Electronic Supporting Information

Electrochemical Sensing of Nitrite using Copper-Titanium Oxide Composite Derived from Hexanuclear Complex

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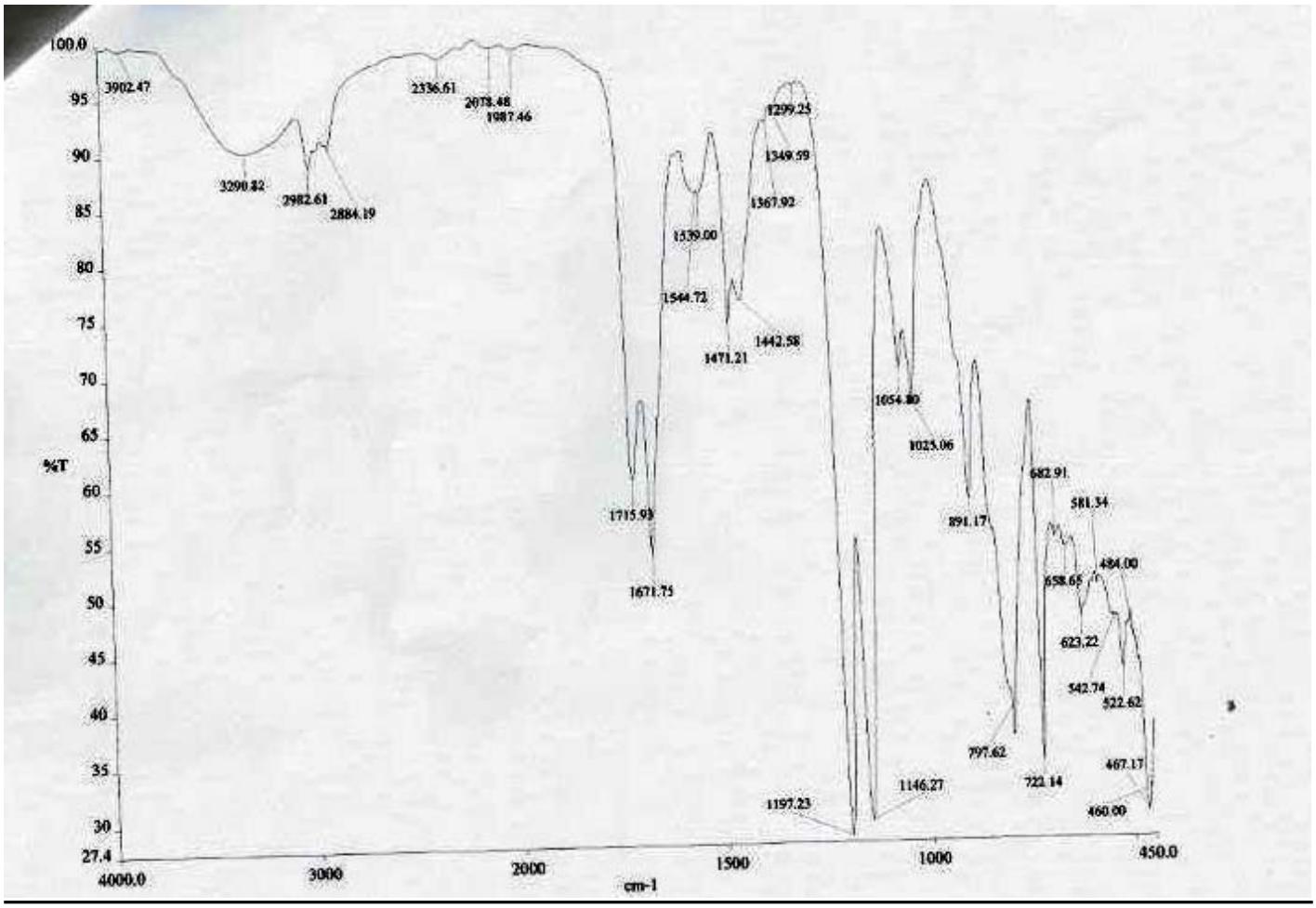
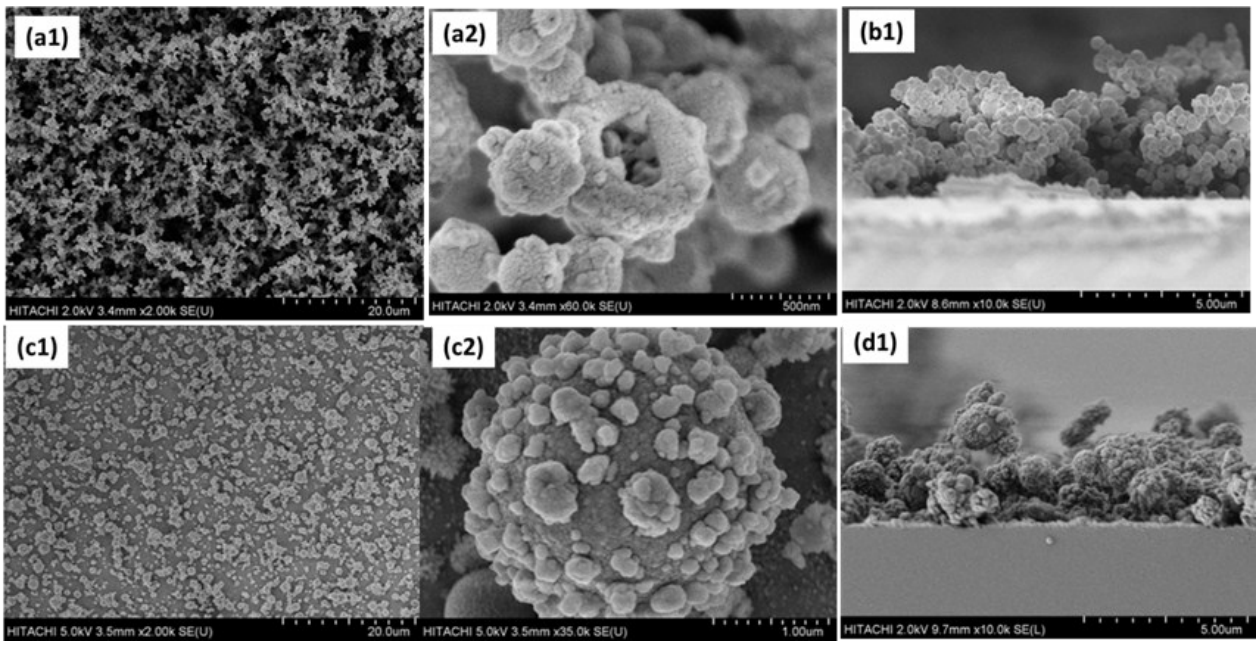
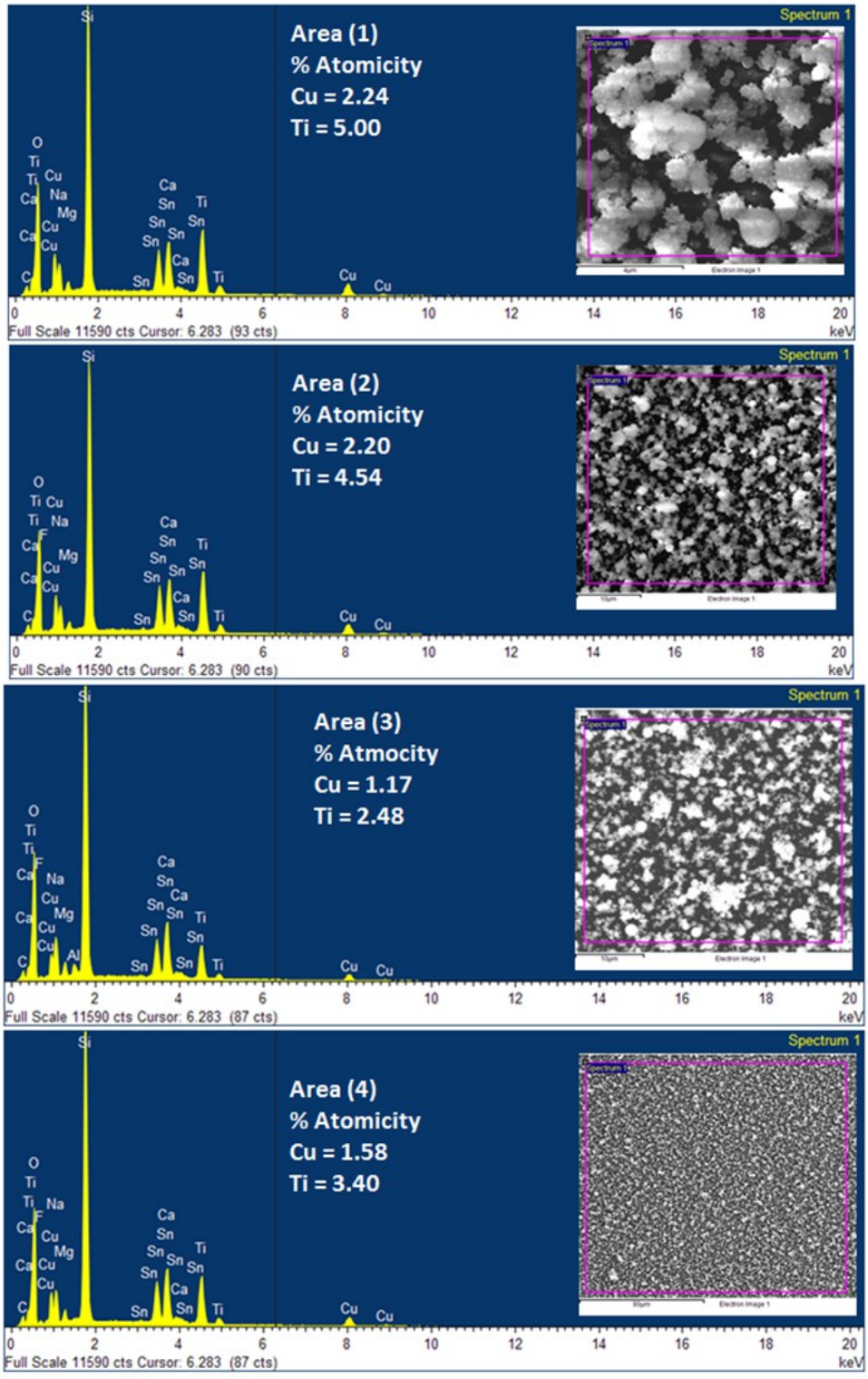


