

Supplementary data A for
[Cu₂(dpyam)₂(μ-C₂O₄)(Cl)₂] (I)

Table A1 Atomic Coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **I**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
Cu(1)	1287(4)	2449(3)	8176(2)	27.2(10)
Cl(1)	4308(8)	3192(6)	6804 (6)	36.9(14)
O(1)	1441(3)	3020(18)	10092(16)	36.5(4)
O(2)	-642 (2)	4749(18)	8492(16)	35.7(4)
N(1)	661(3)	2027(2)	6422(18)	26.8(3)
N(2)	2465(3)	74(2)	8365 (18)	29.5(4)
N(3)	3154(3)	-553(2)	5892(19)	29.7(4)
C(1)	-658(3)	3232(3)	5968(2)	32.4(4)
C(2)	-717(4)	3274(3)	4589(2)	35.9(5)
C(3)	658(4)	2026(3)	3593(2)	36.3(5)
C(4)	1943(4)	761(3)	4034(2)	32.6(4)
C(5)	1891(3)	776(2)	5477(2)	25.5(4)
C(6)	3224(3)	-1025(2)	7238(2)	26.3(4)
C(7)	4146(4)	-2676(3)	7368(3)	36.3(5)
C(8)	4314(4)	-3193(3)	8673(3)	42.8(6)
C(9)	3554(4)	-2058(3)	9847(3)	45.3(6)
C(10)	2646(4)	-475(3)	9646(2)	41.3(5)
C(11)	604(3)	4499(2)	10464(2)	27.9(4)

Table A2 Bond lengths [Å] for [Cu₂(dpyam)₂(μ-C₂O₄)(Cl)₂] **I**

Cu(1)-N(1)	1.9874(16)	Cu(1)-O(1)	2.004(14)
Cu(1)-N(2)	1.9947(17)	Cu(1)-O(2)	2.0252(15)
Cu(1)-Cl(1)	2.4924(6)	O(2)-C(11) ⁱ	1.246(2)
O(1)-C(11)	1.248(3)	N(1)-C(1)	1.357(3)
N(1)-C(5)	1.341(2)	N(2)-C(6)	1.343(3)
N(2)-C(10)	1.356(3)	N(3)-C(5)	1.377(3)
N(3)-C(6)	1.378(3)	C(2)-C(3)	1.391(3)
C(1)-C(2)	1.364(3)	N(3)-H(5)	0.73(3)
C(3)-C(4)	1.365(3)	C(1)-H(1)	0.96(3)
C(4)-C(5)	1.403(3)	C(2)-H(2)	0.94(3)
C(6)-C(7)	1.400(3)	C(3)-H(3)	0.93(3)
C(7)-C(8)	1.368(3)	C(4)-H(4)	0.87(3)
C(8)-C(9)	1.394(4)	C(7)-H(7)	0.90(3)
C(9)-C(10)	1.363(3)	C(8)-H(8)	0.91(3)
C(11)-C(11) ⁱ	1.531(4)	C(9)-H(9)	1.01(3)
C(11)-O(2) ⁱ	1.246(2)	C(10)-H(10)	1.01(3)
Cu(1)-Cu(1) ⁱ	5.256(1)		

ⁱ [-x, -y+1, -z+2]

