

Supplementary data D for
[Cu₂(dpyam)₂(μ-C₂O₄)((CH₃)₂NCOH)₂](ClO₄)₂ (IV)

Table D1 Atomic Coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **IV**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
Cu(1)	5771.6(4)	3298.4(4)	1949.7(3)	33.82(12)
Cl(1)	3652.9(11)	7308.8(10)	2454 (6)	49.3(2)
O(1)	678 (2)	4818(2)	479 (16)	41.4(5)
O(2)	4018(2)	3545(2)	1103.5(15)	39.3(5)
O(3)	7257(3)	1124(3)	1637.8(19)	54.8(6)
O(4)	3231(12)	5762(9)	2827(8)	94(3)
O(5)	4982(17)	7176(18)	3000(14)	78(4)
O(6)	238(2)	8259(18)	2808(16)	101(6)
O(7)	4250(11)	7707(16)	1276(5)	104(3)
N(1)	7379(3)	3527(3)	2731.3(19)	35.3(5)
N(2)	4414(3)	2188(3)	3426.3(18)	34(5)
N(3)	5514(4)	3208(3)	4507(2)	42.5(7)
N(7)	8156(3)	-869(3)	873(2)	48.8(7)
C(1)	8916(4)	3799(4)	2104(3)	43.5(7)
C(2)	1007 (4)	4142(4)	2504(3)	52.1(9)
C(3)	9658(5)	4268(5)	3598(3)	56.1(9)
C(4)	8129(5)	4001(5)	4241(3)	50.9(9)
C(5)	7022(4)	3579(3)	3808(2)	35.6(6)
C(6)	4416(3)	2348(3)	4435(2)	34.9(6)
C(7)	3341(4)	1646(4)	5434(3)	46.9(8)
C(8)	2292(4)	736(4)	5398(3)	52.5(9)
C(9)	2325(4)	518(4)	4367(3)	48.6(8)
C(10)	3380(4)	1260(4)	3415(3)	40.2(7)
C(11)	5800(3)	5370(3)	-179(2)	34.5(6)
C(12)	7188(4)	421(4)	989(3)	48.2(8)
C(13)	9368(7)	-1593(7)	1559(5)	79(14)

Table D2 Bond lengths [Å] for [Cu₂(dpyam)₂(μ-C₂O₄)((CH₃)₂NCOH)₂](ClO₄)₂ **IV**

Cu(1)-N(1)	1.972(2)	C(3)-C(4)	1.357(5)
Cu(1)-N(2)	1.983(2)	C(4)-C(5)	1.384(4)
Cu(1)-O(2)	1.994(2)	C(6)-C(7)	1.392(4)
Cu(1)-O(1)	2.0113(19)	C(7)-C(8)	1.360(5)
Cu(1)-O(3)	2.204(2)	C(8)-C(9)	1.386(5)
Cl(1)-O(6)	1.311(14)	C(9)-C(10)	1.360(4)
Cl(1)-O(7)	1.394(6)	C(11) ⁱ -C(11)	1.535(5)
Cl(1)-O(4)	1.418(7)	C(11) ⁱ -O(2)	1.251(3)
Cl(1)-O(5)	1.440(13)	C(1)-H(1)	0.87(3)
O(1)-C(11)	1.246(3)	C(2)-H(2)	0.82(3)
O(2) ⁱ -C(11)	1.251(3)	C(3)-H(3)	0.94(4)
O(3)-C(12)	1.226(4)	C(4)-H(4)	0.79(3)
N(1)-C(5)	1.339(3)	C(7)-H(6)	0.86(3)
N(1)-C(1)	1.358(4)	C(8)-H(7)	0.84(3)
N(2)-C(6)	1.344(3)	C(9)-H(8)	0.79(3)
N(2)-C(10)	1.350(4)	C(10)-H(9)	0.89(3)
N(3)-C(6)	1.378(4)	C(12)-H(10)	0.90(4)
N(3)-C(5)	1.383(4)	C(14)-H(14)	0.93(5)
N(3)-H(5)	0.66(3)	C(14)-H(15)	0.94(5)
N(7)-C(12)	1.309(4)	C(14)-H(16)	0.90(6)
N(7)-C(13)	1.433(6)	C(13)-H(11)	0.89(5)
N(7)-C(14)	1.454(6)	C(13)-H(13)	0.93(7)
C(1)-C(2)	1.351(5)	C(13)-H(12)	0.94(7)
C(2)-C(3)	1.382(5)		

ⁱ [1-x,1-y,-z]

