Coexisting Ferromagnetic and Ferroelectric Order in a CuCl4-based Organic-Inorganic Hybrid

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# CIF-file generated for C16H24Cl4CuN2                Cmca          a0007
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# 0. AUDIT DETAILS

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_audit_update_record
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 ?
;

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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'Organometallics  Acta Crystallographica
C'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2009-09-21  13:30:04

 Please consider this CIF submission for publication as a
 Regular Structural Paper in Acta Crystallographica E.
 All authors have seen and approved this submission.

 The CIF has passed the Chester CHECKCIF routines and gives
 a satisfactory PRINTCIF file.

 The Structure Factor Listing (in CIF format) and any artwork
 (Schemes, Figures) as HPGL, Postscript, TIFF or encapsulated Postscript files
 will be transferred to Chester by ftp as instructed in Notes for Authors.

 Consider this CIF submission for deposition of the Xray-structure quoted
  in Journal Ref: Inorganica Chimica  Acta 259 (2000) ...
 "A remarkable Lewis acid-base adduct: preparation..."
 Compound : ....
 Your Reference number : ....
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 Please consider this CIF submission for deposition at the  Cambridge Data
 Base.

 Consider this CIF submission for deposition of the first
 X-ray structure of a manuscript to be submitted to : Organometallics
  (Our Compound_Identification_Code : a0007)
;

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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_from_coeditor          ?
_journal_date_accepted               ?

_journal_date_printers_first         ?
_journal_date_printers_final         ?
_journal_date_proofs_out             ?
_journal_date_proofs_in              ?

_journal_coeditor_name               ?
_journal_coeditor_code               ?
_journal_coeditor_notes
;
;

_journal_techeditor_code             ?
_journal_techeditor_notes
;
;

_journal_coden_ASTM                  ?
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_journal_issue                       ?
_journal_page_first                  ?
_journal_page_last                   ?


_journal_suppl_publ_number           ?
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#===============================================================================

# 3. TITLE AND AUTHOR LIST

_publ_section_title
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;
_publ_section_title_footnote
;
;

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


loop_
_publ_author_name
```

```
_publ_author_footnote
_publ_author_address
'?' # author name
;   # author related footnote
;
;   # Address of this author
;
   'Meetsma, Auke'
;
 ? # author related footnote
;
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

#===============================================================================

# 4. TEXT

_publ_section_synopsis
;
 ?
;
_publ_section_abstract
;
 ?
;

# Insert blank lines between paragraphs

_publ_section_comment
;
;
_publ_section_exptl_prep
;
;
_publ_section_exptl_refinement
;
 The hydrogen atoms were generated by geometrical considerations,
  constrained to idealized geometries, and allowed to ride on the
  carrier atom with an  isotropic displacement parameter related to the
  equivalent displacement parameter of their carrier atoms,
  with U~iso~(H) = 1.2U~eq~(C) or 1.5U~eq~(methyl C).
 The amine-group was refined as rigid groups, which were allowed
  to rotate freely.
 Assigned values of bond distances for secondary C-H~2~ = 0.97 \%A,
  aromatic C-H = 0.93 \%A and  N-H = 0.89 \%A

;


_publ_section_related_literature
;
;

# Insert blank lines between references

_publ_section_references
;
 Allen, F.H. (2002). Acta Cryst. B58, 380-388.

