

data_Cu3Cr2O10-phen

```
_audit_creation_method          SHELXL-97
_chemical_name_systematic
;
?
;
_chemical_name_common           ?
_chemical_melting_point         ?
_chemical_formula_moiety        'C12 H8 Cr2 Cu3 N2 O10'
_chemical_formula_sum           'C12 H8 Cr2 Cu3 N2 O10'
_chemical_formula_weight        634.82
```

```
loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
  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'
  Cr Cr -0.1635  2.4439  '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                  5.6292(7)
_cell_length_b                  5.6494(6)
_cell_length_c                  13.7959(13)
_cell_angle_alpha               92.654(7)
_cell_angle_beta               90.330(7)
_cell_angle_gamma              109.093(8)
_cell_volume                    414.05(8)
_cell_formula_units_Z           1
_cell_measurement_temperature   293(2)
_cell_measurement_reflns_used   466
_cell_measurement_theta_min     16.67
_cell_measurement_theta_max     117.68

_exptl_crystal_description      plate
_exptl_crystal_colour           bronze-yellow
_exptl_crystal_size_max         0.12
```

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_exptl_crystal_size_mid      0.08
_exptl_crystal_size_min      0.02
_exptl_crystal_density_meas  ?
_exptl_crystal_density_diffn 2.546
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000         309
_exptl_absorpt_coefficient_mu 15.331
_exptl_absorpt_correction_type empirical
_exptl_absorpt_correction_T_min 0.519
_exptl_absorpt_correction_T_max 1.000
_exptl_absorpt_process_details

'data scaling includes absorption [ABSCOR, Higashi (1995)]'
_exptl_special_details
;
?
;

_diffn_ambient_temperature    293(2)
_diffn_radiation_wavelength    1.54178
_diffn_radiation_type          CuK\alpha
_diffn_radiation_source        'rotating anode'
_diffn_radiation_monochromator 'confocal optics'
_diffn_measurement_device_type  'Rigaku Spider'
_diffn_measurement_device_details 'cureved image plate detector'
_diffn_measurement_method      \w-scans
_diffn_detector_area_resol_mean 10
_diffn_standards_number        0
_diffn_standards_interval_count ?
_diffn_standards_interval_time ?
_diffn_standards_decay_%       0
_diffn_reflns_number           3772
_diffn_reflns_av_R_equivalents 0.1336
_diffn_reflns_av_sigmaI/netI   0.1518
_diffn_reflns_limit_h_min      -5
_diffn_reflns_limit_h_max      6
_diffn_reflns_limit_k_min      -6
_diffn_reflns_limit_k_max      6
_diffn_reflns_limit_l_min      -15
_diffn_reflns_limit_l_max      15
_diffn_reflns_theta_min        8.31
_diffn_reflns_theta_max        58.83
_reflns_number_total           1061
_reflns_number_gt              717
_reflns_threshold_expression    >2sigma(I)

_computing_data_collection      'Crystal Clear (Rigaku, 2005)'
_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)'
_computing_molecular_graphics   'Mercury (Macrae et. al., 2006) and DS Viewpro (Accelrys Inc., 2002)'
_computing_publication_material 'SHELXL-97 (Sheldrick, 2008)'

_refine_special_details
;

