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

Table 1. Crystal data and structure refinement for sad.
Project path: D:\frames\Old_Frames\419Cu\work-ac\sad.*

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 = 7.591(6) A alpha = 90 deg. b = 10.230(8) A beta = 92.799(11) deg. c = 8.184(6) A gamma = 90 deg.
Volume	634.8(8) A^3
Z, Calculated density	2, 1.913 Mg/m^3
Absorption coefficient	1.787 mm^-1
F(000)	374
Crystal size	0.40 x 0.30 x 0.35 mm
Theta range for data collection	2.69 to 28.46 deg.
Limiting indices	-10<=h<=10, -13<=k<=13, -10<=l<=10
Reflections collected / unique	6530 / 3095 [R(int) = 0.0190]
Completeness to theta = 28.46	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7164 and 0.5351
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3095 / 7 / 202
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0240, wR2 = 0.0659
R indices (all data)	R1 = 0.0243, wR2 = 0.0661
Absolute structure parameter	0.026(10)
Largest diff. peak and hole	0.349 and -0.291 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)	2698(1)	2682(1)	2588(1)	27(1)
O(1)	1270(2)	1213(2)	3105(2)	28(1)
O(2)	1354(2)	-914(2)	3565(2)	41(1)
O(3)	4660(2)	1496(1)	3214(2)	32(1)
O(4)	7317(2)	-1307(2)	4851(2)	42(1)
O(5)	8075(3)	-783(2)	2354(2)	39(1)
O(6)	4044(2)	4151(2)	1815(2)	30(1)
O(7)	3762(2)	6242(2)	1101(2)	36(1)
O(8)	720(2)	3780(1)	1834(2)	34(1)
O(9)	-2225(2)	5845(2)	2835(2)	40(1)
O(10)	-2972(2)	6451(2)	283(2)	36(1)
C(1)	2085(3)	154(2)	3448(2)	27(1)
C(2)	4093(2)	224(2)	3739(2)	25(1)
C(3)	5024(3)	-850(2)	2810(3)	30(1)
C(4)	6905(3)	-1012(2)	3456(3)	26(1)
C(5)	3142(3)	5189(2)	1575(2)	26(1)
C(6)	1199(2)	5138(2)	1980(2)	24(1)
C(7)	37(3)	6011(2)	901(2)	30(1)
C(8)	-1818(3)	6081(2)	1471(3)	26(1)
O(1W)	2228(2)	-3082(2)	5441(2)	43(1)
O(2W)	-2536(2)	3281(2)	983(3)	52(1)

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

Cu(1)-O(1)	1.9126(18)
Cu(1)-O(6)	1.9399(18)
Cu(1)-O(8)	1.9506(17)
Cu(1)-O(3)	1.9704(18)
Cu(1)-O(4)#1	2.338(2)
O(1)-C(1)	1.272(3)
O(2)-C(1)	1.231(3)
O(3)-C(2)	1.442(3)
O(3)-H(3C)	0.8200
O(4)-C(4)	1.207(3)
O(4)-Cu(1)#2	2.338(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)	1.439(3)
O(8)-H(8A)	0.8200
O(9)-C(8)	1.197(3)
O(10)-C(8)	1.332(3)
O(10)-H(10A)	0.8200
C(1)-C(2)	1.533(3)
C(2)-C(3)	1.530(3)
C(2)-H(2A)	0.9800
C(3)-C(4)	1.508(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(5)-C(6)	1.529(3)
C(6)-C(7)	1.509(3)
C(6)-H(6A)	0.9800
C(7)-C(8)	1.507(3)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
O(1W)-H(1A)	0.767(16)
O(1W)-H(1B)	0.803(17)
O(2W)-H(2B)	0.810(17)
O(2W)-H(2C)	0.833(17)

O(1)-Cu(1)-O(6)	173.66(7)
O(1)-Cu(1)-O(8)	94.98(8)
O(6)-Cu(1)-O(8)	81.99(8)
O(1)-Cu(1)-O(3)	83.54(8)
O(6)-Cu(1)-O(3)	99.10(8)
O(8)-Cu(1)-O(3)	175.98(7)
O(1)-Cu(1)-O(4)#1	96.99(8)
O(6)-Cu(1)-O(4)#1	88.58(8)
O(8)-Cu(1)-O(4)#1	89.53(8)
O(3)-Cu(1)-O(4)#1	94.36(7)
C(1)-O(1)-Cu(1)	116.32(14)
C(2)-O(3)-Cu(1)	113.58(12)
C(2)-O(3)-H(3C)	109.5
Cu(1)-O(3)-H(3C)	128.8
C(4)-O(4)-Cu(1)#2	161.10(17)
C(4)-O(5)-H(5A)	109.5

