Supplementary data E for

$[Cu_4(dpyam)_2(OCOC_2H_5)_2(\mu\text{-}O_2CC_2H_5)_6(H_2O)_2]$

$[Cu_2(\mu C_2H_5)_4(H_2O)_2](DMF)_2$ (V)

Table E1 Atomic Coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for complex **V**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	**y**	**z**	**U(eq)**
Cu(1)	5536.7(3)	6349.1(3)	8056.5(3)	54.04(13)
Cu(2)	5069.7(4)	9499(3)	5859.2(3)	59.87(14)
Cu(3)	9312.6(3)	5840.1(3)	5512.5(3)	47.3(12)
N(1)	395.1(2)	6266(2)	7941(2)	59.1(7)
N(2)	615(2)	4744(2)	8372(2)	59.2(7)
N(3)	426.5(3)	4777(2)	9010(2)	65.4(8)
N(4)	707(11)	208(8)	991(11)	285(7)
C(1)	320.4(3)	7034(4)	7366(3)	76.7(11)
C(2)	207.3(4)	7105(4)	7283(4)	92.8(14)
C(3)	1647(4)	6379(5)	7801(4)	99.8(15)
C(4)	2373(4)	5628(4)	8400(3)	83.3(12)
C(5)	3537(3)	5575(3)	8436(2)	58.2(8)
C(6)	5481(3)	4278(3)	8911(2)	58.2(8)
C(7)	5964(4)	3290(3)	9394(3)	76.1(11)
C(8)	7152(5)	2775(4)	9290(4)	99(15)
C(9)	7847(4)	3214(4)	8678(4)	99.2(15)
C(10)	7333(3)	4190(3)	8247(3)	77.7(11)
C(11)	7475(3)	6422(3)	8962(3)	63.7(9)
C(12)	8663(4)	6543(5)	8935(3)	97.3(15)
C(13)	9126(5)	6592(6)	9838(4)	139(2)
C(14)	4767(3)	8616(3)	7980(3)	64.3(9)
C(15)	4170(6)	9711(4)	8391(4)	120(2)
C(16)	3507(11)	9827(7)	9256(7)	314(8)
C(17)	2761(3)	10498(3)	5157(3)	58.9(8)
C(18)	1429(3)	10797(3)	5238(3)	73.9(10)
C(19)	940(4)	10219(4)	6033(4)	104.3(16)
C(20)	5246(3)	8267(3)	4205(4)	74.3(11)

Table E1 Atomic Coordinats [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for complex **V**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor (cont.)

	x	y	z	U(eq)
C(21)	5214(14)	7351(12)	3357(14)	124(8)
C(22)	5683(12)	6385(14)	3888(9)	144(5)
C(23)	8376(3)	4195(3)	5197(3)	56.5(8)
C(24)	7425(3)	3695(3)	5333(3)	80.4(12)
C(25)	7868(5)	2531(4)	5550(5)	13(2)
C(26)	9253(3)	5968(3)	3441(2)	58.1(8)
C(27)	8825(4)	6567(4)	2500(3)	89.5(13)
C(28)	8453(7)	7712(4)	2484(4)	142(3)
C(31)	509(8)	-517(6)	1083(7)	169(3)
C(32)	301(9)	1007(7)	523(8)	201(4)
C(33)	1154(10)	465(8)	1971(10)	223(6)
O(1)	5865(3)	6278(3)	6409(2)	58.8(7)
O(2)	70808(19)	6468.3(19)	8124.4(16)	60(6)
O(3)	6971(2)	6262(2)	9742(18)	83.1(8)
O(4)	4739(2)	7823.8(19)	8514.3(17)	67.3(6)
O(5)	5233(2)	8517(2)	7129.1(18)	75.8(7)
O(6)	3334(2)	9943(2)	5836.7(18)	70.2(7)
O(7)	6796(2)	9160(2)	5594.6(18)	70.6(7)
O(8)	4882(2)	10915(2)	6338(2)	78.3(7)
O(9)	5236(3)	8232(2)	5117(2)	80.7(8)
O(10)	8819(2)	6466.8(19)	4225.6(17)	63.1(6)
O(11)	15(2)	4954(2)	6628.8(16)	67.1(6)
O(12)	10681(2)	6324.8(19)	5284.2(18)	64.6(6)
O(13)	8159.1(19)	5083.8(19)	5574.8(18)	62.2(6)
O(14)	8185(2)	7136(2)	6425(2)	57.1(6)
O(15)	2322(11)	-36(10)	.2090(7)	358(7)

