```
#======================================================================
#----------------------------------------------------------------------
data trans-[CuCl2(dmen)2].H2O  (compound 13c)
#----------------------------------------------------------------------
# CHEMICAL DATA
_chemical_formula_sum              'C8 H26 Cl2 Cu N4 O '
_chemical_formula_moiety            'C8 H26 Cl2 Cu N4 O '
_chemical_formula_weight            328.77
_chemical_melting_point             ?
#----------------------------------------------------------------------
# CRYSTAL DATA
_symmetry_cell_setting              monoclinic
_symmetry_space_group_name_H-M      'C 1 2 1'
_symmetry_Int_Tables_number         5
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,y,-z
1/2+x,1/2+y,z
```

```
1/2-x,1/2+y,-z
_cell_length_a                    10.668(8)
_cell_length_b                    8.306(6)
_cell_length_c                    9.478(7)
_cell_angle_alpha                 90
_cell_angle_beta                  122.187(2)
_cell_angle_gamma                 90
_cell_volume                      710.7(9)
_cell_formula_units_Z             2
_cell_measurement_reflns_used     674
_cell_measurement_theta_min       4.7
_cell_measurement_theta_max       26.7
_cell_measurement_temperature     153.2
#-----------------------------------------------------------------------------
_exptl_crystal_description        'block'
_exptl_crystal_colour             'blue'
_exptl_crystal_size_max           0.350
_exptl_crystal_size_mid           0.300
_exptl_crystal_size_min           0.200
_exptl_crystal_size_rad           ?
_exptl_crystal_density_diffrn     1.536
_exptl_crystal_density_meas       ?
_exptl_crystal_density_method     'not measured'
_exptl_absorpt_coefficient_mu     1.900
_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_process_details    'Jacobson, R. (1998) Private
communication'
_exptl_absorpt_correction_T_min   0.684
_exptl_absorpt_correction_T_max   1.000
#-----------------------------------------------------------------------------
# EXPERIMENTAL DATA
_diffrn_radiation_type            'Mo K\a'
_diffrn_radiation_wavelength      0.7107
_diffrn_measurement_device_type   'Rigaku/MSC Mercury CCD'
_diffrn_measurement_method        \w
_diffrn_detector_area_resol_mean  14.71
_diffrn_reflns_number             1587
_diffrn_reflns_av_R_equivalents   0.010
_diffrn_reflns_theta_min          3.00
_diffrn_reflns_theta_max          26.58
_diffrn_reflns_limit_h_min        0
_diffrn_reflns_limit_h_max        13
_diffrn_reflns_limit_k_min        0
_diffrn_reflns_limit_k_max        9
_diffrn_reflns_limit_l_min        -11
_diffrn_reflns_limit_l_max        9
#-----------------------------------------------------------------------------
# REFINEMENT DATA
_refine_special_details
;
```

Refinement using reflections with F^2^ > 2.0 sigma(F^2^). The weighted R-factor (wR) and goodness of fit (S) are based on F^2^. R-factor (gt) are based on F. The threshold expression of F^2^ > 2.0 sigma(F^2^) is used only for calculating R-factor (gt).
;
_reflns_number_total 592
_reflns_number_gt 558
_reflns_threshold_expression >2.0sigma(I)
_refine_ls_structure_factor_coef Fsqd
_refine_ls_R_factor_gt 0.0752
_refine_ls_wR_factor_ref 0.1484
_refine_ls_hydrogen_treatment noref
_refine_ls_number_reflns 558
_refine_ls_number_parameters 75
_refine_ls_goodness_of_fit_ref 1.121
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'w = 1/[\s^2^(Fo^2^) + (0.0445P)^2^+6.1836P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_shift/su_max 0.0351
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details
'Flack, H. D. (1983), Acta Cryst. A39, 876-881. 2580 Friedel Pairs'
_refine_ls_abs_structure_Flack 0.08(6)
_refine_diff_density_max 0.56
_refine_diff_density_min -0.56
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
'C' 'C' 0.003 0.002
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
'H' 'H' 0.000 0.000
;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.4)
;
'Cl' 'Cl' 0.148 0.159
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
'Cu' 'Cu' 0.320 1.265
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
'N' 'N' 0.006 0.003
;International Tables for Crystallography

```
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
  'O' 'O'  0.011 0.006
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
;
#---------------------------------------------------------------------------
# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
loop_
_atom_site_label
_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_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
 Cu(1)  Cu 0.5000     0.1894(2)   1.0000     0.0227(6)   Uani 1.00 d S . .