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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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```
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme        calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.2000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary       direct
_atom_sites_solution_secondary     difmap
_atom_sites_solution_hydrogens     geom
_refine_ls_hydrogen_treatment      mixed
_refine_ls_extinction_method        SHELXL
_refine_ls_extinction_coef          0.014(8)
_refine_ls_extinction_expression
'Fc^*=kFc[1+0.001xFc^2^/l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns           1061
_refine_ls_number_parameters        143
_refine_ls_number_restraints        86
_refine_ls_R_factor_all             0.2269
_refine_ls_R_factor_gt              0.1997
_refine_ls_wR_factor_ref            0.5150
_refine_ls_wR_factor_gt            0.4802
_refine_ls_goodness_of_fit_ref      1.818
_refine_ls_restrained_S_all         1.750
_refine_ls_shift/su_max             0.000
_refine_ls_shift/su_mean            0.000
```

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  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _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
O1 O 0.349(5) 0.644(4) 0.4712(15) 0.066(6) Uani 1 1 d U . .
O5 O 1.120(5) 1.228(4) 0.5950(15) 0.063(6) Uani 1 1 d U . .
Cu1 Cu 0.3922(9) 0.5494(8) 0.6047(3) 0.057(2) Uani 1 1 d . . .
Cu2 Cu 0.5000 1.0000 0.5000 0.060(3) Uani 1 2 d S . .
Cr3 Cr 0.9524(11) 0.9745(9) 0.6500(3) 0.057(3) Uani 1 1 d . . .
O2 O 0.635(4) 0.893(4) 0.6129(13) 0.055(6) Uani 1 1 d U . .
O3 O 1.062(4) 0.744(4) 0.6254(12) 0.050(5) Uani 1 1 d U . .
O4 O 0.977(4) 1.036(4) 0.7649(14) 0.063(6) Uani 1 1 d U . .
N1 N 0.434(5) 0.524(4) 0.7412(15) 0.046(6) Uani 1 1 d DU . .
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```

C1 C 0.328(6) 0.632(6) 0.8094(17) 0.063(9) Uani 1 1 d DU . .
H1 H 0.2229 0.7161 0.7873 0.076 Uiso 1 1 calc R . .
C4 C 0.492(6) 0.493(5) 0.9513(19) 0.055(8) Uani 1 1 d DU . .
C2 C 0.358(7) 0.630(7) 0.9092(19) 0.076(11) Uani 1 1 d DU . .
C7 C 0.559(7) 0.379(7) 0.781(2) 0.078(11) Uani 1 1 d DU . .
H7 H 0.6204 0.2793 0.7396 0.093 Uiso 1 1 calc R . .
C5 C 0.596(8) 0.376(7) 0.881(2) 0.084(12) Uani 1 1 d DU . .
C3 C 0.236(9) 0.751(8) 0.970(3) 0.034(12) Uani 0.50 1 d PDU . .
H3 H 0.1342 0.8334 0.9438 0.041 Uiso 1 1 calc R . .
C6 C 0.736(11) 0.251(11) 0.928(4) 0.065(18) Uani 0.50 1 d PDU . .
H6 H 0.8167 0.1621 0.8897 0.078 Uiso 1 1 calc R . .

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  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_23
  _atom_site_aniso_U_13
  _atom_site_aniso_U_12
O1 0.066(8) 0.067(7) 0.062(7) 0.006(5) -0.001(5) 0.017(5)
O5 0.064(7) 0.062(7) 0.062(7) 0.002(5) 0.005(5) 0.019(5)
Cu1 0.060(4) 0.035(3) 0.056(3) -0.0010(19) 0.006(2) -0.009(2)
Cu2 0.064(6) 0.040(4) 0.057(4) -0.007(3) 0.002(3) -0.006(3)
Cr3 0.054(5) 0.041(4) 0.059(4) 0.002(2) 0.007(3) -0.009(3)
O2 0.056(7) 0.054(7) 0.053(7) 0.004(4) 0.000(5) 0.015(5)
O3 0.051(7) 0.047(7) 0.052(6) -0.002(4) 0.004(4) 0.020(5)
O4 0.062(8) 0.062(7) 0.062(7) -0.002(5) 0.000(5) 0.017(5)
N1 0.048(8) 0.043(7) 0.047(7) -0.001(5) 0.004(5) 0.015(5)
C1 0.063(10) 0.063(10) 0.065(10) 0.006(5) -0.001(5) 0.023(5)
C4 0.056(10) 0.055(9) 0.055(9) 0.000(5) 0.001(5) 0.019(5)
C2 0.078(12) 0.075(12) 0.075(11) 0.002(5) 0.003(5) 0.023(6)
C7 0.077(12) 0.078(12) 0.077(11) 0.003(5) 0.005(5) 0.024(6)
C5 0.084(13) 0.084(13) 0.085(12) 0.005(5) 0.001(5) 0.027(6)
C3 0.035(13) 0.035(13) 0.036(13) 0.004(5) -0.002(5) 0.014(6)
C6 0.066(19) 0.064(19) 0.065(19) 0.002(5) 0.001(5) 0.021(8)

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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_
  _geom_bond_atom_site_label_1
  _geom_bond_atom_site_label_2
  _geom_bond_distance
  _geom_bond_site_symmetry_2
  _geom_bond_publ_flag
O1 Cu2 1.93(2) . ?
O1 Cu1 1.98(2) . ?

