

data\_CuMoO4-phen

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_chemical_name_systematic	
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_chemical_melting_point	?
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_chemical_formula_sum	'C12 H8 Cu2 Mo2 N2 O8'
_chemical_formula_weight	627.17

loop_	
_atom_type_symbol	
_atom_type_description	
_atom_type_scatter_dispersion_real	
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C C 0.0181 0.0091	'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000	'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
N N 0.0311 0.0180	'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0492 0.0322	'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cu Cu -1.9646 0.5888	'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Mo Mo -0.0483 2.7339	'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting	Triclinic
_symmetry_space_group_name_H-M	P-1

loop_	
_symmetry_equiv_pos_as_xyz	
'x, y, z'	
'-x, -y, -z'	

_cell_length_a	7.4173(5)
_cell_length_b	9.2259(7)
_cell_length_c	13.8144(10)
_cell_angle_alpha	72.173(8)
_cell_angle_beta	89.886(6)
_cell_angle_gamma	73.221(7)
_cell_volume	857.75(11)
_cell_formula_units_Z	2
_cell_measurement_temperature	293(2)
_cell_measurement_reflns_used	2315
_cell_measurement_theta_min	13.53
_cell_measurement_theta_max	102.16

_exptl_crystal_description	needle
_exptl_crystal_colour	brown
_exptl_crystal_size_max	0.30
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_exptl_crystal_density_meas	?
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_exptl_absorpt_correction_type      empirical
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'data scaling includes absorption [ABSCOR, Higashi (1995)]'
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_diffrn_ambient_temperature         293(2)
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_diffrn_measurement_device_type       'Rigaku Spider'
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_diffrn_reflns_theta_min              6.76
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_reflns_number_total                  1836
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_reflns_threshold_expression           >2sigma(I)

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_computing_cell_refinement            'FS Process (Rigaku, 1998)'
_computing_data_reduction             'FS Process (Rigaku, 1998)'
_computing_structure_solution         'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement       'SHELXTL-6.10 (Sheldrick, 2008)'
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'Mercury (Macrae et. al., 2006) and DS Viewpro (Accelrys Inc., 2002)'
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Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and goodness of fit S are based on  $F^2$ , conventional R-factors R are based on F, with F set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-

factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
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loop\_

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_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Mo1 Mo 0.2993(7) 0.3138(5) -0.0054(3) 0.0404(19) Uani 1 1 d . . .
Mo2 Mo -0.1284(7) 0.0029(5) 0.1110(4) 0.045(2) Uani 1 1 d . . .
Cu2 Cu 0.3958(10) -0.0655(8) 0.1006(6) 0.038(3) Uani 1 1 d . . .
Cu1 Cu -0.2016(10) 0.3354(8) -0.0737(6) 0.043(3) Uani 1 1 d . . .
O1 O 0.079(5) 0.382(4) -0.086(2) 0.041(10) Uani 1 1 d U . .
O4 O 0.315(4) 0.158(3) 0.101(2) 0.024(9) Uani 1 1 d U . .
O5 O 0.107(5) -0.121(4) 0.099(2) 0.048(11) Uani 1 1 d U . .
O8 O -0.151(5) 0.211(4) 0.072(2) 0.044(10) Uani 1 1 d U . .
O3 O 0.496(4) 0.277(3) -0.071(2) 0.033(9) Uani 1 1 d U . .
O2 O 0.300(5) 0.479(4) 0.034(2) 0.053(11) Uani 1 1 d U . .
N1 N -0.276(6) 0.459(5) -0.220(3) 0.046(13) Uani 1 1 d U . .
C8 C 0.453(7) -0.167(6) 0.424(4) 0.043(16) Uani 1 1 d U . .
H8 H 0.4001 -0.1101 0.4673 0.052 Uiso 1 1 calc R . .
C6 C -0.201(9) 0.405(7) -0.287(5) 0.07(2) Uani 1 1 d U . .
H6 H -0.1042 0.3089 -0.2655 0.081 Uiso 1 1 calc R . .
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C7 C 0.381(8) -0.098(6) 0.315(4) 0.047(17) Uani 1 1 d U . .
H7 H 0.2732 -0.0101 0.2955 0.056 Uiso 1 1 calc R . .
O6 O -0.156(5) -0.057(4) 0.238(3) 0.061(12) Uani 1 1 d U . .
O7 O -0.322(5) -0.038(4) 0.052(2) 0.048(11) Uani 1 1 d U . .
N2 N 0.468(7) -0.160(6) 0.243(4) 0.065(15) Uani 1 1 d U . .
C12 C 0.609(8) -0.309(7) 0.296(4) 0.056(18) Uani 1 1 d U . .
H12 H 0.6778 -0.3665 0.2565 0.067 Uiso 1 1 calc R . .
C4 C -0.251(9) 0.480(7) -0.401(5) 0.061(19) Uani 1 1 d U . .
C1 C -0.388(8) 0.598(7) -0.260(4) 0.058(18) Uani 1 1 d U . .
H1 H -0.4246 0.6584 -0.2166 0.069 Uiso 1 1 calc R . .
C2 C -0.464(8) 0.673(7) -0.364(4) 0.054(17) Uani 1 1 d U . .
H2 H -0.5747 0.7585 -0.3799 0.064 Uiso 1 1 calc R . .
C3 C -0.384(8) 0.626(6) -0.437(5) 0.047(17) Uani 1 1 d U . .
C5 C -0.152(10) 0.406(9) -0.463(5) 0.10(2) Uani 1 1 d U . .
H5 H -0.0629 0.3057 -0.4362 0.118 Uiso 1 1 calc R . .
C10 C 0.648(8) -0.370(7) 0.396(4) 0.047(16) Uani 1 1 d U . .
C11 C 0.808(10) -0.504(8) 0.415(5) 0.09(2) Uani 1 1 d U . .
H11 H 0.8786 -0.5365 0.3656 0.102 Uiso 1 1 calc R . .
C9 C 0.594(7) -0.308(6) 0.465(4) 0.038(15) Uani 1 1 d U . .

