

Supplementary data C for

[Cu₂(dpyam)₂(μ-C₂O₄)((CH₃)₂NCOH)₂](D)_{1.6}(NO₃)_{0.4} (III)

Table C1 Atomic Coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **III**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
Cu(1)	787.1(5)	3414.2(5)	6990.5(3)	31.06(13)
I(1)	8983.3(7)	6947.5(6)	7595(4)	51.5(15)
O(1)	1819(3)	4845(3)	5457(2)	36.1(5)
O(2)	-996(3)	3578(3)	6146.4(19)	34.6(5)
O(3)	2182(4)	1155(3)	6628(2)	52(7)
O(4)	9590(4)	5930(4)	8210(3)	150 (11)
O(5)	8780(4)	6990(4)	6410(3)	135 (10)
O(6)	8380(4)	8050(4)	7730(3)	127 (9)
N(1)	2491(3)	3590(3)	7776(2)	30.5(6)
N(2)	-513(3)	2237(3)	8482(2)	31.4(6)
N(3)	735(4)	3220(4)	9603(2)	37(7)
N(4)	3001(5)	636(4)	-5611(3)	51.7(9)
N(5)	8960(4)	6620(3)	7300(3)	40(1)
C(1)	001(4)	3880(4)	7120(3)	37.5(8)
C(2)	5213(5)	4215(5)	7527(4)	47.8(9)
C(3)	4897(5)	4279(6)	8661(4)	54.9(11)
C(4)	3384(5)	3969(5)	9351(4)	50.6(10)
C(5)	2203(4)	3600(4)	8887(3)	33(7)
C(6)	-429(4)	2378(4)	9511(3)	33.3(7)
C(7)	-1484(5)	1642(5)	10527(3)	43.6(9)
C(8)	-2577(5)	719(5)	10469(3)	48.6(10)
C(9)	-2628(5)	521(5)	9403(3)	46.6(9)
C(10)	-1589(4)	1290(4)	8452(3)	38(8)
C(11)	-815(4)	4635(4)	5194(3)	29.3(7)
C(12)	2199(5)	676(5)	5796(4)	47.7(9)
C(13)	2887(10)	-1154(8)	4619(6)	98(2)
C(14)	3878(8)	-1723(6)	6431(5)	81.8 (17)

Table C2 Bond lengths [Å] for $[\text{Cu}_2(\text{dpyam})_2(\mu\text{-C}_2\text{O}_4)((\text{CH}_3)_2\text{NCOH})_2](\text{I})_{1.6}(\text{NO}_3)_{0.4}$ **III**

Cu(1)-O(1)	2.021(2)	C(11) ⁱ -O(1)	1.243(4)
Cu(1)-O(3)	2.270(3)	C(11) ⁱ -C(11)	1.535(6)
O(4)-I(1)	1.22(4)	O(1) ⁱ -C(11)	1.243(4)
O(4)-N(5)	1.29(5)	O(2)-C(11)	1.255(4)
O(5)-N(5)	1.08(4)	O(3)-C(12)	1.227(5)
O(5)-I(1)	1.34(4)	C(5)-C(4)	1.391(5)
O(6)-I(1)	1.14(3)	C(9)-C(10)	1.357(5)
O(6)-N(5)	1.50(4)	C(9)-C(8)	1.397(6)
C(14)-N(4)	1.421(7)	C(6)-C(7)	1.402(5)
Cu(1)-N(1)	1.970(3)	C(2)-C(3)	1.383(6)
Cu(1)-N(2)	1.987(3)	C(4)-C(3)	1.379(6)
Cu(1)-O(2)	1.992(2)	N(3)-H(5)	0.53(3)
N(1)-C(5)	1.343(4)	C(9)-H(8)	0.93(4)
N(1)-C(1)	1.360(4)	C(8)-H(7)	0.85(5)
N(2)-C(6)	1.338(4)	C(1)-H(1)	0.80(5)
N(2)-C(10)	1.356(4)	C(10)-H(9)	0.84(4)
N(3)-C(5)	1.371(4)	C(7)-H(6)	0.78(5)
N(3)-C(6)	1.379(4)	C(12)-H(10)	0.85(5)
N(4)-C(12)	1.306(5)	C(2)-H(2)	0.84(5)
N(4)-C(13)	1.468(6)	C(4)-H(4)	0.84(5)
C(8)-C(7)	1.365(6)	C(3)-H(3)	0.70(6)
C(1)-C(2)	1.356(5)	Cu(1)-Cu(1) ⁱ	5.219(1)