 Beurskens, P.T., Beurskens, G., Gelder, R. de, Smits, J.M.M.,
```

  Garc\'ia-Granda, S. & Gould, R.O. (2008).
  The DIRDIF08 program system, Technical Report of the Crystallography
  Laboratory, University of Nijmegen, The Netherlands.

 Boeyens, J.C.A. (1978). J. Cryst. Mol. Struct. 8, 317-320.

 Bondi, A. (1964). J. Phys. Chem. 68, 441-451.

 Bruker, (2007). SMART (Version 5.632), SAINT-Plus (Version 7.46a) and
  SADABS (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.

 Hahn, T. (1983). Ed. International Tables for Crystallography,
  Volume A, Space-group symmetry, Kluwer Academic Publishers,
  Dordrecht, The Netherlands.

 Meetsma, A. (2009). Extended version of the program PLUTO.
  University of Groningen, The Netherlands. (unpublished).

 Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

 Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.

 Wilson, A.J.C. (1992). Ed. International Tables for Crystallography,
  Volume C, Kluwer Academic Publishers, Dordrecht, The Netherlands.
;

_publ_section_figure_captions
;

   Fig. 1. Perspective PLUTO drawings of the molecule illustrating the
           configuration and the adopted numbering scheme.

   Fig. 2. Molecular packing viewed down unit cell axes.

   Fig. 3. Perspective ORTEP drawing of the title compound.
           Displacement ellipsoids for non-H atoms are represented at the 50%
           probability level.
           The H-atoms have been omitted to improve clarity.
           The H-atoms are drawn with an arbitrary radius.

   Fig. 4. Portion of the crystal packing, showing
           N-H...Cl hydrogen bonds shown as dashed lines.
;

_publ_section_acknowledgements
;
;

#===

5. CHEMICAL DATA

_chemical_name_systematic
;
;
_chemical_name_common   ?
_chemical_melting_point   ?
_chemical_formula_moiety
'2(C8 H12 N), Cl4 Cu'
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural   ?
_chemical_formula_sum
'C16 H24 Cl4 Cu N2'
_chemical_formula_iupac   ?
_chemical_formula_weight   449.72

```
_chemical_compound_source           'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 N   N    0.0061    0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cu  Cu    0.3201    1.2651
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl  Cl    0.1484    0.1585
 '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'
 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#==============================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting               orthorhombic
_symmetry_space_group_name_Hall      '-C 2bc 2'
_symmetry_space_group_name_H-M       'C m c a'
_symmetry_Int_Tables_number                64

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
   1 x,y,z
   2 -x,1/2-y,1/2+z
   3 x,-y,-z
   4 -x,1/2+y,1/2-z
   5 -x,-y,-z
   6 x,1/2+y,1/2-z
   7 -x,y,z
   8 x,1/2-y,1/2+z
   9 1/2+x,1/2+y,z
  10 1/2-x,-y,1/2+z
  11 1/2+x,1/2-y,-z
  12 1/2-x,y,1/2-z
  13 1/2-x,1/2-y,-z
  14 1/2+x,y,1/2-z
  15 1/2-x,1/2+y,z
  16 1/2+x,-y,1/2+z

_cell_length_a                        39.021(8)
_cell_length_b                         7.3430(15)
_cell_length_c                         7.3939(15)
_cell_angle_alpha                     90
_cell_angle_beta                      90
_cell_angle_gamma                     90
_cell_volume                        2118.6(7)
_cell_formula_units_Z                  4

_cell_measurement_temperature    373(1)
_cell_measurement_reflns_used      2107
_cell_measurement_theta_min        3.13
_cell_measurement_theta_max       23.02
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   2107 reflections after integration using the SAINTPLUS
   software package (Bruker, 2007).
```

```
 Reduced cell calculations did not indicate any higher metric lattice symmetry
   and examination of the final atomic coordinates of the structure did not
   yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description       'block'
_exptl_crystal_colour            'orange'
_exptl_crystal_size_max           0.20
_exptl_crystal_size_mid           0.10
_exptl_crystal_size_min           0.10
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.410
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              924
_exptl_absorpt_coefficient_mu     1.535
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_process_details    '(SADABS, (Bruker, 2007))'
_exptl_absorpt_correction_T_min    0.7256
_exptl_absorpt_correction_T_max    0.8577

#==============================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
;
;
_diffrn_ambient_temperature            373(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method           '\f and \w scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2007)).
;
_diffrn_detector_area_resol_mean     66.06


_diffrn_standards_number              0
_diffrn_standards_interval_count      .
_diffrn_standards_interval_time       .
_diffrn_standards_decay_%             0

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              7895
_diffrn_reflns_av_R_equivalents    0.0313
_diffrn_reflns_av_sigmaI/netI      0.0218
```

```
_diffrn_reflns_limit_h_min        -49
_diffrn_reflns_limit_h_max        49
_diffrn_reflns_limit_k_min        -9
_diffrn_reflns_limit_k_max        9
_diffrn_reflns_limit_l_min        -9
_diffrn_reflns_limit_l_max        9
_diffrn_reflns_theta_min          3.13
_diffrn_reflns_theta_max          26.72
_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.998

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
_reflns_number_total              1146
_reflns_number_gt                 913
_reflns_threshold_expression     I>2\s(I)


