	1.374(14)
Cu(2)-C(29)	2.077(9)	O(5)-C(57)	1.404(13)
Cu(2)-C(35)	2.116(9)	C(57)-C(58)	1.473(15)
Cu(2)-C(30)	2.132(8)	C(58)-C(59)	1.494(17)
Cu(2)-O(4)	2.772(8)	C(59)-C(60)	1.471(17)

O(6)-C(64)	1.354(18)	C(13)-Ti(1)-C(23)	85.3(4)
O(6)-C(61)	1.375(18)	C(6)-Ti(1)-C(15)	78.8(3)
C(61)-C(62)	1.443(18)	C(1)-Ti(1)-C(15)	95.4(3)
C(62)-C(63)	1.441(18)	C(22)-Ti(1)-C(15)	128.2(4)
C(63)-C(64)	1.457(19)	C(13)-Ti(1)-C(15)	56.7(4)
		C(23)-Ti(1)-C(15)	135.3(3)
O(1)-Cu(1)-C(6)	134.6(3)	C(6)-Ti(1)-C(11)	85.3(3)
O(1)-Cu(1)-C(1)	133.2(3)	C(1)-Ti(1)-C(11)	129.7(3)
C(6)-Cu(1)-C(1)	91.2(4)	C(22)-Ti(1)-C(11)	93.6(4)
O(1)-Cu(1)-C(2)	99.6(3)	C(13)-Ti(1)-C(11)	58.0(3)
C(6)-Cu(1)-C(2)	125.3(4)	C(23)-Ti(1)-C(11)	107.3(3)
C(1)-Cu(1)-C(2)	34.1(3)	C(15)-Ti(1)-C(11)	34.6(3)
O(1)-Cu(1)-C(7)	100.5(3)	C(6)-Ti(1)-C(14)	106.5(4)
C(6)-Cu(1)-C(7)	34.4(3)	C(1)-Ti(1)-C(14)	75.6(4)
C(1)-Cu(1)-C(7)	125.7(4)	C(22)-Ti(1)-C(14)	137.4(4)
C(2)-Cu(1)-C(7)	159.7(4)	C(13)-Ti(1)-C(14)	34.3(3)
O(1)-Cu(1)-O(2)	52.6(3)	C(23)-Ti(1)-C(14)	118.7(4)
C(6)-Cu(1)-O(2)	117.3(3)	C(15)-Ti(1)-C(14)	34.2(3)
C(1)-Cu(1)-O(2)	121.8(3)	C(11)-Ti(1)-C(14)	58.1(3)
C(2)-Cu(1)-O(2)	99.8(3)	C(6)-Ti(1)-C(21)	76.3(4)
C(7)-Cu(1)-O(2)	94.9(3)	C(1)-Ti(1)-C(21)	112.8(4)
O(1)-Cu(1)-Ti(1)	172.6(2)	C(22)-Ti(1)-C(21)	34.7(3)
C(6)-Cu(1)-Ti(1)	45.4(3)	C(13)-Ti(1)-C(21)	139.2(4)
C(1)-Cu(1)-Ti(1)	45.9(3)	C(23)-Ti(1)-C(21)	57.2(4)
C(2)-Cu(1)-Ti(1)	79.9(3)	C(15)-Ti(1)-C(21)	142.1(3)
C(7)-Cu(1)-Ti(1)	79.8(3)	C(11)-Ti(1)-C(21)	114.6(3)
O(2)-Cu(1)-Ti(1)	134.77(18)	C(14)-Ti(1)-C(21)	171.4(4)
C(6)-Ti(1)-C(1)	90.3(3)	C(6)-Ti(1)-C(20)	88.9(3)
C(6)-Ti(1)-C(22)	101.5(4)	C(1)-Ti(1)-C(20)	81.0(4)
C(1)-Ti(1)-C(22)	136.2(4)	C(22)-Ti(1)-C(20)	57.6(4)
C(6)-Ti(1)-C(13)	135.4(4)	C(13)-Ti(1)-C(20)	135.7(4)
C(1)-Ti(1)-C(13)	94.8(4)	C(23)-Ti(1)-C(20)	56.8(3)
C(22)-Ti(1)-C(13)	104.9(4)	C(15)-Ti(1)-C(20)	167.1(3)
C(6)-Ti(1)-C(23)	133.0(4)	C(11)-Ti(1)-C(20)	148.7(3)
C(1)-Ti(1)-C(23)	111.8(3)	C(14)-Ti(1)-C(20)	151.8(3)
C(22)-Ti(1)-C(23)	34.7(3)	C(21)-Ti(1)-C(20)	34.5(3)

C(6)-Ti(1)-C(12)	119.4(4)	C(16)-Si(3)-C(11)	106.9(5)
C(1)-Ti(1)-C(12)	129.0(4)	C(18)-Si(3)-C(11)	107.6(5)
C(22)-Ti(1)-C(12)	81.0(4)	C(17)-Si(3)-C(11)	113.3(4)
C(13)-Ti(1)-C(12)	34.7(3)	C(25)-Si(4)-C(24)	112.1(5)
C(23)-Ti(1)-C(12)	78.8(4)	C(25)-Si(4)-C(26)	111.7(5)
C(15)-Ti(1)-C(12)	56.7(3)	C(24)-Si(4)-C(26)	106.9(5)
C(11)-Ti(1)-C(12)	34.7(3)	C(25)-Si(4)-C(19)	108.9(5)
C(14)-Ti(1)-C(12)	57.4(3)	C(24)-Si(4)-C(19)	112.0(4)
C(21)-Ti(1)-C(12)	114.1(4)	C(26)-Si(4)-C(19)	104.9(4)
C(20)-Ti(1)-C(12)	134.6(4)	C(27)-O(1)-Cu(1)	110.7(6)
C(6)-Ti(1)-C(19)	124.0(3)	C(27)-O(2)-Cu(1)	73.3(6)
C(1)-Ti(1)-C(19)	80.3(3)	C(2)-C(1)-Cu(1)	75.0(6)
C(22)-Ti(1)-C(19)	58.0(3)	C(2)-C(1)-Ti(1)	163.9(7)
C(13)-Ti(1)-C(19)	100.5(4)	Cu(1)-C(1)-Ti(1)	88.9(3)
C(23)-Ti(1)-C(19)	34.0(3)	C(1)-C(2)-Si(1)	163.9(8)
C(15)-Ti(1)-C(19)	156.5(3)	C(1)-C(2)-Cu(1)	70.9(6)
C(11)-Ti(1)-C(19)	140.7(3)	Si(1)-C(2)-Cu(1)	125.0(5)
C(14)-Ti(1)-C(19)	123.6(3)	C(7)-C(6)-Cu(1)	76.1(6)
C(21)-Ti(1)-C(19)	58.1(3)	C(7)-C(6)-Ti(1)	165.6(8)
C(20)-Ti(1)-C(19)	35.2(3)	Cu(1)-C(6)-Ti(1)	89.6(4)
C(12)-Ti(1)-C(19)	108.5(3)	C(6)-C(7)-Si(2)	165.0(8)
C(3)-Si(1)-C(2)	107.9(5)	C(6)-C(7)-Cu(1)	69.4(6)
C(3)-Si(1)-C(5)	109.8(5)	Si(2)-C(7)-Cu(1)	124.9(5)
C(2)-Si(1)-C(5)	106.9(5)	C(15)-C(11)-C(12)	105.9(8)
C(3)-Si(1)-C(4)	112.4(6)	C(15)-C(11)-Si(3)	125.8(8)
C(2)-Si(1)-C(4)	110.8(5)	C(12)-C(11)-Si(3)	127.2(7)
C(5)-Si(1)-C(4)	108.9(5)	C(15)-C(11)-Ti(1)	72.6(5)
C(8)-Si(2)-C(7)	111.2(5)	C(12)-C(11)-Ti(1)	73.4(5)
C(8)-Si(2)-C(9)	111.3(5)	Si(3)-C(11)-Ti(1)	128.2(4)
C(7)-Si(2)-C(9)	110.6(5)	C(13)-C(12)-C(11)	107.8(9)
C(8)-Si(2)-C(10)	109.3(6)	C(13)-C(12)-Ti(1)	71.1(5)
C(7)-Si(2)-C(10)	104.7(5)	C(11)-C(12)-Ti(1)	71.9(5)
C(9)-Si(2)-C(10)	109.4(5)	C(14)-C(13)-C(12)	109.2(9)
C(16)-Si(3)-C(18)	110.1(5)	C(14)-C(13)-Ti(1)	74.0(6)
C(16)-Si(3)-C(17)	109.6(5)	C(12)-C(13)-Ti(1)	74.2(6)
C(18)-Si(3)-C(17)	109.4(5)	C(13)-C(14)-C(15)	106.5(9)

C(13)-C(14)-Ti(1)	71.7(6)	C(29)-Ti(2)-C(41)	113.6(4)
C(15)-C(14)-Ti(1)	72.4(5)	C(34)-Ti(2)-C(41)	76.0(4)
C(14)-C(15)-C(11)	110.5(9)	C(49)-Ti(2)-C(41)	133.9(4)
C(14)-C(15)-Ti(1)	73.4(6)	C(42)-Ti(2)-C(41)	33.4(4)
C(11)-C(15)-Ti(1)	72.7(5)	C(48)-Ti(2)-C(41)	112.7(4)
C(23)-C(19)-C(20)	105.7(8)	C(29)-Ti(2)-C(43)	113.1(4)
C(23)-C(19)-Si(4)	126.1(7)	C(34)-Ti(2)-C(43)	132.6(4)
C(20)-C(19)-Si(4)	127.3(7)	C(49)-Ti(2)-C(43)	81.7(4)
C(23)-C(19)-Ti(1)	71.8(5)	C(42)-Ti(2)-C(43)	34.5(4)
C(20)-C(19)-Ti(1)	72.3(5)	C(48)-Ti(2)-C(43)	81.7(4)
Si(4)-C(19)-Ti(1)	129.3(5)	C(41)-Ti(2)-C(43)	57.0(4)
C(21)-C(20)-C(19)	108.5(9)	C(29)-Ti(2)-C(51)	89.5(4)
C(21)-C(20)-Ti(1)	72.6(5)	C(34)-Ti(2)-C(51)	81.1(4)
C(19)-C(20)-Ti(1)	72.5(5)	C(49)-Ti(2)-C(51)	57.5(4)
C(22)-C(21)-C(20)	107.3(9)	C(42)-Ti(2)-C(51)	134.1(4)
C(22)-C(21)-Ti(1)	70.5(5)	C(48)-Ti(2)-C(51)	56.8(4)
C(20)-C(21)-Ti(1)	72.9(5)	C(41)-Ti(2)-C(51)	146.8(4)
C(23)-C(22)-C(21)	107.9(9)	C(43)-Ti(2)-C(51)	136.7(4)
C(23)-C(22)-Ti(1)	73.9(5)	C(29)-Ti(2)-C(50)	75.9(4)
C(21)-C(22)-Ti(1)	74.7(6)	C(34)-Ti(2)-C(50)	112.9(4)
C(19)-C(23)-C(22)	110.5(9)	C(49)-Ti(2)-C(50)	33.9(4)
C(19)-C(23)-Ti(1)	74.2(5)	C(42)-Ti(2)-C(50)	134.3(5)
C(22)-C(23)-Ti(1)	71.4(5)	C(48)-Ti(2)-C(50)	56.4(4)
O(2)-C(27)-O(1)	123.2(9)	C(41)-Ti(2)-C(50)	167.7(4)
O(2)-C(27)-C(28)	120.6(11)	C(43)-Ti(2)-C(50)	112.9(4)
O(1)-C(27)-C(28)	116.2(10)	C(51)-Ti(2)-C(50)	35.1(3)
C(29)-Ti(2)-C(34)	89.2(4)	C(29)-Ti(2)-C(40)	81.8(4)
C(29)-Ti(2)-C(49)	100.0(4)	C(34)-Ti(2)-C(40)	88.5(4)
C(34)-Ti(2)-C(49)	137.2(4)	C(49)-Ti(2)-C(40)	134.1(4)
C(29)-Ti(2)-C(42)	136.1(4)	C(42)-Ti(2)-C(40)	56.3(4)
C(34)-Ti(2)-C(42)	101.0(4)	C(48)-Ti(2)-C(40)	136.3(4)
C(49)-Ti(2)-C(42)	100.7(5)	C(41)-Ti(2)-C(40)	34.8(3)
C(29)-Ti(2)-C(48)	131.6(4)	C(43)-Ti(2)-C(40)	56.7(4)
C(34)-Ti(2)-C(48)	114.9(4)	C(51)-Ti(2)-C(40)	166.5(4)
C(49)-Ti(2)-C(48)	34.1(3)	C(50)-Ti(2)-C(40)	148.5(4)
C(42)-Ti(2)-C(48)	82.3(4)	C(29)-Ti(2)-C(47)	124.3(4)

