Supplementary Material (ESI) for *Journal of Materials Chemistry*

Table 1. Crystal data and structure refinement for sad.
Project path: D:\frames\Old_Frames\426Cu\work-ac\sad.* (Cu-L-malate)

Identification code	sad
Empirical formula	C8 H14 Cu O12
Formula weight	365.73
Temperature	298(11) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 7.584(4) A alpha = 90 deg. b = 10.214(5) A beta = 92.778(7) deg. c = 8.169(4) A gamma = 90 deg.
Volume	632.1(5) A^3
Z, Calculated density	2, 1.921 Mg/m^3
Absorption coefficient	1.794 mm^-1
F(000)	374
Crystal size	0.40 x 0.20 x 0.15 mm
Theta range for data collection	2.69 to 28.34 deg.
Limiting indices	-9<=h<=10, -13<=k<=13, -10<=l<=10
Reflections collected / unique	6473 / 3072 [R(int) = 0.0178]
Completeness to theta = 28.34	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7746 and 0.5339
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3072 / 7 / 202
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0241, wR2 = 0.0663
R indices (all data)	R1 = 0.0245, wR2 = 0.0666
Absolute structure parameter	0.009(9)
Largest diff. peak and hole	0.428 and -0.332 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sad.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	7301(1)	7317(1)	7412(1)	26(1)
O(1)	8726(2)	8788(2)	6894(2)	28(1)
O(2)	8645(2)	10915(2)	6441(2)	40(1)
O(3)	5337(2)	8506(2)	6784(2)	31(1)
O(4)	2683(2)	11306(2)	5153(2)	41(1)
O(5)	1921(3)	10781(2)	7651(2)	39(1)
O(6)	5958(2)	5848(2)	8187(2)	29(1)
O(7)	6239(2)	3754(2)	8897(2)	35(1)
O(8)	9278(2)	6221(2)	8165(2)	33(1)
O(9)	12225(2)	4155(2)	7162(2)	39(1)
O(10)	12975(2)	3549(2)	9717(2)	35(1)
C(1)	7912(3)	9846(2)	6553(3)	26(1)
C(2)	5905(2)	9778(2)	6263(3)	25(1)
C(3)	4971(3)	10853(2)	7192(3)	29(1)
C(4)	3090(3)	11011(2)	6545(3)	25(1)
C(5)	6861(2)	4809(2)	8424(2)	24(1)
C(6)	8802(2)	4862(2)	8019(2)	23(1)
C(7)	9966(3)	3990(2)	9100(2)	28(1)
C(8)	11822(3)	3921(2)	8531(3)	25(1)
O(1W)	7773(2)	13083(2)	4560(2)	42(1)
O(2W)	12533(2)	6721(2)	9014(3)	51(1)

Table 3. Bond lengths [A] and angles [deg] for sad.

Cu(1)-O(1)	1.9101(16)
Cu(1)-O(6)	1.9369(17)
Cu(1)-O(8)	1.9473(16)
Cu(1)-O(3)	1.9698(17)
Cu(1)-O(4)#1	2.336(2)
O(1)-C(1)	1.269(3)
O(2)-C(1)	1.230(3)
O(3)-C(2)	1.440(3)
O(3)-H(3C)	0.8200
O(4)-C(4)	1.202(3)
O(4)-Cu(1)#2	2.336(2)
O(5)-C(4)	1.317(3)
O(5)-H(5A)	0.8200
O(6)-C(5)	1.273(3)
O(7)-C(5)	1.245(3)
O(8)-C(6)	1.438(3)
O(8)-H(8A)	0.8200
O(9)-C(8)	1.198(3)
O(10)-C(8)	1.329(3)
O(10)-H(10A)	0.8200
C(1)-C(2)	1.531(3)
C(2)-C(3)	1.528(3)
C(2)-H(2A)	0.9800
C(3)-C(4)	1.506(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(5)-C(6)	1.526(3)
C(6)-C(7)	1.509(3)
C(6)-H(6A)	0.9800
C(7)-C(8)	1.505(3)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
O(1W)-H(1A)	0.777(16)
O(1W)-H(1B)	0.805(17)
O(2W)-H(2B)	0.829(18)
O(2W)-H(2C)	0.825(17)
O(1)-Cu(1)-O(6)	173.60(7)
O(1)-Cu(1)-O(8)	94.98(7)
O(6)-Cu(1)-O(8)	81.98(7)
O(1)-Cu(1)-O(3)	83.48(7)
O(6)-Cu(1)-O(3)	99.18(7)
O(8)-Cu(1)-O(3)	175.98(7)
O(1)-Cu(1)-O(4)#1	96.98(7)
O(6)-Cu(1)-O(4)#1	88.66(7)
O(8)-Cu(1)-O(4)#1	89.53(7)
O(3)-Cu(1)-O(4)#1	94.33(7)
C(1)-O(1)-Cu(1)	116.36(14)
C(2)-O(3)-Cu(1)	113.59(12)
C(2)-O(3)-H(3C)	109.5
Cu(1)-O(3)-H(3C)	128.9
C(4)-O(4)-Cu(1)#2	161.24(17)
C(4)-O(5)-H(5A)	109.5