_computing_data_collection          'SMART (Bruker, 2007)'
_computing_cell_refinement          'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction           'SAINT-Plus'
_computing_structure_solution
;
 DIRDIF-08 (Beurskens et al., 2008)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics
;
 PLATON (Spek, 2003)
 PLUTO (Meetsma, 2009)
;
_computing_publication_material      'PLATON (Spek, 2003)'

#=============================================================================

# 8. REFINEMENT DATA


_refine_special_details
;
 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^ > 2sigma(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.
;

_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^)+(0.1044P)^2^+0.6794P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
```

```
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  '.'

_refine_ls_abs_structure_Flack    ?
_refine_ls_number_reflns          1146
_refine_ls_number_parameters      68
_refine_ls_number_restraints      2
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0653
_refine_ls_R_factor_gt            0.0544
_refine_ls_wR_factor_ref          0.1597
_refine_ls_wR_factor_gt           0.1481
_refine_ls_goodness_of_fit_ref    1.119
_refine_ls_restrained_S_all       1.128
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.756
_refine_diff_density_min         -0.723
_refine_diff_density_rms          0.104

_vrn_publ_code_void_volume         128.1
_vrn_publ_code_number_frames       1800
_vrn_publ_code_frame_time_sec      10.0
_vrn_publ_code_meas_time_hour       7.8


#===============================================================================

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
N1 N Uani 0.05465(14) 0.500   0.00000 1.000 0.077(2) . .
C1 C Uani 0.0895(3) 0.500   0.00000 1.000 0.161(8) . .
C2 C Uani 0.1196(2) 0.455(2) -0.1085(16) 0.5   0.185(10) . .
C3 C Uani 0.1505(3) 0.500   0.00000 1.000 0.201(9) . .
C4 C Uani 0.1699(2) 0.6185(16) -0.1079(16) 1.0   0.210(7) . .
C5 C Uani 0.2045(2) 0.6148(16) -0.0941(17) 1.0   0.183(6) . .
C6 C Uani 0.2197(4) 0.500   0.00000 1.000 0.180(10) . .
Cu1 Cu Uani 0.000   0.50000 0.50000 1.000 0.0495(3) . .
Cl1 Cl Uani -0.05866(4) 0.500   0.50000 1.000 0.0764(6) . .
Cl2 Cl Uani 0.000   0.27901(16) 0.28124(16) 1.000 0.0671(5) . .
H1 H Uiso 0.09425 0.43231 0.10982 0.5   0.1945 . .
H1' H Uiso 0.09425 0.62571 0.03151 0.5   0.1945 . .
H2 H Uiso 0.11946 0.52552 -0.21974 0.5   0.2200 . .
H2' H Uiso 0.11946 0.32705 -0.13938 0.5   0.2200 . .
H4 H Uiso 0.15919 0.69821 -0.18753 1.0   0.2522 . .
H5 H Uiso 0.21733 0.70086 -0.15703 1.0   0.2197 . .
H6 H Uiso 0.24355 0.500   0.00000 1.000 0.2171 . .
H9 H Uiso 0.04704 0.54756 0.10319 0.5   0.1152 . .
H9' H Uiso 0.04704 0.38624 -0.01069 0.5   0.1152 . .
H9" H Uiso 0.04704 0.56620 -0.09250 0.5   0.1152 . .

loop_
_atom_site_aniso_label
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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
N1 0.070(4) 0.078(4) 0.082(4) -0.004(3) 0.036(8) -0.017(10)
C1 0.080(7) 0.163(13) 0.24(2) 0.074(10) 0.085(15) 0.043(15)
C2 0.152(15) 0.232(18) 0.17(2) -0.088(16) -0.050(14) 0.061(14)
C3 0.050(5) 0.262(19) 0.29(2) 0.134(14) 0.00   0.0000
C4 0.133(8) 0.260(14) 0.237(13) 0.153(13) 0.014(6) 0.003(7)
C5 0.097(7) 0.202(12) 0.250(13) 0.033(11) 0.038(7) -0.025(6)
C6 0.081(8) 0.22(2) 0.24(2) -0.036(12) 0.00   0.0000
Cu1 0.0626(6) 0.0447(5) 0.0412(5) -0.0076(3) 0.00   0.0000
Cl1 0.0604(9) 0.0866(11) 0.0822(11) 0.0013(6) 0.00   0.0000
Cl2 0.1076(10) 0.0485(6) 0.0451(7) -0.0088(5) 0.00   0.0000