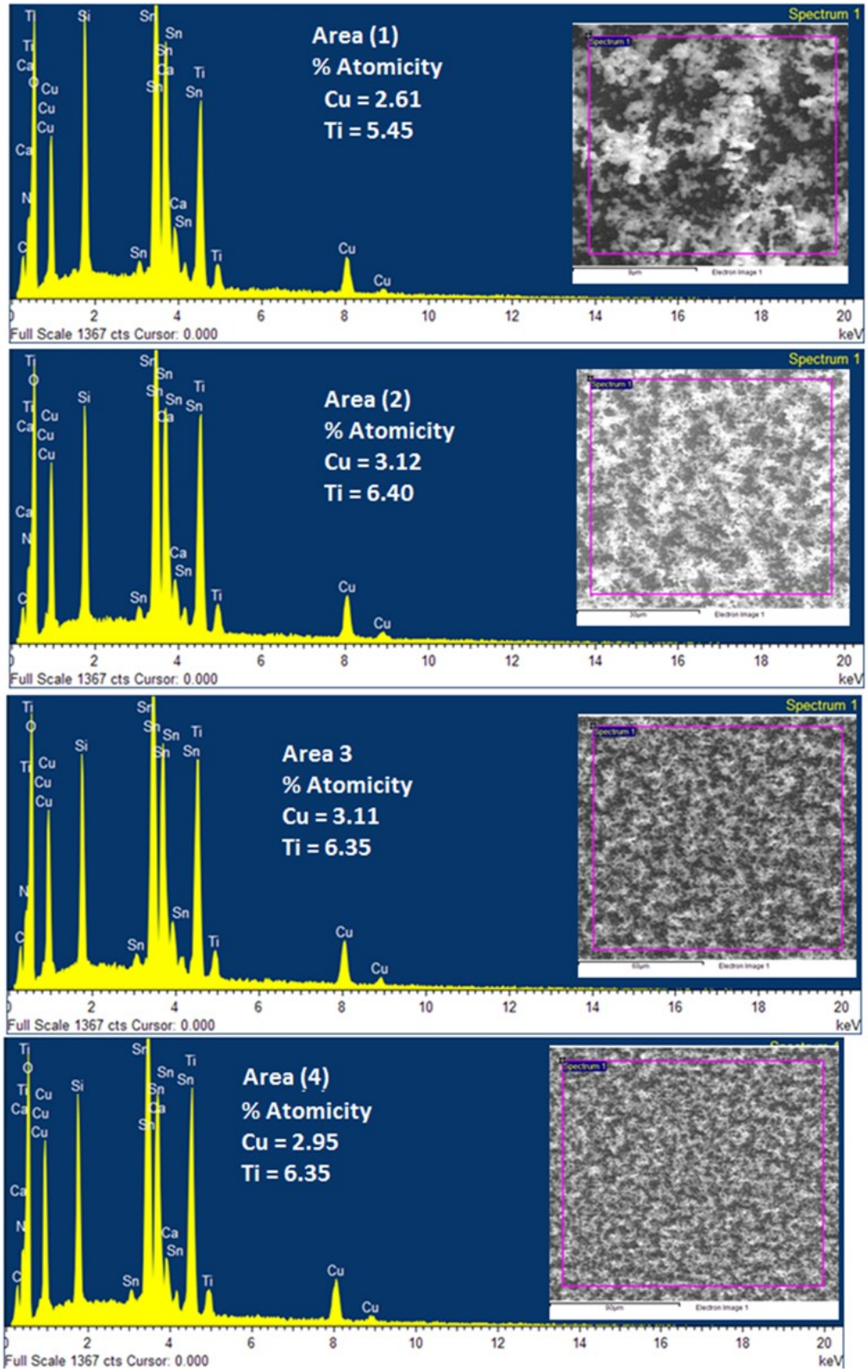
SI. Figure 1: ATR-FTIR spectrum of complex $[Cu_2Ti_4(O)_2(OH)_4(TFA)_8(THF)_6]\cdot THF$ (**1**)



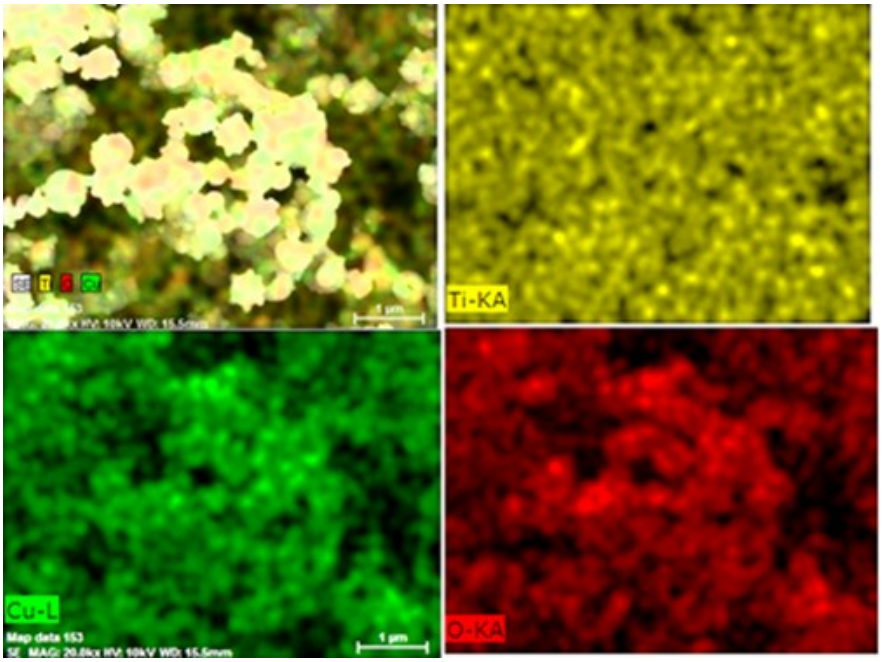
SI. Figure 2: (**a1**), (**a2**), (**c1**) and (**c2**) show surface ; (**b1**) and (**d1**) indicate the cross section SEM images of CuO-2TiO_2 composite thin films deposited on FTO glass substrate at 550 °C from solution of precursor (**1**) in (**a, b**) ethanol and (**c, d**) methanol and respectively.



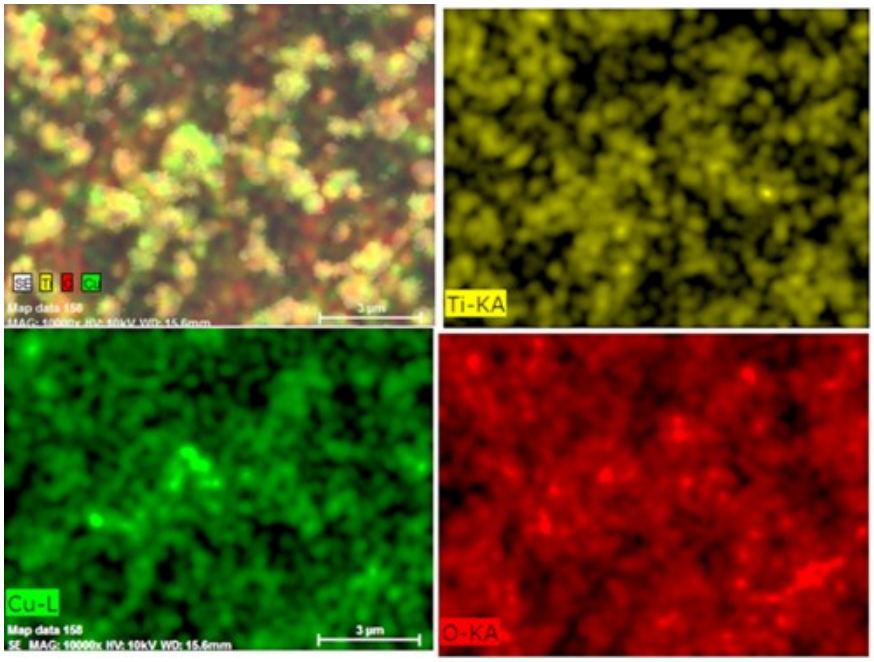
SI. Figure 3a: EDX spectrum recorded from different areas of $CuO\text{-}2TiO_2$ composite oxide film deposited from methanol solution of (**1**) on FTO substrate at 550 ˚C in air atmosphere.



SI. Figure 3b: EDX spectrum recorded from different areas of CuO-2TiO_2 composite oxide film deposited from ethanol solution of (**1**) on FTO substrate at 550 ˚C in air atmosphere.



SI. Figure 4a: EDX Elemental map showing the distribution of Cu, Ti and O atoms in CuO–2TiO_2 composite thin film deposited from ethanol solution of precursor (**1**).