Table A3 Bond angle [°] for [Cu₂(dpyam)₂(μ-C₂O₄)(Cl)₂] **I**

N(1)-Cu(1)-N(2)	91.98(7)	O(1)-Cu(1)-O(2)	81.84(6)
N(1)-Cu(1)-O(1)	170.79(7)	O(1)-Cu(1)-Cl(1)	93.59(5)
N(2)-Cu(1)-O(1)	91.89(6)	O(2)-Cu(1)-Cl(1)	95.88(5)
N(1)-Cu(1)-O(2)	91.95(6)	C(11)-O(1)-Cu(1)	112.19(12)
N(2)-Cu(1)-O(2)	161.74(8)	C(11)A-O(2)-Cu(1)	111.73(13)
N(1)-Cu(1)-Cl(1)	93.81(5)	C(5)-N(1)-C(1)	117.71(17)
N(2)-Cu(1)-Cl(1)	101.65(6)	C(5)-N(1)-Cu(1)	120.38(14)
C(1)-N(1)-Cu(1)	119.31(13)	C(6)-N(2)-C(10)	117.29(18)
C(6)-N(2)-Cu(1)	122.39(14)	C(10)-N(2)-Cu(1)	120.19(14)
C(5)-N(3)-C(6)	130.94(18)	C(5)-N(3)-H(5)	113.6(19)
C(6)-N(3)-H(5)	114.0(19)	N(1)-C(1)-C(2)	123.4(2)
N(1)-C(1)-H(1)	117.8(18)	C(2)-C(1)-H(1)	118.8(18)
C(1)-C(2)-C(3)	118.3(2)	C(1)-C(2)-H(2)	121.6(17)
C(3)-C(2)-H(2)	119.9(17)	C(4)-C(3)-C(2)	119.5(2)
C(4)-C(3)-H(3)	118.3(18)	C(2)-C(3)-H(3)	121.9(18)
C(3)-C(4)-C(5)	119.1(2)	C(3)-C(4)-H(4)	120.5(19)
C(5)-C(4)-H(4)	120.4(19)	N(1)-C(5)-N(3)	120.97(17)
N(1)-C(5)-C(4)	121.74(19)	N(3)-C(5)-C(4)	117.29(18)
N(2)-C(6)-N(3)	120.72(18)	N(2)-C(6)-C(7)	121.89(19)
N(3)-C(6)-C(7)	117.38(18)	C(8)-C(7)-C(6)	119.5(2)
C(8)-C(7)-H(7)	122.8(18)	C(6)-C(7)-H(7)	117.7(18)
C(7)-C(8)-C(9)	119.1(2)	C(7)-C(8)-H(8)	115.0(19)
C(9)-C(8)-H(8)	125.9(19)	C(10)-C(9)-C(8)	118.2(2)
C(10)-C(9)-H(9)	118.8(18)	C(8)-C(9)-H(9)	122.9(18)
N(2)-C(10)-C(9)	124.0(2)	N(2)-C(10)-H(10)	115.5(17)
C(9)-C(10)-H(10)	120.4(17)	O(2)#1-C(11)-O(1)	127.20(18)
O(2)-C(11)-C(11) ⁱ	116.3(2)	O(1)-C(11)-C(11) ⁱ	116.5(2)

ⁱ [-x, -y+1, -z+2]

Table A4 Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **I**.
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
Cu(1)	38(17)	20(15)	21(14)	-4(9)	-3(10)	1(1)
Cl(1)	38(3)	32(3)	36(3)	-7(2)	-6(2)	-9(2)
O(1)	53 (9)	23 (7)	26 (7)	-6(6)	-19(7)	4(7)
O(2)	49.4(9)	25.7(7)	27.6(7)	-7.6(6)	-20.4(7)	3.5(7)
N(1)	33.0(8)	23.7(8)	23.0(8)	-2.3(6)	-11.6(7)	-4.9(7)
N(2)	39.6(9)	21.5(8)	24.7(8)	-1.0(6)	-12.2(7)	-3.3(7)
N(3)	37.4(9)	22.6(8)	22.0(8)	-6.6(7)	-7.9(7)	-0.1(7)
C(1)	36.1(11)	28.2(10)	32.7(10)	-3.5(8)	-16.9(9)	-3.0(9)
C(2)	45.5(12)	31.4(11)	35.7(11)	3.7(9)	-23.7(10)	-8.0(10)
C(3)	51.1(13)	38.2(12)	24.1(10)	3.9(9)	-17.2(9)	-14.9(10)
C(4)	41.8(11)	31.7(11)	22.4(9)	-4.6(8)	-8.9(8)	-9.3(9)
C(5)	31.1(9)	24.3(9)	22.4(9)	-0.3(7)	-9.7(7)	-9.0(8)
C(6)	28.3(9)	23.3(9)	26.2(9)	-0.9(7)	-9.7(7)	-5.2(8)
C(7)	45.0(12)	23.7(10)	35.2(11)	-5.1(8)	-14.7(10)	-1.0(9)
C(8)	55.3(15)	24.1(11)	44.3(13)	4.1(9)	-20.6(11)	-1.2(10)
C(9)	66.8(17)	32.2(12)	33.4(12)	6.3(9)	-22.6(12)	-4.6(11)
C(10)	64.3(15)	27.3(11)	27.7(10)	-0.9(8)	-18.5(10)	-3.8(10)
C(11)	33.5(10)	25.2(10)	20.1(9)	-1.6(7)	-10.0(8)	-0.5(8)

Table A5 Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Cu}_2(\text{dpyam})_2(\mu\text{-C}_2\text{O}_4)(\text{Cl})_2] \text{ I}$

	x	y	z	U(eq)
H(1)	-1580(4)	4100(4)	6660(3)	50(8)
H(2)	-1590(4)	4160(4)	4290(3)	41(7)
H(3)	660(4)	1980(4)	2650(3)	49(8)
H(4)	2750(4)	-60(4)	3440(3)	41(7)
H(5)	3740(4)	-1200(3)	5310(3)	23(6)
H(7)	4620(4)	-3350(4)	6580(3)	43(7)
H(8)	4920(4)	-4280(4)	8680(3)	45(7)
H(9)	3700(5)	-2350(4)	820(3)	55(8)
H(10)	1990(4)	360(4)	480(3)	50(8)