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

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
 Cu1     Cl2      2.9192(13)                    .     2_555                yes
 Cu1     Cl1      2.2890(16)                    .       .                  yes
 Cu1     Cl2      2.2912(13)                    .       .                  yes
 Cu1     Cl1      2.2890(16)                    .     5_566                yes
 Cu1     Cl2      2.2912(13)                    .     3_566                yes
 Cu1     Cl2      2.9192(13)                    .     4_555                yes
 N1      C1        1.360(13)                    .       .                  yes
 N1      H9"          0.89                      .     3_565                no
 N1      H9"          0.89                      .       .                  no
 N1      H9           0.89                      .       .                  no
 N1      H9'          0.89                      .       .                  no
 N1      H9           0.89                      .     3_565                no
 N1      H9'          0.89                      .     3_565                no
 C1      C2        1.460(13)                    .       .                  no
 C1      C2        1.460(13)                    .     3_565                no
 C2      C3        1.486(13)                    .       .                  no
 C3      C4        1.402(12)                    .       .                  no
 C3      C4        1.402(12)                    .     3_565                no
 C4      C5        1.354(11)                    .       .                  no
 C5      C6        1.244(14)                    .       .                  no
 C1      H1'          0.97                      .       .                  no
 C1      H1           0.97                      .       .                  no
 C1      H1           0.97                      .     3_565                no
 C1      H1'          0.97                      .     3_565                no
 C2      H2           0.97                      .       .                  no
 C2      H2'          0.97                      .       .                  no
 C4      H4           0.93                      .       .                  no
 C5      H5           0.93                      .       .                  no
 C6      H6           0.93                      .       .                  no
```

```
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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_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 Cl1     Cu1     Cl2          90              .       .       .          yes
 Cl1     Cu1     Cl2          90              .       .     2_555        yes
 Cl1     Cu1     Cl2          90              .       .     3_566        yes
 Cl1     Cu1     Cl2          90              .       .     4_555        yes
 Cl1     Cu1     Cl1         180              .       .     5_566        yes
 Cl2     Cu1     Cl2       90.33(4)           .       .     2_555        yes
 Cl2     Cu1     Cl2         180              .       .     3_566        yes
 Cl2     Cu1     Cl2       89.67(4)           .       .     4_555        yes
 Cl1     Cu1     Cl2          90            5_566     .       .          yes
 Cl2     Cu1     Cl2       89.67(4)         2_555     .     3_566        yes
 Cl2     Cu1     Cl2         180            2_555     .     4_555        yes
 Cl1     Cu1     Cl2          90            5_566     .     2_555        yes
 Cl2     Cu1     Cl2       90.33(4)         3_566     .     4_555        yes
 Cl1     Cu1     Cl2          90            5_566     .     3_566        yes
 Cl1     Cu1     Cl2          90            5_566     .     4_555        yes
 Cu1     Cl2     Cu1      179.48(5)           .       .     2_554        yes
 C1      N1      H9           109             .       .     3_565        no
 C1      N1      H9'          109             .       .     3_565        no
 C1      N1      H9"          109             .       .     3_565        no
 H9      N1      H9'          109             .       .       .          no
 H9      N1      H9"          109             .       .       .          no
 H9      N1      H9           141             .       .     3_565        no
 H9      N1      H9'           56             .       .     3_565        no
 H9      N1      H9"           56             .       .     3_565        no
 H9'     N1      H9"          109             .       .       .          no
 H9      N1      H9'           56           3_565     .       .          no
 H9'     N1      H9'          141             .       .     3_565        no
 H9'     N1      H9"           56             .       .     3_565        no
 H9      N1      H9"           56           3_565     .       .          no
 H9'     N1      H9"           56           3_565     .       .          no
 H9"     N1      H9"          141             .       .     3_565        no
 H9      N1      H9'          109           3_565     .     3_565        no
 H9      N1      H9"          109           3_565     .     3_565        no
 H9'     N1      H9"          109           3_565     .     3_565        no
 C1      N1      H9"          109             .       .       .          no
 C1      N1      H9           109             .       .       .          no
 C1      N1      H9'          109             .       .       .          no
 C2      C1      C2          72.9(8)          .       .     3_565        no
 N1      C1      C2         143.6(5)          .       .     3_565        yes
 N1      C1      C2         143.6(5)          .       .       .          yes
 C1      C2      C3         107.8(9)          .       .       .          no
 C2      C3      C2          71.5(8)          .       .     3_565        no
 C2      C3      C4         105.6(7)          .       .       .          no
 C2      C3      C4         127.4(7)        3_565     .       .          no
 C4      C3      C4        114.7(10)          .       .     3_565        no
 C2      C3      C4         127.4(8)          .       .     3_565        no
 C2      C3      C4         105.6(7)        3_565     .     3_565        no
 C3      C4      C5        118.9(10)          .       .       .          no
 C4      C5      C6        122.1(12)          .       .       .          no
 C5      C6      C5        123.0(14)          .       .     3_565        no
 C2      C1      H1'          101           3_565     .     3_565        no
 H1      C1      H1'          104           3_565     .     3_565        no
 N1      C1      H1           101             .       .     3_565        no
 N1      C1      H1'          101             .       .     3_565        no
 C2      C1      H1           101             .       .       .          no
 C2      C1      H1'          101             .       .       .          no
```