 Cl(1)  Cl 0.8113(2)  0.1915(6)   1.1168(2)  0.0273(6)   Uani 1.00 d . . .
 O(1)   O  1.0000     0.103(3)    1.5000     0.093(6)    Uani 1.00 d S . .
 N(1)   N  0.518(1)   0.028(2)    1.170(1)   0.029(3)    Uani 1.00 d . . .
 N(2)   N  0.525(1)   0.360(2)    1.172(1)   0.035(3)    Uani 1.00 d . . .
 C(1)   C  0.636(2)   -0.106(3)   1.226(3)   0.062(6)    Uani 1.00 d . . .
 C(2)   C  0.494(1)   0.122(2)    1.290(1)   0.040(3)    Uani 1.00 d . . .
 C(3)   C  0.580(1)   0.277(2)    1.329(1)   0.044(3)    Uani 1.00 d . . .
 C(4)   C  0.642(2)   0.462(2)    1.231(2)   0.048(5)    Uani 1.00 d . . .
 H(1)   H  0.3942     0.1451      1.2443     0.0507      Uiso 1.00 calc . . .
 H(2)   H  0.5328     0.0633      1.3924     0.0507      Uiso 1.00 calc . . .
 H(3)   H  0.6833     0.2539      1.3781     0.0540      Uiso 1.00 calc . . .
 H(4)   H  0.5667     0.3411      1.4010     0.0540      Uiso 1.00 calc . . .
 H(5)   H  0.6208     -0.1847     1.2875     0.0861      Uiso 1.00 calc . . .
 H(6)   H  0.6319     -0.1509     1.1335     0.0861      Uiso 1.00 calc . . .
 H(7)   H  0.7316     -0.0570     1.2981     0.0861      Uiso 1.00 calc . . .
 H(8)   H  0.7323     0.4093      1.2720     0.0614      Uiso 1.00 calc . . .
 H(9)   H  0.6261     0.5351      1.1420     0.0614      Uiso 1.00 calc . . .
 H(10)  H  0.6481     0.5299      1.3174     0.0614      Uiso 1.00 calc . . .
 H(11)  H  0.4283     -0.0340     1.1091     0.0385      Uiso 1.00 calc . . .
 H(12)  H  0.4343     0.4113      1.1371     0.0406      Uiso 1.00 calc . . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
```

```
_atom_site_aniso_U_23
 Cu(1)  0.0331(8)   0.0223(9)   0.0159(7)   0.0000     0.0151(5)   0.0000
 Cl(1)  0.0197(9)   0.035(1)    0.0269(9)   0.000(2)    0.0120(7)   0.001(2)
 O(1)   0.12(1)     0.08(1)     0.034(6)    0.0000      0.014(7)    0.0000
 N(1)   0.037(7)    0.030(7)    0.022(6)    0.002(6)    0.017(6)    0.000(6)
 N(2)   0.037(7)    0.038(8)    0.025(6)    0.012(6)    0.014(5)    -0.007(6)
 C(1)   0.031(8)    0.05(1)     0.09(1)     0.003(6)    0.019(8)    0.042(8)
 C(2)   0.047(6)    0.056(7)    0.027(5)    -0.006(6)   0.025(4)    0.002(5)
 C(3)   0.040(6)    0.062(7)    0.033(5)    -0.004(6)   0.021(4)    -0.017(5)
 C(4)   0.037(8)    0.06(1)     0.045(8)    0.010(7)    0.017(7)    -0.025(7)
#-------------------------------------------------------------------------------
_computing_data_collection          'CRYSTALCLEAR'
_computing_cell_refinement          'CRYSTALCLEAR'
_computing_data_reduction           'teXsan Ver. 1.11'
_computing_structure_solution         SIR92
_computing_structure_refinement      'SHELXL93'
_computing_publication_material      'teXsan Ver. 1.11'
_computing_molecular_graphics        'ORTEP-II'
#-------------------------------------------------------------------------------
_geom_special_details
;
 ?