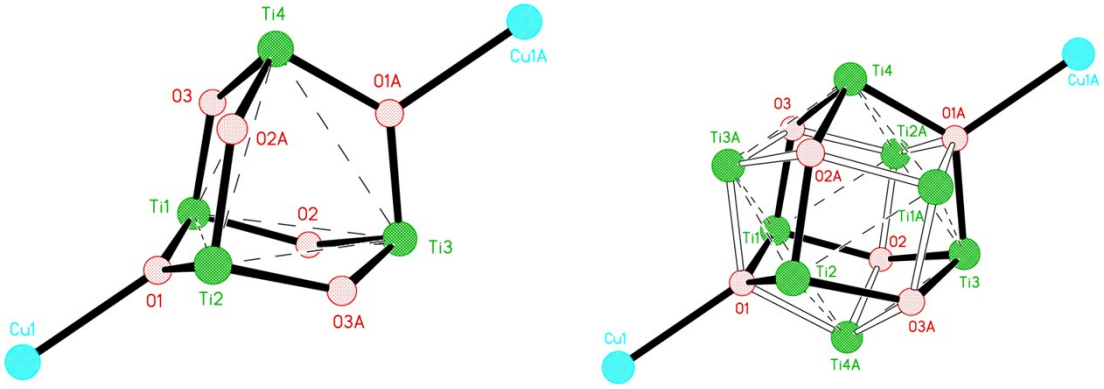


SI. Figure 4b: EDX Elemental map showing distribution of Cu, Ti and O atoms in CuO–2TiO_2 composite thin film deposited from methanol solution of precursor (**1**).

X-ray Crystallography of $[Cu_2Ti_4(O)_2(OH)_4(CF_3COO)_8(THF)_6]\cdot THF$ (1)

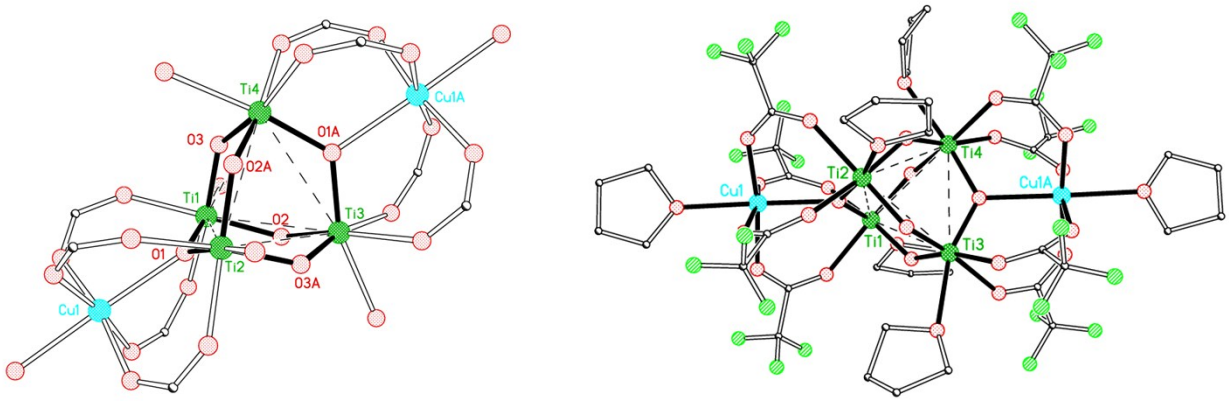
The structure was refined in space group *Pbca* with a disorder about the centre of symmetry which was not reduced by reducing the symmetry of the system to $Pca2_1$ or $P2_12_12_1$.

The core of the molecule consists of a tetrahedron of Ti(II) ions. Each edge of the tetrahedron is bridged by an oxygen atom, generating a Ti_4O_6 adamantane cage. Four of the bridging species are hydroxo ions; the remaining two are oxo ions which are also coordinated to Cu(II) ions. The disorder arises from Ti ions occupying alternative sites, generating an overlapping adamantine with the oxygen atoms in the same positions.



SI. Figure 5: Left $Cu_2Ti_4O_6$ adamantane core, lines show the "tetrahedron" of Ti ions; right core showing disorder of the Ti ions, dashed lines show the "cube" of 50% occupancy Ti ions.

Four trifluoroacetate ions are bonded to each copper ion, each bridging to a titanium ion. All of the metal ions are six-coordinate, the last binding site being filled by one THF ligand for each metal ion. There is also a (disordered) non-coordinated THF solvate molecule in the lattice.



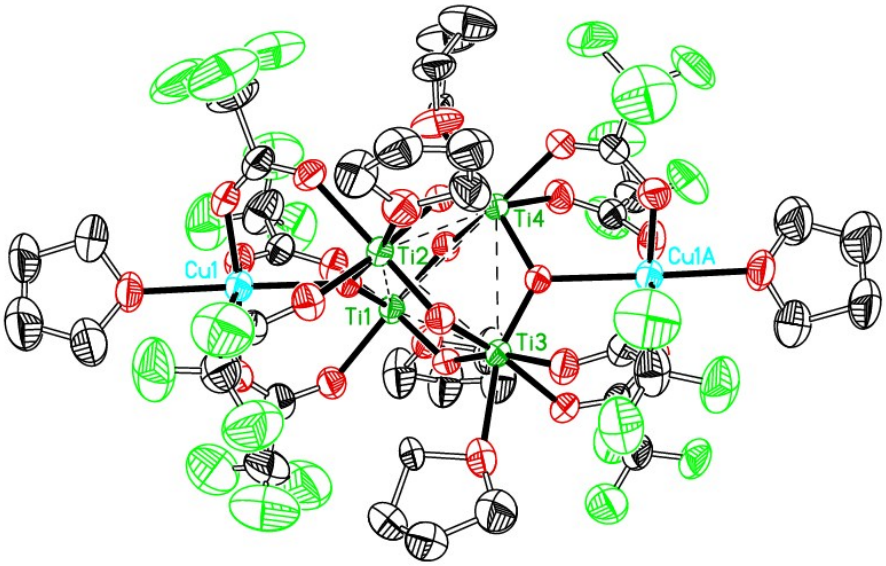
SI. Figure 6: *Core of the $[Cu_2Ti_4(O)_2(OH)_4(CF_3COO)_8(THF)_6]$ molecule. CF_3COO^- ions are*

represented by OCO links; THF molecules by terminal O atoms. Bold bonds highlight the $Ti_4O_2(OH)_4$ adamantane core; right complete molecule, disorder and H atoms omitted for clarity.

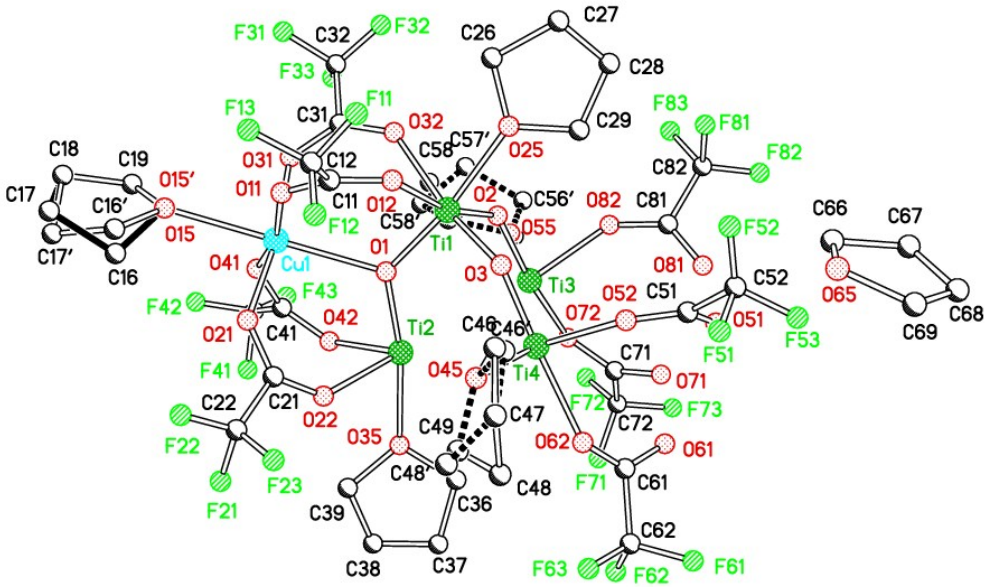
The copper, hydroxo and oxo ions are refined with full occupancy. The carbon atoms of the THF molecule coordinated to copper and those coordinated to Ti3 and Ti4 were disordered and were refined with equal occupancy of two overlapping positions. The titanium ions and their CF_3COO^- and

THF ligands are disordered about the centre of symmetry and were refined with 50% occupancy.

The extensive disorder results in a low data:parameter ratio in the refinement.



SI. Figure 7: *$[Cu_2Ti_4(O)_2(OH)_4(CF_3COO)_8(THF)_6]$ molecule50% displacement ellipsoids. Disorder and*
H-atoms omitted for clarity, dashed lines highlight the Ti_4 tetrahedron.



