

Supplementary data I for
[Cu₂(μ-O₂CCH₃)₄(C₇H₇NO)₂] (IX)

Table I1 Atomic Coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **IX**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
Cu(1)	4053.17(16)	306.77(13)	4039(2)	3128(8)
N(1)	2550.7(12)	885.5(10)	1206.4(16)	358(3)
O(1)	4833.1(12)	1661.6(9)	5460(18)	503(3)
O(2)	3359.7(12)	528.5(11)	-1905.9(15)	500(3)
O(3)	3561.1(12)	-1143.3(9)	1194(17)	467(3)
O(4)	5029.1(12)	-17.8(12)	2575.7(14)	467(3)
O(5)	-0368.2(18)	3055.9(16)	2929(3)	912(6)
C(2)	1666.7(16)	284.6(13)	1351(2)	400(4)
C(3)	714.5(14)	1670.7(14)	2310(2)	402(4)
C(4)	2533.1(17)	1872.8(13)	1641(2)	427(4)
C(5)	1636.5(17)	2295.2(14)	2173(2)	444(4)
C(6)	741.1(15)	648.9(15)	1904(2)	426(4)
C(7)	-1073(2)	1437(3)	3466(4)	916(9)
C(8)	5810.2(15)	1816.8(12)	277(2)	390(3)
C(9)	3940 (17)	0352.2(11)	-2900(2)	379(4)
C(10)	-261.4(18)	2138.7(19)	2905(3)	582(5)
C(11)	6261(2)	2911.5(15)	434(3)	622(6)
C(12)	3342(2)	556.2(17)	-4638(2)	558(5)

Table I2 Bond lengths [Å] for [Cu₂(μ-O₂CCH₃)₄(C₇H₇NO)₂] **IX**

C(10)-O(5)	1.198(3)	N(1)-C(2)	1.332(2)
C(10)-C(7)	1.492(4)	N(1)-C(4)	1.338(2)
C(10)-C(3)	1.506(2)	O(4)-C(9) ⁱ	1.246(2)
Cu(1)-O(3)	1.9653(12)	C(2)-C(6)	1.385(3)
Cu(1)-O(4)	1.9677(12)	C(3)-C(6)	1.375(3)
Cu(1)-O(2)	1.9682(12)	C(3)-C(5)	1.384(3)
Cu(1)-O(1)	1.9720(12)	C(4)-C(5)	1.373(2)
Cu(1)-N(1)	2.1976(13)	C(9)-O(4) ⁱ	1.246(2)
Cu(1)-Cu(1) ⁱ	2.6307(4)	C(9)-C(12)	1.504(2)
O(3)-C(8) ⁱ	1.251(2)	C(8)-O(3) ⁱ	1.251(2)
O(1)-C(8)	1.248(2)	C(8)-C(11)	1.510(2)
O(2)-C(9)	1.255(2)		

ⁱ [1-x,-y,-z]

Table I3 Bond angle [°] for [Cu₂(μ-O₂CCH₃)₄(C₇H₇NO)₂] **IX**

O(5)-C(10)-C(7)	121.5(2)	C(8)-O(1)-Cu(1)	124.62(11)
O(5)-C(10)-C(3)	120.0(2)	C(9)-O(2)-Cu(1)	121.19(12)
C(7)-C(10)-C(3)	118.6(2)	C(2)-N(1)-C(4)	117.58(14)
O(3)-Cu(1)-O(4)	89.49(6)	C(2)-N(1)-Cu(1)	122.93(11)
O(30)-Cu(1)-O(2)	89.15(6)	C(4)-N(1)-Cu(1)	119.42(11)
O(4)-Cu(1)-O(2)	168.19(5)	C(9) ⁱ -O(4)-Cu(1)	124.84(11)
O(3)-Cu(1)-O(1)	168.07(5)	N(1)-C(2)-C(6)	122.56(16)
O(4)-Cu(1)-O(1)	89.41(6)	C(6)-C(3)-C(5)	118.07(16)
O(2)-Cu(1)-O(1)	89.51(6)	C(6)-C(3)-C(10)	123.28(18)
O(3)-Cu(1)-N(1)	97.62(5)	C(5)-C(3)-C(10)	118.64(17)
O(4)-Cu(1)-N(1)	94.71(5)	N(1)-C(4)-C(5)	123.26(17)
O(2)-Cu(1)-N(1) ⁱ	97.09(5)	C(4)-C(5)-C(3)	118.99(17)
O(1)-Cu(1)-N(1) ⁱ	94.31(5)	C(3)-C(6)-C(2)	119.50(16)
O(3)-Cu(1)-Cu(1) ⁱ	85.31(4)	O(4) ⁱ -C(9)-O(2)	125.75(16)
O(4)-Cu(1)-Cu(1) ⁱ	82.65(4)	O(4) ⁱ -C(9)-C(12)	116.80(16)
O(2)-Cu(1)-Cu(1)	85.55(4)	O(2)-C(9)-C(12)	117.44(17)
O(1)-Cu(1)-Cu(1)	82.76(4)	O(1)-C(8)-O(3) ⁱ	125.43(16)
N(1)-Cu(1)-Cu(1) ⁱ	176.07(4)	O(1)-C(8)-C(11)	116.95(15)
C(8) ⁱ -O(3)-Cu(1)	121.88(11)	O(3)-C(8)-C(11) ⁱ	117.62(15)

