Supplementary data H for

$[Cu_2(\mu\text{-}O_2CC_6H_4OH)_4(C_7H_7NO)_2](H_2O)_6$ (VIII)

Table H1 Atomic Coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for complex **VIII**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	**y**	**z**	**U(eq)**
Cu(1)	38881(3)	5113.08(15)	9189.7(3)	287.5(12)
N(1)	1983(2)	5295.6(10)	7934(2)	333(5)
O(1)	3316(3)	5678.1(10)	10454.5(19)	539(6)
O(2)	2956(2)	4452.7(10)	10037.2(19)	473(6)
O(3)	4839(2)	4514.2(10)	8183.6(19)	500(6)
O(4)	5200(2)	5729.4(10)	8598(2)	517(6)
O(5)	-1570(3)	5895.8(12)	4510(2)	644(7)
O(6)	7718(5)	6409(2)	2143(4)	727(13)
O(7)	7861(3)	7600.2(15)	1901(3)	652(8)
O(8)	8753(5)	8009(2)	4214(3)	821(11)
O(9)	2746(3)	2804.4(11)	14318(2)	524(6)
O(10)	5674(3)	3133.5(12)	4725(2)	519(6)
C(1)	0715(3)	5019.2(15)	8056(3)	444(8)
C(2)	-511(3)	5091.2(15)	7273(3)	431(8)
C(3)	-447(3)	5472(12)	6292(3)	339(6)
C(4)	856(3)	5768.8(15)	6167(3)	428(7)
C(5)	2036(3)	5671.9(14)	6990(3)	399(7)
C(6)	-1717(3)	5566.3(14)	5364(3)	437(8)
C(7)	-3133(4)	5241(2)	5522(4)	574(10)
C(8)	3517(3)	4177.6(12)	10950(2)	311(6)
C(9)	2603(3)	3721.4(12)	11537(2)	312(6)
C(10)	1198(3)	3581.1(14)	11059(3)	399(7)
C(11)	350(4)	3187.6(15)	11674(3)	475(8)
C(12)	869(4)	2933.6(15)	12765(3)	457(8)
C(13)	3139(3)	3455.7(13)	12623(3)	326(6)

Table H1 Atomic Coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for complex **VIII**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor (cont.)

	x	**y**	**z**	**U(eq)**
C(14)	2269(3)	3067.7(13)	13233(3)	381(7)
C(16)	6656(3)	3821.1(12)	7659(2)	323(6)
C(17)	5884(3)	3663.1(13)	6575(3)	343(7)
C(18)	6489(3)	3278.8(13)	5770(2)	352(7)
C(15)	6012(3)	4248.3(12)	8525(2)	328(6)
C(21)	8053(3)	3587.6(14)	7916(3)	400(7)
C(19)	7892(3)	3053.6(14)	6028(3)	404(7)
C(20)	8662(3)	3208.9(15)	7104(3)	451(8)

Table H2 Bond lengths [Å] for $[Cu_2(\mu\text{-}O_2CC_6H_4OH)_4(C_7H_7NO)_2](H_2O)_6$ **VIII**

Cu(1)-O(4)	1.958(2)	C(8)-O(4)[i]	1.256(3)
Cu(1)-O(2)	1.962(2)	C(8)-C(9)	1.487(4)
Cu(1)-O(3)	1.969(2)	C(3)-C(4)	1.374(4)
Cu(1)-O(1)	1.970(2)	C(3)-C(6)	1.504(4)
Cu(1)-N(1)	2.181(2)	C(13)-C(14)	1.377(4)
Cu(1)-Cu(1)[i]	2.6539(6)	C(13)-C(9)	1.390(4)
O(2)-C(8)	1.254(3)	C(17)-C(18)	1.372(4)
O(3)-C(15)	1.256(3)	C(9)-C(10)	1.386(4)
N(1)-C(1)	1.324(4)	O(5)-C(6)	1.206(4)
N(1)-C(5)	1.337(4)	C(18)-C(19)	1.385(4)
O(4)-C(8)[i]	1.256(3)	C(4)-C(5)	1.374(4)
O(1)-C(15)[i]	1.252(3)	C(11)-C(10)	1.375(4)
O(10)-C(18)	1.364(3)	C(11)-C(12)	1.380(5)
C(2)-C(1)	1.372(4)	C(14)-C(12)	1.375(4)
C(2)-C(3)	1.376(4)	C(15)-O(1)[i]	1.252(3)
O(9)-C(14)	1.372(4)	C(21)-C(20)	1.372(4)
C(16)-C(21)	1.386(4)	C(19)-C(20)	1.377(4)
C(16)-C(17)	1.387(4)	C(6)-C(7)	1.499(5)
C(16)-C(15)	1.493(4)		

[i] [1-x,1-y,2-z]