C(34)-Ti(2)-C(47)	82.5(4)	C(34)-Cu(2)-Ti(2)	45.6(3)
C(49)-Ti(2)-C(47)	57.7(4)	C(29)-Cu(2)-Ti(2)	45.4(3)
C(42)-Ti(2)-C(47)	99.5(4)	C(35)-Cu(2)-Ti(2)	80.0(3)
C(48)-Ti(2)-C(47)	34.4(3)	C(30)-Cu(2)-Ti(2)	79.4(3)
C(41)-Ti(2)-C(47)	117.3(4)	O(4)-Cu(2)-Ti(2)	131.04(18)
C(43)-Ti(2)-C(47)	112.6(4)	C(32)-Si(5)-C(31)	111.9(6)
C(51)-Ti(2)-C(47)	34.8(3)	C(32)-Si(5)-C(33)	109.4(6)
C(50)-Ti(2)-C(47)	57.9(4)	C(31)-Si(5)-C(33)	109.0(6)
C(40)-Ti(2)-C(47)	152.0(3)	C(32)-Si(5)-C(30)	110.3(5)
C(29)-Ti(2)-C(39)	81.5(4)	C(31)-Si(5)-C(30)	109.7(5)
C(34)-Ti(2)-C(39)	122.5(4)	C(33)-Si(5)-C(30)	106.5(5)
C(49)-Ti(2)-C(39)	100.2(4)	C(36)-Si(6)-C(35)	111.0(5)
C(42)-Ti(2)-C(39)	57.0(4)	C(36)-Si(6)-C(37)	110.3(6)
C(48)-Ti(2)-C(39)	113.1(4)	C(35)-Si(6)-C(37)	109.3(5)
C(41)-Ti(2)-C(39)	57.5(4)	C(36)-Si(6)-C(38)	109.3(6)
C(43)-Ti(2)-C(39)	34.4(3)	C(35)-Si(6)-C(38)	105.4(5)
C(51)-Ti(2)-C(39)	154.2(4)	C(37)-Si(6)-C(38)	111.4(6)
C(50)-Ti(2)-C(39)	119.1(4)	C(45)-Si(7)-C(46)	111.8(6)
C(40)-Ti(2)-C(39)	34.2(3)	C(45)-Si(7)-C(44)	109.5(7)
C(47)-Ti(2)-C(39)	146.4(3)	C(46)-Si(7)-C(44)	107.8(6)
O(3)-Cu(2)-C(34)	134.2(4)	C(45)-Si(7)-C(39)	107.3(5)
O(3)-Cu(2)-C(29)	134.4(4)	C(46)-Si(7)-C(39)	113.5(5)
C(34)-Cu(2)-C(29)	91.0(4)	C(44)-Si(7)-C(39)	106.7(6)
O(3)-Cu(2)-C(35)	99.8(4)	C(52)-Si(8)-C(54)	111.3(6)
C(34)-Cu(2)-C(35)	34.4(4)	C(52)-Si(8)-C(53)	109.9(6)
C(29)-Cu(2)-C(35)	125.4(5)	C(54)-Si(8)-C(53)	107.5(6)
O(3)-Cu(2)-C(30)	100.6(3)	C(52)-Si(8)-C(47)	109.4(5)
C(34)-Cu(2)-C(30)	125.0(4)	C(54)-Si(8)-C(47)	111.7(5)
C(29)-Cu(2)-C(30)	34.0(3)	C(53)-Si(8)-C(47)	106.9(5)
C(35)-Cu(2)-C(30)	159.3(4)	C(55)-O(3)-Cu(2)	110.3(6)
O(3)-Cu(2)-O(4)	52.8(3)	C(55)-O(4)-Cu(2)	72.4(6)
C(34)-Cu(2)-O(4)	117.5(3)	C(30)-C(29)-Cu(2)	75.5(6)
C(29)-Cu(2)-O(4)	118.9(3)	C(30)-C(29)-Ti(2)	165.0(8)
C(35)-Cu(2)-O(4)	97.2(4)	Cu(2)-C(29)-Ti(2)	89.6(4)
C(30)-Cu(2)-O(4)	98.1(3)	C(29)-C(30)-Si(5)	165.5(8)
O(3)-Cu(2)-Ti(2)	176.1(2)	C(29)-C(30)-Cu(2)	70.5(6)

Si(5)-C(30)-Cu(2)	123.9(5)	C(48)-C(47)-Ti(2)	70.9(5)
C(35)-C(34)-Cu(2)	75.8(7)	C(51)-C(47)-Ti(2)	71.5(5)
C(35)-C(34)-Ti(2)	166.0(8)	Si(8)-C(47)-Ti(2)	127.7(5)
Cu(2)-C(34)-Ti(2)	90.2(4)	C(49)-C(48)-C(47)	110.8(9)
C(34)-C(35)-Si(6)	163.6(9)	C(49)-C(48)-Ti(2)	72.5(6)
C(34)-C(35)-Cu(2)	69.8(6)	C(47)-C(48)-Ti(2)	74.8(5)
Si(6)-C(35)-Cu(2)	126.5(6)	C(48)-C(49)-C(50)	108.5(10)
C(40)-C(39)-C(43)	106.2(9)	C(48)-C(49)-Ti(2)	73.4(6)
C(40)-C(39)-Si(7)	128.0(8)	C(50)-C(49)-Ti(2)	74.5(6)
C(43)-C(39)-Si(7)	125.5(8)	C(49)-C(50)-C(51)	107.6(10)
C(40)-C(39)-Ti(2)	71.8(5)	C(49)-C(50)-Ti(2)	71.6(6)
C(43)-C(39)-Ti(2)	71.2(5)	C(51)-C(50)-Ti(2)	72.3(6)
Si(7)-C(39)-Ti(2)	126.0(5)	C(47)-C(51)-C(50)	107.9(10)
C(39)-C(40)-C(41)	108.7(10)	C(47)-C(51)-Ti(2)	73.7(6)
C(39)-C(40)-Ti(2)	74.0(5)	C(50)-C(51)-Ti(2)	72.6(6)
C(41)-C(40)-Ti(2)	71.9(6)	O(4)-C(55)-O(3)	124.4(10)
C(42)-C(41)-C(40)	107.1(10)	O(4)-C(55)-C(56)	121.2(11)
C(42)-C(41)-Ti(2)	72.5(6)	O(3)-C(55)-C(56)	114.4(11)
C(40)-C(41)-Ti(2)	73.3(6)	C(60)-O(5)-C(57)	110.7(14)
C(41)-C(42)-C(43)	110.3(10)	O(5)-C(57)-C(58)	109.0(13)
C(41)-C(42)-Ti(2)	74.1(6)	C(57)-C(58)-C(59)	103.9(15)
C(43)-C(42)-Ti(2)	73.7(6)	C(60)-C(59)-C(58)	106.4(15)
C(42)-C(43)-C(39)	107.6(10)	O(5)-C(60)-C(59)	107.6(16)
C(42)-C(43)-Ti(2)	71.8(6)	C(64)-O(6)-C(61)	114(3)
C(39)-C(43)-Ti(2)	74.4(6)	O(6)-C(61)-C(62)	99(2)
C(48)-C(47)-C(51)	105.1(9)	C(63)-C(62)-C(61)	106(2)
C(48)-C(47)-Si(8)	126.9(8)	C(62)-C(63)-C(64)	107(2)
C(51)-C(47)-Si(8)	127.6(8)	O(6)-C(64)-C(63)	95(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Torsion angles [°] for 3a.

C(6)-Cu(1)-O(1)-C(27)	90.9(7)
C(1)-Cu(1)-O(1)-C(27)	-103.5(7)
C(2)-Cu(1)-O(1)-C(27)	-97.4(7)
C(7)-Cu(1)-O(1)-C(27)	85.8(7)
O(2)-Cu(1)-O(1)-C(27)	-2.4(6)
Ti(1)-Cu(1)-O(1)-C(27)	177.2(13)
O(1)-Cu(1)-O(2)-C(27)	2.4(6)
C(6)-Cu(1)-O(2)-C(27)	-124.5(6)
C(1)-Cu(1)-O(2)-C(27)	125.1(6)
C(2)-Cu(1)-O(2)-C(27)	97.1(6)
C(7)-Cu(1)-O(2)-C(27)	-97.0(6)
Ti(1)-Cu(1)-O(2)-C(27)	-177.5(5)
O(1)-Cu(1)-C(1)-C(2)	10.7(8)
C(6)-Cu(1)-C(1)-C(2)	-179.5(7)
C(7)-Cu(1)-C(1)-C(2)	179.4(6)
O(2)-Cu(1)-C(1)-C(2)	-55.9(7)
Ti(1)-Cu(1)-C(1)-C(2)	-179.5(8)
O(1)-Cu(1)-C(1)-Ti(1)	-169.8(3)
C(6)-Cu(1)-C(1)-Ti(1)	0.0(4)
C(2)-Cu(1)-C(1)-Ti(1)	179.5(8)
C(7)-Cu(1)-C(1)-Ti(1)	-1.1(5)
O(2)-Cu(1)-C(1)-Ti(1)	123.6(3)
C(6)-Ti(1)-C(1)-C(2)	2(3)
C(22)-Ti(1)-C(1)-C(2)	-105(3)
C(13)-Ti(1)-C(1)-C(2)	138(3)
C(23)-Ti(1)-C(1)-C(2)	-136(3)
C(15)-Ti(1)-C(1)-C(2)	81(3)
C(11)-Ti(1)-C(1)-C(2)	86(3)
C(14)-Ti(1)-C(1)-C(2)	109(3)
C(21)-Ti(1)-C(1)-C(2)	-73(3)
C(20)-Ti(1)-C(1)-C(2)	-87(3)
C(12)-Ti(1)-C(1)-C(2)	131(3)
C(19)-Ti(1)-C(1)-C(2)	-123(3)
C(6)-Ti(1)-C(1)-Cu(1)	0.0(4)

