Kupfer(II)-oximat

Empirical formula	C8 H16 Cu N2 O8
Formula weight	331.77
Temperature	299(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 6.109(1) A alpha = 102.02(2) deg. b = 7.008(1) A beta = 95.06(1) deg. c = 9.152(2) A gamma = 112.48(2) deg.
Volume	347.94(11) A^3
Z, Calculated density	1, 1.583 Mg/m^3
Absorption coefficient	1.604 mm^-1
F(000)	171
Crystal size	0.30 x 0.20 x 0.06 mm
Theta range for data collection	3.26 to 26.36 deg.
Limiting indices	-7<=h<=7, -7<=k<=8, -9<=l<=11
Reflections collected / unique	2162 / 1422 [R(int) = 0.0116]
Completeness to theta = 26.36	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9099 and 0.6447
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1422 / 2 / 94
Goodness-of-fit on F^2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0299, wR2 = 0.0802
R indices (all data)	R1 = 0.0319, wR2 = 0.0828
Largest diff. peak and hole	0.360 and -0.322 e.A^-3

Atomic parameters					
Atom	**Wyck**	**Site**	**x/a**	**y/b**	**z/c**
C1	2i	1	0.9775(4)	0.8085(3)	0.0768(3)
C2	2i	1	0.8876(4)	0.9022(4)	0.2111(3)
C3	2i	1	1.0425(6)	1.1171(5)	0.3131(3)
H3A	2i	1	1.07960	1.22140	0.25520
H3B	2i	1	1.18920	1.11580	0.35910
H3C	2i	1	0.95880	1.15320	0.39100
C4	2i	1	0.3797(6)	0.7115(5)	0.3679(4)
H4A	2i	1	0.40820	0.59220	0.38610
H4B	2i	1	0.25890	0.66370	0.27810
H4C	2i	1	0.32500	0.77260	0.45330
Cu1	1e	-1	1/2	1/2	0
N1	2i	1	0.6768(4)	0.7817(3)	0.2232(2)
O1	2i	1	0.5827(3)	0.3001(3)	0.1076(2)
H11	2i	1	0.668(5)	0.254(5)	0.061(3)
H12	2i	1	0.465(4)	0.194(4)	0.104(4)
O2	2i	1	0.8327(3)	0.6370(2)	-0.01778(19)
O3	2i	1	1.1906(3)	0.9043(3)	0.0669(2)
O4	2i	1	0.5975(4)	0.8687(3)	0.3475(2)

Anisotropic displacement parameters, in Å^2						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{12}**	**U_{13}**	**U_{23}**
C1	0.0243(10)	0.0253(10)	0.0437(12)	0.0102(9)	0.0093(9)	0.0151(9)
C2	0.0331(12)	0.0281(11)	0.0346(12)	0.0075(9)	0.0066(9)	0.0072(9)
C3	0.0527(16)	0.0400(15)	0.0431(14)	-0.0026(12)	0.0097(12)	0.0004(12)
C4	0.0511(17)	0.0505(17)	0.0528(16)	0.0092(14)	0.0276(14)	0.0051(13)
Cu1	0.0214(2)	0.0212(2)	0.0374(2)	0.00579(15)	0.00990(14)	0.00504(15)
N1	0.0351(10)	0.0294(10)	0.0397(11)	0.0111(8)	0.0149(8)	0.0049(8)
O1	0.0309(9)	0.0276(9)	0.0595(11)	0.0086(7)	0.0145(8)	0.0119(8)
O2	0.0255(8)	0.0258(8)	0.0444(9)	0.0083(6)	0.0143(7)	0.0058(7)
O3	0.0227(8)	0.0317(9)	0.0652(11)	0.0067(7)	0.0127(7)	0.0139(8)
O4	0.0533(12)	0.0366(10)	0.0472(10)	0.0083(9)	0.0259(9)	-0.0012(8)

Selected geometric informations

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
C1—O3	1.237(3)	C4—H4C	0.9600
C1—O2	1.263(3)	Cu1—O2	1.9264(16)
C1—C2	1.518(3)	Cu1—O2^{i}	1.9264(16)
C2—N1	1.271(3)	Cu1—O1^{i}	2.0533(19)
C2—C3	1.484(3)	Cu1—O1	2.0533(19)
C3—H3A	0.9600	Cu1—N1	2.353(2)
C3—H3B	0.9600	Cu1—N1^{i}	2.353(2)
C3—H3C	0.9600	N1—O4	1.390(3)
C4—O4	1.424(3)	O1—H11	0.814(18)
C4—H4A	0.9600	O1—H12	0.803(18)
C4—H4B	0.9600		

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
O3—C1—O2	123.6(2)	O2—Cu1—O1	89.84(7)
O3—C1—C2	117.8(2)	O2^{i}—Cu1—O1	90.16(7)
O2—C1—C2	118.60(19)	O1^{i}—Cu1—O1	180.00(5)
N1—C2—C3	126.2(2)	O2—Cu1—N1	75.49(7)
N1—C2—C1	113.88(19)	O2^{i}—Cu1—N1	104.51(7)
C3—C2—C1	120.0(2)	O1^{i}—Cu1—N1	89.95(8)
C2—C3—H3A	109.500	O1—Cu1—N1	90.05(8)
C2—C3—H3B	109.500	O2—Cu1—N1^{i}	104.51(7)
H3A—C3—H3B	109.500	O2^{i}—Cu1—N1^{i}	75.49(7)
C2—C3—H3C	109.500	O1^{i}—Cu1—N1^{i}	90.05(8)
H3A—C3—H3C	109.500	O1—Cu1—N1^{i}	89.95(8)
H3B—C3—H3C	109.500	N1—Cu1—N1^{i}	180.000
O4—C4—H4A	109.500	C2—N1—O4	113.28(19)
O4—C4—H4B	109.500	C2—N1—Cu1	109.04(15)
H4A—C4—H4B	109.500	O4—N1—Cu1	136.38(15)
O4—C4—H4C	109.500	Cu1—O1—H11	109.(2)
H4A—C4—H4C	109.500	Cu1—O1—H12	111.(2)
H4B—C4—H4C	109.500	H11—O1—H12	104.(3)
O2—Cu1—O2^{i}	180.0(1)	C1—O2—Cu1	121.68(14)
O2—Cu1—O1^{i}	90.16(7)	N1—O4—C4	109.80(19)
O2^{i}—Cu1—O1^{i}	89.84(7)		

Selected hydrogen bonds

Atoms D,H,A	Dist. D,H [Å	Dist. H,A [Å]	Dist. D,A [Å]	Angle D,H,A [°]
O1—H11—O3^{i}	0.814(18)	1.932(19)	2.734(3)	168.(3)
O1—H12—O3^{ii}	0.803(18)	2.016(19)	2.811(2)	170.(3)

(i) 2-x, 1-y, -z; (ii) -1+x, -1+y, z.