C(5)-O(6)-Cu(1)	114.10(14)
C(6)-O(8)-Cu(1)	110.00(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)	123.82(19)
O(2)-C(1)-C(2)	118.56(19)
O(1)-C(1)-C(2)	117.62(18)
O(3)-C(2)-C(3)	110.36(16)
O(3)-C(2)-C(1)	107.78(16)
C(3)-C(2)-C(1)	111.67(17)
O(3)-C(2)-H(2A)	109.0
C(3)-C(2)-H(2A)	109.0
C(1)-C(2)-H(2A)	109.0
C(4)-C(3)-C(2)	110.94(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)	122.7(2)
O(4)-C(4)-C(3)	123.80(19)
O(5)-C(4)-C(3)	113.53(19)
O(7)-C(5)-O(6)	124.15(19)
O(7)-C(5)-C(6)	118.71(18)
O(6)-C(5)-C(6)	117.07(18)
O(8)-C(6)-C(7)	112.62(16)
O(8)-C(6)-C(5)	104.92(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)	112.05(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)	123.2(2)
O(9)-C(8)-C(7)	124.49(19)
O(10)-C(8)-C(7)	112.30(18)
H(1A)-O(1W)-H(1B)	116(2)
H(2B)-O(2W)-H(2C)	108(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)	20(1)	22(1)	39(1)	4(1)	0(1)	0(1)
O(1)	20(1)	27(1)	39(1)	4(1)	1(1)	0(1)
O(2)	22(1)	30(1)	71(1)	12(1)	-1(1)	-2(1)
O(3)	20(1)	24(1)	50(1)	4(1)	-6(1)	-2(1)
O(4)	39(1)	52(1)	34(1)	7(1)	-1(1)	5(1)
O(5)	23(1)	54(1)	41(1)	4(1)	5(1)	-3(1)
O(6)	20(1)	26(1)	42(1)	4(1)	3(1)	2(1)
O(7)	21(1)	29(1)	59(1)	12(1)	2(1)	0(1)
O(8)	18(1)	25(1)	58(1)	4(1)	-6(1)	-1(1)
O(9)	30(1)	59(1)	32(1)	3(1)	5(1)	2(1)
O(10)	21(1)	47(1)	40(1)	11(1)	1(1)	1(1)
C(1)	20(1)	30(1)	31(1)	1(1)	2(1)	0(1)
C(2)	19(1)	24(1)	33(1)	1(1)	1(1)	0(1)
C(3)	22(1)	30(1)	37(1)	-6(1)	0(1)	0(1)
C(4)	24(1)	19(1)	34(1)	-2(1)	1(1)	1(1)
C(5)	20(1)	26(1)	31(1)	0(1)	-1(1)	0(1)
C(6)	17(1)	26(1)	30(1)	2(1)	0(1)	-1(1)
C(7)	20(1)	34(1)	34(1)	8(1)	4(1)	5(1)
C(8)	20(1)	23(1)	35(1)	1(1)	3(1)	1(1)
O(1W)	33(1)	40(1)	55(1)	9(1)	-5(1)	4(1)
O(2W)	24(1)	50(1)	80(1)	-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)	5620	1670	3665	38
H(5A)	9071	-900	2763	47
H(8A)	-350	3718	1665	41
H(10A)	-3834	5968	271	43
H(2A)	4388	128	4912	30
H(3A)	4396	-1669	2922	36
H(3B)	5008	-630	1656	36
H(6A)	1096	5407	3121	29
H(7A)	538	6883	898	35
H(7B)	9	5681	-211	35
H(1A)	1400(30)	-3370(30)	5800(40)	51
H(1B)	2100(40)	-2380(20)	5000(30)	51
H(2B)	-2640(40)	2620(20)	430(40)	62
H(2C)	-3530(30)	3480(30)	1300(40)	62

Table 6. Torsion angles [deg] for sad.

O(8)-Cu(1)-O(1)-C(1)	170.27(15)
O(3)-Cu(1)-O(1)-C(1)	-5.97(15)
O(4)#1-Cu(1)-O(1)-C(1)	-99.60(15)
O(1)-Cu(1)-O(3)-C(2)	-1.12(13)
O(6)-Cu(1)-O(3)-C(2)	-175.30(13)
O(4)#1-Cu(1)-O(3)-C(2)	95.44(14)
O(8)-Cu(1)-O(6)-C(5)	15.38(15)
O(3)-Cu(1)-O(6)-C(5)	-168.53(15)
O(4)#1-Cu(1)-O(6)-C(5)	-74.34(15)
O(1)-Cu(1)-O(8)-C(6)	155.80(13)
O(6)-Cu(1)-O(8)-C(6)	-29.81(13)
O(4)#1-Cu(1)-O(8)-C(6)	58.82(13)
Cu(1)-O(1)-C(1)-O(2)	-168.66(18)
Cu(1)-O(1)-C(1)-C(2)	11.6(2)
Cu(1)-O(3)-C(2)-C(3)	128.64(15)
Cu(1)-O(3)-C(2)-C(1)	6.46(19)
O(2)-C(1)-C(2)-O(3)	168.52(19)
O(1)-C(1)-C(2)-O(3)	-11.8(3)
O(2)-C(1)-C(2)-C(3)	47.1(3)
O(1)-C(1)-C(2)-C(3)	-133.1(2)
O(3)-C(2)-C(3)-C(4)	76.0(2)
C(1)-C(2)-C(3)-C(4)	-164.18(17)
Cu(1)#2-O(4)-C(4)-O(5)	-141.9(4)
Cu(1)#2-O(4)-C(4)-C(3)	39.1(6)
C(2)-C(3)-C(4)-O(4)	60.2(3)
C(2)-C(3)-C(4)-O(5)	-118.8(2)
Cu(1)-O(6)-C(5)-O(7)	179.03(17)
Cu(1)-O(6)-C(5)-C(6)	2.1(2)
Cu(1)-O(8)-C(6)-C(7)	159.52(13)
Cu(1)-O(8)-C(6)-C(5)	35.88(17)
O(7)-C(5)-C(6)-O(8)	157.53(19)
O(6)-C(5)-C(6)-O(8)	-25.4(2)
O(7)-C(5)-C(6)-C(7)	34.3(3)
O(6)-C(5)-C(6)-C(7)	-148.58(19)
O(8)-C(6)-C(7)-C(8)	68.9(2)
C(5)-C(6)-C(7)-C(8)	-172.26(17)
C(6)-C(7)-C(8)-O(9)	22.2(3)
C(6)-C(7)-C(8)-O(10)	-158.43(18)

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