Table D3 Bond angle [°] for [Cu₂(dpyam)₂(μ-C₂O₄)((CH₃)₂NCOH)₂](ClO₄)₂ **IV**

N(1)-Cu(1)-N(2)	91.22(9)	O(2) ⁱ -C(11)-C(11) ⁱ	116.4(3)
N(1)-Cu(1)-O(2)	168.16(9)	O(3)-C(12)-N(7)	124.7(4)
N(2)-Cu(1)-O(2)	92.59(9)	O(3)-C(12)-H(10)	125(2)
N(1)-Cu(1)-O(1)	91.25(9)	O(2)-Cu(1)-O(3)	99.10(9)
N(2)-Cu(1)-O(1)	67.84(9)	O(1)-Cu(1)-O(3)	97.26(9)
N(1)-Cu(1)-O(3)	91.76(9)	O(6)-Cl(1)-O(7)	115.6(10)
N(2)-Cu(1)-O(3)	94.56(9)	O(6)-Cl(1)-O(5)	110.0(11)
O(2)-Cu(1)-O(1)	82.76(8)	O(7)-Cl(1)-O(5)	109.1(7)
O(6)-Cl(1)-O(4)	109.3(9)	C(6)-N(2)-Cu(1)	123.9(2)
O(7)-Cl(1)-O(4)	107.6(6)	C(10)-N(2)-Cu(1)	118.21(19)
C(11)-O(1)-Cu(1)	111.31(17)	C(6)-N(3)-C(5)	130.6(3)
C(11) ⁱ -O(2)-Cu(1)	111.74(18)	C(6)-N(3)-H(5)	113(3)
C(12)-O(3)-Cu(1)	130.3(2)	C(12)-N(7)-C(13)	120.2(4)
C(5)-N(1)-C(1)	117.3(3)	C(13)-N(7)-C(14)	118.2(4)
C(5)-N(1)-Cu(1)	124.7(2)	C(3)-C(4)-C(5)	120.0(3)
C(1)-N(1)-Cu(1)	117.7(2)	C(3)-C(4)-H(4)	122(3)
C(6)-N(2)-C(10)	117.8(2)	C(5)-C(4)-H(4)	118(3)
C(5)-N(3)-H(5)	113(3)	N(1)-C(1)-H(1)	115.5(19)
C(12)-N(7)-C(14)	121.5(4)	N(1)-C(5)-N(3)	119.6(3)
C(2)-C(1)-N(1)	123.5(3)	N(1)-C(5)-C(4)	121.5(3)
C(2)-C(1)-H(1)	121.1(19)	N(3)-C(5)-C(4)	118.9(3)
C(1)-C(2)-C(3)	118.6(3)	N(2)-C(6)-N(3)	120.3(2)
C(1)-C(2)-H(2)	118(3)	N(2)-C(6)-C(7)	121.7(3)
C(3)-C(2)-H(2)	123(3)	N(3)-C(6)-C(7)	118.1(3)
C(4)-C(3)-C(2)	119.0(4)	N(2)-C(10)-C(9)	123.1(3)
C(4)-C(3)-H(3)	120(2)	N(2)-C(10)-H(9)	118(2)
C(2)-C(3)-H(3)	121(2)	N(7)-C(12)-H(10)	111(2)
C(8)-C(7)-C(6)	119.3(3)	N(7)-C(14)-H(14)	110(4)
C(8)-C(7)-H(6)	124(2)	N(7)-C(14)-H(15)	110(3)
C(6)-C(7)-H(6)	117(2)	H(14)-C(14)-H(15)	103(5)

ⁱ [1-x,1-y,-z]

Table D3 Bond angle [°] for [Cu₂(dpyam)₂(μ-C₂O₄)((CH₃)₂NCOH)₂](ClO₄)₂
IV (cont.)

O(1)-C(11)-O(2) ⁱ	127.0(3)	C(7)-C(8)-C(9)	119.3(3)
C(7)-C(8)-H(7)	121(2)	H(14)-C(14)-H(16)	106(5)
C(9)-C(8)-H(7)	120(2)	N(7)-C(13)-H(11)	109(3)
C(10)-C(9)-C(8)	118.7(3)	N(7)-C(13)-H(13)	109(4)
C(10)-C(9)-H(8)	122(2)	N(7)-C(13)-H(12)	104(4)
C(8)-C(9)-H(8)	119(2)	H(15)-C(14)-H(16)	116(5)
C(9)-C(10)-H(9)	119(2)	H(11)-C(13)-H(13)	114(5)
O(1)-C(11)-C(11) ⁱ	116.5(3)	H(11)-C(13)-H(12)	101(5)
N(7)-C(14)-H(16)	111(4)	H(13)-C(13)-H(12)	118(6)