C(22)-Ti(1)-C(1)-Cu(1)	-107.0(5)
C(13)-Ti(1)-C(1)-Cu(1)	135.7(4)
C(23)-Ti(1)-C(1)-Cu(1)	-137.5(3)
C(15)-Ti(1)-C(1)-Cu(1)	78.8(4)
C(11)-Ti(1)-C(1)-Cu(1)	84.1(5)
C(14)-Ti(1)-C(1)-Cu(1)	107.0(4)
C(21)-Ti(1)-C(1)-Cu(1)	-75.2(4)
C(20)-Ti(1)-C(1)-Cu(1)	-88.8(3)
C(12)-Ti(1)-C(1)-Cu(1)	129.4(4)
C(19)-Ti(1)-C(1)-Cu(1)	-124.5(4)
Cu(1)-C(1)-C(2)-Si(1)	-173(3)
Ti(1)-C(1)-C(2)-Si(1)	-175.4(15)
Ti(1)-C(1)-C(2)-Cu(1)	-2(3)
C(3)-Si(1)-C(2)-C(1)	113(3)
C(5)-Si(1)-C(2)-C(1)	-5(3)
C(4)-Si(1)-C(2)-C(1)	-123(3)
C(3)-Si(1)-C(2)-Cu(1)	-59.0(8)
C(5)-Si(1)-C(2)-Cu(1)	-177.0(6)
C(4)-Si(1)-C(2)-Cu(1)	64.5(8)
O(1)-Cu(1)-C(2)-C(1)	-172.1(6)
C(6)-Cu(1)-C(2)-C(1)	0.7(8)
C(7)-Cu(1)-C(2)-C(1)	-1.4(14)
O(2)-Cu(1)-C(2)-C(1)	134.4(6)
Ti(1)-Cu(1)-C(2)-C(1)	0.4(6)
O(1)-Cu(1)-C(2)-Si(1)	5.7(7)
C(6)-Cu(1)-C(2)-Si(1)	178.5(5)
C(1)-Cu(1)-C(2)-Si(1)	177.8(11)
C(7)-Cu(1)-C(2)-Si(1)	176.4(8)
O(2)-Cu(1)-C(2)-Si(1)	-47.8(6)
Ti(1)-Cu(1)-C(2)-Si(1)	178.2(6)
O(1)-Cu(1)-C(6)-C(7)	-8.8(8)
C(1)-Cu(1)-C(6)-C(7)	-178.4(6)
C(2)-Cu(1)-C(6)-C(7)	-178.8(6)
O(2)-Cu(1)-C(6)-C(7)	54.4(7)
Ti(1)-Cu(1)-C(6)-C(7)	-178.4(8)
O(1)-Cu(1)-C(6)-Ti(1)	169.6(3)

C(1)-Cu(1)-C(6)-Ti(1)	0.0(4)
C(2)-Cu(1)-C(6)-Ti(1)	-0.4(5)
C(7)-Cu(1)-C(6)-Ti(1)	178.4(8)
O(2)-Cu(1)-C(6)-Ti(1)	-127.2(3)
C(1)-Ti(1)-C(6)-C(7)	6(3)
C(22)-Ti(1)-C(6)-C(7)	144(3)
C(13)-Ti(1)-C(6)-C(7)	-91(3)
C(23)-Ti(1)-C(6)-C(7)	127(3)
C(15)-Ti(1)-C(6)-C(7)	-89(3)
C(11)-Ti(1)-C(6)-C(7)	-124(3)
C(14)-Ti(1)-C(6)-C(7)	-69(3)
C(21)-Ti(1)-C(6)-C(7)	120(3)
C(20)-Ti(1)-C(6)-C(7)	87(3)
C(12)-Ti(1)-C(6)-C(7)	-130(3)
C(19)-Ti(1)-C(6)-C(7)	85(3)
C(1)-Ti(1)-C(6)-Cu(1)	0.0(4)
C(22)-Ti(1)-C(6)-Cu(1)	137.5(3)
C(13)-Ti(1)-C(6)-Cu(1)	-97.1(5)
C(23)-Ti(1)-C(6)-Cu(1)	120.8(4)
C(15)-Ti(1)-C(6)-Cu(1)	-95.4(3)
C(11)-Ti(1)-C(6)-Cu(1)	-129.8(3)
C(14)-Ti(1)-C(6)-Cu(1)	-75.0(4)
C(21)-Ti(1)-C(6)-Cu(1)	113.4(4)
C(20)-Ti(1)-C(6)-Cu(1)	81.0(3)
C(12)-Ti(1)-C(6)-Cu(1)	-136.4(3)
C(19)-Ti(1)-C(6)-Cu(1)	78.5(4)
Cu(1)-C(6)-C(7)-Si(2)	-163(3)
Ti(1)-C(6)-C(7)-Si(2)	-169.8(16)
Ti(1)-C(6)-C(7)-Cu(1)	-6(3)
C(8)-Si(2)-C(7)-C(6)	-147(3)
C(9)-Si(2)-C(7)-C(6)	88(3)
C(10)-Si(2)-C(7)-C(6)	-29(3)
C(8)-Si(2)-C(7)-Cu(1)	51.9(7)
C(9)-Si(2)-C(7)-Cu(1)	-72.4(7)
C(10)-Si(2)-C(7)-Cu(1)	169.8(6)
O(1)-Cu(1)-C(7)-C(6)	173.6(6)

C(1)-Cu(1)-C(7)-C(6)	2.0(8)
C(2)-Cu(1)-C(7)-C(6)	2.9(14)
O(2)-Cu(1)-C(7)-C(6)	-133.5(6)
Ti(1)-Cu(1)-C(7)-C(6)	1.2(5)
O(1)-Cu(1)-C(7)-Si(2)	-11.6(6)
C(6)-Cu(1)-C(7)-Si(2)	174.8(10)
C(1)-Cu(1)-C(7)-Si(2)	176.8(5)
C(2)-Cu(1)-C(7)-Si(2)	177.7(8)
O(2)-Cu(1)-C(7)-Si(2)	41.3(6)
Ti(1)-Cu(1)-C(7)-Si(2)	176.0(6)
C(16)-Si(3)-C(11)-C(15)	3.0(10)
C(18)-Si(3)-C(11)-C(15)	121.2(9)
C(17)-Si(3)-C(11)-C(15)	-117.8(9)
C(16)-Si(3)-C(11)-C(12)	-163.2(8)
C(18)-Si(3)-C(11)-C(12)	-45.0(10)
C(17)-Si(3)-C(11)-C(12)	76.0(10)
C(16)-Si(3)-C(11)-Ti(1)	98.7(7)
C(18)-Si(3)-C(11)-Ti(1)	-143.1(6)
C(17)-Si(3)-C(11)-Ti(1)	-22.1(8)
C(6)-Ti(1)-C(11)-C(15)	77.1(6)
C(1)-Ti(1)-C(11)-C(15)	-9.3(7)
C(22)-Ti(1)-C(11)-C(15)	178.3(6)
C(13)-Ti(1)-C(11)-C(15)	-76.4(6)
C(23)-Ti(1)-C(11)-C(15)	-149.2(6)
C(14)-Ti(1)-C(11)-C(15)	-35.7(6)
C(21)-Ti(1)-C(11)-C(15)	149.6(6)
C(20)-Ti(1)-C(11)-C(15)	157.0(7)
C(12)-Ti(1)-C(11)-C(15)	-113.1(8)
C(19)-Ti(1)-C(11)-C(15)	-141.2(6)
C(6)-Ti(1)-C(11)-C(12)	-169.8(6)
C(1)-Ti(1)-C(11)-C(12)	103.7(6)
C(22)-Ti(1)-C(11)-C(12)	-68.6(6)
C(13)-Ti(1)-C(11)-C(12)	36.7(6)
C(23)-Ti(1)-C(11)-C(12)	-36.1(6)
C(15)-Ti(1)-C(11)-C(12)	113.1(8)
C(14)-Ti(1)-C(11)-C(12)	77.4(6)

C(21)-Ti(1)-C(11)-C(12)	-97.3(6)
C(20)-Ti(1)-C(11)-C(12)	-89.9(8)
C(19)-Ti(1)-C(11)-C(12)	-28.2(8)
C(6)-Ti(1)-C(11)-Si(3)	-45.2(6)
C(1)-Ti(1)-C(11)-Si(3)	-131.6(5)
C(22)-Ti(1)-C(11)-Si(3)	56.0(6)
C(13)-Ti(1)-C(11)-Si(3)	161.4(8)
C(23)-Ti(1)-C(11)-Si(3)	88.5(6)
C(15)-Ti(1)-C(11)-Si(3)	-122.3(9)
C(14)-Ti(1)-C(11)-Si(3)	-158.0(8)
C(21)-Ti(1)-C(11)-Si(3)	27.3(7)
C(20)-Ti(1)-C(11)-Si(3)	34.8(10)
C(12)-Ti(1)-C(11)-Si(3)	124.6(9)
C(19)-Ti(1)-C(11)-Si(3)	96.5(7)
C(15)-C(11)-C(12)-C(13)	3.5(10)
Si(3)-C(11)-C(12)-C(13)	171.8(7)
Ti(1)-C(11)-C(12)-C(13)	-62.4(7)
C(15)-C(11)-C(12)-Ti(1)	65.9(6)
Si(3)-C(11)-C(12)-Ti(1)	-125.7(7)
C(6)-Ti(1)-C(12)-C(13)	128.5(6)
C(1)-Ti(1)-C(12)-C(13)	11.0(8)
C(22)-Ti(1)-C(12)-C(13)	-133.3(7)
C(23)-Ti(1)-C(12)-C(13)	-98.1(7)
C(15)-Ti(1)-C(12)-C(13)	78.1(7)
C(11)-Ti(1)-C(12)-C(13)	116.9(9)
C(14)-Ti(1)-C(12)-C(13)	37.1(6)
C(21)-Ti(1)-C(12)-C(13)	-144.1(6)
C(20)-Ti(1)-C(12)-C(13)	-109.9(7)
C(19)-Ti(1)-C(12)-C(13)	-81.5(7)
C(6)-Ti(1)-C(12)-C(11)	11.6(7)
C(1)-Ti(1)-C(12)-C(11)	-105.9(6)
C(22)-Ti(1)-C(12)-C(11)	109.8(6)
C(13)-Ti(1)-C(12)-C(11)	-116.9(9)
C(23)-Ti(1)-C(12)-C(11)	145.0(6)
C(15)-Ti(1)-C(12)-C(11)	-38.7(5)
C(14)-Ti(1)-C(12)-C(11)	-79.8(6)

C(21)-Ti(1)-C(12)-C(11)	99.0(6)
C(20)-Ti(1)-C(12)-C(11)	133.2(6)
C(19)-Ti(1)-C(12)-C(11)	161.6(5)
C(11)-C(12)-C(13)-C(14)	-3.4(11)
Ti(1)-C(12)-C(13)-C(14)	-66.3(7)
C(11)-C(12)-C(13)-Ti(1)	62.9(7)
C(6)-Ti(1)-C(13)-C(14)	39.6(8)
C(1)-Ti(1)-C(13)-C(14)	-55.6(6)
C(22)-Ti(1)-C(13)-C(14)	163.9(6)
C(23)-Ti(1)-C(13)-C(14)	-167.2(6)
C(15)-Ti(1)-C(13)-C(14)	37.7(6)
C(11)-Ti(1)-C(13)-C(14)	79.1(6)
C(21)-Ti(1)-C(13)-C(14)	170.8(6)
C(20)-Ti(1)-C(13)-C(14)	-137.6(6)
C(12)-Ti(1)-C(13)-C(14)	115.9(9)
C(19)-Ti(1)-C(13)-C(14)	-136.6(6)
C(6)-Ti(1)-C(13)-C(12)	-76.2(8)
C(1)-Ti(1)-C(13)-C(12)	-171.4(6)
C(22)-Ti(1)-C(13)-C(12)	48.1(7)
C(23)-Ti(1)-C(13)-C(12)	77.0(6)
C(15)-Ti(1)-C(13)-C(12)	-78.2(6)
C(11)-Ti(1)-C(13)-C(12)	-36.8(6)
C(14)-Ti(1)-C(13)-C(12)	-115.9(9)
C(21)-Ti(1)-C(13)-C(12)	54.9(8)
C(20)-Ti(1)-C(13)-C(12)	106.6(7)
C(19)-Ti(1)-C(13)-C(12)	107.5(6)
C(12)-C(13)-C(14)-C(15)	2.0(11)
Ti(1)-C(13)-C(14)-C(15)	-64.5(7)
C(12)-C(13)-C(14)-Ti(1)	66.4(7)
C(6)-Ti(1)-C(14)-C(13)	-152.2(6)
C(1)-Ti(1)-C(14)-C(13)	121.9(6)
C(22)-Ti(1)-C(14)-C(13)	-23.3(8)
C(23)-Ti(1)-C(14)-C(13)	14.6(7)
C(15)-Ti(1)-C(14)-C(13)	-114.8(9)
C(11)-Ti(1)-C(14)-C(13)	-78.7(6)
C(21)-Ti(1)-C(14)-C(13)	-45(3)