Table H3 Bond angle [°] for $[Cu_2(\mu\text{-}O_2CC_6H_4OH)_4(C_7H_7NO)_2](H_2O)_6$ **VIII**

O(4)-Cu(1)-O(2)	167.04(8)	C(4)-C(3)-C(2)	117.1(3)
O(4)-Cu(1)-O(3)	89.06(10)	C(4)-C(3)-C(6)	119.7(3)
O(2)-Cu(1)-O(3)	89.03(10)	C(2)-C(3)-C(6)	123.1(3)
O(4)-Cu(1)-O(1)	89.20(11)	C(14)-C(13)-C(9)	120.2(3)
O(2) -Cu(1)-O(1)	89.83(10)	C(18)-C(17)-C(16)	120.6(3)
O(3) -Cu(1)-O(1)	167.21(9)	C(10)-C(9)-C(13)	119.5(3)
O(4) -Cu(1)-N(1)	97.93(8)	C(10)-C(9)-C(8)	121.3(3)
O(2) -Cu(1)-N(1)	95.03(8)	C(13)-C(9)-C(8)	119.2(2)
O(3) -Cu(1)-N(1)	97.59(9)	O(10)-C(18)-C(17)	118.1(3)
O(1)-Cu(1)-N(1)	95.20(9)	O(10)-C(18)-C(19)	122.0(3)
O(4)-Cu(1)-Cu(1)^{i}	84.22(6)	C(17)-C(18)-C(19)	120.0(3)
O(2)-Cu(1)-Cu(1)^{i}	82.84(6)	C(5)-C(4)-C(3)	120.2(3)
O(3)-Cu(1)-Cu(1)^{i}	84.48(6)	C(10)-C(11)-C(12)	121.1(3)
O(1)-Cu(1)-Cu(1)^{i}	82.74(6)	O(9)-C(14)-C(12)	117.7(3)
N(1)-Cu(1)-Cu(1)^{i}	177.02(6)	O(9)-C(14)-C(13)	122.1(3)
C(8)-O(2)-Cu(1)	125.33(18)	C(12)-C(14)-C(13)	120.3(3)
C(15)-O(3)-Cu(1)	123.26(19)	O(1)^{i}-C(15)-O(3)	124.1(3)
C(1)-N(1)-C(5)	116.5(3)	O(1)^{i}-C(15)-C(16)	117.7(2)
C(1)-N(1)-Cu(1)	120.84(19)	O(3)-C(15)-C(16)	118.2(2)
C(5)-N(1)-Cu(1)	122.59(19)	C(11)-C(10)-C(9)	119.5(3)
C(8)^{i}-O(4)-Cu(1)	123.86(18)	N(1)-C(5)-C(4)	122.8(3)
C(15)^{i}-O(1)-Cu(1)	125.39(19)	C(20)-C(21)-C(16)	120.3(3)
C(1)-C(2)-C(3)	119.2(3)	C(14)-C(12)-C(11)	119.4(3)
C(21)-C(16)-C(17)	119.1(3)	C(20)-C(19)-C(18)	119.7(3)
C(21)-C(16)-C(15)	120.3(3)	O(5)-C(6)-C(7)	121.6(3)
C(17)-C(16)-C(15)	120.6(3)	O(5)-C(6)-C(3)	119.4(3)
O(2)-C(8)-O(4)^{i}	123.6(3)	C(7)-C(6)-C(3)	118.9(3)
O(2)-C(8)-C(9)	118.0(2)	N(1)-C(1)-C(2)	124.2(3)
O(4)^{i}-C(8)-C(9)	118.3(2)	C(21)-C(20)-C(19)	120.5(3)

[1] [1-x,1-y,2-z]