```
 C2      C1      H1           60              .       .     3_565         no
 C2      C1      H1'          60              .       .     3_565         no
 H1      C1      H1'         104              .       .       .           no
 C2      C1      H1           60           3_565      .       .           no
 H1      C1      H1          158              .       .     3_565         no
 H1      C1      H1'          71              .       .     3_565         no
 C2      C1      H1'          60           3_565      .       .           no
 H1'     C1      H1'         158              .       .     3_565         no
 C2      C1      H1          101           3_565      .     3_565         no
 N1      C1      H1          101              .       .       .           no
 N1      C1      H1'         101              .       .       .           no
 H1      C1      H1'          71           3_565      .       .           no
 C1      C2      H2          110              .       .       .           no
 C3      C2      H2          110              .       .       .           no
 C3      C2      H2'         110              .       .       .           no
 C1      C2      H2'         110              .       .       .           no
 H2      C2      H2'         109              .       .       .           no
 C5      C4      H4          121              .       .       .           no
 C3      C4      H4          121              .       .       .           no
 C4      C5      H5          119              .       .       .           no
 C6      C5      H5          119              .       .       .           no
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 C2      C1      C2      C3           0.0(8)     .       .     3_565     .   no
 C1      C2      C3      C4        -124.9(9)     .       .       .       .   no
 C1      C2      C3      C2           0.0(8)     .       .       .     3_565 no
 C1      C2      C3      C4         95.8(11)     .       .       .     3_565 no
 C2      C3      C4      C5       -148.0(11)     .       .       .       .   no
 C2      C3      C4      C5        133.6(11)   3_565     .       .       .   no
 C4      C3      C4      C5         -2.8(13)   3_565     .       .       .   no
 C3      C4      C5      C6          5.9(17)     .       .       .       .   no
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 Cl1     Cl2     3.2387(15)                    .     3_566               no
 Cl1     Cl2     3.2387(15)                    .     3_566               no
 Cl2     N1        3.371(4)                    .     2_555               no
 Cl2     N1        3.371(4)                    .     4_545               no
 Cl2     N1        3.392(4)                    .       .                 no
 Cl2     N1        3.392(4)                    .       .                 no
 Cl2     N1        3.392(4)                    .     5_565               no
 Cl2     Cl1     3.2387(15)                    .       .                 no
 Cl2     Cl1     3.2387(15)                    .     5_566               no
 Cl2     N1        3.392(4)                    .     7_555               no
 Cl2     Cl1     3.2387(15)                    .     5_566               no
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Cl1	H9"	3.09	.	5_565	no
Cl1	H9'	2.87	.	4_555	no
Cl1	H1'	3.09	.	4_545	no
Cl1	H9"	3.09	.	7_556	no
Cl1	H9	2.99	.	5_566	no
Cl1	H1'	3.09	.	2_565	no
Cl1	H9	2.99	.	7_555	no
Cl1	H9'	2.87	.	2_555	no
Cl2	H9	2.64	.	4_545	no
Cl2	H9'	2.94	.	.	no
Cl2	H9'	2.68	.	2_555	no
Cl2	H9"	2.57	.	5_565	no
Cl2	H9	3.00	.	.	no
Cl2	H9'	2.94	.	7_555	no
Cl2	H9	3.00	.	7_555	no
Cl2	H9"	2.57	.	3_565	no
N1	Cl2	3.392(4)	.	3_565	no
N1	Cl2	3.371(4)	.	2_554	no
N1	Cl2	3.392(4)	.	.	no
N1	Cl2	3.371(4)	.	2_554	no
N1	Cl2	3.392(4)	.	5_565	no
N1	Cl2	3.371(4)	.	4_555	no
N1	Cl2	3.371(4)	.	4_555	no
N1	Cl2	3.392(4)	.	.	no
C2	H4	2.87	.	6_544	no
C4	H1	2.98	.	3_565	no
H1	C4	2.98	.	3_565	no
H1'	Cl1	3.09	.	2_564	no
H1'	Cl1	3.09	.	4_555	no
H2	H4	2.02	.	.	no
H2'	H4	2.22	.	6_544	no
H4	C2	2.87	.	6_554	no
H4	H2'	2.22	.	6_554	no
H4	H2	2.02	.	.	no
H9	Cl1	2.99	.	5_566	no
H9	Cl2	3.00	.	.	no
H9	Cl1	2.99	.	5_566	no
H9	Cl2	3.00	.	.	no
H9	Cl2	2.64	.	4_555	no
H9	Cl2	2.64	.	4_555	no
H9'	Cl2	2.94	.	.	no
H9'	Cl2	2.68	.	2_554	no
H9'	Cl2	2.68	.	2_554	no
H9'	Cl1	2.87	.	2_554	no
H9'	Cl1	2.87	.	2_554	no
H9'	Cl2	2.94	.	.	no
H9"	Cl2	2.57	.	5_565	no
H9"	Cl1	3.09	.	7_554	no
H9"	Cl1	3.09	.	5_565	no
H9"	Cl2	2.57	.	3_565	no

