

**Supplementary data G for**  
**{[Cu<sub>4</sub>(phen)<sub>2</sub>(μ-O<sub>2</sub>CC<sub>2</sub>H<sub>5</sub>)<sub>8</sub>](H<sub>2</sub>O)}<sub>n</sub> (VII)**

**Table G1** Atomic Coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for complex **VII**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor

	<b>x</b>	<b>y</b>	<b>z</b>	<b>U(eq)</b>
Cu(1)	32893(4)	10030.6(3)	4573.1(3)	1.97(14)
Cu(2)	8099(5)	6166.9(4)	7671(4)	66.39(16)
N(1)	3332(3)	10550(3)	6155(2)	55.4(6)
N(2)	1021(3)	8777(3)	4260(3)	56.5(7)
O(1)	5519(2)	11241.1(19)	5055(2)	53.6(5)
O(2)	4883(3)	12786(2)	5038(3)	77.4(8)
O(3)	2934(3)	10048(2)	3047(2)	66.6(6)
O(4)	2104(3)	8002(2)	2079(2)	69.1(7)
O(5)	2304(4)	5590(3)	1335(3)	94.7(10)
O(6)	1719(4)	6625(3)	-336(3)	87.6(9)
O(7)	-950(4)	6382(3)	-27(3)	94(9)
O(8)	-347(4)	5339(3)	1635(3)	91.1(10)
O(9)	4668(17)	4671(12)	4113(12)	183(5)
C(1)	2504(4)	9153(4)	2143(3)	64.2(9)
C(2)	2435(11)	9533(6)	1105(5)	121(2)
C(4)	4511(5)	11462(4)	7087(3)	68.4(10)
C(5)	2998(6)	11019(5)	8196(4)	92.6(14)
C(6)	1948(4)	9854(3)	6221(3)	55.2(7)
C(7)	1697(5)	10050(4)	7213(4)	73.7(10)
C(8)	181(6)	9281(6)	7185(5)	93.4(15)
C(9)	-1002(6)	8381(5)	6216(5)	81.8(12)
C(10)	-778(4)	8159(3)	5189(4)	64.7(9)
C(11)	694(4)	8902(3)	5193(3)	53.9(7)
C(12)	-1966(4)	7235(4)	4155(4)	73.3(11)
C(13)	-1626(5)	7101(4)	3227(4)	78.9(12)
C(14)	-0125(4)	7890(4)	3299(4)	70.8(10)

**Table G1** Atomic Coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for complex **VII**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor (cont.)

	<b>x</b>	<b>y</b>	<b>z</b>	<b>U(eq)</b>
C(15)	2107(7)	4487(6)	868(5)	91.1(14)
C(16)	1329(5)	5836(4)	-1281(4)	76.6(11)
C(17)	2230(4)	6300(3)	-2080(2)	116(8)
C(19)	4383(6)	11709(5)	8118(4)	87.5(14)
C(20)	3484(14)	4275(12)	1372(11)	114(3)
C(21)	3870(2)	4360(2)	2330(18)	225(10)
C(22)	2120(4)	7500(2)	-2211(17)	180(13)
C(23)	5848(4)	12421(3)	5133(3)	58.6(8)
C(24)	1270(4)	9630(4)	550(2)	186(16)
C(25)	7548(5)	13342(4)	5381(5)	84.7(13)
C(26)	7893(8)	14620(6)	5249(8)	137(3)

**Table G2** Bond lengths [Å] for {[Cu<sub>4</sub>(phen)<sub>2</sub>(μ-O<sub>2</sub>CC<sub>2</sub>H<sub>5</sub>)<sub>8</sub>](H<sub>2</sub>O)}<sub>n</sub> **VII**