;
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Cu(1)    Cl(1)    2.887(3)   . . yes
 Cu(1)    Cl(1)    2.887(3)   . 2_657 yes
 Cu(1)    N(1)     2.02(1)    . . yes
 Cu(1)    N(1)     2.02(1)    . 2_657 yes
 Cu(1)    N(2)     2.06(1)    . . yes
 Cu(1)    N(2)     2.06(1)    . 2_657 yes
 N(1)     C(1)     1.55(2)    . . yes
 N(1)     C(2)     1.51(2)    . . yes
 N(2)     C(3)     1.45(2)    . . yes
 N(2)     C(4)     1.35(2)    . . yes
 C(2)     C(3)     1.50(2)    . . yes
#-------------------------------------------------------------------------------
loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
```

```
_geom_angle_publ_flag
  Cl(1)    Cu(1)    Cl(1)    179.3(2)   . . 2_657 yes
  Cl(1)    Cu(1)    N(1)     95.6(4)    . . . yes
  Cl(1)    Cu(1)    N(1)     84.9(4)    . . 2_657 yes
  Cl(1)    Cu(1)    N(2)     93.0(4)    . . . yes
  Cl(1)    Cu(1)    N(2)     86.5(4)    . . 2_657 yes
  Cl(1)    Cu(1)    N(1)     84.9(4)    2_657 . . yes
  Cl(1)    Cu(1)    N(1)     95.6(4)    2_657 . 2_657 yes
  Cl(1)    Cu(1)    N(2)     86.5(4)    2_657 . . yes
  Cl(1)    Cu(1)    N(2)     93.0(4)    2_657 . 2_657 yes
  N(1)     Cu(1)    N(1)     96.9(8)    . . 2_657 yes
  N(1)     Cu(1)    N(2)     84.9(6)    . . . yes
  N(1)     Cu(1)    N(2)     177.3(6)   . . 2_657 yes
  N(1)     Cu(1)    N(2)     177.3(6)   2_657 . . yes
  N(1)     Cu(1)    N(2)     84.9(6)    2_657 . 2_657 yes
  N(2)     Cu(1)    N(2)     93.2(8)    . . 2_657 yes
  Cu(1)    N(1)     C(1)     117(1)     . . . yes
  Cu(1)    N(1)     C(2)     105.7(9)   . . . yes
  C(1)     N(1)     C(2)     123(1)     . . . yes
  Cu(1)    N(2)     C(3)     107.1(10)  . . . yes
  Cu(1)    N(2)     C(4)     117(1)     . . . yes
  C(3)     N(2)     C(4)     95(1)      . . . yes
  N(1)     C(2)     C(3)     107(1)     . . . yes
  N(2)     C(3)     C(2)     107.1(9)   . . . yes
  N(1)     Cu(1)    N(1)     96.9(8)    . . 2_657 yes
  N(1)     Cu(1)    N(2)     84.9(6)    . . . yes
  N(1)     Cu(1)    N(2)     177.3(6)   . . 2_657 yes
  N(1)     Cu(1)    Cl(1)    95.6(4)    . . . yes
  N(1)     Cu(1)    Cl(1)    84.9(4)    . . 2_657 yes
  N(1)     Cu(1)    N(2)     177.3(6)   2_657 . . yes
  N(1)     Cu(1)    N(2)     84.9(6)    2_657 . 2_657 yes
  N(1)     Cu(1)    Cl(1)    84.9(4)    2_657 . . yes
  N(1)     Cu(1)    Cl(1)    95.6(4)    2_657 . 2_657 yes
  N(2)     Cu(1)    N(2)     93.2(8)    . . 2_657 yes
  N(2)     Cu(1)    Cl(1)    93.0(4)    . . . yes
  N(2)     Cu(1)    Cl(1)    86.5(4)    . . 2_657 yes
  N(2)     Cu(1)    Cl(1)    86.5(4)    2_657 . . yes
  N(2)     Cu(1)    Cl(1)    93.0(4)    2_657 . 2_657 yes
  Cl(1)    Cu(1)    Cl(1)    179.3(2)   . . 2_657 yes
#------------------------------------------------------------------------------
#===END of compound 13c
#------------------------------------------------------------------------------
#==============================================================================
==================

#===CIF END

#==============================================================================
==================
```