C(20)-Ti(1)-C(14)-C(13)	87.2(9)
C(12)-Ti(1)-C(14)-C(13)	-37.4(6)
C(19)-Ti(1)-C(14)-C(13)	54.2(7)
C(6)-Ti(1)-C(14)-C(15)	-37.3(7)
C(1)-Ti(1)-C(14)-C(15)	-123.3(6)
C(22)-Ti(1)-C(14)-C(15)	91.5(7)
C(13)-Ti(1)-C(14)-C(15)	114.8(9)
C(23)-Ti(1)-C(14)-C(15)	129.5(6)
C(11)-Ti(1)-C(14)-C(15)	36.1(6)
C(21)-Ti(1)-C(14)-C(15)	70(3)
C(20)-Ti(1)-C(14)-C(15)	-157.9(7)
C(12)-Ti(1)-C(14)-C(15)	77.4(6)
C(19)-Ti(1)-C(14)-C(15)	169.0(5)
C(13)-C(14)-C(15)-C(11)	0.2(11)
Ti(1)-C(14)-C(15)-C(11)	-63.8(7)
C(13)-C(14)-C(15)-Ti(1)	64.0(7)
C(12)-C(11)-C(15)-C(14)	-2.3(11)
Si(3)-C(11)-C(15)-C(14)	-170.9(7)
Ti(1)-C(11)-C(15)-C(14)	64.2(7)
C(12)-C(11)-C(15)-Ti(1)	-66.5(6)
Si(3)-C(11)-C(15)-Ti(1)	125.0(7)
C(6)-Ti(1)-C(15)-C(14)	143.6(7)
C(1)-Ti(1)-C(15)-C(14)	54.4(6)
C(22)-Ti(1)-C(15)-C(14)	-120.5(6)
C(13)-Ti(1)-C(15)-C(14)	-37.8(6)
C(23)-Ti(1)-C(15)-C(14)	-74.3(7)
C(11)-Ti(1)-C(15)-C(14)	-118.4(9)
C(21)-Ti(1)-C(15)-C(14)	-166.8(6)
C(20)-Ti(1)-C(15)-C(14)	127.2(15)
C(12)-Ti(1)-C(15)-C(14)	-79.5(6)
C(19)-Ti(1)-C(15)-C(14)	-23.6(11)
C(6)-Ti(1)-C(15)-C(11)	-98.0(6)
C(1)-Ti(1)-C(15)-C(11)	172.8(6)
C(22)-Ti(1)-C(15)-C(11)	-2.1(8)
C(13)-Ti(1)-C(15)-C(11)	80.6(6)
C(23)-Ti(1)-C(15)-C(11)	44.1(8)

C(14)-Ti(1)-C(15)-C(11)	118.4(9)
C(21)-Ti(1)-C(15)-C(11)	-48.4(8)
C(20)-Ti(1)-C(15)-C(11)	-114.4(15)
C(12)-Ti(1)-C(15)-C(11)	38.8(5)
C(19)-Ti(1)-C(15)-C(11)	94.8(9)
C(25)-Si(4)-C(19)-C(23)	-168.7(8)
C(24)-Si(4)-C(19)-C(23)	66.7(9)
C(26)-Si(4)-C(19)-C(23)	-49.0(9)
C(25)-Si(4)-C(19)-C(20)	-1.6(10)
C(24)-Si(4)-C(19)-C(20)	-126.2(8)
C(26)-Si(4)-C(19)-C(20)	118.2(9)
C(25)-Si(4)-C(19)-Ti(1)	95.7(7)
C(24)-Si(4)-C(19)-Ti(1)	-28.9(8)
C(26)-Si(4)-C(19)-Ti(1)	-144.5(6)
C(6)-Ti(1)-C(19)-C(23)	118.2(6)
C(1)-Ti(1)-C(19)-C(23)	-158.1(6)
C(22)-Ti(1)-C(19)-C(23)	36.1(6)
C(13)-Ti(1)-C(19)-C(23)	-65.0(6)
C(15)-Ti(1)-C(19)-C(23)	-77.0(10)
C(11)-Ti(1)-C(19)-C(23)	-13.7(8)
C(14)-Ti(1)-C(19)-C(23)	-92.7(6)
C(21)-Ti(1)-C(19)-C(23)	77.3(6)
C(20)-Ti(1)-C(19)-C(23)	113.8(8)
C(12)-Ti(1)-C(19)-C(23)	-30.1(7)
C(6)-Ti(1)-C(19)-C(20)	4.3(7)
C(1)-Ti(1)-C(19)-C(20)	88.1(6)
C(22)-Ti(1)-C(19)-C(20)	-77.7(6)
C(13)-Ti(1)-C(19)-C(20)	-178.8(6)
C(23)-Ti(1)-C(19)-C(20)	-113.8(8)
C(15)-Ti(1)-C(19)-C(20)	169.2(8)
C(11)-Ti(1)-C(19)-C(20)	-127.5(6)
C(14)-Ti(1)-C(19)-C(20)	153.5(6)
C(21)-Ti(1)-C(19)-C(20)	-36.6(6)
C(12)-Ti(1)-C(19)-C(20)	-143.9(6)
C(6)-Ti(1)-C(19)-Si(4)	-119.7(6)
C(1)-Ti(1)-C(19)-Si(4)	-36.0(6)

C(22)-Ti(1)-C(19)-Si(4)	158.2(8)
C(13)-Ti(1)-C(19)-Si(4)	57.1(7)
C(23)-Ti(1)-C(19)-Si(4)	122.1(9)
C(15)-Ti(1)-C(19)-Si(4)	45.1(12)
C(11)-Ti(1)-C(19)-Si(4)	108.5(7)
C(14)-Ti(1)-C(19)-Si(4)	29.4(8)
C(21)-Ti(1)-C(19)-Si(4)	-160.6(8)
C(20)-Ti(1)-C(19)-Si(4)	-124.0(9)
C(12)-Ti(1)-C(19)-Si(4)	92.0(6)
C(23)-C(19)-C(20)-C(21)	-0.4(10)
Si(4)-C(19)-C(20)-C(21)	-169.6(7)
Ti(1)-C(19)-C(20)-C(21)	64.2(7)
C(23)-C(19)-C(20)-Ti(1)	-64.5(6)
Si(4)-C(19)-C(20)-Ti(1)	126.3(7)
C(6)-Ti(1)-C(20)-C(21)	67.0(6)
C(1)-Ti(1)-C(20)-C(21)	157.4(7)
C(22)-Ti(1)-C(20)-C(21)	-37.4(6)
C(13)-Ti(1)-C(20)-C(21)	-115.0(7)
C(23)-Ti(1)-C(20)-C(21)	-79.0(6)
C(15)-Ti(1)-C(20)-C(21)	83.1(17)
C(11)-Ti(1)-C(20)-C(21)	-12.0(10)
C(14)-Ti(1)-C(20)-C(21)	-168.6(7)
C(12)-Ti(1)-C(20)-C(21)	-65.0(8)
C(19)-Ti(1)-C(20)-C(21)	-116.6(9)
C(6)-Ti(1)-C(20)-C(19)	-176.4(6)
C(1)-Ti(1)-C(20)-C(19)	-86.0(6)
C(22)-Ti(1)-C(20)-C(19)	79.2(6)
C(13)-Ti(1)-C(20)-C(19)	1.6(8)
C(23)-Ti(1)-C(20)-C(19)	37.6(5)
C(15)-Ti(1)-C(20)-C(19)	-160.3(14)
C(11)-Ti(1)-C(20)-C(19)	104.6(8)
C(14)-Ti(1)-C(20)-C(19)	-52.0(10)
C(21)-Ti(1)-C(20)-C(19)	116.6(9)
C(12)-Ti(1)-C(20)-C(19)	51.6(7)
C(19)-C(20)-C(21)-C(22)	-1.5(11)
Ti(1)-C(20)-C(21)-C(22)	62.6(6)

C(19)-C(20)-C(21)-Ti(1)	-64.1(6)
C(6)-Ti(1)-C(21)-C(22)	135.4(7)
C(1)-Ti(1)-C(21)-C(22)	-140.2(6)
C(13)-Ti(1)-C(21)-C(22)	-11.6(9)
C(23)-Ti(1)-C(21)-C(22)	-38.1(6)
C(15)-Ti(1)-C(21)-C(22)	85.1(8)
C(11)-Ti(1)-C(21)-C(22)	57.2(7)
C(14)-Ti(1)-C(21)-C(22)	26(3)
C(20)-Ti(1)-C(21)-C(22)	-115.9(9)
C(12)-Ti(1)-C(21)-C(22)	19.0(7)
C(19)-Ti(1)-C(21)-C(22)	-78.6(6)
C(6)-Ti(1)-C(21)-C(20)	-108.7(7)
C(1)-Ti(1)-C(21)-C(20)	-24.3(7)
C(22)-Ti(1)-C(21)-C(20)	115.9(9)
C(13)-Ti(1)-C(21)-C(20)	104.3(7)
C(23)-Ti(1)-C(21)-C(20)	77.8(6)
C(15)-Ti(1)-C(21)-C(20)	-158.9(6)
C(11)-Ti(1)-C(21)-C(20)	173.2(6)
C(14)-Ti(1)-C(21)-C(20)	142(2)
C(12)-Ti(1)-C(21)-C(20)	135.0(6)
C(19)-Ti(1)-C(21)-C(20)	37.4(6)
C(20)-C(21)-C(22)-C(23)	2.8(11)
Ti(1)-C(21)-C(22)-C(23)	67.0(7)
C(20)-C(21)-C(22)-Ti(1)	-64.2(7)
C(6)-Ti(1)-C(22)-C(23)	-158.4(6)
C(1)-Ti(1)-C(22)-C(23)	-55.8(8)
C(13)-Ti(1)-C(22)-C(23)	57.9(7)
C(15)-Ti(1)-C(22)-C(23)	116.9(6)
C(11)-Ti(1)-C(22)-C(23)	115.7(6)
C(14)-Ti(1)-C(22)-C(23)	71.2(8)
C(21)-Ti(1)-C(22)-C(23)	-114.3(9)
C(20)-Ti(1)-C(22)-C(23)	-77.2(6)
C(12)-Ti(1)-C(22)-C(23)	83.3(6)
C(19)-Ti(1)-C(22)-C(23)	-35.3(6)
C(6)-Ti(1)-C(22)-C(21)	-44.1(6)
C(1)-Ti(1)-C(22)-C(21)	58.5(8)