O(5)-C(15)	1.258(6)	C(10)-C(9)	1.420(6)
O(5)-Cu(2)	1.952(3)	O(6)-C(16)	1.254(5)
C(20)-C(21)	1.18(2)	O(8)-C(16) <sup>i</sup>	1.241(5)
C(20)-C(15)	1.527(11)	O(7)-C(15) <sup>i</sup>	1.240(6)
C(19)-C(5)	1.358(7)	C(1)-C(2)	1.500(7)
C(19)-C(4)	1.380(6)	C(12)-C(13)	1.351(7)
C(19)-H(7)	0.81(6)	C(12)-H(3)	0.91(4)
Cu(1)-O(3)	1.931(3)	C(7)-C(5)	1.415(6)
Cu(1)-O(1) <sup>j</sup>	1.960(2)	C(7)-C(8)	1.424(6)
Cu(1)-N(1)	2.031(3)	C(4)-H(8)	0.83(4)
Cu(1)-N(2)	2.044(3)	C(14)-C(13)	1.395(6)
Cu(1)-O(1)	2.354(2)	C(14)-H(1)	0.86(4)
Cu(2)-O(7)	1.960(3)	C(9)-C(8)	1.343(7)
Cu(2)-O(6)	1.962(3)	C(9)-H(4)	0.88(5)
Cu(2)-O(8)	1.962(3)	C(13)-H(2)	1.03(5)
Cu(2)-O(4)	2.120(2)	C(16)-O(8) <sup>i</sup>	1.241(5)
Cu(2)-Cu(2) <sup>i</sup>	2.6233(8)	C(16)-C(17)	1.60(3)
N(2)-C(14)	1.323(5)	C(5)-H(6)	1.05(5)
N(2)-C(11)	1.350(4)	C(8)-H(5)	0.96(6)
N(1)-C(4)	1.321(5)	C(17)-C(22)	1.52(3)
N(1)-C(6)	1.350(4)	C(15)-O(7) <sup>i</sup>	1.240(6)
O(3)-C(1)	1.266(4)	C(2)-C(24)	1.28(3)
O(4)-C(1)	1.246(4)	O(1)-C(23)	1.289(4)
C(11)-C(10)	1.395(5)	O(1)-Cu(1) <sup>j</sup>	2.354(2)
C(11)-C(6)	1.424(5)	C(23)-O(2)	1.223(4)
C(6)-C(7)	1.389(5)	C(23)-C(25)	1.522(5)
C(10)-C(12)	1.401(6)	C(25)-C(26)	1.479(7)

<sup>i</sup> [-x,1-y,-z]; <sup>j</sup> [1-x,2-y,1-z]

**Table G3** Bond angle [°] for  $\{[\text{Cu}_4(\text{phen})_2(\mu\text{-O}_2\text{CC}_2\text{H}_5)_8](\text{H}_2\text{O})\}_n$  **VII**

C(15)-O(5)-Cu(2)	123.1(3)	C(12)-C(10)-C(9)	123.6(4)
C(21)-C(20)-(15)	117.5(14)	C(16)-O(6)-Cu(2)	124.1(3)
C(5)-C(19)-C(4)	120.0(4)	C(16) <sup>i</sup> -O(8)-Cu(2)	123.1(3)
C(5)-C(19)-H(7)	117(4)	C(15) <sup>i</sup> -O(7)-Cu(2)	122.9(3)
C(4)-C(19)-H(7)	123(4)	O(4)-C(1)-O(3)	123.6(3)
O(3)-Cu(1)-O(1) <sup>j</sup>	90.15(11)	O(4)-C(1)-C(2)	120.1(4)
O(3)-Cu(1)-N(1)	155.97(12)	O(3)-C(1)-C(2)	116.3(4)
O(1)-Cu(1)-N(1)	93.47(10)	C(13)-C(12)-C(10)	118.8(4)
O(3)-Cu(1)-N(2)	96.45(12)	C(13)-C(12)-H(3)	125(3)
O(1)-Cu(1)-N(2)	173.39(11)	C(10)-C(12)-H(3)	116(3)
N(1)-Cu(1)-N(2)	80.44(11)	C(6)-C(7)-C(5)	116.4(4)
O(3)-Cu(1)-O(1)	109.45(10)	C(6)-C(7)-C(8)	119.1(4)
O(1)-Cu(1)-O(1) <sup>j</sup>	76.01(9)	C(5)-C(7)-C(8)	124.5(4)
N(1)-Cu(1)-O(1) <sup>j</sup>	94.46(10)	N(1)-C(4)-C(19)	122.5(4)
N(2)-Cu(1)-O(1) <sup>j</sup>	101.75(9)	N(1)-C(4)-H(8)	124(3)
O(5)-Cu(2)-O(7)	168.25(13)	C(19)-C(4)-H(8)	114(3)
O(5)-Cu(2)-O(6)	89.09(16)	N(2)-C(14)-C(13)	122.5(4)
O(7)-Cu(2)-O(6)	90.19(16)	N(2)-C(14)-H(1)	114(3)
O(5)-Cu(2)-O(8)	89.34(16)	C(13)-C(14)-H(1)	123(3)
O(7)-Cu(2)-O(8)	88.91(16)	C(8)-C(9)-C(10)	121.0(4)
O(6)-Cu(2)-O(8)	167.93(12)	C(8)-C(9)-H(4)	127(3)
O(5)-Cu(2)-O(4)	94.49(12)	C(10)-C(9)-H(4)	112(3)
O(7)-Cu(2)-O(4)	97.19(12)	C(12)-C(13)-C(14)	120.4(4)
O(6)-Cu(2)-O(4)	99.53(11)	C(12)-C(13)-H(2)	123(3)
O(8)-Cu(2)-O(4)	92.52(11)	C(14)-C(13)-H(2)	115(3)
O(5)-Cu(2)-Cu(2) <sup>i</sup>	84.03(10)	O(8) <sup>i</sup> -C(16)-O(6)	124.8(4)
O(7)-Cu(2)-Cu(2) <sup>i</sup>	84.24(10)	O(8) <sup>i</sup> -C(16)-C(17)	115.4(10)
O(6)-Cu(2)-Cu(2) <sup>i</sup>	83.42(8)	O(6)-C(16)-C(17)	119.6(10)
O(8)-Cu(2)-Cu(2) <sup>i</sup>	84.52(9)	C(19)-C(5)-C(7)	119.3(4)