SI. Figure 8: *Fig. Independent atoms – showing labelling and including disorder but not inversion symmetry*

Crystal data

$C_{40}H_{52}Cu_2F_{24}O_{28}Ti_4 \cdot C_4H_8O$	D_x = 1.769 Mg m^{-3}
M_r = 1827.60	Mo $K\alpha$ radiation, λ = 0.71073 Å
Orthorhombic, *Pbca*	Cell parameters from 4831 reflections
a = 18.8071 (11) Å	θ = 2.2–20.4°
b = 17.3656 (10) Å	μ = 1.20 mm^{-1}
c = 21.0146 (12) Å	T = 150 K
V = 6863.3 (7) Å^3	Irreg, blue
Z = 4	0.43 × 0.32 × 0.24 mm
F(000) = 3672	

Data collection

Bruker APEX 2 CCD diffractometer	4097 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.101
ω rotation with narrow frames scans	θ_{max} = 26.5°, θ_{min} = 1.9°
Absorption correction: multi-scan *SADABS* v2012/1, (Krause et al., 2015)	h = -23→23
T_{min} = 0.592, T_{max} = 0.745	k = -21→21
59386 measured reflections	l = -26→26
7057 independent reflections	

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Secondary atom site location: diff
$R[F^2 > 2\sigma(F^2)] = 0.067$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.217$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.1115P)^2 + 12.7671P]$ where $P = (F_o^2 + 2F_c^2)/3$
7057 reflections	$(\Delta/\sigma)_{max} = 0.001$
910 parameters	$\Delta\rangle_{max} = 0.65$ e Å^{-3}
1810 restraints	$\Delta\rangle_{min} = -0.67$ e Å^{-3}

Computer Programs Used:

Data collection: *APEX2* v.2010.1-2 (Bruker Nonius, 2010); cell refinement: *SAINT* v.7.68a (Bruker, 2010); data reduction: *SAINT* v.7.68a (Bruker, 2010); program(s) used to solve structure: SHELXT (Sheldrick 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: Bruker *SHELXTL*, *Mercury* (Macrae at al., 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.58852 (4)	0.33059 (4)	0.62937 (3)	0.0446 (2)	
O15	0.6372 (3)	0.2420 (2)	0.7010 (2)	0.0672 (12)	0.5
C16	0.5952 (13)	0.1775 (11)	0.7187 (12)	0.143 (11)	0.5
H16A	0.5796	0.1478	0.6810	0.172*	0.5
H16B	0.5529	0.1934	0.7436	0.172*	0.5
C17	0.6482 (15)	0.1303 (9)	0.7603 (12)	0.140 (10)	0.5
H17A	0.6229	0.0970	0.7911	0.168*	0.5
H17B	0.6800	0.0982	0.7337	0.168*	0.5
C18	0.6860 (9)	0.1890 (6)	0.7913 (6)	0.190 (7)	0.5
H18A	0.7378	0.1794	0.7882	0.228*	0.5
H18B	0.6727	0.1909	0.8368	0.228*	0.5
C19	0.6682 (6)	0.2614 (5)	0.7604 (4)	0.122 (4)	0.5
H19A	0.6341	0.2911	0.7867	0.146*	0.5
H19B	0.7114	0.2930	0.7540	0.146*	0.5
O15'	0.6372 (3)	0.2420 (2)	0.7010 (2)	0.0672 (12)	0.5
C16'	0.6209 (13)	0.1633 (7)	0.7028 (9)	0.101 (7)	0.5

H16C	0.6565	0.1325	0.6793	0.122*	0.5
H16D	0.5730	0.1530	0.6852	0.122*	0.5
C17'	0.6240 (17)	0.1469 (15)	0.7764 (11)	0.199 (12)	0.5
H17C	0.5817	0.1672	0.7989	0.239*	0.5
H17D	0.6295	0.0914	0.7857	0.239*	0.5
C18'	0.6860 (9)	0.1890 (6)	0.7913 (6)	0.190 (7)	0.5
H18C	0.7291	0.1653	0.7727	0.228*	0.5
H18D	0.6923	0.1952	0.8378	0.228*	0.5
C19'	0.6682 (6)	0.2614 (5)	0.7604 (4)	0.122 (4)	0.5
H19C	0.6341	0.2911	0.7867	0.146*	0.5
H19D	0.7114	0.2930	0.7540	0.146*	0.5
Ti1	0.59907 (10)	0.45013 (11)	0.49293 (9)	0.0375 (4)	0.5
Ti2	0.44911 (10)	0.45252 (10)	0.57682 (9)	0.0367 (4)	0.5
Ti3	0.50852 (10)	0.61396 (10)	0.51090 (9)	0.0389 (5)	0.5
Ti4	0.44471 (11)	0.47352 (10)	0.41941 (9)	0.0399 (5)	0.5
O1	0.54034 (18)	0.42158 (18)	0.55985 (16)	0.0369 (8)	
O2	0.58593 (18)	0.55510 (19)	0.50271 (16)	0.0391 (8)	
H2	0.6291	0.5835	0.5036	0.047*	
O3	0.53502 (19)	0.44177 (19)	0.42908 (16)	0.0396 (8)	
H3	0.5529	0.4149	0.3931	0.048*	
O11	0.6376 (10)	0.2696 (11)	0.5652 (6)	0.054 (4)	0.5
O12	0.6366 (4)	0.3370 (4)	0.4756 (4)	0.0516 (19)	0.5
C11	0.6442 (7)	0.2768 (6)	0.5079 (6)	0.052 (3)	0.5
C12	0.6622 (10)	0.2046 (8)	0.4713 (8)	0.092 (5)	0.5
F11	0.7044 (9)	0.2228 (10)	0.4242 (7)	0.130 (6)	0.5
F12	0.6110 (9)	0.1667 (10)	0.4448 (9)	0.153 (6)	0.5
F13	0.7017 (10)	0.1586 (10)	0.5064 (10)	0.138 (7)	0.5
O21	0.5086 (7)	0.2612 (10)	0.6232 (8)	0.055 (4)	0.5
O22	0.4163 (4)	0.3388 (4)	0.5981 (4)	0.0486 (18)	0.5
C21	0.4458 (8)	0.2752 (8)	0.6099 (11)	0.063 (5)	0.5
C22	0.3985 (9)	0.2057 (8)	0.6088 (10)	0.111 (6)	0.5
F21	0.3438 (9)	0.2149 (9)	0.6467 (9)	0.169 (6)	0.5
F22	0.4234 (9)	0.1416 (7)	0.6242 (10)	0.167 (6)	0.5
F23	0.3676 (10)	0.1920 (11)	0.5538 (8)	0.163 (7)	0.5
O31	0.6771 (10)	0.3907 (8)	0.6452 (7)	0.052 (4)	0.5
O32	0.6900 (4)	0.4548 (5)	0.5524 (4)	0.0495 (18)	0.5
C31	0.7071 (8)	0.4344 (10)	0.6074 (8)	0.061 (4)	0.5
C32	0.7752 (8)	0.4711 (10)	0.6306 (8)	0.106 (5)	0.5
F31	0.8169 (10)	0.4185 (12)	0.6560 (10)	0.161 (8)	0.5
F32	0.8122 (9)	0.5017 (13)	0.5871 (8)	0.164 (6)	0.5
F33	0.7652 (9)	0.5219 (11)	0.6766 (9)	0.188 (6)	0.5

O41	0.5589 (16)	0.3840 (13)	0.7048 (14)	0.058 (5)	0.5
O42	0.4669 (4)	0.4584 (4)	0.6757 (4)	0.0498 (18)	0.5
C41	0.5106 (7)	0.4310 (7)	0.7145 (6)	0.049 (3)	0.5
C42	0.5081 (10)	0.4624 (10)	0.7811 (7)	0.069 (4)	0.5
F41	0.4408 (8)	0.4547 (10)	0.7951 (10)	0.123 (6)	0.5
F42	0.5268 (10)	0.4121 (10)	0.8230 (8)	0.118 (6)	0.5
F43	0.5189 (10)	0.5352 (9)	0.7907 (10)	0.134 (6)	0.5
O51	0.4458 (19)	0.6159 (12)	0.2925 (14)	0.065 (6)	0.5
O52	0.4640 (5)	0.4917 (4)	0.3219 (4)	0.056 (2)	0.5
C51	0.4641 (7)	0.5485 (7)	0.2846 (5)	0.048 (3)	0.5
C52	0.4871 (8)	0.5289 (10)	0.2176 (6)	0.056 (4)	0.5
F51	0.4486 (8)	0.4664 (10)	0.2052 (10)	0.119 (5)	0.5
F52	0.5496 (6)	0.5085 (9)	0.2050 (7)	0.093 (4)	0.5
F53	0.4492 (7)	0.5675 (10)	0.1758 (7)	0.088 (4)	0.5
O61	0.3170 (9)	0.6237 (7)	0.3729 (7)	0.049 (4)	0.5
O62	0.3373 (4)	0.4966 (4)	0.3922 (4)	0.0541 (19)	0.5
C61	0.3001 (7)	0.5558 (8)	0.3828 (9)	0.050 (4)	0.5
C62	0.2210 (6)	0.5394 (7)	0.3768 (6)	0.065 (3)	0.5
F61	0.1987 (7)	0.5628 (10)	0.3197 (5)	0.094 (4)	0.5
F62	0.1841 (6)	0.5741 (9)	0.4200 (6)	0.132 (4)	0.5
F63	0.2076 (6)	0.4650 (6)	0.3827 (8)	0.101 (4)	0.5
O71	0.3821 (9)	0.7412 (11)	0.4378 (5)	0.044 (3)	0.5
O72	0.4345 (4)	0.7023 (4)	0.5274 (3)	0.0472 (17)	0.5
C71	0.3896 (6)	0.7397 (7)	0.4954 (5)	0.048 (3)	0.5
C72	0.3446 (8)	0.7972 (8)	0.5328 (6)	0.070 (4)	0.5
F71	0.2832 (8)	0.7667 (11)	0.5472 (8)	0.131 (5)	0.5
F72	0.3760 (7)	0.8192 (8)	0.5842 (5)	0.089 (4)	0.5
F73	0.3301 (8)	0.8590 (7)	0.4979 (7)	0.092 (4)	0.5
O81	0.5034 (6)	0.7247 (10)	0.3616 (7)	0.049 (3)	0.5
O82	0.5600 (4)	0.6983 (4)	0.4547 (4)	0.0498 (18)	0.5
C81	0.5532 (7)	0.7281 (9)	0.3999 (8)	0.048 (4)	0.5
C82	0.6136 (6)	0.7789 (7)	0.3790 (6)	0.061 (3)	0.5
F81	0.6587 (6)	0.7330 (7)	0.3441 (6)	0.108 (3)	0.5
F82	0.5985 (5)	0.8335 (6)	0.3405 (5)	0.073 (3)	0.5
F83	0.6587 (6)	0.7981 (9)	0.4245 (6)	0.093 (4)	0.5
O25	0.6795 (6)	0.4750 (8)	0.4220 (6)	0.051 (3)	0.5
C26	0.7526 (8)	0.4609 (11)	0.4233 (8)	0.087 (6)	0.5
H26A	0.7623	0.4051	0.4269	0.105*	0.5
H26B	0.7751	0.4876	0.4597	0.105*	0.5
C27	0.7811 (9)	0.4927 (13)	0.3600 (10)	0.093 (7)	0.5
H27A	0.8292	0.5146	0.3655	0.111*	0.5