ⁱ [1-x,1-y,-z]

Table D4 Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **IV**.
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)	39.1(2)	37.1(2)	24.04(18)	-5.48(14)	-6.68(14)	-8.93(15)
Cl(1)	65.3(5)	52.1(5)	36(4)	-16(4)	-15.5(4)	-9.2(4)
O(1)	41(11)	49.4(13)	29.8(10)	-0.3(9)	-9.2(9)	-14.8(10)
O(2)	44.4(11)	44.8(12)	26.6(9)	-1(9)	-7(9)	-18.3(10)
O(3)	65.8(15)	50.2(14)	53.2(14)	-26.8(12)	-17.5(12)	6.2(12)
O(7)	116(6)	156(9)	31(3)	-29(5)	-12(3)	-9(7)
O(6)	104(12)	97(7)	127(15)	-82(9)	-49(10)	43(7)
O(5)	81(6)	106(7)	74(7)	-26(5)	-27(5)	-55(6)
O(4)	123(7)	62(4)	123(6)	-23(5)	-61(6)	-29(4)
N(1)	35.1(12)	36.6(13)	31.9(12)	-8.9(10)	-6.7(10)	-3.3(10)
N(2)	38.9(13)	34.6(13)	25.7(11)	-4 (10)	-7.5(10)	-6.6(11)
N(3)	51.1(16)	54.3(17)	22.8(13)	-11.1(12)	-5 (12)	-13.1(13)
N(7)	52.9(17)	39.8(15)	53.7(16)	-19.9(13)	-3.7(14)	-6.2(13)
C(1)	39.7(17)	48.1(19)	36.4(16)	-10.3(14)	-7.3(14)	1.6(14)
C(2)	33.8(17)	58(2)	56(2)	-5.2(17)	-11.1(16)	-6.5(16)
C(3)	55(2)	63(2)	56(2)	-9.1(18)	-27.8(18)	-15.2(18)
C(4)	60(2)	60(2)	38.9(18)	-10.5(16)	-18.2(17)	-19.1(18)
C(5)	41.4(16)	31.5(15)	32.1(14)	-6.6(12)	-10.2(12)	-3.4(12)
C(6)	35.7(15)	35.9(15)	29.9(14)	-7.4(12)	-6.3(12)	-3.6(12)
C(7)	53(2)	56(2)	30.1(15)	-9.8(14)	-5.4(14)	-14 (16)
C(8)	48.4(19)	63(2)	35.9(17)	-0.5(16)	-1.1(15)	-19.8(17)
C(9)	52(2)	42.8(19)	49.3(19)	-5.1(15)	-9.3(16)	-19.2(17)
C(10)	47.5(18)	39.5(17)	33.7(15)	-4.9(13)	-12.7(14)	-10.9(14)
C(11)	38.2(15)	39.2(16)	26.5(13)	-11.8(12)	-1.9(12)	-9.2(13)
C(12)	52(2)	48(2)	43.8(18)	-14.0(16)	-11.2(16)	-3.5(16)
C(14)	112(5)	85(4)	114(5)	-68(4)	-24(4)	-7(4)
C(13)	77(3)	61(3)	82(3)	-17(3)	-18(3)	19(3)

Table D5 Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Cu}_2(\text{dpyam})_2(\mu\text{-C}_2\text{O}_4)((\text{CH}_3)_2\text{NCOH})_2](\text{ClO}_4)_2$ **IV**

	x	y	z	U(eq)
H(1)	9130(3)	3730(3)	1410(3)	32(8)
H(2)	10990(4)	4240(4)	2090(3)	54(11)
H(3)	10380(4)	4620(4)	3880(3)	60(11)
H(4)	7840(4)	4060(4)	4870(3)	52(11)
H(5)	5430(4)	3230(3)	5030(3)	23(8)
H(6)	3390(4)	1810(4)	6050(3)	40(9)
H(7)	1650(4)	290(4)	5990(3)	54(10)
H(8)	1760(4)	-60(4)	4360(3)	42(10)
H(9)	3430(4)	1110(4)	2760(3)	40(8)
H(10)	6520(4)	0770(4)	480(3)	57(11)
H(11)	10270(6)	-1990(5)	1150(4)	85(15)
H(12)	8960(8)	-2520(8)	2070(6)	15(3)
H(13)	9540(8)	-860(9)	1860(6)	17(3)
H(14)	7740(7)	-2660(7)	490(4)	12(2)
H(15)	9020(7)	-1820(6)	-390(5)	11(2)
H(16)	7150(8)	-1140(7)	-250(5)	13(3)