**Table G3** Bond angle [°] for {[Cu<sub>4</sub>(phen)<sub>2</sub>(μ-O<sub>2</sub>CC<sub>2</sub>H<sub>5</sub>)<sub>8</sub>](H<sub>2</sub>O)}<sub>n</sub> **VII** (cont.)

O(4)-Cu(2)-Cu(2) <sup>i</sup>	176.70(8)	C(19)-C(5)-H(6)	121(3)
C(14)-N(2)-C(11)	117.4(3)	C(7)-C(5)-H(6)	120(3)
C(14)-N(2)-Cu(1)	129.5(3)	C(9)-C(8)-C(7)	121.1(5)
C(11)-N(2)-Cu(1)	113.0(2)	C(9)-C(8)-H(5)	128(3)
C(4)-N(1)-C(6)	118.2(3)	C(7)-C(8)-H(5)	111(4)
C(4)-N(1)-Cu(1)	128.4(3)	C(22)-C(17)-C(16)	106(2)
C(6)-N(1)-Cu(1)	113.4(2)	O(7) <sup>i</sup> -C(15)-O(5)	125.8(5)
C(1)-O(3)-Cu(1)	130.6(3)	O(7) <sup>i</sup> -C(15)-C(20)	119.2(7)
C(1)-O(4)-Cu(2)	136.2(2)	O(5)-C(15)-C(20)	114.9(6)
N(2)-C(11)-(10)	123.6(3)	C(24)-C(2)-C(1)	120.9(12)
N(2)-C(11)-C(6)	116.5(3)	C(23)-O(1)-Cu(1) <sup>j</sup>	141.7(2)
C(10)-C(11)-C(6)	119.9(3)	Cu(1)-O(1)-Cu(1) <sup>j</sup>	103.99(9)
N(1)-C(6)-C(7)	123.6(3)	O(2)-C(23)-O(1)	123.0(3)
N(1)-C(6)-C(11)	116.6(3)	O(2)-C(23)-C(25)	122.2(3)
C(7)-C(6)-C(11)	119.8(3)	O(1)-C(23)-C(25)	114.8(3)
C(11)-C(10)-(12)	117.4(4)	C(26)-C(25)-C(23)	115.8(4)
C(11)-C(10)-C(9)	119.0(4)		

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<sup>i</sup> [-x,1-y,-z]; <sup>j</sup> [1-x,2-y,1-z]

**Table G4** Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for complex **VII**.  
The anisotropic displacement factor exponent takes the form:  
 $-2\pi^2[(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$