C(13)-Ti(1)-C(22)-C(21)	172.2(6)
C(23)-Ti(1)-C(22)-C(21)	114.3(9)
C(15)-Ti(1)-C(22)-C(21)	-128.8(6)
C(11)-Ti(1)-C(22)-C(21)	-130.0(6)
C(14)-Ti(1)-C(22)-C(21)	-174.5(6)
C(20)-Ti(1)-C(22)-C(21)	37.1(5)
C(12)-Ti(1)-C(22)-C(21)	-162.5(6)
C(19)-Ti(1)-C(22)-C(21)	79.0(6)
C(20)-C(19)-C(23)-C(22)	2.2(11)
Si(4)-C(19)-C(23)-C(22)	171.5(7)
Ti(1)-C(19)-C(23)-C(22)	-62.7(7)
C(20)-C(19)-C(23)-Ti(1)	64.8(6)
Si(4)-C(19)-C(23)-Ti(1)	-125.8(7)
C(21)-C(22)-C(23)-C(19)	-3.2(11)
Ti(1)-C(22)-C(23)-C(19)	64.4(7)
C(21)-C(22)-C(23)-Ti(1)	-67.6(7)
C(6)-Ti(1)-C(23)-C(19)	-89.1(7)
C(1)-Ti(1)-C(23)-C(19)	23.3(7)
C(22)-Ti(1)-C(23)-C(19)	-118.6(9)
C(13)-Ti(1)-C(23)-C(19)	116.6(6)
C(15)-Ti(1)-C(23)-C(19)	146.5(6)
C(11)-Ti(1)-C(23)-C(19)	171.0(5)
C(14)-Ti(1)-C(23)-C(19)	108.4(6)
C(21)-Ti(1)-C(23)-C(19)	-80.4(6)
C(20)-Ti(1)-C(23)-C(19)	-39.1(5)
C(12)-Ti(1)-C(23)-C(19)	151.0(6)
C(6)-Ti(1)-C(23)-C(22)	29.6(8)
C(1)-Ti(1)-C(23)-C(22)	141.9(6)
C(13)-Ti(1)-C(23)-C(22)	-124.8(6)
C(15)-Ti(1)-C(23)-C(22)	-94.8(7)
C(11)-Ti(1)-C(23)-C(22)	-70.4(7)
C(14)-Ti(1)-C(23)-C(22)	-133.0(6)
C(21)-Ti(1)-C(23)-C(22)	38.2(6)
C(20)-Ti(1)-C(23)-C(22)	79.6(7)
C(12)-Ti(1)-C(23)-C(22)	-90.4(6)
C(19)-Ti(1)-C(23)-C(22)	118.6(9)

Cu(1)-O(2)-C(27)-O(1)	-3.5(8)
Cu(1)-O(2)-C(27)-C(28)	176.4(10)
Cu(1)-O(1)-C(27)-O(2)	5.1(12)
Cu(1)-O(1)-C(27)-C(28)	-174.8(7)
C(29)-Ti(2)-Cu(2)-O(3)	89(3)
C(34)-Ti(2)-Cu(2)-O(3)	-88(3)
C(49)-Ti(2)-Cu(2)-O(3)	150(3)
C(42)-Ti(2)-Cu(2)-O(3)	-30(3)
C(48)-Ti(2)-Cu(2)-O(3)	-164(3)
C(41)-Ti(2)-Cu(2)-O(3)	-27(3)
C(43)-Ti(2)-Cu(2)-O(3)	18(3)
C(51)-Ti(2)-Cu(2)-O(3)	-174(3)
C(50)-Ti(2)-Cu(2)-O(3)	154(3)
C(40)-Ti(2)-Cu(2)-O(3)	5(3)
C(47)-Ti(2)-Cu(2)-O(3)	-148(3)
C(39)-Ti(2)-Cu(2)-O(3)	31(3)
C(29)-Ti(2)-Cu(2)-C(34)	177.3(5)
C(49)-Ti(2)-Cu(2)-C(34)	-121.7(5)
C(42)-Ti(2)-Cu(2)-C(34)	58.4(5)
C(48)-Ti(2)-Cu(2)-C(34)	-75.8(6)
C(41)-Ti(2)-Cu(2)-C(34)	61.1(5)
C(43)-Ti(2)-Cu(2)-C(34)	106.6(6)
C(51)-Ti(2)-Cu(2)-C(34)	-85.4(4)
C(50)-Ti(2)-Cu(2)-C(34)	-118.2(5)
C(40)-Ti(2)-Cu(2)-C(34)	93.5(4)
C(47)-Ti(2)-Cu(2)-C(34)	-60.2(5)
C(39)-Ti(2)-Cu(2)-C(34)	119.3(4)
C(34)-Ti(2)-Cu(2)-C(29)	-177.3(5)
C(49)-Ti(2)-Cu(2)-C(29)	61.0(5)
C(42)-Ti(2)-Cu(2)-C(29)	-118.9(5)
C(48)-Ti(2)-Cu(2)-C(29)	106.9(6)
C(41)-Ti(2)-Cu(2)-C(29)	-116.2(5)
C(43)-Ti(2)-Cu(2)-C(29)	-70.7(6)
C(51)-Ti(2)-Cu(2)-C(29)	97.3(5)
C(50)-Ti(2)-Cu(2)-C(29)	64.5(5)
C(40)-Ti(2)-Cu(2)-C(29)	-83.9(4)

C(47)-Ti(2)-Cu(2)-C(29)	122.4(5)
C(39)-Ti(2)-Cu(2)-C(29)	-58.1(4)
C(29)-Ti(2)-Cu(2)-C(35)	176.8(5)
C(34)-Ti(2)-Cu(2)-C(35)	-0.5(5)
C(49)-Ti(2)-Cu(2)-C(35)	-122.2(5)
C(42)-Ti(2)-Cu(2)-C(35)	57.9(5)
C(48)-Ti(2)-Cu(2)-C(35)	-76.3(5)
C(41)-Ti(2)-Cu(2)-C(35)	60.6(4)
C(43)-Ti(2)-Cu(2)-C(35)	106.1(5)
C(51)-Ti(2)-Cu(2)-C(35)	-85.9(4)
C(50)-Ti(2)-Cu(2)-C(35)	-118.7(4)
C(40)-Ti(2)-Cu(2)-C(35)	92.9(4)
C(47)-Ti(2)-Cu(2)-C(35)	-60.8(4)
C(39)-Ti(2)-Cu(2)-C(35)	118.8(4)
C(29)-Ti(2)-Cu(2)-C(30)	-0.8(5)
C(34)-Ti(2)-Cu(2)-C(30)	-178.1(5)
C(49)-Ti(2)-Cu(2)-C(30)	60.2(4)
C(42)-Ti(2)-Cu(2)-C(30)	-119.7(5)
C(48)-Ti(2)-Cu(2)-C(30)	106.1(5)
C(41)-Ti(2)-Cu(2)-C(30)	-117.0(4)
C(43)-Ti(2)-Cu(2)-C(30)	-71.5(5)
C(51)-Ti(2)-Cu(2)-C(30)	96.5(4)
C(50)-Ti(2)-Cu(2)-C(30)	63.7(4)
C(40)-Ti(2)-Cu(2)-C(30)	-84.6(4)
C(47)-Ti(2)-Cu(2)-C(30)	121.7(4)
C(39)-Ti(2)-Cu(2)-C(30)	-58.8(4)
C(29)-Ti(2)-Cu(2)-O(4)	-92.3(4)
C(34)-Ti(2)-Cu(2)-O(4)	90.3(4)
C(49)-Ti(2)-Cu(2)-O(4)	-31.4(4)
C(42)-Ti(2)-Cu(2)-O(4)	148.7(4)
C(48)-Ti(2)-Cu(2)-O(4)	14.5(5)
C(41)-Ti(2)-Cu(2)-O(4)	151.4(4)
C(43)-Ti(2)-Cu(2)-O(4)	-163.1(5)
C(51)-Ti(2)-Cu(2)-O(4)	4.9(3)
C(50)-Ti(2)-Cu(2)-O(4)	-27.8(4)
C(40)-Ti(2)-Cu(2)-O(4)	-176.2(3)

C(47)-Ti(2)-Cu(2)-O(4)	30.1(3)
C(39)-Ti(2)-Cu(2)-O(4)	-150.4(3)
C(34)-Cu(2)-O(3)-C(55)	94.0(7)
C(29)-Cu(2)-O(3)-C(55)	-96.2(7)
C(35)-Cu(2)-O(3)-C(55)	91.4(7)
C(30)-Cu(2)-O(3)-C(55)	-92.4(7)
O(4)-Cu(2)-O(3)-C(55)	-0.2(6)
Ti(2)-Cu(2)-O(3)-C(55)	178(100)
O(3)-Cu(2)-O(4)-C(55)	0.2(6)
C(34)-Cu(2)-O(4)-C(55)	-126.0(7)
C(29)-Cu(2)-O(4)-C(55)	125.9(7)
C(35)-Cu(2)-O(4)-C(55)	-96.7(7)
C(30)-Cu(2)-O(4)-C(55)	97.3(7)
Ti(2)-Cu(2)-O(4)-C(55)	-179.7(5)
O(3)-Cu(2)-C(29)-C(30)	6.8(9)
C(34)-Cu(2)-C(29)-C(30)	179.4(7)
C(35)-Cu(2)-C(29)-C(30)	177.5(6)
O(4)-Cu(2)-C(29)-C(30)	-58.0(7)
Ti(2)-Cu(2)-C(29)-C(30)	-178.7(8)
O(3)-Cu(2)-C(29)-Ti(2)	-174.6(3)
C(34)-Cu(2)-C(29)-Ti(2)	-1.9(4)
C(35)-Cu(2)-C(29)-Ti(2)	-3.9(6)
C(30)-Cu(2)-C(29)-Ti(2)	178.7(8)
O(4)-Cu(2)-C(29)-Ti(2)	120.6(3)
C(34)-Ti(2)-C(29)-C(30)	7(3)
C(49)-Ti(2)-C(29)-C(30)	-131(3)
C(42)-Ti(2)-C(29)-C(30)	112(3)
C(48)-Ti(2)-C(29)-C(30)	-117(3)
C(41)-Ti(2)-C(29)-C(30)	81(3)
C(43)-Ti(2)-C(29)-C(30)	144(3)
C(51)-Ti(2)-C(29)-C(30)	-74(3)
C(50)-Ti(2)-C(29)-C(30)	-107(3)
C(40)-Ti(2)-C(29)-C(30)	95(3)
C(47)-Ti(2)-C(29)-C(30)	-73(3)
C(39)-Ti(2)-C(29)-C(30)	130(3)
C(34)-Ti(2)-C(29)-Cu(2)	1.9(4)

