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

Table 1. Crystal data and structure refinement for sad.
Project path: D:\frames\Old_Frames\725Cu\work-ac\sad.* (Cu-DL-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)/c
Unit cell dimensions	a = 8.478(6) A alpha = 90 deg. b = 7.430(5) A beta = 102.581(9) deg. c = 10.295(7) A gamma = 90 deg.
Volume	632.9(7) A^3
Z, Calculated density	2, 1.919 Mg/m^3
Absorption coefficient	1.792 mm^-1
F(000)	374
Crystal size	0.70 x 0.50 x 0.50 mm
Theta range for data collection	3.41 to 28.37 deg.
Limiting indices	-11<=h<=11, -9<=k<=9, -13<=l<=13
Reflections collected / unique	6116 / 1556 [R(int) = 0.0244]
Completeness to theta = 28.37	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4678 and 0.3669
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1556 / 3 / 103
Goodness-of-fit on F^2	1.130
Final R indices [I>2sigma(I)]	R1 = 0.0294, wR2 = 0.0777
R indices (all data)	R1 = 0.0318, wR2 = 0.0806
Largest diff. peak and hole	0.460 and -0.353 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)	5000	5000	0	27(1)
O(1)	5377(2)	3057(2)	-1111(1)	31(1)
O(2)	6697(2)	507(2)	-1153(1)	37(1)
O(3)	6618(2)	3760(2)	1342(1)	28(1)
O(4)	8947(2)	1002(2)	3518(1)	39(1)
O(5)	11128(2)	2163(2)	2963(2)	45(1)
C(1)	6316(2)	1830(2)	-550(2)	26(1)
C(2)	7025(2)	1998(2)	953(2)	25(1)
C(3)	8851(2)	1770(3)	1233(2)	31(1)
C(4)	9614(2)	1603(2)	2693(2)	28(1)
O(1W)	2725(2)	3175(2)	509(2)	35(1)

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

Cu(1)-O(1)#1	1.9115(15)
Cu(1)-O(1)	1.9115(15)
Cu(1)-O(3)#1	1.9536(14)
Cu(1)-O(3)	1.9536(14)
Cu(1)-O(1W)	2.5047(19)
O(1)-C(1)	1.264(2)
O(2)-C(1)	1.243(2)
O(3)-C(2)	1.433(2)
O(3)-H(3C)	0.8200
O(4)-C(4)	1.203(2)
O(5)-C(4)	1.321(2)
O(5)-H(5A)	0.8200
C(1)-C(2)	1.537(2)
C(2)-C(3)	1.522(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
O(1W)-H(1A)	0.797(16)
O(1W)-H(1B)	0.779(16)
O(1)#1-Cu(1)-O(1)	180.00(6)
O(1)#1-Cu(1)-O(3)#1	83.32(7)
O(1)-Cu(1)-O(3)#1	96.68(7)
O(1)#1-Cu(1)-O(3)	96.68(7)
O(1)-Cu(1)-O(3)	83.32(7)
O(3)#1-Cu(1)-O(3)	180.00(7)
O(1)#1-Cu(1)-O(1W)	92.70(7)
O(1)-Cu(1)-O(1W)	87.30(7)
O(3)#1-Cu(1)-O(1W)	87.09(7)
O(3)-Cu(1)-O(1W)	92.91(7)
C(1)-O(1)-Cu(1)	116.22(12)
C(2)-O(3)-Cu(1)	114.05(10)
C(2)-O(3)-H(3C)	109.5
Cu(1)-O(3)-H(3C)	127.2
C(4)-O(5)-H(5A)	109.5
O(2)-C(1)-O(1)	123.24(16)
O(2)-C(1)-C(2)	118.70(15)
O(1)-C(1)-C(2)	118.06(15)
O(3)-C(2)-C(3)	110.20(14)
O(3)-C(2)-C(1)	106.91(13)
C(3)-C(2)-C(1)	109.90(14)
O(3)-C(2)-H(2A)	109.9
C(3)-C(2)-H(2A)	109.9
C(1)-C(2)-H(2A)	109.9
C(4)-C(3)-C(2)	113.36(15)
C(4)-C(3)-H(3A)	108.9
C(2)-C(3)-H(3A)	108.9
C(4)-C(3)-H(3B)	108.9
C(2)-C(3)-H(3B)	108.9
H(3A)-C(3)-H(3B)	107.7
O(4)-C(4)-O(5)	123.59(17)
O(4)-C(4)-C(3)	124.66(17)

O(5)-C(4)-C(3)	111.73(16)
Cu(1)-O(1W)-H(1A)	114.3(19)
Cu(1)-O(1W)-H(1B)	100(2)
H(1A)-O(1W)-H(1B)	113(2)

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

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)	29(1)	32(1)	18(1)	-2(1)	-1(1)	8(1)
O(1)	35(1)	36(1)	18(1)	-3(1)	-1(1)	8(1)
O(2)	55(1)	30(1)	23(1)	-3(1)	4(1)	8(1)
O(3)	36(1)	32(1)	16(1)	-1(1)	0(1)	8(1)
O(4)	38(1)	53(1)	26(1)	2(1)	6(1)	-4(1)
O(5)	32(1)	63(1)	35(1)	14(1)	-2(1)	-5(1)
C(1)	27(1)	30(1)	19(1)	-2(1)	3(1)	-2(1)
C(2)	29(1)	27(1)	19(1)	0(1)	3(1)	2(1)
C(3)	29(1)	40(1)	23(1)	2(1)	4(1)	5(1)
C(4)	29(1)	28(1)	25(1)	1(1)	2(1)	6(1)
O(1W)	36(1)	35(1)	34(1)	3(1)	8(1)	4(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)	6713	3790	2152	34
H(5A)	11568	1859	3721	54
H(2A)	6549	1083	1436	30
H(3A)	9106	702	777	37
H(3B)	9319	2796	873	37
H(1A)	2990(30)	2220(20)	840(20)	42
H(1B)	2420(30)	3830(30)	990(20)	42

Table 6. Torsion angles [deg] for sad.

O(3)#1-Cu(1)-O(1)-C(1)	-174.95(13)
O(3)-Cu(1)-O(1)-C(1)	5.05(13)
O(1W)-Cu(1)-O(1)-C(1)	-88.20(14)
O(1)#1-Cu(1)-O(3)-C(2)	169.52(11)
O(1)-Cu(1)-O(3)-C(2)	-10.48(11)
O(1W)-Cu(1)-O(3)-C(2)	76.46(12)
Cu(1)-O(1)-C(1)-O(2)	-178.42(14)
Cu(1)-O(1)-C(1)-C(2)	1.2(2)
Cu(1)-O(3)-C(2)-C(3)	132.15(12)
Cu(1)-O(3)-C(2)-C(1)	12.74(16)
O(2)-C(1)-C(2)-O(3)	170.39(16)
O(1)-C(1)-C(2)-O(3)	-9.3(2)
O(2)-C(1)-C(2)-C(3)	50.8(2)
O(1)-C(1)-C(2)-C(3)	-128.86(17)
O(3)-C(2)-C(3)-C(4)	72.15(19)
C(1)-C(2)-C(3)-C(4)	-170.28(15)
C(2)-C(3)-C(4)-O(4)	28.2(3)
C(2)-C(3)-C(4)-O(5)	-153.15(17)

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