ⁱ [1-x,-y,-z]

Table I4 Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **IX**.
The anisotropic displacement factor exponent takes the form:
 $-2\pi^2[(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
C(10)	39.2(9)	77.5(15)	0.061.1(12)	-13.4(10)	19(9)	9.5(9)
Cu(1)	33.14(12)	30.21(12)	34.66(13)	2.01(6)	16.29(8)	4.81(7)
O(3)	46.2(7)	34.2(6)	67.3(8)	-4.3(5)	28.5(6)	-1(5)
O(1)	51.4(7)	33.4(6)	77.7(9)	-2(6)	37.5(7)	-2.6(5)
O(2)	49.7(8)	64.1(8)	37.6(6)	7.7(6)	14.2(5)	19.8(6)
N(1)	36.1(7)	35.7(7)	39.7(7)	0.6(5)	17.4(5)	4.5(5)
O(4)	48.2(7)	59.6(7)	34.9(6)	4.2(6)	15.5(5)	12.9(6)
C(2)	40.7(9)	36.5(9)	45.4(9)	-6(6)	15.9(7)	-1.9(6)
C(3)	32.5(8)	51.5(10)	38.5(8)	-1.9(7)	12.6(6)	6.9(7)
C(4)	42.2(9)	33.7(8)	59.7(11)	3.1(7)	26.7(8)	0.7(7)
C(5)	45.2(9)	35.1(8)	57.9(11)	-1.2(7)	22.4(8)	6(7)
C(6)	32.5(8)	49.3(9)	48.6(9)	-5.2(8)	15.1(7)	-6.8(7)
O(5)	77.1(12)	77.5(12)	134.6(18)	-18.7(12)	55.3(12)	24.8(10)
C97)	61.2(15)	125(3)	108(2)	-14.6(19)	55.8(15)	-2.3(16)
C(9)	50.1(10)	30.4(7)	33.4(8)	1.6(6)	11.6(7)	4.5(6)
C(8)	43.5(9)	32.8(7)	44.8(9)	3.7(6)	19(7)	0.1(7)
C(12)	71.6(14)	56.4(11)	34.7(9)	3.4(8)	6.3(9)	20(10)
C(11)	63.5(13)	35.4(9)	98.9(17)	-3.5(10)	41.2(12)	-7.4(9)

Table I5 Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Cu}_2(\mu\text{-O}_2\text{CCH}_3)_4(\text{C}_7\text{H}_7\text{NO})_2]$ **IX**

	x	y	z	U(eq)
H(13)	-1520(3)	1810(3)	3890(4)	114(12)
H(12)	-1540(4)	1000(3)	2660(6)	142(17)
H(11)	-550(4)	1040(4)	4360(5)	139(16)
H(1)	1784(18)	-387(14)	1110(2)	300(5)
H(4)	3187(18)	2232(16)	1650(2)	450(5)
H(2)	150(2)	233(15)	1930(3)	470(6)
H(3)	1600(2)	2930(2)	2410(3)	650(7)
H(8)	7080(3)	2990(2)	0750(3)	860(9)
H(9)	6020(3)	3280(3)	1150(4)	1230(13)
H(10)	6140(4)	3130(4)	-530(5)	1500(19)