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  _atom_site_aniso_U_13
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Mo1 0.041(4) 0.028(3) 0.044(4) -0.007(3) 0.008(3) -0.003(3)
Mo2 0.043(4) 0.031(3) 0.047(4) -0.007(3) 0.004(3) 0.002(3)
Cu2 0.029(6) 0.023(5) 0.054(6) -0.007(4) 0.011(4) -0.003(4)
Cu1 0.024(6) 0.023(5) 0.069(6) -0.012(4) 0.011(4) 0.009(4)
O1 0.044(11) 0.039(11) 0.042(11) -0.016(6) 0.001(5) -0.012(6)
O4 0.023(10) 0.023(9) 0.024(9) -0.009(5) 0.006(5) -0.005(5)
O5 0.049(12) 0.048(11) 0.046(11) -0.016(6) 0.005(5) -0.015(6)
O8 0.042(11) 0.045(11) 0.046(11) -0.014(6) 0.004(5) -0.015(6)
O3 0.035(10) 0.030(10) 0.035(10) -0.012(6) 0.001(5) -0.009(5)
O2 0.053(12) 0.053(12) 0.053(12) -0.016(6) 0.005(5) -0.017(6)
N1 0.046(14) 0.045(14) 0.046(14) -0.014(6) 0.004(5) -0.013(6)
C8 0.044(17) 0.043(17) 0.043(17) -0.014(7) 0.004(5) -0.013(7)
C6 0.07(2) 0.07(2) 0.07(2) -0.022(8) 0.006(5) -0.021(8)
C7 0.048(17) 0.047(17) 0.046(17) -0.014(7) 0.005(5) -0.015(7)
O6 0.062(13) 0.060(13) 0.062(13) -0.020(6) 0.007(5) -0.018(6)
O7 0.047(12) 0.046(12) 0.048(12) -0.016(6) 0.007(5) -0.012(6)
N2 0.066(16) 0.064(16) 0.066(16) -0.022(7) 0.006(5) -0.020(7)
C12 0.056(19) 0.056(19) 0.056(19) -0.017(8) 0.006(5) -0.017(7)
C4 0.062(19) 0.061(19) 0.061(19) -0.020(8) 0.005(5) -0.018(7)
C1 0.058(19) 0.057(19) 0.058(19) -0.020(8) 0.005(5) -0.016(7)
C2 0.054(18) 0.054(18) 0.053(18) -0.017(7) 0.006(5) -0.017(7)
C3 0.047(17) 0.047(17) 0.047(17) -0.015(7) 0.005(5) -0.013(7)
C5 0.10(3) 0.10(2) 0.10(3) -0.031(9) 0.009(6) -0.029(9)
C10 0.046(17) 0.047(17) 0.047(17) -0.014(7) 0.005(5) -0.015(7)
C11 0.09(2) 0.09(2) 0.08(2) -0.027(9) 0.008(6) -0.026(8)
C9 0.039(16) 0.038(16) 0.038(16) -0.013(7) 0.004(5) -0.010(7)

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_geom_special_details
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All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

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Mo1 O4 1.69(3) . ?  
Mo1 O3 1.72(3) . ?  
Mo1 O2 1.77(3) . ?  
Mo1 O1 1.82(3) . ?  
Mo2 O6 1.70(4) . ?  
Mo2 O8 1.79(3) . ?  
Mo2 O5 1.83(3) . ?  
Mo2 O7 1.83(4) . ?  
Cu2 N2 1.89(5) . ?  
Cu2 O4 1.97(3) . ?  
Cu2 O7 2.03(3) 2 ?  
Cu2 O3 2.05(3) 2\_655 ?  
Cu2 O7 2.26(4) 1\_655 ?  
Cu2 O5 2.34(4) . ?  
Cu1 O2 1.90(3) 2\_565 ?  
Cu1 O8 1.96(3) . ?  
Cu1 N1 1.98(4) . ?  
Cu1 O5 2.04(3) 2 ?  
Cu1 O1 2.24(4) . ?  
O5 Cu1 2.04(3) 2 ?  
O3 Cu2 2.05(3) 2\_655 ?  
O2 Cu1 1.90(3) 2\_565 ?  
N1 C6 1.24(6) . ?  
N1 C1 1.26(6) . ?  
C8 C9 1.37(6) . ?  
C8 C7 1.47(6) . ?  
C6 C4 1.50(7) . ?  
C7 N2 1.37(6) . ?  
O7 Cu2 2.03(3) 2 ?  
O7 Cu2 2.26(4) 1\_455 ?  
N2 C12 1.44(6) . ?  
C12 C10 1.32(6) . ?  
C4 C5 1.35(7) . ?  
C4 C3 1.36(7) . ?  
C1 C2 1.42(7) . ?  
C2 C3 1.29(6) . ?  
C3 C9 1.29(6) 1\_464 ?  
C5 C11 1.62(8) 1\_464 ?  
C10 C9 1.26(6) . ?  
C10 C11 1.40(7) . ?  
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C9 C3 1.29(6) 1\_646 ?