H27B	0.7832	0.4515	0.3274	0.111*	0.5
C28	0.7325 (11)	0.5500 (11)	0.3421 (8)	0.083 (6)	0.5
H28A	0.7232	0.5476	0.2957	0.099*	0.5
H28B	0.7516	0.6017	0.3524	0.099*	0.5
C29	0.6670 (10)	0.5357 (16)	0.3777 (13)	0.074 (7)	0.5
H29A	0.6524	0.5830	0.4005	0.088*	0.5
H29B	0.6283	0.5211	0.3481	0.088*	0.5
O35	0.3437 (6)	0.4740 (8)	0.6090 (7)	0.056 (3)	0.5
C36	0.2965 (9)	0.5200 (14)	0.5726 (10)	0.068 (5)	0.5
H36A	0.2937	0.5004	0.5284	0.082*	0.5
H36B	0.3134	0.5739	0.5714	0.082*	0.5
C37	0.2239 (8)	0.5158 (10)	0.6041 (10)	0.074 (4)	0.5
H37A	0.2070	0.5680	0.6153	0.089*	0.5
H37B	0.1889	0.4918	0.5750	0.089*	0.5
C38	0.2324 (8)	0.4708 (11)	0.6591 (8)	0.071 (4)	0.5
H38A	0.1947	0.4311	0.6613	0.086*	0.5
H38B	0.2289	0.5036	0.6975	0.086*	0.5
C39	0.3021 (8)	0.4344 (10)	0.6561 (8)	0.072 (4)	0.5
H39A	0.3258	0.4375	0.6981	0.086*	0.5
H39B	0.2970	0.3795	0.6445	0.086*	0.5
O45	0.4264 (6)	0.3420 (7)	0.4065 (7)	0.086 (3)	0.25
C46	0.4585 (14)	0.305 (3)	0.3548 (17)	0.051 (6)	0.25
H46A	0.4993	0.2730	0.3688	0.061*	0.25
H46B	0.4750	0.3425	0.3226	0.061*	0.25
C47	0.3968 (10)	0.2537 (13)	0.3283 (9)	0.107 (8)	0.25
H47A	0.3957	0.2549	0.2812	0.128*	0.25
H47B	0.4018	0.1996	0.3426	0.128*	0.25
C48	0.3342 (11)	0.289 (3)	0.3547 (12)	0.103 (10)	0.25
H48A	0.2947	0.2510	0.3571	0.124*	0.25
H48B	0.3188	0.3332	0.3289	0.124*	0.25
C49	0.3561 (6)	0.3127 (7)	0.4178 (6)	0.068 (3)	0.25
H49A	0.3243	0.3532	0.4348	0.082*	0.25
H49B	0.3569	0.2687	0.4478	0.082*	0.25
O45'	0.4264 (6)	0.3420 (7)	0.4065 (7)	0.086 (3)	0.25
C46'	0.454 (2)	0.313 (3)	0.350 (2)	0.077 (16)	0.25
H46C	0.5005	0.2873	0.3575	0.093*	0.25
H46D	0.4604	0.3542	0.3181	0.093*	0.25
C47'	0.3968 (10)	0.2537 (13)	0.3283 (9)	0.107 (8)	0.25
H47C	0.3690	0.2744	0.2921	0.128*	0.25
H47D	0.4194	0.2048	0.3149	0.128*	0.25
C48'	0.352 (2)	0.2415 (17)	0.3820 (16)	0.107 (12)	0.25

H48C	0.3695	0.1977	0.4078	0.129*	0.25
H48D	0.3027	0.2309	0.3685	0.129*	0.25
C49'	0.3561 (6)	0.3127 (7)	0.4178 (6)	0.068 (3)	0.25
H49C	0.3197	0.3497	0.4028	0.082*	0.25
H49D	0.3485	0.3029	0.4637	0.082*	0.25
O55	0.5625 (6)	0.6941 (6)	0.5819 (5)	0.072 (3)	0.25
C56	0.557 (2)	0.7610 (12)	0.6216 (12)	0.090 (7)	0.25
H56A	0.5070	0.7776	0.6260	0.108*	0.25
H56B	0.5853	0.8041	0.6040	0.108*	0.25
C57	0.5876 (19)	0.7343 (17)	0.6864 (11)	0.078 (7)	0.25
H57A	0.6146	0.7761	0.7074	0.094*	0.25
H57B	0.5492	0.7168	0.7153	0.094*	0.25
C58	0.6335 (16)	0.6716 (15)	0.6692 (13)	0.078 (7)	0.25
H58A	0.6440	0.6377	0.7059	0.093*	0.25
H58B	0.6784	0.6897	0.6499	0.093*	0.25
C59	0.5872 (8)	0.6340 (6)	0.6226 (6)	0.055 (3)	0.25
H59A	0.6140	0.5950	0.5980	0.065*	0.25
H59B	0.5468	0.6084	0.6441	0.065*	0.25
O55'	0.5625 (6)	0.6941 (6)	0.5819 (5)	0.072 (3)	0.25
C56'	0.5985 (19)	0.7624 (11)	0.6052 (14)	0.086 (7)	0.25
H56C	0.5637	0.8004	0.6214	0.103*	0.25
H56D	0.6268	0.7867	0.5710	0.103*	0.25
C57'	0.6476 (18)	0.7337 (17)	0.6598 (16)	0.085 (8)	0.25
H57C	0.6950	0.7186	0.6435	0.102*	0.25
H57D	0.6534	0.7733	0.6932	0.102*	0.25
C58'	0.6089 (18)	0.6687 (14)	0.6827 (9)	0.077 (7)	0.25
H58C	0.5674	0.6844	0.7087	0.092*	0.25
H58D	0.6395	0.6336	0.7078	0.092*	0.25
C59'	0.5872 (8)	0.6340 (6)	0.6226 (6)	0.055 (3)	0.25
H59C	0.6280	0.6071	0.6028	0.065*	0.25
H59D	0.5488	0.5960	0.6300	0.065*	0.25
O65	0.5058 (7)	0.3627 (7)	0.0252 (5)	0.100 (4)	0.5
C66	0.5287 (11)	0.4280 (10)	0.0599 (9)	0.099 (5)	0.5
H66A	0.5801	0.4241	0.0694	0.118*	0.5
H66B	0.5024	0.4316	0.1007	0.118*	0.5
C67	0.514 (3)	0.496 (2)	0.020 (2)	0.20 (2)	0.5
H67A	0.4925	0.5366	0.0469	0.244*	0.5
H67B	0.5598	0.5161	0.0034	0.244*	0.5
C68	0.4707 (16)	0.4790 (16)	-0.0283 (13)	0.113 (7)	0.5
H68A	0.4908	0.4968	-0.0693	0.136*	0.5
H68B	0.4234	0.5028	-0.0222	0.136*	0.5