Table E2 Bond lengths [Å] for $[Cu_4(dpyam)_2(OCOC_2H_5)_2(\mu\text{-}O_2CC_2H_5)_6(H_2O)_2]$ $[Cu_2(\mu C_2H_5)_4(H_2O)_2](DMF)_2$ **V**

Cu(3)-Cu(3)[i]	2.6474(7)	N(4)-C(31)	1.072(10)
Cu(1)-O(2)	1.942(2)	N(4)-C(32)	1.182(10)
Cu(1)-O(4)	1.963(2)	N(4)-C(33)	1.595(16)
Cu(1)-N(1)	1.983(3)	N(1)-C(5)	1.322(4)
Cu(1)-N(2)	2.033(3)	N(1)-C(1)	1.369(5)
Cu(1)-O(1)	2.259(3)	N(2)-C(6)	1.332(4)
Cu(2)-O(5)	2.100(2)	N(2)-C(10)	1.356(4)
Cu(2)-Cu(2)[j]	2.6323(8)	N(3)-C(5)	1.379(4)
C(18)-C(17)	1.511(5)	N(3)-C(6)	1.379(4)
C(17)-O(7)[j]	1.254(4)	C(21)-C(20)	1.75(2)
C(17)-O(6)	1.257(4)	C(22)-C(21)	1.400(18)
C(24)-C(23)	1.513(5)	C(27)-C(28)	1.427(6)
C(20)-O(9)	1.249(5)	C(27)-C(26)	1.514(5)
C(20)-O(8)[j]	1.255(5)	C(13)-C(12)	1.422(6)
C(23)-O(13)	1.249(4)	C(25)-C(24)	1.471(6)
C(23)-O(12)[i]	1.251(4)	C(19)-C(18)	1.495(5)
O(2)-C(11)	1.278(4)	C(11)-O(3)	1.226(4)
O(4)-C(14)	1.259(4)	C(11)-C(12)	1.499(5)
O(6)-Cu(2)	1.973(2)	C(6)-C(7)	1.393(5)
O(7)-C(17)[j]	1.254(4)	C(5)-C(4)	1.391(5)
O(7)-Cu(2)	1.976(2)	C(10)-C(9)	1.354(6)
O(9)-Cu(2)	1.958(3)	C(1)-C(2)	1.354(5)
O(8)-C(20)[j]	1.255(5)	C(7)-C(8)	1.353(6)
O(8)-Cu(2)	1.960(3)	C(4)-C(3)	1.368(6)
O(13)-Cu(3)	1.984(2)	C(3)-C(2)	1.381(6)
O(11)-C(26)[i]	1.234(4)	C(9)-C(8)	1.382(6)
O(11)-Cu(3)	1.948(2)	C(26)-O(11)[j]	1.234(4)
O(10)-C(26)	1.265(4)	C(14)-C(15)	1.493(6)

Table E2 Bond lengths [Å] for $[Cu_4(dpyam)_2(OCOC_2H_5)_2(\mu\text{-}O_2CC_2H_5)_6(H_2O)_2]$ $[Cu_2(\mu C_2H_5)_4(H_2O)_2](DMF)_2$ **V** (cont.)

O(10)-Cu(3)	1.964(2)	C(15)-C(16)	1.352(8)
O(14)-Cu(3)	2.156(2)	C(33)-O(15)	1.354(12)
O(12)-C(23)[i]	1.251(4)	O(1)-H(1)	0.66(4)
O(12)-Cu(3)[i]	1.973(2)	O(1)-H(2)	0.74(5)
O(5)-C(14)	1.239(4)	O(14)-H(3)	0.64(4)
O(14)-H(4)	0.86(4)		

[I] [2-x,1-y,1-z] ;[J] [1-x,2-y,1-z]

Table E3 Bond angle [˚] for $[Cu_4(dpyam)_2(OCOC_2H_5)_2(\mu\text{-}O_2CC_2H_5)_6(H_2O)_2]$ $[Cu_2(\mu C_2H_5)_4(H_2O)_2](DMF)_2$ **V**