C(5)-O(6)-Cu(1)	114.10(13)
C(6)-O(8)-Cu(1)	110.01(12)
C(6)-O(8)-H(8A)	109.5
Cu(1)-O(8)-H(8A)	138.5
C(8)-O(10)-H(10A)	109.5
O(2)-C(1)-O(1)	123.74(19)
O(2)-C(1)-C(2)	118.55(19)
O(1)-C(1)-C(2)	117.71(18)
O(3)-C(2)-C(3)	110.49(16)
O(3)-C(2)-C(1)	107.73(16)
C(3)-C(2)-C(1)	111.83(17)
O(3)-C(2)-H(2A)	108.9
C(3)-C(2)-H(2A)	108.9
C(1)-C(2)-H(2A)	108.9
C(4)-C(3)-C(2)	110.90(17)
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.0
O(4)-C(4)-O(5)	122.9(2)
O(4)-C(4)-C(3)	123.7(2)
O(5)-C(4)-C(3)	113.44(18)
O(7)-C(5)-O(6)	124.04(19)
O(7)-C(5)-C(6)	118.85(18)
O(6)-C(5)-C(6)	117.04(18)
O(8)-C(6)-C(7)	112.56(16)
O(8)-C(6)-C(5)	104.93(16)
C(7)-C(6)-C(5)	113.28(16)
O(8)-C(6)-H(6A)	108.6
C(7)-C(6)-H(6A)	108.6
C(5)-C(6)-H(6A)	108.6
C(8)-C(7)-C(6)	112.08(17)
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7B)	109.2
C(6)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
O(9)-C(8)-O(10)	123.3(2)
O(9)-C(8)-C(7)	124.33(19)
O(10)-C(8)-C(7)	112.36(18)
H(1A)-O(1W)-H(1B)	114(3)
H(2B)-O(2W)-H(2C)	107(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+1 #2 -x+1,y+1/2,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for sad.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	19(1)	22(1)	38(1)	4(1)	0(1)	0(1)
O(1)	19(1)	26(1)	38(1)	4(1)	0(1)	1(1)
O(2)	21(1)	30(1)	69(1)	12(1)	-1(1)	-2(1)
O(3)	19(1)	24(1)	48(1)	3(1)	-7(1)	-2(1)
O(4)	38(1)	50(1)	35(1)	6(1)	-2(1)	4(1)
O(5)	21(1)	55(1)	40(1)	4(1)	4(1)	-4(1)
O(6)	19(1)	26(1)	42(1)	4(1)	3(1)	2(1)
O(7)	20(1)	29(1)	58(1)	12(1)	2(1)	-1(1)
O(8)	18(1)	25(1)	57(1)	4(1)	-6(1)	-1(1)
O(9)	28(1)	59(1)	31(1)	2(1)	5(1)	2(1)
O(10)	19(1)	45(1)	41(1)	12(1)	0(1)	1(1)
C(1)	18(1)	28(1)	32(1)	2(1)	3(1)	0(1)
C(2)	19(1)	23(1)	32(1)	1(1)	0(1)	1(1)
C(3)	21(1)	30(1)	37(1)	-6(1)	0(1)	-1(1)
C(4)	23(1)	19(1)	33(1)	-2(1)	1(1)	1(1)
C(5)	19(1)	24(1)	29(1)	0(1)	-1(1)	0(1)
C(6)	17(1)	24(1)	28(1)	2(1)	0(1)	-1(1)
C(7)	19(1)	32(1)	34(1)	8(1)	3(1)	4(1)
C(8)	18(1)	22(1)	34(1)	1(1)	1(1)	0(1)
O(1W)	30(1)	39(1)	56(1)	9(1)	-5(1)	4(1)
O(2W)	23(1)	48(1)	81(2)	-30(1)	-1(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sad.