C69	0.4661 (12)	0.3951 (12)	-0.0263 (9)	0.111 (6)	0.5
H69A	0.4156	0.3798	-0.0220	0.133*	0.5
H69B	0.4842	0.3739	-0.0669	0.133*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0525 (4)	0.0366 (4)	0.0447 (4)	0.0027 (3)	-0.0052 (3)	0.0041 (3)
O15	0.103 (3)	0.046 (2)	0.053 (2)	0.006 (2)	-0.018 (2)	0.0118 (19)
C16	0.184 (15)	0.100 (11)	0.145 (17)	-0.041 (11)	-0.078 (13)	0.069 (12)
C17	0.21 (2)	0.078 (8)	0.132 (16)	-0.006 (8)	-0.090 (16)	0.045 (8)
C18	0.302 (15)	0.102 (6)	0.166 (9)	-0.025 (7)	-0.134 (10)	0.048 (6)
C19	0.188 (10)	0.085 (5)	0.093 (5)	-0.002 (5)	-0.060 (6)	0.014 (4)
O15'	0.103 (3)	0.046 (2)	0.053 (2)	0.006 (2)	-0.018 (2)	0.0118 (19)
C16'	0.149 (16)	0.040 (5)	0.115 (11)	0.011 (6)	-0.065 (11)	0.016 (6)
C17'	0.32 (2)	0.148 (15)	0.127 (13)	-0.083 (16)	-0.094 (13)	0.056 (11)
C18'	0.302 (15)	0.102 (6)	0.166 (9)	-0.025 (7)	-0.134 (10)	0.048 (6)
C19'	0.188 (10)	0.085 (5)	0.093 (5)	-0.002 (5)	-0.060 (6)	0.014 (4)
Ti1	0.0407 (10)	0.0338 (9)	0.0381 (10)	0.0036 (8)	-0.0018 (8)	0.0036 (8)
Ti2	0.0387 (10)	0.0322 (9)	0.0392 (10)	0.0006 (8)	-0.0019 (8)	0.0044 (8)
Ti3	0.0496 (11)	0.0270 (9)	0.0401 (10)	-0.0007 (8)	-0.0103 (8)	0.0011 (8)
Ti4	0.0525 (11)	0.0275 (9)	0.0398 (10)	-0.0017 (8)	-0.0157 (9)	-0.0005 (8)
O1	0.0431 (18)	0.0302 (16)	0.0373 (18)	0.0013 (14)	-0.0062 (14)	0.0008 (14)
O2	0.0401 (19)	0.0332 (17)	0.044 (2)	-0.0044 (14)	-0.0068 (15)	0.0012 (15)
O3	0.049 (2)	0.0345 (18)	0.0352 (18)	0.0045 (15)	-0.0036 (15)	-0.0036 (15)
O11	0.066 (10)	0.038 (6)	0.058 (5)	0.006 (6)	0.000 (4)	0.004 (4)
O12	0.062 (5)	0.041 (3)	0.052 (4)	0.007 (3)	0.003 (3)	0.006 (3)
C11	0.060 (8)	0.038 (5)	0.060 (5)	0.004 (5)	-0.004 (5)	0.003 (4)
C12	0.131 (11)	0.050 (7)	0.094 (8)	0.014 (6)	0.024 (7)	-0.010 (6)
F11	0.168 (12)	0.106 (9)	0.117 (9)	0.018 (8)	0.043 (8)	-0.007 (7)
F12	0.167 (11)	0.122 (10)	0.170 (14)	-0.013 (7)	0.007 (9)	-0.047 (10)
F13	0.182 (14)	0.089 (9)	0.143 (10)	0.049 (9)	0.003 (9)	-0.009 (7)
O21	0.065 (5)	0.035 (6)	0.063 (8)	-0.001 (4)	-0.006 (5)	0.015 (5)
O22	0.046 (4)	0.038 (3)	0.062 (5)	-0.007 (3)	-0.001 (3)	0.008 (3)
C21	0.068 (6)	0.035 (5)	0.084 (12)	-0.004 (4)	-0.014 (6)	0.012 (5)
C22	0.105 (9)	0.056 (6)	0.171 (14)	-0.035 (6)	-0.014 (8)	0.006 (7)
F21	0.155 (10)	0.116 (10)	0.234 (15)	-0.056 (9)	0.030 (10)	-0.001 (10)
F22	0.149 (11)	0.059 (6)	0.294 (18)	-0.034 (6)	-0.033 (11)	0.023 (8)
F23	0.171 (14)	0.118 (10)	0.198 (13)	-0.080 (10)	-0.031 (9)	-0.009 (8)
O31	0.058 (6)	0.053 (6)	0.046 (6)	0.001 (5)	-0.013 (4)	0.002 (5)
O32	0.043 (4)	0.055 (4)	0.051 (4)	-0.003 (3)	-0.004 (3)	0.011 (3)
C31	0.062 (7)	0.062 (9)	0.058 (6)	0.002 (6)	-0.010 (5)	0.011 (5)

C32	0.083 (8)	0.121 (11)	0.114 (10)	-0.028 (7)	-0.036 (7)	0.008 (7)
F31	0.101 (10)	0.171 (12)	0.211 (17)	-0.011 (8)	-0.059 (10)	0.029 (11)
F32	0.122 (11)	0.210 (15)	0.159 (12)	-0.067 (11)	-0.011 (8)	0.025 (10)
F33	0.199 (13)	0.181 (12)	0.184 (11)	-0.043 (10)	-0.037 (10)	-0.057 (9)
O41	0.062 (8)	0.061 (8)	0.051 (8)	0.014 (6)	-0.010 (5)	0.004 (5)
O42	0.053 (4)	0.052 (4)	0.044 (4)	0.006 (3)	-0.001 (3)	0.001 (3)
C41	0.050 (6)	0.049 (6)	0.048 (5)	-0.004 (5)	-0.004 (4)	0.011 (4)
C42	0.083 (9)	0.074 (7)	0.050 (6)	-0.004 (6)	0.006 (5)	0.001 (5)
F41	0.103 (7)	0.155 (13)	0.110 (9)	-0.025 (7)	0.020 (6)	-0.004 (9)
F42	0.182 (14)	0.114 (9)	0.057 (6)	0.025 (9)	0.006 (8)	0.011 (6)
F43	0.163 (15)	0.097 (7)	0.141 (11)	-0.018 (8)	-0.007 (11)	-0.019 (6)
O51	0.105 (15)	0.049 (6)	0.040 (8)	0.020 (7)	-0.003 (7)	0.005 (5)
O52	0.077 (5)	0.050 (4)	0.040 (4)	0.003 (4)	-0.012 (3)	0.000 (3)
C51	0.058 (8)	0.045 (5)	0.042 (5)	-0.002 (5)	-0.010 (4)	0.002 (4)
C52	0.053 (6)	0.069 (8)	0.046 (6)	0.000 (5)	-0.004 (4)	-0.007 (5)
F51	0.094 (8)	0.131 (8)	0.131 (10)	-0.030 (6)	0.005 (7)	-0.035 (6)
F52	0.066 (5)	0.135 (11)	0.079 (7)	0.010 (6)	0.000 (5)	-0.015 (8)
F53	0.081 (7)	0.135 (9)	0.049 (5)	0.020 (6)	-0.017 (5)	-0.014 (5)
O61	0.044 (5)	0.045 (5)	0.058 (9)	0.003 (4)	-0.006 (6)	-0.002 (5)
O62	0.054 (4)	0.046 (4)	0.063 (5)	-0.007 (3)	-0.024 (3)	0.009 (3)
C61	0.047 (5)	0.047 (5)	0.056 (9)	-0.005 (4)	-0.017 (5)	0.006 (5)
C62	0.046 (6)	0.076 (6)	0.073 (7)	-0.008 (4)	-0.020 (4)	0.018 (5)
F61	0.058 (6)	0.138 (10)	0.086 (6)	-0.006 (6)	-0.035 (5)	0.016 (6)
F62	0.099 (7)	0.154 (9)	0.141 (8)	0.003 (7)	0.040 (6)	-0.010 (7)
F63	0.061 (6)	0.086 (5)	0.156 (11)	-0.028 (4)	-0.012 (6)	0.013 (6)
O71	0.049 (8)	0.035 (6)	0.050 (4)	-0.003 (5)	-0.005 (4)	0.003 (4)
O72	0.062 (4)	0.038 (4)	0.041 (4)	0.008 (3)	-0.004 (3)	0.002 (3)
C71	0.054 (6)	0.040 (5)	0.050 (5)	0.001 (5)	0.000 (4)	0.004 (4)
C72	0.087 (7)	0.066 (7)	0.056 (6)	0.033 (5)	0.006 (5)	0.000 (5)
F71	0.114 (7)	0.155 (11)	0.123 (11)	-0.004 (7)	0.026 (7)	-0.017 (9)
F72	0.113 (8)	0.094 (7)	0.059 (5)	0.039 (6)	0.003 (5)	-0.013 (5)
F73	0.136 (10)	0.058 (6)	0.083 (6)	0.043 (6)	-0.003 (6)	-0.007 (4)
O81	0.051 (6)	0.043 (7)	0.054 (7)	0.004 (4)	0.002 (5)	0.005 (5)
O82	0.053 (4)	0.037 (4)	0.060 (4)	-0.008 (3)	-0.008 (3)	0.010 (3)
C81	0.051 (6)	0.035 (7)	0.059 (6)	-0.002 (5)	-0.003 (4)	0.015 (5)
C82	0.050 (5)	0.061 (6)	0.072 (6)	-0.012 (4)	0.001 (4)	0.030 (5)
F81	0.093 (6)	0.105 (7)	0.125 (7)	0.010 (6)	0.040 (5)	0.017 (6)
F82	0.075 (6)	0.060 (5)	0.085 (6)	-0.014 (4)	0.004 (4)	0.036 (4)
F83	0.077 (6)	0.106 (8)	0.097 (6)	-0.033 (5)	-0.010 (5)	0.028 (6)
O25	0.053 (5)	0.051 (5)	0.050 (5)	0.000 (4)	0.010 (4)	0.005 (4)
C26	0.055 (6)	0.118 (13)	0.089 (9)	0.017 (7)	0.029 (6)	0.049 (9)