ⁱ [-x,1-y,1-z]

Table C3 Bond angle [°] for $[\text{Cu}_2(\text{dpyam})_2(\mu\text{-C}_2\text{O}_4)((\text{CH}_3)_2\text{NCOH})_2](\text{I})_{1.6}(\text{NO}_3)_{0.4}$ **III**

N(1)-Cu(1)-N(2)	91.35(11)	C(5)-N(1)-C(1)	118.3(3)
N(1)-Cu(1)-O(1)	92.95(10)	C(5)-N(3)-C(6)	130.3(3)
N(1)-Cu(1)-O(2)	171.66(11)	C(6)-N(2)-C(10)	118.2(3)
N(2)-Cu(1)-O(2)	92.09(10)	C(6)-N(2)-Cu(1)	123.4(2)
N(1)-Cu(1)-O(3)	90.29(11)	C(11)-O(2)-Cu(1)	111.7(2)
N(2)-Cu(1)-O(1)	171.67(11)	C(10)-C(9)-C(8)	117.9(4)
N(2)-Cu(1)-O(3)	92.85(11)	C(12)-N(4)-C(14)	121.4(4)
O(1)-Cu(1)-O(3)	94.26(11)	C(12)-N(4)-C(13)	121.8(4)
O(2)-Cu(1)-O(1)	82.74(9)	C(14)-N(4)-C(13)	116.4(4)
O(2)-Cu(1)-O(3)	97.12(11)	C(7)-C(8)-C(9)	119.6(3)
C(1)-N(1)-Cu(1)	117.7(2)	C(2)-C(1)-N(1)	123.2(3)
C(11) ⁱ -O(1)-Cu(1)	110.7(2)	C(8)-C(7)-C(6)	119.3(4)
C(5)-N(1)-Cu(1)	123.7(2)	C(1)-C(2)-C(3)	118.5(4)
C(10)-N(2)-Cu(1)	118.4(2)	C(3)-C(4)-C(5)	119.1(4)
C(12)-O(3)-Cu(1)	126.6(3)	C(4)-C(3)-C(2)	119.6(4)
I(1)-O(4)-N(5)	18.3(13)	C(5)-N(3)-H(5)	113(4)
I(1)-O(6)-N(5)	8.3(12)	C(6)-N(3)-H(5)	114(4)
O(6)-I(1)-O(4)	114(2)	C(10)-C(9)-H(8)	118(3)
O(6)-I(1)-O(5)	113(2)	C(8)-C(9)-H(8)	124(3)
O(4)-I(1)-O(5)	133(2)	C(7)-C(8)-H(7)	122(3)
N(5)-O(5)-I(1)	15.1(16)	C(9)-C(8)-H(7)	119(3)
O(5)-N(5)-O(4)	162(4)	C(2)-C(1)-H(1)	119(3)
O(5)-N(5)-O(6)	105(3)	C(9)-C(10)-H(9)	118(2)
O(4)-N(5)-O(6)	90(3)	C(8)-C(7)-H(6)	130(3)
O(1) ⁱ -C(11)-O(2)	126.9(3)	C(6)-C(7)-H(6)	111(3)
O(1) ⁱ -C(11)-C(11) ⁱ	117.0(3)	C(1)-C(2)-H(2)	116(3)
O(2)-C(11)-C(11) ⁱ	116.1(4)	C(3)-C(2)-H(2)	126(3)
N(1)-C(5)-N(3)	120.5(3)	C(3)-C(4)-H(4)	120(3)
N(1)-C(5)-C(4)	121.3(3)	C(5)-C(4)-H(4)	121(3)

Table C3 Bond angle [°] for $[\text{Cu}_2(\text{dpyam})_2(\mu\text{-C}_2\text{O}_4)((\text{CH}_3)_2\text{NCOH})_2](\text{I})_{1.6}(\text{NO}_3)_{0.4}$ **III** (cont.)