C(31)-N(4)-C(32)	132.6(13)	O(9)-Cu(2)-O(6)	88.67(12)
C(31)-N(4)-C(33)	110.6(12)	O(8)-Cu(2)-O(6)	89.99(12)
C(32)-N(4)-C(33)	110.2(11)	O(9)-Cu(2)-O(7)	88.31(12)
C(28)-C(27)-C(26)	118.0(4)	O(8)-Cu(2)-O(5)	104.21(11)
C(22)-C(21)-C(20)	100.2(14)	O(6)-Cu(2)-O(5)	97.19(10)
C(19)-C(18)-C(17)	115.4(3)	O(7)-Cu(2)-O(5)	94.21(10)
$O(7)^{j}$-C(17)-O(6)	125.2(3)	O(8)-Cu(2)-O(7)	90.62(12)
$O(7)^{j}$-C(17)-C(18)	116.2(3)	O(9)-Cu(2)-O(5)	87.53(11)
O(6)-C(17)-C(18)	118.6(3)	O(7)-Cu(2)-O(5)	94.21(10)
C(25)-C(24)-C(23)	114.5(4)	O(6)-Cu(2)-O(7)	168.07(10)
C(11)-O(2)-Cu(1)	118.9(2)	O(9)-Cu(8)-O(7)	168.26(12)
O(9)-C(20)-$O(8)^{j}$	126.0(4)	O(9)-Cu(2)-Cu(2)	85.13(9)
O(9)-C(20)-C(21)	132.8(6)	O(8)-Cu(2)-$Cu(2)^{j}$	83.13(8)
$O(8)^{j}$-C(20)-C(21)	100.5(6)	O(6)-Cu(2)-$Cu(2)^{j}$	83.55(7)
O(13)-C(23)-$O(12)^{i}$	125.5(3)	O(7)-Cu(2)-$Cu(2)^{j}$	84.69(7)
O(13)-C(23)-C(24)	117.7(3)	O(5)-Cu(2)-$Cu(2)^{j}$	172.60(8)
$O(12)^{i}$-C(23)-C(24)	116.8(3)	C(14)-O(4)-Cu(1)	120.8(2)
$C(17)^{j}$-O(6)-Cu(2)	124.0(2)	C(5)-N(1)-C(1)	118.0(3)
C(17)-O(7)-Cu(2)	122.5(2)	C(5)-N(1)-Cu(1)	124.6(2)
C(20)-O(9)-Cu(2)	121.8(3)	C(1)-N(1)-Cu(1)	117.2(2)
$C(20)^{j}$-O(8)-Cu(2)	123.9(3)	Cu(1)-O(1)-H(2)	120(3)
C(23)-O(13)-Cu(3)	123.5(2)	Cu(1)-O(1)-H(1)	114(4)
$C(26)^{i}$-O(11)-Cu(3)	123.7(2)	C(6)-N(2)-C(10)	117.7(3)
C(26)-O(10)-Cu(3)	122.1(2)	C(6)-N(2)-Cu(1)	121.3(2)
Cu(3)-O(14)-H(3)	117(3)	C(10)-N(2)-Cu(1)	118.9(2)
Cu(3)-O(14)-H(4)	121(2)	C(5)-N(3)-C(6)	129.5(3)
$C(23)^{i}$-O(12)-Cu(3)	123.3(2)	O(3)-C(11)-O(2)	124.8(3)
O(11)-Cu(3)-O(10)	167.78(10)	O(3)-C(11)-C(12)	120.5(3)
O(11)-Cu(3)-O(12)	90.51(11)	O(2)-C(11)-C(12)	114.6(3)
O(10)-Cu(3)-O(12)	88.36(11)	C(8)-C(7)-C(6)	118.6(4)

Table E3 Bond angle [˚] for $[Cu_4(dpyam)_2(OCOC_2H_5)_2(\mu\text{-}O_2CC_2H_5)_6(H_2O)_2]$ $[Cu_2(\mu C_2H_5)_4(H_2O)_2](DMF)_2$ **V**