C(49)-Ti(2)-C(29)-Cu(2)	-136.1(4)
C(42)-Ti(2)-C(29)-Cu(2)	106.9(6)
C(48)-Ti(2)-C(29)-Cu(2)	-121.6(4)
C(41)-Ti(2)-C(29)-Cu(2)	76.2(5)
C(43)-Ti(2)-C(29)-Cu(2)	138.8(4)
C(51)-Ti(2)-C(29)-Cu(2)	-79.3(4)
C(50)-Ti(2)-C(29)-Cu(2)	-112.0(4)
C(40)-Ti(2)-C(29)-Cu(2)	90.4(4)
C(47)-Ti(2)-C(29)-Cu(2)	-78.5(5)
C(39)-Ti(2)-C(29)-Cu(2)	125.0(4)
Cu(2)-C(29)-C(30)-Si(5)	-179(100)
Ti(2)-C(29)-C(30)-Si(5)	175.4(16)
Ti(2)-C(29)-C(30)-Cu(2)	-5(3)
C(32)-Si(5)-C(30)-C(29)	-112(4)
C(31)-Si(5)-C(30)-C(29)	125(4)
C(33)-Si(5)-C(30)-C(29)	7(4)
C(32)-Si(5)-C(30)-Cu(2)	68.9(7)
C(31)-Si(5)-C(30)-Cu(2)	-54.7(7)
C(33)-Si(5)-C(30)-Cu(2)	-172.5(6)
O(3)-Cu(2)-C(30)-C(29)	-175.1(6)
C(34)-Cu(2)-C(30)-C(29)	-0.7(8)
C(35)-Cu(2)-C(30)-C(29)	-5.8(14)
O(4)-Cu(2)-C(30)-C(29)	131.4(6)
Ti(2)-Cu(2)-C(30)-C(29)	1.0(6)
O(3)-Cu(2)-C(30)-Si(5)	4.7(6)
C(34)-Cu(2)-C(30)-Si(5)	179.2(5)
C(29)-Cu(2)-C(30)-Si(5)	179.8(10)
C(35)-Cu(2)-C(30)-Si(5)	174.0(8)
O(4)-Cu(2)-C(30)-Si(5)	-48.8(6)
Ti(2)-Cu(2)-C(30)-Si(5)	-179.2(6)
O(3)-Cu(2)-C(34)-C(35)	-4.5(9)
C(29)-Cu(2)-C(34)-C(35)	-177.2(7)
C(30)-Cu(2)-C(34)-C(35)	-176.8(6)
O(4)-Cu(2)-C(34)-C(35)	59.2(7)
Ti(2)-Cu(2)-C(34)-C(35)	-179.1(8)
O(3)-Cu(2)-C(34)-Ti(2)	174.6(3)

C(29)-Cu(2)-C(34)-Ti(2)	1.9(4)
C(35)-Cu(2)-C(34)-Ti(2)	179.1(8)
C(30)-Cu(2)-C(34)-Ti(2)	2.3(5)
O(4)-Cu(2)-C(34)-Ti(2)	-121.7(3)
C(29)-Ti(2)-C(34)-C(35)	2(4)
C(49)-Ti(2)-C(34)-C(35)	106(4)
C(42)-Ti(2)-C(34)-C(35)	-135(4)
C(48)-Ti(2)-C(34)-C(35)	138(3)
C(41)-Ti(2)-C(34)-C(35)	-113(4)
C(43)-Ti(2)-C(34)-C(35)	-119(3)
C(51)-Ti(2)-C(34)-C(35)	91(4)
C(50)-Ti(2)-C(34)-C(35)	76(4)
C(40)-Ti(2)-C(34)-C(35)	-80(4)
C(47)-Ti(2)-C(34)-C(35)	127(4)
C(39)-Ti(2)-C(34)-C(35)	-77(4)
C(29)-Ti(2)-C(34)-Cu(2)	-1.9(4)
C(49)-Ti(2)-C(34)-Cu(2)	102.0(5)
C(42)-Ti(2)-C(34)-Cu(2)	-138.9(4)
C(48)-Ti(2)-C(34)-Cu(2)	134.7(4)
C(41)-Ti(2)-C(34)-Cu(2)	-116.5(4)
C(43)-Ti(2)-C(34)-Cu(2)	-123.2(5)
C(51)-Ti(2)-C(34)-Cu(2)	87.7(4)
C(50)-Ti(2)-C(34)-Cu(2)	72.5(4)
C(40)-Ti(2)-C(34)-Cu(2)	-83.7(4)
C(47)-Ti(2)-C(34)-Cu(2)	122.9(4)
C(39)-Ti(2)-C(34)-Cu(2)	-81.2(4)
Cu(2)-C(34)-C(35)-Si(6)	175(3)
Ti(2)-C(34)-C(35)-Si(6)	171.4(17)
Ti(2)-C(34)-C(35)-Cu(2)	-4(3)
C(36)-Si(6)-C(35)-C(34)	-125(3)
C(37)-Si(6)-C(35)-C(34)	113(3)
C(38)-Si(6)-C(35)-C(34)	-7(3)
C(36)-Si(6)-C(35)-Cu(2)	49.7(8)
C(37)-Si(6)-C(35)-Cu(2)	-72.2(8)
C(38)-Si(6)-C(35)-Cu(2)	168.0(7)
O(3)-Cu(2)-C(35)-C(34)	176.8(6)

C(29)-Cu(2)-C(35)-C(34)	3.5(8)
C(30)-Cu(2)-C(35)-C(34)	7.4(14)
O(4)-Cu(2)-C(35)-C(34)	-129.8(6)
Ti(2)-Cu(2)-C(35)-C(34)	0.7(6)
O(3)-Cu(2)-C(35)-Si(6)	-1.6(7)
C(34)-Cu(2)-C(35)-Si(6)	-178.4(11)
C(29)-Cu(2)-C(35)-Si(6)	-174.9(5)
C(30)-Cu(2)-C(35)-Si(6)	-170.9(8)
O(4)-Cu(2)-C(35)-Si(6)	51.8(7)
Ti(2)-Cu(2)-C(35)-Si(6)	-177.7(7)
C(45)-Si(7)-C(39)-C(40)	-2.9(10)
C(46)-Si(7)-C(39)-C(40)	121.2(9)
C(44)-Si(7)-C(39)-C(40)	-120.2(10)
C(45)-Si(7)-C(39)-C(43)	170.9(9)
C(46)-Si(7)-C(39)-C(43)	-65.0(10)
C(44)-Si(7)-C(39)-C(43)	53.6(10)
C(45)-Si(7)-C(39)-Ti(2)	-97.4(7)
C(46)-Si(7)-C(39)-Ti(2)	26.7(8)
C(44)-Si(7)-C(39)-Ti(2)	145.3(7)
C(29)-Ti(2)-C(39)-C(40)	-87.9(6)
C(34)-Ti(2)-C(39)-C(40)	-4.4(7)
C(49)-Ti(2)-C(39)-C(40)	173.4(6)
C(42)-Ti(2)-C(39)-C(40)	77.2(7)
C(48)-Ti(2)-C(39)-C(40)	140.3(6)
C(41)-Ti(2)-C(39)-C(40)	37.3(6)
C(43)-Ti(2)-C(39)-C(40)	115.0(9)
C(51)-Ti(2)-C(39)-C(40)	-158.6(7)
C(50)-Ti(2)-C(39)-C(40)	-156.5(6)
C(47)-Ti(2)-C(39)-C(40)	128.6(7)
C(29)-Ti(2)-C(39)-C(43)	157.1(7)
C(34)-Ti(2)-C(39)-C(43)	-119.3(7)
C(49)-Ti(2)-C(39)-C(43)	58.4(7)
C(42)-Ti(2)-C(39)-C(43)	-37.8(6)
C(48)-Ti(2)-C(39)-C(43)	25.3(7)
C(41)-Ti(2)-C(39)-C(43)	-77.7(7)
C(51)-Ti(2)-C(39)-C(43)	86.4(10)

C(50)-Ti(2)-C(39)-C(43)	88.5(7)
C(40)-Ti(2)-C(39)-C(43)	-115.0(9)
C(47)-Ti(2)-C(39)-C(43)	13.6(10)
C(29)-Ti(2)-C(39)-Si(7)	36.3(6)
C(34)-Ti(2)-C(39)-Si(7)	119.8(6)
C(49)-Ti(2)-C(39)-Si(7)	-62.4(7)
C(42)-Ti(2)-C(39)-Si(7)	-158.6(8)
C(48)-Ti(2)-C(39)-Si(7)	-95.5(6)
C(41)-Ti(2)-C(39)-Si(7)	161.5(8)
C(43)-Ti(2)-C(39)-Si(7)	-120.8(10)
C(51)-Ti(2)-C(39)-Si(7)	-34.4(12)
C(50)-Ti(2)-C(39)-Si(7)	-32.3(8)
C(40)-Ti(2)-C(39)-Si(7)	124.2(9)
C(47)-Ti(2)-C(39)-Si(7)	-107.2(7)
C(43)-C(39)-C(40)-C(41)	-0.7(11)
Si(7)-C(39)-C(40)-C(41)	174.0(7)
Ti(2)-C(39)-C(40)-C(41)	-64.1(7)
C(43)-C(39)-C(40)-Ti(2)	63.4(7)
Si(7)-C(39)-C(40)-Ti(2)	-121.9(8)
C(29)-Ti(2)-C(40)-C(39)	86.9(6)
C(34)-Ti(2)-C(40)-C(39)	176.3(6)
C(49)-Ti(2)-C(40)-C(39)	-9.1(8)
C(42)-Ti(2)-C(40)-C(39)	-79.4(7)
C(48)-Ti(2)-C(40)-C(39)	-58.1(8)
C(41)-Ti(2)-C(40)-C(39)	-116.4(9)
C(43)-Ti(2)-C(40)-C(39)	-37.7(6)
C(51)-Ti(2)-C(40)-C(39)	137.0(14)
C(50)-Ti(2)-C(40)-C(39)	41.8(10)
C(47)-Ti(2)-C(40)-C(39)	-112.8(8)
C(29)-Ti(2)-C(40)-C(41)	-156.7(7)
C(34)-Ti(2)-C(40)-C(41)	-67.3(7)
C(49)-Ti(2)-C(40)-C(41)	107.3(8)
C(42)-Ti(2)-C(40)-C(41)	37.0(7)
C(48)-Ti(2)-C(40)-C(41)	58.3(9)
C(43)-Ti(2)-C(40)-C(41)	78.6(7)
C(51)-Ti(2)-C(40)-C(41)	-106.6(16)

C(50)-Ti(2)-C(40)-C(41)	158.2(8)
C(47)-Ti(2)-C(40)-C(41)	3.5(12)
C(39)-Ti(2)-C(40)-C(41)	116.4(9)
C(39)-C(40)-C(41)-C(42)	0.3(11)
Ti(2)-C(40)-C(41)-C(42)	-65.1(7)
C(39)-C(40)-C(41)-Ti(2)	65.4(7)
C(29)-Ti(2)-C(41)-C(42)	139.9(7)
C(34)-Ti(2)-C(41)-C(42)	-137.3(8)
C(49)-Ti(2)-C(41)-C(42)	6.8(10)
C(48)-Ti(2)-C(41)-C(42)	-25.8(8)
C(43)-Ti(2)-C(41)-C(42)	36.9(7)
C(51)-Ti(2)-C(41)-C(42)	-89.5(9)
C(50)-Ti(2)-C(41)-C(42)	0(2)
C(40)-Ti(2)-C(41)-C(42)	114.6(10)
C(47)-Ti(2)-C(41)-C(42)	-63.5(8)
C(39)-Ti(2)-C(41)-C(42)	78.0(7)
C(29)-Ti(2)-C(41)-C(40)	25.3(8)
C(34)-Ti(2)-C(41)-C(40)	108.1(7)
C(49)-Ti(2)-C(41)-C(40)	-107.8(8)
C(42)-Ti(2)-C(41)-C(40)	-114.6(10)
C(48)-Ti(2)-C(41)-C(40)	-140.4(7)
C(43)-Ti(2)-C(41)-C(40)	-77.7(7)
C(51)-Ti(2)-C(41)-C(40)	155.9(7)
C(50)-Ti(2)-C(41)-C(40)	-114.2(18)
C(47)-Ti(2)-C(41)-C(40)	-178.1(6)
C(39)-Ti(2)-C(41)-C(40)	-36.6(6)
C(40)-C(41)-C(42)-C(43)	0.3(12)
Ti(2)-C(41)-C(42)-C(43)	-65.4(8)
C(40)-C(41)-C(42)-Ti(2)	65.7(7)
C(29)-Ti(2)-C(42)-C(41)	-58.3(10)
C(34)-Ti(2)-C(42)-C(41)	42.1(7)
C(49)-Ti(2)-C(42)-C(41)	-175.0(7)
C(48)-Ti(2)-C(42)-C(41)	156.1(8)
C(43)-Ti(2)-C(42)-C(41)	-117.3(10)
C(51)-Ti(2)-C(42)-C(41)	130.3(7)
C(50)-Ti(2)-C(42)-C(41)	-179.9(7)