N(3)-C(5)-C(4)	118.2(3)	C(4)-C(3)-H(3)	121(5)
N(2)-C(6)-N(3)	120.6(3)	C(2)-C(3)-H(3)	120(5)
N(2)-C(6)-C(7)	121.2(3)	N(1)-C(1)-H(1)	118(3)
N(3)-C(6)-C(7)	118.2(3)	N(2)-C(10)-H(9)	118(2)
N(2)-C(10)-C(9)	123.7(3)	O(3)-C(12)-H(10)	120(3)
O(3)-C(12)-N(4)	125.5(4)	N(4)-C(12)-H(10)	114(3)

¹ -x,1-y,1-z

Table C4 Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for complex **III**.
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)	31.8(2)	39.(2)	20.(2)	-1.84(16)	-7.97(15)	-8.04(17)
I(1)	65.6(2)	55.(3)	35.(2)	-16 (17)	-12.63(1)	-3.5(2)
N(1)	30.7(14)	33.(14)	25.9(14)	-6.6(11)	-9.1(11)	1(11)
N(2)	35.7(14)	33.(14)	22.5(13)	-1.2(11)	-9 (11)	-4.4(11)
N(3)	42.2(16)	49.2(18)	21.9(14)	-11(12)	-5.9(12)	-10.2(13)
N(4)	58(2)	39.7(18)	58(2)	-21.2(16)	-3.4(17)	-5.6(15)
O(1)	31.3(12)	47 (14)	26.4(12)	1.2(10)	-10.7(10)	-9.1(10)
O(2)	38(12)	41.(13)	21.(11)	1.9(9)	-9.4(9)	-11.3(10)
O(3)	65.8(18)	45 (15)	45.3(16)	-18.8(13)	-14.7(14)	10.4(13)
C(1)	31(17)	44(2)	34.4(18)	-10(15)	-7.1(14)	1.8(14)
C(2)	30.2(18)	57(2)	53(2)	-11.1(19)	-9.4(17)	-3.9(16)
C(3)	49(2)	72(3)	54(3)	-16(2)	-.22(2)	-21(2)
C(4)	54(2)	68(3)	38(2)	-17.8(19)	-13.1(18)	-1.8(2)
C(5)	39 (18)	31 (17)	29.9(17)	-8(13)	-11.5(14)	-0.3(14)
C(6)	34.1(17)	35 (18)	26.5(16)	-2.4(13)	-9.4(13)	0.3(14)
C(7)	45(2)	55(2)	25.4(17)	-3 (16)	-5.5(15)	-7.5(17)
C(8)	43(2)	56(2)	34(2)	6.9(17)	-4.1(16)	-13.9(18)
C(9)	46(2)	44(2)	45(2)	4.9(17)	-15.6(17)	-13.3(17)
C(10)	44 (19)	383(19)	32.6(18)	-1.2(14)	-16.9(15)	-9.8(15)
C(11)	30.9(16)	34.7(17)	22.9(15)	-9.2(13)	-2.2(13)	-7.1(13)
C(12)	54(2)	44(2)	48(2)	-18(18)	-12.2(19)	-1.3(18)
C(13)	137(6)	83(4)	102(5)	-65(4)	-35(4)	0(4)
C(14)	101(4)	47(3)	74(4)	-7(2)	-2(3)	15(3)

Table C5 Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Cu}_2(\text{dpyam})_2(\mu\text{-C}_2\text{O}_4)((\text{CH}_3)_2\text{NCOH})_2](\text{I})_{1.6}(\text{NO}_3)_{0.4}$ **III**

	x	y	z	U(eq)
H(1)	4210(5)	3740(5)	6500(4)	46(12)
H(2)	6090(6)	4400(5)	7050(4)	52(12)
H(3)	5480(7)	4510(7)	8870(5)	74(18)
H(4)	3190(5)	3980(5)	10050(4)	46(11)
H(5)	660(4)	3320(4)	10(3)	20(9)
H(6)	-1360(5)	1870(5)	11050(4)	50(13)
H(7)	-3230(6)	260(5)	11060(4)	55(13)
H(8)	-3280(5)	-160(5)	9310(4)	48(11)
H(9)	-1590(4)	1150(4)	7810(3)	26 (8)
H(10)	1690(5)	1230(5)	5260(4)	48(12)