O(10)-Cu(3)-O(13)	90.24(10)	N(2)-C(6)-C(7)	122.4(3)
O(11)-Cu(3)-O(13)	88.26(11)	N(2)-C(6)-N(3)	120.1(3)
O(12)-Cu(3)-O(13)	167.65(9)	N(1)-C(5)-C(4)	121.9(4)
O(11)-Cu(3)-O(14)	92.92(11)	N(3)-C(5)-C(4)	118.2(3)
O(10)-Cu(3)-O(14)	99.29(11)	C(9)-C(10)-N(2)	122.4(4)
O(12)-Cu(3)-O(14)	97.85(10)	C(2)-C(1)-N(1)	122.7(4)
O(13)-Cu(3)-O(14)	94.49(10)	C(13)-C(12)-C(11)	118.5(4)
O(11)-Cu(3)-Cu(3)^{i}	83.85(7)	C(3)-C(4)-C(5)	119.5(4)
O(10)-Cu(3)-Cu(3)^{i}	83.94(7)	C(4)-C(3)-C(2)	118.8(4)
O(12)-Cu(3)-Cu(3)^{i}	84.14(7)	C(10)-C(9)-C(8)	119.2(4)
O(13)-Cu(3)-Cu(3)^{i}	83.51(7)	C(1)-C(2)-C(3)	119.1(4)
O(14)-Cu(3)-Cu(3)^{i}	176.23(8)	C(7)-C(8)-C(9)	119.6(4)
O(11)-Cu(3)-O(13)	88.26(11)	O(10)-Cu(3)-O(13)	90.24(10)
O(11)-Cu(3)-O(14)	92.92(11)	O(10)-Cu(3)-O(14)	99.29(11)
O(12)-Cu(3)-O(14)	97.85(10)	O(13)-Cu(3)-O(14)	94.49(10)
O(11)-Cu(3)-Cu(3)^{i}	83.85(7)	O(10)-Cu(3)-Cu(3)^{i}	83.94(7)
O(12)-Cu(3)-Cu(3)^{i}	84.14(7)	N(1)-C(5)-N(3)	119.9(3)
O(2)-Cu(1)O(4)	90.99(10)	C(14)-O(5)-Cu(2)	136.1(2)
O(2)-Cu(1)-N(1)	177.73(10)	O(11)^{i}-C(26)-O(10)	126.4(3)
O(4)-Cu(1)-N(1)	88.32(11)	O(11)^{i}-C(26)-C(27)	117.3(3)
O(2)-Cu(1)-N(2)	93.03(11)	O(10)-C(26)-C(27)	116.3(3)
O(4)-Cu(1)-N(2)	148.68(10)	O(5)-C(14)-O(4)	122.5(3)
O(2)-Cu(1)-O(1)	89.34(10)	O(5)-C(14)-C(15)	119.9(3)
O(4)-Cu(1)-O(1)	112.57(11)	O(4)-C(14)-C(15)	117.6(3)
N(1)-Cu(1)-N(2)	88.68(12)	C(16)-C(15)-C(14)	119.6(5)
N(1)-Cu(1)-O(1)	88.92(11)	O(15)-C(33)-N(4)	115.9(10)
N(2)-Cu(1)-O(1)	98.54(12)	H(2)-O(1)-H(1)	105(5)
N(3)-C(6)-C(7)	117.5(3)	H(3)-O(14)-H(4)	104(4)

[I] [2-x,1-y,1-z] ;[J] [1-x,2-y,1-z]