C(40)-Ti(2)-C(42)-C(41)	-38.6(6)
C(47)-Ti(2)-C(42)-C(41)	126.3(7)
C(39)-Ti(2)-C(42)-C(41)	-79.7(7)
C(29)-Ti(2)-C(42)-C(43)	59.1(10)
C(34)-Ti(2)-C(42)-C(43)	159.5(7)
C(49)-Ti(2)-C(42)-C(43)	-57.7(8)
C(48)-Ti(2)-C(42)-C(43)	-86.6(8)
C(41)-Ti(2)-C(42)-C(43)	117.3(10)
C(51)-Ti(2)-C(42)-C(43)	-112.3(7)
C(50)-Ti(2)-C(42)-C(43)	-62.5(9)
C(40)-Ti(2)-C(42)-C(43)	78.8(7)
C(47)-Ti(2)-C(42)-C(43)	-116.4(7)
C(39)-Ti(2)-C(42)-C(43)	37.6(6)
C(41)-C(42)-C(43)-C(39)	-0.7(12)
Ti(2)-C(42)-C(43)-C(39)	-66.3(7)
C(41)-C(42)-C(43)-Ti(2)	65.6(8)
C(40)-C(39)-C(43)-C(42)	0.8(11)
Si(7)-C(39)-C(43)-C(42)	-174.0(7)
Ti(2)-C(39)-C(43)-C(42)	64.6(7)
C(40)-C(39)-C(43)-Ti(2)	-63.8(7)
Si(7)-C(39)-C(43)-Ti(2)	121.4(7)
C(29)-Ti(2)-C(43)-C(42)	-139.7(7)
C(34)-Ti(2)-C(43)-C(42)	-27.9(10)
C(49)-Ti(2)-C(43)-C(42)	122.9(8)
C(48)-Ti(2)-C(43)-C(42)	88.4(8)
C(41)-Ti(2)-C(43)-C(42)	-35.7(7)
C(51)-Ti(2)-C(43)-C(42)	104.3(8)
C(50)-Ti(2)-C(43)-C(42)	136.4(7)
C(40)-Ti(2)-C(43)-C(42)	-77.5(7)
C(47)-Ti(2)-C(43)-C(42)	73.1(8)
C(39)-Ti(2)-C(43)-C(42)	-115.0(10)
C(29)-Ti(2)-C(43)-C(39)	-24.7(7)
C(34)-Ti(2)-C(43)-C(39)	87.1(8)
C(49)-Ti(2)-C(43)-C(39)	-122.1(7)
C(42)-Ti(2)-C(43)-C(39)	115.0(10)
C(48)-Ti(2)-C(43)-C(39)	-156.6(7)

C(41)-Ti(2)-C(43)-C(39)	79.3(7)
C(51)-Ti(2)-C(43)-C(39)	-140.7(6)
C(50)-Ti(2)-C(43)-C(39)	-108.6(6)
C(40)-Ti(2)-C(43)-C(39)	37.5(6)
C(47)-Ti(2)-C(43)-C(39)	-171.9(6)
C(52)-Si(8)-C(47)-C(48)	172.9(9)
C(54)-Si(8)-C(47)-C(48)	-63.4(10)
C(53)-Si(8)-C(47)-C(48)	53.9(10)
C(52)-Si(8)-C(47)-C(51)	1.6(10)
C(54)-Si(8)-C(47)-C(51)	125.2(9)
C(53)-Si(8)-C(47)-C(51)	-117.4(9)
C(52)-Si(8)-C(47)-Ti(2)	-93.5(7)
C(54)-Si(8)-C(47)-Ti(2)	30.1(8)
C(53)-Si(8)-C(47)-Ti(2)	147.5(6)
C(29)-Ti(2)-C(47)-C(48)	-115.3(7)
C(34)-Ti(2)-C(47)-C(48)	160.8(7)
C(49)-Ti(2)-C(47)-C(48)	-35.8(6)
C(42)-Ti(2)-C(47)-C(48)	60.9(7)
C(41)-Ti(2)-C(47)-C(48)	90.9(7)
C(43)-Ti(2)-C(47)-C(48)	27.6(7)
C(51)-Ti(2)-C(47)-C(48)	-114.0(9)
C(50)-Ti(2)-C(47)-C(48)	-76.1(7)
C(40)-Ti(2)-C(47)-C(48)	88.6(10)
C(39)-Ti(2)-C(47)-C(48)	19.3(9)
C(29)-Ti(2)-C(47)-C(51)	-1.4(8)
C(34)-Ti(2)-C(47)-C(51)	-85.2(6)
C(49)-Ti(2)-C(47)-C(51)	78.2(7)
C(42)-Ti(2)-C(47)-C(51)	174.8(7)
C(48)-Ti(2)-C(47)-C(51)	114.0(9)
C(41)-Ti(2)-C(47)-C(51)	-155.2(6)
C(43)-Ti(2)-C(47)-C(51)	141.5(6)
C(50)-Ti(2)-C(47)-C(51)	37.9(6)
C(40)-Ti(2)-C(47)-C(51)	-157.5(7)
C(39)-Ti(2)-C(47)-C(51)	133.2(7)
C(29)-Ti(2)-C(47)-Si(8)	122.3(6)
C(34)-Ti(2)-C(47)-Si(8)	38.4(6)

C(49)-Ti(2)-C(47)-Si(8)	-158.2(8)
C(42)-Ti(2)-C(47)-Si(8)	-61.5(7)
C(48)-Ti(2)-C(47)-Si(8)	-122.4(10)
C(41)-Ti(2)-C(47)-Si(8)	-31.5(8)
C(43)-Ti(2)-C(47)-Si(8)	-94.8(7)
C(51)-Ti(2)-C(47)-Si(8)	123.6(10)
C(50)-Ti(2)-C(47)-Si(8)	161.5(8)
C(40)-Ti(2)-C(47)-Si(8)	-33.8(11)
C(39)-Ti(2)-C(47)-Si(8)	-103.1(8)
C(51)-C(47)-C(48)-C(49)	0.3(11)
Si(8)-C(47)-C(48)-C(49)	-172.6(7)
Ti(2)-C(47)-C(48)-C(49)	64.1(7)
C(51)-C(47)-C(48)-Ti(2)	-63.8(6)
Si(8)-C(47)-C(48)-Ti(2)	123.3(8)
C(29)-Ti(2)-C(48)-C(49)	-26.2(9)
C(34)-Ti(2)-C(48)-C(49)	-139.2(6)
C(42)-Ti(2)-C(48)-C(49)	122.2(7)
C(41)-Ti(2)-C(48)-C(49)	136.2(7)
C(43)-Ti(2)-C(48)-C(49)	87.4(7)
C(51)-Ti(2)-C(48)-C(49)	-79.7(7)
C(50)-Ti(2)-C(48)-C(49)	-37.3(6)
C(40)-Ti(2)-C(48)-C(49)	104.5(7)
C(47)-Ti(2)-C(48)-C(49)	-118.2(9)
C(39)-Ti(2)-C(48)-C(49)	73.3(7)
C(29)-Ti(2)-C(48)-C(47)	92.0(7)
C(34)-Ti(2)-C(48)-C(47)	-21.0(7)
C(49)-Ti(2)-C(48)-C(47)	118.2(9)
C(42)-Ti(2)-C(48)-C(47)	-119.6(7)
C(41)-Ti(2)-C(48)-C(47)	-105.6(7)
C(43)-Ti(2)-C(48)-C(47)	-154.4(7)
C(51)-Ti(2)-C(48)-C(47)	38.5(6)
C(50)-Ti(2)-C(48)-C(47)	80.9(7)
C(40)-Ti(2)-C(48)-C(47)	-137.3(6)
C(39)-Ti(2)-C(48)-C(47)	-168.5(6)
C(47)-C(48)-C(49)-C(50)	1.2(12)
Ti(2)-C(48)-C(49)-C(50)	66.7(7)

C(47)-C(48)-C(49)-Ti(2)	-65.5(7)
C(29)-Ti(2)-C(49)-C(48)	160.4(7)
C(34)-Ti(2)-C(49)-C(48)	60.7(9)
C(42)-Ti(2)-C(49)-C(48)	-58.5(7)
C(41)-Ti(2)-C(49)-C(48)	-62.3(8)
C(43)-Ti(2)-C(49)-C(48)	-87.4(7)
C(51)-Ti(2)-C(49)-C(48)	77.5(7)
C(50)-Ti(2)-C(49)-C(48)	115.3(10)
C(40)-Ti(2)-C(49)-C(48)	-111.3(7)
C(47)-Ti(2)-C(49)-C(48)	36.1(6)
C(39)-Ti(2)-C(49)-C(48)	-116.5(7)
C(29)-Ti(2)-C(49)-C(50)	45.2(7)
C(34)-Ti(2)-C(49)-C(50)	-54.6(9)
C(42)-Ti(2)-C(49)-C(50)	-173.8(7)
C(48)-Ti(2)-C(49)-C(50)	-115.3(10)
C(41)-Ti(2)-C(49)-C(50)	-177.6(6)
C(43)-Ti(2)-C(49)-C(50)	157.3(7)
C(51)-Ti(2)-C(49)-C(50)	-37.8(6)
C(40)-Ti(2)-C(49)-C(50)	133.4(7)
C(47)-Ti(2)-C(49)-C(50)	-79.2(7)
C(39)-Ti(2)-C(49)-C(50)	128.2(7)
C(48)-C(49)-C(50)-C(51)	-2.2(12)
Ti(2)-C(49)-C(50)-C(51)	63.8(7)
C(48)-C(49)-C(50)-Ti(2)	-66.0(7)
C(29)-Ti(2)-C(50)-C(49)	-133.9(7)
C(34)-Ti(2)-C(50)-C(49)	143.0(6)
C(42)-Ti(2)-C(50)-C(49)	8.5(9)
C(48)-Ti(2)-C(50)-C(49)	37.5(6)
C(41)-Ti(2)-C(50)-C(49)	8(2)
C(43)-Ti(2)-C(50)-C(49)	-24.5(8)
C(51)-Ti(2)-C(50)-C(49)	116.2(9)
C(40)-Ti(2)-C(50)-C(49)	-87.6(9)
C(47)-Ti(2)-C(50)-C(49)	78.7(7)
C(39)-Ti(2)-C(50)-C(49)	-62.3(7)
C(29)-Ti(2)-C(50)-C(51)	109.9(7)
C(34)-Ti(2)-C(50)-C(51)	26.9(7)