Table H4 Anisotropic displacement parameters [$Å^2$ x 10^3] for complex **VIII**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+\ldots+ 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	27.61(19)	28.45(19)	29.33(19)	1.57(14)	-4.31(13)	-0.67(14)
N(1)	30(12)	35(13)	34.2(13)	3.1(10)	-3.2(10)	1.3(10)
O(1)	56.8(14)	59.9(15)	42.5(13)	-17.3(11)	-14.9(11)	21(12)
O(2)	38.5(12)	53.3(14)	48.2(13)	21.9(11)	-10.1(10)	-11.6(10)
O(3)	43.6(13)	610(15)	43.8(13)	-16.7(11)	-8.0(10)	16.9(11)
O(4)	37.4(12)	56.5(14)	58.4(14)	26.3(11)	-16.6(10)	-18(10)
O(5)	65(16)	73.7(18)	51.2(15)	21.0(13)	-18.3(12)	0.1(13)
O(6)	92(3)	62(3)	61(3)	15(2)	-22(2)	-22(2)
O(7)	68.4(19)	80(2)	47.7(19)	11.7(16)	0086(15)	-0.1(16)
O(8)	109(3)	70(3)	70(2)	8.2(18)	0233(19)	-30(2)
O(9)	56.3(17)	54.1(15)	46.5(14)	18.6(11)	1.1(12)	-8.4(13)
O(10)	51.9(15)	68.7(17)	34.2(13)	-11.7(12)	-3.6(11)	12.6(13)
C(1)	38.7(18)	50(2)	43(18)	20.6(15)	-4.8(14)	-3.9(14)
C(2)	29.4(16)	47.2(19)	52(2)	12.4(15)	-3.9(14)	-7.5(14)
C(3)	31.8(15)	33.1(16)	36.1(16)	0.6(12)	-2.4(12)	5.4(12)
C(4)	42.9(18)	46.7(19)	37.6(18)	13.3(15)	-5.2(14)	-1.8(15)
C(5)	32.4(16)	42(18)	44.7(18)	6.3(14)	-1.9(14)	-5.7(14)
C(6)	40(17)	44(18)	45.1(19)	-4.3(15)	-11.1(14)	7.3(14)
C(7)	40(2)	69(3)	60(3)	-1(2)	-17.2(19)	1.6(18)
C(8)	32.3(15)	28.6(14)	32.3(15)	-0.3(12)	0.8(12)	0.8(12)
C(9)	29.7(14)	29.9(15)	33.9(15)	-2.2(12)	2.2(12)	-0.10(12)
C(10)	37(17)	43.6(18)	38.1(18)	4.5(14)	-4.4(14)	-3.3(14)
C(11)	31.7(17)	51(2)	59(2)	-2.3(16)	-0.1(16)	-11.1(15)
C(12)	40.1(18)	42.4(19)	56(2)	5.2(16)	10.2(16)	-12.6(15)
C(13)	29.4(15)	32.1(15)	35.8(16)	2.3(12)	-0.7(12)	-2.9(12)
C(14)	43.7(17)	34.3(16)	36.7(16)	0.3(13)	6.7(14)	-1.2(13)

Table H4 Anisotropic displacement parameters [$Å^2$ x 10^3] for complex **VIII**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2 U_{11}+\ldots+ 2hka^*b^*U_{12}]$ (cont.)

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(15)	33.7(15)	29.7(15)	34.7(16)	3.2(12)	1.1(13)	-3.4(12)
C(16)	33.4(15)	29.1(15)	34.4(15)	2.8(12)	2.1(12)	-2.9(12)
C(17)	29.7(16)	36.8(17)	36.1(16)	3.8(13)	0.4(13)	5.6(13)
C(18)	36.8(16)	36.8(17)	31.6(16)	2.4(12)	-0.2(13)	0.1(12)
C(19)	39.9(17)	40.4(18)	42(18)	-4.4(14)	9.4(14)	4.3(14)
C(20)	27.8(16)	51(2)	56(2)	-1.6(16)	-1.2(15)	7.5(14)
C(21)	33.9(16)	43.3(18)	41.6(18)	-2.9(14)	-5.3(14)	-0.7(13)

Table H5 Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for $[Cu_2(\mu\text{-}O_2CC_6H_4OH)_4(C_7H_7NO)_2](H_2O)_6$ (**VIII**)

	x	y	z	U(eq)
H(1)	690(4)	4773(15)	8680(3)	550(10)
H(2)	-1330(3)	4902(13)	7410(3)	360(8)
H(3)	900(3)	6015(14)	5520(3)	490(9)
H(4)	2930(4)	5847(16)	6870(3)	59(010)
H(5)	-3500(5)	5350(2)	6210(4)	1070(19)
H(6)	-2920(5)	4820(2)	5570(4)	830(14)
H(7)	-3700(4)	5308(17)	4840(4)	760(13)
H(8)	8580(3)	3678(13)	8560(3)	330(8)
H(9)	9600(4)	3039(14)	7300(3)	510(9)
H(10)	8260(3)	2788(13)	5520(3)	360(8)
H(11)	6060(5)	2948(18)	4290(4)	700(14)
H(12)	5060(3)	3798(13)	6430(3)	390(9)
H(13)	880(3)	3750(14)	10330(3)	450(9)
H(14)	-560(4)	3115(15)	11390(3)	560(10)
H(15)	340(3)	2689(13)	13170(3)	380(8)
H(16)	3530(4)	2892(18)	14480(3)	630(14)
H(17)	4050(3)	3544(12)	12940(2)	0280(7)
H(18)	8100(3)	7721(14)	2430(3)	170(9)
H(19)	7880(9)	6290(4)	2590(7)	400(3)
H(20)	8370(6)	7860(2)	4560(4)	800(2)
H(21)	8760(8)	8330(3)	4360(6)	1800(4)