```

O1 Cu1 2.32(3) 2_666 ?
 O5 Cr3 1.66(2) . ?
 O5 Cu1 1.95(2) 1_665 ?
 Cu1 N1 1.91(2) . ?
 Cu1 O5 1.95(2) 1_445 ?
 Cu1 O2 1.97(2) . ?
 Cu1 O1 2.32(3) 2_666 ?
 Cu2 O1 1.93(2) 2_676 ?
 Cu2 O2 1.93(2) . ?
 Cu2 O2 1.93(2) 2_676 ?
 Cu2 Cu1 2.877(4) 2_676 ?
 Cr3 O4 1.601(19) . ?
 Cr3 O3 1.64(2) . ?
 Cr3 O2 1.76(2) . ?
 N1 C1 1.343(18) . ?
 N1 C7 1.366(19) . ?
 C1 C2 1.388(18) . ?
 C4 C4 1.34(5) 2_667 ?
 C4 C2 1.386(19) . ?
 C4 C5 1.387(19) . ?
 C2 C3 1.38(2) . ?
 C7 C5 1.397(19) . ?
 C5 C6 1.40(2) . ?
 C3 C6 1.42(7) 2_667 ?
 C6 C3 1.42(7) 2_667 ?

loop_
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 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
 Cu2 O1 Cu1 94.8(9) . . ?
 Cu2 O1 Cu1 115.3(11) . 2_666 ?
 Cu1 O1 Cu1 97.5(11) . 2_666 ?
 Cr3 O5 Cu1 147.4(14) . 1_665 ?
 N1 Cu1 O5 91.8(9) . 1_445 ?
 N1 Cu1 O2 90.1(9) . . ?
 O5 Cu1 O2 173.0(10) 1_445 . ?
 N1 Cu1 O1 168.5(9) . . ?
 O5 Cu1 O1 95.9(9) 1_445 . ?
 O2 Cu1 O1 81.3(8) . . ?
 N1 Cu1 O1 106.3(9) . 2_666 ?
 O5 Cu1 O1 88.6(9) 1_445 2_666 ?
 O2 Cu1 O1 97.3(9) . 2_666 ?
 O1 Cu1 O1 82.5(11) . 2_666 ?
 O1 Cu2 O1 180.000(5) 2_676 . ?
 O1 Cu2 O2 96.5(9) 2_676 . ?
 O1 Cu2 O2 83.5(9) . . ?
 O1 Cu2 O2 83.5(9) 2_676 2_676 ?
 O1 Cu2 O2 96.5(9) . 2_676 ?
 O2 Cu2 O2 180.000(7) . 2_676 ?
 O1 Cu2 Cu1 43.2(6) 2_676 2_676 ?
 O1 Cu2 Cu1 136.8(6) . 2_676 ?
 O2 Cu2 Cu1 136.9(6) . 2_676 ?
 O2 Cu2 Cu1 43.1(6) 2_676 2_676 ?

O4 Cr3 O3 108.3(11) . . ?
 O4 Cr3 O5 108.7(11) . . ?
 O3 Cr3 O5 110.0(11) . . ?
 O4 Cr3 O2 109.3(11) . . ?
 O3 Cr3 O2 111.2(11) . . ?
 O5 Cr3 O2 109.3(11) . . ?
 Cr3 O2 Cu2 127.6(11) . . ?
 Cr3 O2 Cu1 125.0(13) . . ?
 Cu2 O2 Cu1 94.8(8) . . ?
 C1 N1 C7 112(3) . . ?
 C1 N1 Cu1 124(2) . . ?
 C7 N1 Cu1 124.2(18) . . ?
 N1 C1 C2 127(3) . . ?
 C4 C4 C2 117(3) 2_667 . ?
 C4 C4 C5 133(3) 2_667 . ?
 C2 C4 C5 111(3) . . ?
 C3 C2 C4 118(3) . . ?
 C3 C2 C1 120(3) . . ?
 C4 C2 C1 122(3) . . ?
 N1 C7 C5 122(3) . . ?
 C4 C5 C6 108(4) . . ?
 C4 C5 C7 125(3) . . ?
 C6 C5 C7 127(4) . . ?
 C2 C3 C6 120(4) . 2_667 ?
 C5 C6 C3 125(5) . 2_667 ?

_diffn_measured_fraction_theta_max	0.891
_diffn_reflns_theta_full	58.83
_diffn_measured_fraction_theta_full	0.891
_refine_diff_density_max	1.345
_refine_diff_density_min	-1.855
_refine_diff_density_rms	0.337