loop\_

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O3 Mo1 O2 106.0(15) . . ?
O4 Mo1 O1 114.2(15) . . ?
O3 Mo1 O1 113.1(14) . . ?
O2 Mo1 O1 104.5(14) . . ?
O6 Mo2 O8 107.7(16) . . ?
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O6 Mo2 O7 103.9(16) . . ?
O8 Mo2 O7 112.4(15) . . ?
O5 Mo2 O7 113.9(15) . . ?
N2 Cu2 O4 96.0(17) . . ?
N2 Cu2 O7 178.9(19) . 2 ?
O4 Cu2 O7 83.4(12) . 2 ?
N2 Cu2 O3 93.6(17) . 2_655 ?
O4 Cu2 O3 167.5(12) . 2_655 ?
O7 Cu2 O3 86.8(12) 2 2_655 ?
N2 Cu2 O7 97.5(17) . 1_655 ?
O4 Cu2 O7 89.5(12) . 1_655 ?
O7 Cu2 O7 81.6(14) 2 1_655 ?
O3 Cu2 O7 81.3(12) 2_655 1_655 ?
N2 Cu2 O5 97.7(17) . . ?
O4 Cu2 O5 102.0(12) . . ?
O7 Cu2 O5 83.3(13) 2 . ?
O3 Cu2 O5 84.5(12) 2_655 . ?
O7 Cu2 O5 159.8(12) 1_655 . ?
O2 Cu1 O8 87.6(14) 2_565 . ?
O2 Cu1 N1 92.0(17) 2_565 . ?
O8 Cu1 N1 174.7(17) . . ?
O2 Cu1 O5 172.8(14) 2_565 2 ?
O8 Cu1 O5 86.1(13) . 2 ?
N1 Cu1 O5 93.9(16) . 2 ?
O2 Cu1 O1 89.4(14) 2_565 . ?
O8 Cu1 O1 94.7(13) . . ?
N1 Cu1 O1 90.5(15) . . ?
O5 Cu1 O1 94.6(13) 2 . ?
Mo1 O1 Cu1 136.6(17) . . ?
Mo1 O4 Cu2 122.3(16) . . ?
Mo2 O5 Cu1 132.8(19) . 2 ?
Mo2 O5 Cu2 128.6(17) . . ?
Cu1 O5 Cu2 98.5(14) 2 . ?
Mo2 O8 Cu1 118.9(18) . . ?
Mo1 O3 Cu2 122.1(17) . 2_655 ?
Mo1 O2 Cu1 158(2) . 2_565 ?
C6 N1 C1 110(5) . . ?
C6 N1 Cu1 121(4) . . ?
C1 N1 Cu1 129(4) . . ?
C9 C8 C7 125(5) . . ?
N1 C6 C4 127(6) . . ?
N2 C7 C8 122(5) . . ?

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Mo2 O7 Cu2 119.2(17) . 2 ?  
 Mo2 O7 Cu2 134.0(17) . 1\_455 ?  
 Cu2 O7 Cu2 98.4(14) 2 1\_455 ?  
 C7 N2 C12 107(5) . . ?  
 C7 N2 Cu2 124(4) . . ?  
 C12 N2 Cu2 129(4) . . ?  
 C10 C12 N2 125(6) . . ?  
 C5 C4 C3 123(6) . . ?  
 C5 C4 C6 118(6) . . ?  
 C3 C4 C6 119(6) . . ?  
 N1 C1 C2 128(6) . . ?  
 C3 C2 C1 122(6) . . ?  
 C2 C3 C9 132(6) . 1\_464 ?  
 C2 C3 C4 112(6) . . ?  
 C9 C3 C4 116(6) 1\_464 . ?  
 C4 C5 C11 118(6) . 1\_464 ?  
 C9 C10 C12 130(6) . . ?  
 C9 C10 C11 121(6) . . ?  
 C12 C10 C11 107(6) . . ?  
 C10 C11 C5 109(6) . 1\_646 ?  
 C10 C9 C3 130(6) . 1\_646 ?  
 C10 C9 C8 110(6) . . ?  
 C3 C9 C8 118(6) 1\_646 . ?

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