	x	y	z	U(eq)
H(3C)	4377	8332	6331	37
H(5A)	924	10898	7243	46
H(8A)	10350	6285	8334	40
H(10A)	13839	4033	9729	42
H(2A)	5611	9876	5088	30
H(3A)	4987	10634	8348	35
H(3B)	5597	11674	7078	35
H(6A)	8906	4592	6876	28
H(7A)	9993	4321	10214	34
H(7B)	9468	3116	9105	34
H(1A)	8620(30)	13350(30)	4190(40)	51
H(1B)	7910(40)	12390(20)	5030(30)	51
H(2B)	12620(40)	7410(20)	9550(40)	61
H(2C)	13540(30)	6530(30)	8740(40)	61

Table 6. Torsion angles [deg] for sad.

O(8)-Cu(1)-O(1)-C(1)	-170.23(15)
O(3)-Cu(1)-O(1)-C(1)	6.05(15)
O(4)#1-Cu(1)-O(1)-C(1)	99.64(16)
O(1)-Cu(1)-O(3)-C(2)	0.94(13)
O(6)-Cu(1)-O(3)-C(2)	175.06(13)
O(4)#1-Cu(1)-O(3)-C(2)	-95.60(14)
O(8)-Cu(1)-O(6)-C(5)	-15.52(15)
O(3)-Cu(1)-O(6)-C(5)	168.37(15)
O(4)#1-Cu(1)-O(6)-C(5)	74.20(15)
O(1)-Cu(1)-O(8)-C(6)	-155.81(13)
O(6)-Cu(1)-O(8)-C(6)	29.86(13)
O(4)#1-Cu(1)-O(8)-C(6)	-58.85(14)
Cu(1)-O(1)-C(1)-O(2)	168.52(18)
Cu(1)-O(1)-C(1)-C(2)	-11.6(2)
Cu(1)-O(3)-C(2)-C(3)	-128.64(14)
Cu(1)-O(3)-C(2)-C(1)	-6.2(2)
O(2)-C(1)-C(2)-O(3)	-168.53(19)
O(1)-C(1)-C(2)-O(3)	11.6(3)
O(2)-C(1)-C(2)-C(3)	-46.9(3)
O(1)-C(1)-C(2)-C(3)	133.2(2)
O(3)-C(2)-C(3)-C(4)	-75.7(2)
C(1)-C(2)-C(3)-C(4)	164.32(18)
Cu(1)#2-O(4)-C(4)-O(5)	142.0(4)
Cu(1)#2-O(4)-C(4)-C(3)	-38.7(6)
C(2)-C(3)-C(4)-O(4)	-60.5(3)
C(2)-C(3)-C(4)-O(5)	118.9(2)
Cu(1)-O(6)-C(5)-O(7)	-178.89(17)
Cu(1)-O(6)-C(5)-C(6)	-1.9(2)
Cu(1)-O(8)-C(6)-C(7)	-159.50(13)
Cu(1)-O(8)-C(6)-C(5)	-35.88(17)
O(7)-C(5)-C(6)-O(8)	-157.64(19)
O(6)-C(5)-C(6)-O(8)	25.2(2)
O(7)-C(5)-C(6)-C(7)	-34.5(3)
O(6)-C(5)-C(6)-C(7)	148.39(18)
O(8)-C(6)-C(7)-C(8)	-68.9(2)
C(5)-C(6)-C(7)-C(8)	172.27(17)
C(6)-C(7)-C(8)-O(9)	-22.3(3)
C(6)-C(7)-C(8)-O(10)	158.66(18)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+1 #2 -x+1,y+1/2,-z+1