	<b>U11</b>	<b>U22</b>	<b>U33</b>	<b>U23</b>	<b>U13</b>	<b>U12</b>
O(5)	82(2)	78(2)	86(2)	7.6(17)	22(16)	34.9(17)
C(20)	99(7)	113(8)	07(8)	21(6)	2(6)	63(6)
C(19)	83(3)	88(3)	57(2)	2(2)	19(2)	27(3)
Cu(1)	45.6(2)	40.4(2)	55.5(2)	4.1(16)	1663(17)	15.84(16)
Cu(2)	68.1(3)	47.8(2)	54.7(3)	0.6(18)	158(2)	15.9(2)
N(2)	44.9(13)	45.4(14)	67.1(18)	10.0(12)	164(12)	18.8(11)
N(1)	50.9(14)	48.8(14)	57.9(16)	8.6(12)	188(12)	22.7(12)
O(3)	80.6(16)	45.6(12)	59(14)	7.8(10)	265(13)	23(12)
O(4)	77.7(16)	46.8(13)	54.7(14)	0.8(10)	159(12)	19.3(12)
C(11)	50.9(16)	44.1(16)	71(2)	20.2(15)	233(15)	26.9(13)
C(6)	56.9(17)	48.1(17)	62(2)	15.4(14)	241(15)	28.5(14)
C(10)	53.3(18)	53.4(19)	92(3)	28.2(19)	292(19)	28.9(16)
O(6)	99(2)	59.8(16)	67(17)	2.9(13)	348(16)	13.2(15)
O(8)	113(2)	59.5(17)	70.4(18)	4.3(14)	438(17)	182(16)
O(7)	96(2)	69.9(19)	95(2)	9.1(17)	167(19)	44(17)
C(1)	68(2)	53(2)	52.3(19)	7(15)	174(16)	209(16)
C(12)	52.1(19)	55(2)	101(3)	24(2)	25(2)	20.6(17)
C(7)	74(2)	78(3)	72(2)	26(2)	37(2)	36(2)
C(4)	59(2)	64(2)	62(2)	5.6(17)	183(17)	215(18)
C(14)	534(19)	63(2)	72(3)	6.2(19)	167(19)	198(17)
C99)	70(3)	78(3)	107(4)	39(3)	51(3)	33(2)
C(13)	525(19)	59(2)	88(3)	7(2)	11(2)	13(17)
C(16)	90(3)	58(2)	65(2)	11(18)	32(2)	24(2)
C(5)	92(3)	100(4)	63(3)	13(2)	35(2)	31(3)
C(8)	86(3)	108(4)	94(4)	35(3)	55(3)	42(3)
C(17)	185(18)	93(12)	143(16)	0.069(11)	123(14)	84(13)

**Table G4** Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for complex **VII**.  
The anisotropic displacement factor exponent takes the form:  
 $-2\pi^2[(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$  (cont.)

	<b>U11</b>	<b>U22</b>	<b>U33</b>	<b>U23</b>	<b>U13</b>	<b>U12</b>
C(15)	85(3)	94(4)	86(3)	0.028(3)	17(3)	49(3)
C(2)	212(8)	82(4)	78(3)	0.029(3)	73(5)	70(4)
O(1)	47.9(11)	35.1(10)	65.9(14)	0.0089(9)	196(10)	153(9)
C(22)	370(4)	113(15)	134(17)	0.073(13)	14(2)	14(2)
C(21)	240(2)	21(2)	178(19)	-0.015(15)	6(16)	159(19)
C(23)	58.2(18)	43.1(17)	64(2)	0.0122(14)	190(16)	21.7(14)
C(24)	180(3)	34(5)	99(17)	0.15(3)	62(17)	15(3)
O(2)	72.2(16)	51.5(14)	105(2)	0.0175(14)	291(15)	34.3(13)
C(25)	64(2)	49(2)	121(4)	0.029(2)	27(2)	15.8(17)
C(26)	118(4)	76(3)	221(8)	0.073(5)	82(5)	033(3)
O(9)	221(13)	154(10)	219(13)	0.083(10)	107(11)	112(10)



**Table G5** Hydrogen coordinates [ $\times 10^4$ ] and isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $\{[\text{Cu}_4(\text{phen})_2(\mu\text{-O}_2\text{CC}_2\text{H}_5)_8](\text{H}_2\text{O})\}_n$  **VII**

	<b>x</b>	<b>y</b>	<b>z</b>	<b>U(eq)</b>
H(1)	110(4)	791(4)	2710(3)	61(11)
H(2)	-2460(6)	6550(5)	2420(4)	93(14)
H(3)	-2940(5)	6810(4)	4150(4)	78(12)
H(4)	-1980(6)	7910(5)	6120(4)	89(14)
H(5)	170(7)	9490(6)	7930(5)	122(19)
H(6)	2890(5)	11170(4)	8980(4)	87(13)
H(7)	5120(7)	12220(6)	8710(5)	120(2)
H(8)	5380(5)	11950(4)	7110(4)	72(12)