C27	0.074 (8)	0.108 (14)	0.096 (12)	0.020 (8)	0.040 (8)	0.042 (10)
C28	0.075 (10)	0.094 (11)	0.080 (9)	0.012 (8)	0.028 (8)	0.027 (9)
C29	0.070 (9)	0.076 (11)	0.075 (10)	0.019 (8)	0.025 (7)	0.029 (9)
O35	0.042 (4)	0.059 (6)	0.067 (7)	0.001 (4)	0.004 (4)	0.002 (5)
C36	0.052 (7)	0.076 (10)	0.076 (8)	0.009 (7)	-0.008 (6)	-0.001 (7)
C37	0.053 (7)	0.067 (9)	0.103 (11)	0.006 (6)	-0.001 (6)	-0.006 (8)
C38	0.043 (7)	0.069 (10)	0.102 (9)	0.003 (6)	0.007 (6)	-0.005 (7)
C39	0.048 (7)	0.076 (8)	0.092 (9)	0.012 (6)	0.019 (6)	0.014 (7)
O45	0.094 (6)	0.063 (6)	0.101 (7)	-0.031 (5)	0.009 (5)	-0.038 (5)
C46	0.082 (9)	0.025 (9)	0.045 (9)	-0.009 (7)	-0.010 (7)	0.006 (7)
C47	0.103 (9)	0.111 (14)	0.107 (11)	-0.051 (9)	0.016 (7)	-0.058 (11)
C48	0.089 (10)	0.14 (2)	0.081 (12)	-0.034 (9)	-0.003 (7)	-0.045 (13)
C49	0.077 (6)	0.055 (7)	0.072 (7)	-0.025 (5)	-0.006 (5)	-0.015 (5)
O45'	0.094 (6)	0.063 (6)	0.101 (7)	-0.031 (5)	0.009 (5)	-0.038 (5)
C46'	0.085 (13)	0.07 (3)	0.079 (16)	-0.024 (17)	0.004 (13)	-0.027 (19)
C47'	0.103 (9)	0.111 (14)	0.107 (11)	-0.051 (9)	0.016 (7)	-0.058 (11)
C48'	0.117 (18)	0.083 (12)	0.122 (17)	-0.052 (13)	0.028 (15)	-0.047 (13)
C49'	0.077 (6)	0.055 (7)	0.072 (7)	-0.025 (5)	-0.006 (5)	-0.015 (5)
O55	0.094 (6)	0.059 (4)	0.063 (4)	0.003 (4)	-0.031 (4)	0.012 (3)
C56	0.109 (14)	0.074 (8)	0.087 (9)	0.006 (8)	-0.020 (9)	-0.003 (6)
C57	0.087 (13)	0.075 (10)	0.073 (9)	-0.012 (9)	-0.014 (8)	0.000 (7)
C58	0.086 (11)	0.081 (10)	0.066 (10)	-0.006 (8)	-0.028 (8)	-0.001 (7)
C59	0.071 (7)	0.045 (4)	0.047 (5)	-0.002 (4)	-0.027 (5)	0.012 (4)
O55'	0.094 (6)	0.059 (4)	0.063 (4)	0.003 (4)	-0.031 (4)	0.012 (3)
C56'	0.103 (13)	0.070 (7)	0.085 (11)	-0.009 (7)	-0.024 (10)	0.010 (7)
C57'	0.095 (12)	0.081 (10)	0.080 (11)	-0.012 (9)	-0.028 (9)	0.008 (8)
C58'	0.091 (13)	0.077 (9)	0.062 (7)	-0.010 (9)	-0.025 (7)	0.003 (6)
C59'	0.071 (7)	0.045 (4)	0.047 (5)	-0.002 (4)	-0.027 (5)	0.012 (4)
O65	0.130 (10)	0.091 (7)	0.080 (7)	-0.011 (6)	-0.020 (6)	-0.021 (5)
C66	0.113 (12)	0.091 (8)	0.092 (9)	-0.005 (8)	-0.026 (9)	-0.029 (7)
C67	0.32 (4)	0.103 (11)	0.19 (2)	-0.043 (11)	-0.16 (3)	0.005 (10)
C68	0.135 (17)	0.111 (11)	0.094 (12)	-0.015 (10)	-0.030 (12)	-0.013 (9)
C69	0.134 (14)	0.113 (10)	0.086 (9)	-0.017 (10)	-0.033 (10)	-0.011 (8)

Geometric parameters (Å, º) for (ct)

Cu1—O41	1.92 (2)	C42—F42	1.288 (14)
Cu1—O21	1.930 (16)	C42—F43	1.297 (14)
Cu1—O11	1.947 (18)	C42—F41	1.305 (15)
Cu1—O31	1.994 (16)	O51—C51	1.231 (13)
Cu1—O1	2.335 (3)	O52—C51	1.259 (11)
Cu1—O15	2.339 (4)	C51—C52	1.512 (12)

Cu1—O15'	2.339 (4)	C52—F52	1.256 (13)
O15—C19	1.419 (8)	C52—F53	1.316 (13)
O15—C16	1.420 (14)	C52—F51	1.331 (14)
C16—C17	1.559 (16)	O61—C61	1.239 (12)
C17—C18	1.403 (15)	O62—C61	1.259 (13)
C18—C19	1.454 (10)	C61—C62	1.519 (12)
O15'—C16'	1.400 (12)	C62—F62	1.292 (13)
O15'—C19'	1.419 (8)	C62—F63	1.323 (13)
C16'—C17'	1.575 (17)	C62—F61	1.336 (12)
C17'—C18'	1.411 (17)	O71—C71	1.218 (11)
C18'—C19'	1.454 (10)	O72—C71	1.260 (11)
Ti1—O3	1.809 (4)	C71—C72	1.527 (12)
Ti1—O2	1.851 (4)	C72—F72	1.290 (13)
Ti1—O1	1.856 (4)	C72—F71	1.306 (13)
Ti1—O32	2.119 (7)	C72—F73	1.327 (12)
Ti1—O12	2.120 (7)	O81—C81	1.236 (12)
Ti1—O25	2.167 (10)	O82—C81	1.270 (13)
Ti1—Ti4	3.314 (3)	C81—C82	1.505 (12)
Ti1—Ti2	3.326 (3)	C82—F82	1.278 (11)
Ti1—Ti3	3.337 (3)	C82—F83	1.321 (12)
Ti2—O1	1.833 (4)	C82—F81	1.375 (13)
Ti2—O42	2.107 (8)	O25—C26	1.397 (13)
Ti2—O22	2.117 (7)	O25—C29	1.427 (14)
Ti2—O35	2.128 (11)	C26—C27	1.537 (14)
Ti2—Ti3	3.321 (3)	C27—C28	1.403 (15)
Ti2—Ti4	3.329 (3)	C28—C29	1.463 (15)
Ti3—O2	1.787 (4)	O35—C36	1.419 (14)
Ti3—O72	2.100 (7)	O35—C39	1.436 (13)
Ti3—O82	2.115 (7)	C36—C37	1.518 (15)
Ti3—O55	2.278 (10)	C37—C38	1.405 (15)
Ti3—Ti4	3.329 (3)	C38—C39	1.457 (14)
Ti4—O3	1.797 (4)	O45—C46	1.400 (15)
Ti4—O52	2.105 (8)	O45—C49	1.436 (11)
Ti4—O62	2.138 (8)	C46—C47	1.565 (16)
Ti4—O45	2.326 (11)	C47—C48	1.437 (17)
O11—C11	1.218 (11)	C48—C49	1.450 (16)
O12—C11	1.254 (11)	O45'—C46'	1.392 (15)
C11—C12	1.509 (12)	O45'—C49'	1.436 (11)
C12—F12	1.292 (14)	C46'—C47'	1.559 (17)
C12—F11	1.308 (14)	C47'—C48'	1.423 (17)
C12—F13	1.317 (13)	C48'—C49'	1.448 (16)

O21—C21	1.239 (12)	O55—C59	1.427 (11)
O22—C21	1.260 (13)	O55—C56	1.435 (15)
C21—C22	1.500 (13)	C56—C57	1.548 (17)
C22—F22	1.251 (13)	C57—C58	1.436 (18)
C22—F21	1.311 (15)	C58—C59	1.463 (16)
C22—F23	1.316 (14)	O55'—C59'	1.427 (11)
O31—C31	1.235 (13)	O55'—C56'	1.451 (15)
O32—C31	1.252 (13)	C56'—C57'	1.554 (18)
C31—C32	1.511 (13)	C57'—C58'	1.427 (18)
C32—F32	1.266 (14)	C58'—C59'	1.458 (16)
C32—F31	1.317 (14)	O65—C69	1.43 (2)
C32—F33	1.323 (14)	O65—C66	1.415 (18)
O41—C41	1.237 (14)	C66—C67	1.47 (4)
O42—C41	1.253 (11)	C67—C68	1.34 (3)
C41—C42	1.503 (12)	C68—C69	1.46 (3)
O41—Cu1—O21	97.5 (12)	Ti1—O1—Cu1	115.09 (17)
O41—Cu1—O11	166.6 (9)	Ti3—O2—Ti1	133.1 (2)
O21—Cu1—O11	89.0 (7)	Ti4—O3—Ti1	133.5 (2)
O41—Cu1—O31	81.5 (12)	C11—O11—Cu1	132.7 (15)
O21—Cu1—O31	171.2 (7)	C11—O12—Ti1	135.9 (7)
O11—Cu1—O31	90.3 (7)	O11—C11—O12	127.5 (13)
O41—Cu1—O1	94.4 (7)	O11—C11—C12	116.2 (13)
O21—Cu1—O1	94.5 (5)	O12—C11—C12	116.3 (11)
O11—Cu1—O1	96.8 (5)	F12—C12—F11	104.5 (15)
O31—Cu1—O1	94.3 (5)	F12—C12—F13	110.6 (14)
O41—Cu1—O15	84.3 (7)	F11—C12—F13	103.2 (15)
O21—Cu1—O15	86.4 (5)	F12—C12—C11	118.4 (14)
O11—Cu1—O15	84.4 (5)	F11—C12—C11	108.7 (13)
O31—Cu1—O15	84.8 (5)	F13—C12—C11	110.2 (13)
O1—Cu1—O15	178.50 (14)	C21—O21—Cu1	129.4 (13)
C19—O15—C16	100.7 (10)	C21—O22—Ti2	136.9 (8)
C19—O15—Cu1	124.8 (4)	O21—C21—O22	129.6 (13)
C16—O15—Cu1	118.0 (7)	O21—C21—C22	114.3 (13)
O15—C16—C17	101.9 (13)	O22—C21—C22	116.1 (11)
C18—C17—C16	101.6 (12)	F22—C22—F21	104.2 (15)
C17—C18—C19	107.8 (9)	F22—C22—F23	103.3 (15)
O15—C19—C18	106.3 (7)	F21—C22—F23	102.1 (15)
C16'—O15'—C19'	107.4 (8)	F22—C22—C21	119.4 (14)
C16'—O15'—Cu1	125.0 (7)	F21—C22—C21	111.1 (15)
C19'—O15'—Cu1	124.8 (4)	F23—C22—C21	114.9 (15)