C(49)-Ti(2)-C(50)-C(51)	-116.2(9)
C(42)-Ti(2)-C(50)-C(51)	-107.6(7)
C(48)-Ti(2)-C(50)-C(51)	-78.6(7)
C(41)-Ti(2)-C(50)-C(51)	-107.9(18)
C(43)-Ti(2)-C(50)-C(51)	-140.7(6)
C(40)-Ti(2)-C(50)-C(51)	156.2(7)
C(47)-Ti(2)-C(50)-C(51)	-37.5(6)
C(39)-Ti(2)-C(50)-C(51)	-178.4(6)
C(48)-C(47)-C(51)-C(50)	-1.6(10)
Si(8)-C(47)-C(51)-C(50)	171.2(7)
Ti(2)-C(47)-C(51)-C(50)	-65.0(7)
C(48)-C(47)-C(51)-Ti(2)	63.4(6)
Si(8)-C(47)-C(51)-Ti(2)	-123.8(8)
C(49)-C(50)-C(51)-C(47)	2.4(11)
Ti(2)-C(50)-C(51)-C(47)	65.8(7)
C(49)-C(50)-C(51)-Ti(2)	-63.4(7)
C(29)-Ti(2)-C(51)-C(47)	178.9(6)
C(34)-Ti(2)-C(51)-C(47)	89.6(6)
C(49)-Ti(2)-C(51)-C(47)	-78.9(6)
C(42)-Ti(2)-C(51)-C(47)	-7.1(9)
C(48)-Ti(2)-C(51)-C(47)	-38.1(6)
C(41)-Ti(2)-C(51)-C(47)	42.9(10)
C(43)-Ti(2)-C(51)-C(47)	-56.9(9)
C(50)-Ti(2)-C(51)-C(47)	-115.3(9)
C(40)-Ti(2)-C(51)-C(47)	129.5(14)
C(39)-Ti(2)-C(51)-C(47)	-112.2(9)
C(29)-Ti(2)-C(51)-C(50)	-65.8(6)
C(34)-Ti(2)-C(51)-C(50)	-155.1(7)
C(49)-Ti(2)-C(51)-C(50)	36.4(6)
C(42)-Ti(2)-C(51)-C(50)	108.2(8)
C(48)-Ti(2)-C(51)-C(50)	77.3(7)
C(41)-Ti(2)-C(51)-C(50)	158.3(8)
C(43)-Ti(2)-C(51)-C(50)	58.4(9)
C(40)-Ti(2)-C(51)-C(50)	-115.2(15)
C(47)-Ti(2)-C(51)-C(50)	115.3(9)
C(39)-Ti(2)-C(51)-C(50)	3.2(11)

Cu(2)-O(4)-C(55)-O(3)	-0.3(9)
Cu(2)-O(4)-C(55)-C(56)	179.1(10)
Cu(2)-O(3)-C(55)-O(4)	0.4(12)
Cu(2)-O(3)-C(55)-C(56)	-179.0(7)
C(60)-O(5)-C(57)-C(58)	4(2)
O(5)-C(57)-C(58)-C(59)	6(2)
C(57)-C(58)-C(59)-C(60)	-13(2)
C(57)-O(5)-C(60)-C(59)	-12(2)
C(58)-C(59)-C(60)-O(5)	16(3)
C(64)-O(6)-C(61)-C(62)	39(5)
O(6)-C(61)-C(62)-C(63)	-12(4)
C(61)-C(62)-C(63)-C(64)	-14(4)
C(61)-O(6)-C(64)-C(63)	-46(5)
C(62)-C(63)-C(64)-O(6)	33(5)

Symmetry transformations used to generate equivalent atoms:

Table 8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3a.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cu(1)	36(1)	32(1)	26(1)	-4(1)	12(1)	-1(1)
Ti(1)	33(1)	28(1)	27(1)	-3(1)	11(1)	-2(1)
Si(1)	43(2)	47(2)	29(2)	0(1)	9(1)	4(2)
Si(2)	56(2)	40(2)	28(2)	-7(1)	17(1)	-12(2)
Si(3)	40(2)	40(2)	41(2)	7(1)	15(1)	4(1)
Si(4)	50(2)	41(2)	31(2)	2(1)	18(1)	2(2)
O(1)	46(4)	40(5)	43(4)	-10(3)	24(4)	-5(4)
O(2)	61(5)	41(5)	65(5)	-1(4)	35(4)	-1(4)
C(1)	38(6)	40(6)	16(5)	-10(5)	16(5)	-5(5)
C(2)	38(6)	40(6)	29(6)	-5(5)	12(5)	7(6)
C(3)	48(7)	84(9)	53(7)	16(7)	10(6)	26(7)
C(4)	82(9)	48(8)	47(7)	2(6)	17(7)	6(7)

C(5)	49(7)	69(8)	39(7)	-9(6)	10(6)	11(6)
C(6)	35(6)	37(6)	28(6)	0(5)	16(5)	-10(5)
C(7)	34(6)	45(7)	21(5)	4(5)	7(5)	0(5)
C(8)	93(10)	58(8)	44(7)	-12(6)	37(7)	-21(7)
C(9)	56(7)	55(7)	58(7)	-12(6)	32(6)	-18(6)
C(10)	81(9)	74(9)	33(7)	-11(6)	3(6)	-15(7)
C(11)	31(6)	28(6)	42(6)	1(5)	16(5)	-4(5)
C(12)	46(7)	21(6)	60(7)	-2(5)	29(6)	-1(5)
C(13)	52(7)	29(6)	46(7)	-4(5)	16(6)	-5(5)
C(14)	37(6)	36(6)	40(7)	7(5)	9(5)	-6(5)
C(15)	36(6)	31(6)	48(7)	6(5)	27(5)	2(5)
C(16)	45(7)	55(8)	63(8)	-2(6)	22(6)	7(6)
C(17)	40(7)	72(9)	46(7)	13(6)	6(6)	-5(6)
C(18)	57(7)	46(7)	55(7)	11(6)	15(6)	3(6)
C(19)	35(6)	39(6)	31(6)	3(5)	24(5)	-5(5)
C(20)	38(6)	35(6)	46(7)	-8(5)	21(5)	-12(5)
C(21)	30(6)	49(7)	33(6)	2(5)	12(5)	-17(5)
C(22)	39(6)	48(8)	45(7)	4(6)	20(6)	-9(5)
C(23)	47(6)	43(7)	37(6)	5(5)	36(6)	13(5)
C(24)	54(7)	63(8)	35(6)	-9(6)	20(6)	-3(6)
C(25)	52(7)	62(8)	46(7)	15(6)	23(6)	4(6)
C(26)	70(8)	62(8)	39(6)	-6(6)	35(6)	3(6)
C(27)	44(7)	49(8)	27(6)	-9(5)	14(5)	5(6)
C(28)	67(8)	43(7)	59(8)	-9(6)	25(7)	14(6)
Ti(2)	39(1)	31(1)	33(1)	6(1)	16(1)	4(1)
Cu(2)	35(1)	36(1)	28(1)	-2(1)	12(1)	-1(1)
Si(5)	39(2)	44(2)	31(2)	1(1)	5(1)	5(1)
Si(6)	49(2)	56(2)	28(2)	-11(2)	12(2)	-15(2)
Si(7)	84(2)	37(2)	35(2)	-5(2)	20(2)	-13(2)
Si(8)	41(2)	55(2)	53(2)	14(2)	14(2)	4(2)
O(3)	34(4)	45(5)	50(4)	-7(4)	20(4)	0(3)
O(4)	65(6)	52(5)	88(6)	-11(4)	49(5)	-11(4)
C(29)	47(7)	36(6)	25(6)	-5(5)	18(5)	-1(6)
C(30)	42(6)	26(6)	20(5)	-13(4)	9(5)	-1(5)
C(31)	34(7)	111(11)	62(8)	12(8)	18(6)	10(7)
C(32)	58(8)	53(8)	65(8)	15(6)	8(7)	8(6)

C(33)	89(10)	86(10)	34(7)	-16(7)	2(7)	21(8)
C(34)	27(6)	47(7)	29(6)	5(5)	9(5)	-3(5)
C(35)	37(6)	59(8)	27(6)	9(6)	6(5)	-8(6)
C(36)	87(9)	86(10)	40(7)	-34(7)	31(7)	-38(8)
C(37)	84(9)	45(8)	64(8)	-14(6)	26(7)	-11(7)
C(38)	95(10)	84(10)	29(7)	-8(7)	-1(7)	-10(8)
C(39)	41(7)	28(6)	41(6)	2(5)	23(5)	-4(5)
C(40)	48(7)	35(6)	45(7)	13(5)	28(6)	2(5)
C(41)	65(8)	44(7)	41(7)	11(6)	21(7)	-14(6)
C(42)	49(7)	37(7)	66(9)	22(6)	10(7)	1(6)
C(43)	80(9)	20(6)	76(9)	0(6)	55(8)	-9(6)
C(44)	220(20)	53(9)	65(10)	-16(8)	61(12)	-24(11)
C(45)	56(8)	110(12)	50(8)	15(8)	5(6)	-31(8)
C(46)	99(10)	46(7)	25(6)	0(5)	27(6)	4(7)
C(47)	28(6)	37(6)	57(7)	6(6)	26(5)	3(5)
C(48)	29(6)	50(8)	76(9)	2(6)	40(6)	14(5)
C(49)	55(7)	44(8)	46(7)	-4(6)	33(6)	-7(6)
C(50)	57(7)	51(8)	44(7)	7(6)	30(6)	0(6)
C(51)	34(6)	53(7)	54(7)	13(6)	35(6)	6(5)
C(52)	55(8)	58(8)	68(8)	-1(7)	20(7)	-16(6)
C(53)	53(8)	92(10)	81(10)	17(8)	27(7)	13(7)
C(54)	59(8)	69(9)	52(7)	22(6)	7(6)	-3(7)
C(55)	29(6)	44(8)	42(7)	-19(6)	1(5)	0(6)
C(56)	69(8)	49(8)	88(9)	-12(7)	41(8)	14(6)
O(5)	99(9)	120(10)	143(11)	-32(8)	30(8)	-5(7)
C(57)	86(11)	86(11)	91(11)	-23(9)	32(9)	-7(9)
C(58)	180(20)	160(20)	95(14)	-22(13)	79(15)	-117(18)
C(59)	66(14)	280(40)	160(20)	70(20)	-9(15)	-44(19)
C(60)	80(15)	170(20)	200(20)	90(20)	55(15)	46(14)
O(6)	200(20)	240(30)	360(40)	30(30)	-60(30)	-60(20)
C(61)	280(40)	320(50)	130(20)	20(30)	10(20)	210(40)
C(62)	230(30)	130(20)	150(20)	-16(18)	40(20)	-60(20)
C(63)	170(30)	420(60)	250(40)	-200(40)	100(30)	-130(30)
C(64)	360(60)	150(30)	260(40)	-100(30)	60(40)	-50(30)

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

$$9.8061 (0.0940) x + 14.8315 (0.0381) y - 6.3028 (0.1124) z = 2.0855 (0.0539)$$

* 0.0168 (0.0057) C11

* -0.0200 (0.0060) C12

* 0.0158 (0.0061) C13

* -0.0050 (0.0059) C14

* -0.0075 (0.0058) C15

2.0459 (0.0044) Ti1

-0.2200 (0.0152) Si3

Rms deviation of fitted atoms = 0.0142

$$16.4111 (0.0304) x + 10.6475 (0.0260) y - 11.0996 (0.0519) z = 6.0071 (0.0266)$$

Angle to previous plane (with approximate esd) = 23.14 (0.42)

* -0.0012 (0.0036) Ti1

* -0.0080 (0.0070) C1

* 0.0020 (0.0055) C2

* 0.0134 (0.0068) C6

* -0.0130 (0.0052) C7

* 0.0070 (0.0044) Cu1

-0.0447 (0.0112) Si1

0.0857 (0.0108) Si2

-0.2366 (0.0103) O1

1.9584 (0.0109) O2

Rms deviation of fitted atoms = 0.0088