Table E4 Anisotropic displacement parameters [$Å^2$ x 10^3] for complex **V**. 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)	44.4(2)	63.7(3)	53.2(2)	9.51(18)	2.75(16)	-21.43(1)
Cu(2)	53.3(2)	52.3(2)	62.1(3)	12.47(19)	4.09(19)	-8.32(19)
Cu(3)	42.6(2)	50.2(2)	46.2(2)	0.50(16)	3.13(15)	-14.70(1)
O(1)	52.6(16)	60.7(18)	56.3(15)	6.4(14)	8.8(12)	-16.0(14)
O(2)	51.4(13)	78(16)	54.7(14)	13.2(11)	-1.3(10)	-30.6(12)
O(3)	85.5(19)	115(2)	587(15)	20(15)	5.9(13)	-54.0(17)
O(4)	70.3(16)	62.1(15)	64.8(15)	8.8(12)	9.8(12)	-23.2(13)
O(5)	84.8(19)	615(16)	63.4(16)	16.8(12)	6.8(13)	-9.9(13)
O(6)	52.4(14)	75.4(17)	71.8(16)	20.4(13)	1.6(12)	-14.2(12)
O(7)	52.1(14)	73.7(17)	70.7(16)	17.6(13)	4(12)	-8.5(12)
O(8)	88(2)	64.9(17)	76(17)	-8.4(14)	3.4(14)	-20.9(15)
O(9)	92(2)	52.1(15)	89(2)	3.7(14)	6.7(16)	-18.7(14)
O(10)	65.1(15)	59.9(14)	55(14)	7.0(11)	-7.3(11)	-11.5(12)
O(11)	75.3(16)	63.4(16)	50.2(13)	3.4(11)	-6.4(11)	-9.6(13)
O(12)	49.4(13)	65.4(15)	79.7(16)	-17.6(12)	13.3(12)	-23.4(11)
O(13)	47.7(13)	61.1(15)	77.4(16)	-8.9(12)	14(11)	-22.6(11)
O(14)	54.1(15)	53.9(15)	52.4(15)	5.2(12)	12.9(12)	-11.0(12)
O(15)	309(12)	414(15)	277(10)	-153(10)	-62(9)	-6(10)
N(1)	50.2(15)	72.4(19)	55.7(16)	5.5(14)	4.9(12)	-26.2(14)
N(2)	55.3(16)	62.7(18)	56.6(16)	2.3(13)	5.1(13)	-20.0(14)
N(3)	68.4(19)	75(2)	55.1(16)	4.2(15)	19.0(14)	-35.4(17)
N(4)	304(13)	150(9)	421(17)	109(11)	-220(12)	-75(9)
C(1)	54(2)	98(3)	75(2)	20(2)	-0.2(18)	-28(2)
C(2)	54(2)	121(4)	96(3)	17(3)	-11(2)	-23(2)
C(3)	50(2)	151(5)	103(4)	4(3)	3(2)	-44(3)
C(4)	62(2)	112(4)	87(3)	5(3)	10(2)	-49(2)
C(5)	55(2)	73(2)	491(18)	-4.2(16)	10.7(15)	-28.8(18)

Table E4 Anisotropic displacement parameters [$Å^2$ x 10^3] for complex **V**. 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(6)	69(2)	57(2)	483(18)	-4(15)	7.8(16)	-24.2(17)
C(7)	92(3)	63(2)	68(2)	6.6(19)	9(2)	-26(2)
C(8)	108(4)	67(3)	103(4)	18(2)	-7(3)	-10(3)
C(9)	71(3)	77(3)	123(4)	8(3)	8(3)	0(2)
C(10)	61(2)	69(3)	94(3)	4(2)	5(2)	-16(2)
C(11)	63(2)	75(2)	57(2)	15.4(18)	-3.1(17)	-32.3(19)
C(12)	89(3)	161(5)	70(3)	22(3)	-13(2)	-79(3)
C(13)	129(5)	250(8)	78(3)	13(4)	-19(3)	-117(5)
C(14)	58(2)	65(2)	64(2)	9.7(18)	0.5(17)	-17.6(18)
C(15)	169(5)	72(3)	90(3)	0(3)	32(3)	-17(3)
C(16)	500(19)	121(6)	166(8)	7(6)	148(10)	32(9)
C(17)	520(19)	49.3(19)	69(2)	-1.2(17)	3.7(17)	-12.8(16)
C(18)	55(2)	76(3)	84(3)	8(2)	-0.9(19)	-18.1(19)
C(19)	74(3)	99(4)	141(4)	25(3)	4(3)	-40(3)
C(20)	53(2)	55(2)	108(4)	-18(2)	12(2)	-13.8(18)
C(21)	76(9)	95(11)	17(2)	60(13)	5(11)	-1(7)
C(22)	118(10)	211(17)	99(9)	-32(11)	4(7)	-53(12)
C(23)	48.7(19)	62(2)	61(2)	0.4(17)	0.5(15)	-23.0(16)
C(24)	61(2)	81(3)	107(3)	-22(2)	15(2)	-37(2)
C(25)	108(4)	90(4)	195(6)	-1(4)	34(4)	-50(3)
C(26)	63(2)	64(2)	48.5(19)	7.1(16)	-7.3(16)	-24.3(19)
C(27)	104(3)	91(3)	58(2)	14(2)	-17(2)	-16(3)
C(28)	233(7)	74(3)	75(3)	15(3)	-14(4)	-1(4)
C(31)	202(8)	83(5)	214(8)	46(5)	-62(6)	-38(5)
C(32)	247(11)	122(7)	259(11)	36(7)	-64(9)	-91(7)
C(33)	163(9)	158(8)	295(15)	14(9)	86(10)	-21(7)