O15'—C16'—C17'	101.2 (12)	C31—O31—Cu1	126.5 (13)
C18'—C17'—C16'	98.9 (14)	C31—O32—Ti1	137.8 (8)
C17'—C18'—C19'	99.1 (13)	O31—C31—O32	130.6 (14)
O15'—C19'—C18'	106.3 (7)	O31—C31—C32	116.0 (13)
O3—Ti1—O2	94.16 (17)	O32—C31—C32	113.3 (11)
O3—Ti1—O1	98.30 (18)	F32—C32—F31	104.9 (16)
O2—Ti1—O1	95.71 (17)	F32—C32—F33	109.0 (16)
O3—Ti1—O32	167.8 (3)	F31—C32—F33	104.5 (15)
O2—Ti1—O32	90.3 (3)	F32—C32—C31	114.2 (14)
O1—Ti1—O32	92.5 (2)	F31—C32—C31	110.1 (14)
O3—Ti1—O12	91.1 (3)	F33—C32—C31	113.4 (15)
O2—Ti1—O12	167.6 (3)	C41—O41—Cu1	132 (2)
O1—Ti1—O12	94.6 (2)	C41—O42—Ti2	136.7 (8)
O32—Ti1—O12	82.4 (3)	O41—C41—O42	128.6 (16)
O3—Ti1—O25	88.3 (4)	O41—C41—C42	114.6 (15)
O2—Ti1—O25	88.5 (4)	O42—C41—C42	116.6 (11)
O1—Ti1—O25	171.9 (3)	F42—C42—F43	120.9 (15)
O32—Ti1—O25	80.5 (4)	F42—C42—F41	92.4 (14)
O12—Ti1—O25	80.4 (4)	F43—C42—F41	102.5 (14)
O3—Ti1—Ti4	23.17 (12)	F42—C42—C41	112.4 (14)
O2—Ti1—Ti4	79.29 (12)	F43—C42—C41	119.5 (14)
O1—Ti1—Ti4	82.22 (12)	F41—C42—C41	101.6 (14)
O32—Ti1—Ti4	167.7 (2)	C51—O52—Ti4	136.3 (8)
O12—Ti1—Ti4	109.0 (2)	O51—C51—O52	131.4 (16)
O25—Ti1—Ti4	105.5 (3)	O51—C51—C52	114.8 (15)
O3—Ti1—Ti2	80.18 (13)	O52—C51—C52	113.7 (10)
O2—Ti1—Ti2	79.38 (13)	F52—C52—F53	120.7 (13)
O1—Ti1—Ti2	25.44 (11)	F52—C52—F51	103.8 (12)
O32—Ti1—Ti2	111.8 (2)	F53—C52—F51	89.3 (13)
O12—Ti1—Ti2	112.6 (2)	F52—C52—C51	122.0 (12)
O25—Ti1—Ti2	162.5 (3)	F53—C52—C51	110.6 (12)
Ti4—Ti1—Ti2	60.18 (6)	F51—C52—C51	102.1 (13)
O3—Ti1—Ti3	79.20 (12)	C61—O62—Ti4	136.1 (7)
O2—Ti1—Ti3	23.04 (11)	O61—C61—O62	131.4 (13)
O1—Ti1—Ti3	80.69 (12)	O61—C61—C62	114.5 (12)
O32—Ti1—Ti3	108.2 (2)	O62—C61—C62	113.8 (10)
O12—Ti1—Ti3	168.4 (2)	F62—C62—F63	106.7 (12)
O25—Ti1—Ti3	105.3 (3)	F62—C62—F61	108.7 (12)
Ti4—Ti1—Ti3	60.08 (5)	F63—C62—F61	108.7 (13)
Ti2—Ti1—Ti3	59.78 (6)	F62—C62—C61	112.4 (12)
O1—Ti2—O42	93.3 (2)	F63—C62—C61	111.3 (10)

O1—Ti2—O22	92.3 (2)	F61—C62—C61	108.9 (11)
O42—Ti2—O22	83.3 (3)	C71—O72—Ti3	137.1 (7)
O1—Ti2—O35	170.2 (4)	O71—C71—O72	128.2 (13)
O42—Ti2—O35	79.9 (5)	O71—C71—C72	115.7 (12)
O22—Ti2—O35	79.9 (4)	O72—C71—C72	115.7 (9)
O1—Ti2—Ti3	81.45 (12)	F72—C72—F71	109.4 (13)
O42—Ti2—Ti3	108.5 (2)	F72—C72—F73	108.5 (12)
O22—Ti2—Ti3	166.9 (3)	F71—C72—F73	105.9 (13)
O35—Ti2—Ti3	107.4 (4)	F72—C72—C71	111.8 (11)
O1—Ti2—Ti1	25.78 (11)	F71—C72—C71	110.1 (13)
O42—Ti2—Ti1	112.9 (2)	F73—C72—C71	111.0 (11)
O22—Ti2—Ti1	110.4 (2)	C81—O82—Ti3	138.0 (7)
O35—Ti2—Ti1	163.9 (3)	O81—C81—O82	130.3 (13)
Ti3—Ti2—Ti1	60.27 (6)	O81—C81—C82	114.2 (12)
O1—Ti2—Ti4	82.07 (12)	O82—C81—C82	115.4 (10)
O42—Ti2—Ti4	168.1 (2)	F82—C82—F83	114.5 (11)
O22—Ti2—Ti4	107.8 (2)	F82—C82—F81	103.3 (10)
O35—Ti2—Ti4	105.9 (4)	F83—C82—F81	97.8 (11)
Ti3—Ti2—Ti4	60.09 (5)	F82—C82—C81	116.8 (10)
Ti1—Ti2—Ti4	59.72 (6)	F83—C82—C81	114.9 (11)
O2—Ti3—O72	166.8 (3)	F81—C82—C81	106.4 (12)
O2—Ti3—O82	88.2 (3)	C26—O25—C29	107.7 (11)
O72—Ti3—O82	83.7 (3)	C26—O25—Ti1	129.7 (9)
O2—Ti3—O55	92.8 (3)	C29—O25—Ti1	118.8 (10)
O72—Ti3—O55	75.0 (3)	O25—C26—C27	105.3 (11)
O82—Ti3—O55	74.9 (4)	C28—C27—C26	105.1 (11)
O2—Ti3—Ti2	80.29 (13)	C27—C28—C29	106.9 (11)
O72—Ti3—Ti2	108.9 (2)	O25—C29—C28	108.7 (12)
O82—Ti3—Ti2	166.2 (2)	C36—O35—C39	107.4 (11)
O55—Ti3—Ti2	113.1 (3)	C36—O35—Ti2	120.7 (10)
O2—Ti3—Ti4	79.58 (13)	C39—O35—Ti2	130.0 (10)
O72—Ti3—Ti4	113.0 (2)	O35—C36—C37	107.5 (11)
O82—Ti3—Ti4	110.4 (2)	C38—C37—C36	106.5 (11)
O55—Ti3—Ti4	170.4 (2)	C37—C38—C39	107.9 (11)
Ti2—Ti3—Ti4	60.08 (6)	O35—C39—C38	108.2 (11)
O2—Ti3—Ti1	23.91 (12)	C46—O45—C49	111.3 (9)
O72—Ti3—Ti1	168.4 (2)	C46—O45—Ti4	118.5 (18)
O82—Ti3—Ti1	107.1 (2)	C49—O45—Ti4	117.7 (9)
O55—Ti3—Ti1	111.5 (3)	O45—C46—C47	102.6 (11)
Ti2—Ti3—Ti1	59.94 (6)	C48—C47—C46	103.3 (14)
Ti4—Ti3—Ti1	59.61 (6)	C47—C48—C49	104.0 (13)

O3—Ti4—O52	89.6 (3)	O45—C49—C48	102.3 (13)
O3—Ti4—O62	168.8 (3)	C46'—O45'—C49'	111.0 (10)
O52—Ti4—O62	82.8 (3)	O45'—C46'—C47'	103.3 (11)
O3—Ti4—O45	81.5 (4)	C48'—C47'—C46'	105.8 (15)
O52—Ti4—O45	93.4 (4)	C47'—C48'—C49'	104.8 (13)
O62—Ti4—O45	90.8 (4)	O45'—C49'—C48'	105.3 (13)
O3—Ti4—Ti1	23.33 (12)	C59—O55—C56	105.4 (11)
O52—Ti4—Ti1	108.7 (3)	C59—O55—Ti3	95.3 (7)
O62—Ti4—Ti1	167.4 (3)	C56—O55—Ti3	147.6 (16)
O45—Ti4—Ti1	93.7 (4)	O55—C56—C57	104.1 (13)
O3—Ti4—Ti2	80.25 (13)	C58—C57—C56	103.2 (15)
O52—Ti4—Ti2	168.4 (3)	C57—C58—C59	98.6 (15)
O62—Ti4—Ti2	108.1 (3)	O55—C59—C58	105.6 (13)
O45—Ti4—Ti2	90.7 (4)	C59'—O55'—C56'	104.1 (10)
Ti1—Ti4—Ti2	60.10 (5)	O55'—C56'—C57'	105.3 (13)
O3—Ti4—Ti3	79.56 (13)	C58'—C57'—C56'	101.6 (16)
O52—Ti4—Ti3	113.0 (2)	C57'—C58'—C59'	100.2 (16)
O62—Ti4—Ti3	111.0 (2)	O55'—C59'—C58'	108.0 (12)
O45—Ti4—Ti3	147.1 (4)	C69—O65—C66	103.5 (14)
Ti1—Ti4—Ti3	60.31 (6)	O65—C66—C67	107.2 (17)
Ti2—Ti4—Ti3	59.83 (6)	C68—C67—C66	112 (2)
Ti2—O1—Ti1	128.8 (2)	C67—C68—C69	103.4 (19)
Ti2—O1—Cu1	116.10 (17)	O65—C69—C68	112.6 (17)

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