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_geom_hbond_distance_DA
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#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
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N1      H9      Cl2         0.8900     2.6400   3.371(4)     140      4_555 yes
N1      H9'     Cl2         0.8900     2.6800   3.371(4)     135      2_554 yes
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N1      H9"     Cl2         0.8900     2.5700   3.392(4)     154      3_565 yes

#===END of Crystallographic Information File

# CIF-file generated for C16H24Cl4CuN2                Pbca          q1311
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# 0. AUDIT DETAILS

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 SHELXL97-2 & Manual Editing
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_audit_update_record
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?

2008-05-06 # Formatted by publCIF
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#==============================================================================

# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
  Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;
_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'JACS'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2008-05-06  15:01:04


 Consider this CIF submission for deposition of the fifth
 X-ray structure of a manuscript to be submitted to : JACS
  (Our Compound_Identification_Code : q1311)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic        ?
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_journal_date_from_coeditor         ?
_journal_date_accepted              ?

_journal_date_printers_first        ?
_journal_date_printers_final        ?
_journal_date_proofs_out            ?
_journal_date_proofs_in             ?

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_journal_page_first                 ?
_journal_page_last                  ?


_journal_suppl_publ_number          ?
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#==============================================================================

# 3. TITLE AND AUTHOR LIST

_publ_section_title
;
Title (type here to add)
;
_publ_section_title_footnote
.

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'?' # author name
;   # author related footnote
;
;   # Address of this author
;
   'Meetsma, Auke'
;
 ? # author related footnote
;
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
```

```
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

#===============================================================================

# 4. TEXT

_publ_section_synopsis
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_publ_section_abstract
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# Insert blank lines between paragraphs

_publ_section_comment
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(type here to add)
;
_publ_section_exptl_prep
;

;
_publ_section_exptl_refinement
;
The hydrogen atoms were generated by geometrical considerations, constrained to
idealized geometries, and allowed to ride on the carrier atom with an
isotropic displacement parameter related to the equivalent displacement
parameter of their carrier atoms, with <i>U</i>~iso~(H) = 1.2<i>U</i>~eq~(C)
or 1.5<i>U</i>~eq~(methyl C). The methyl-groups were refined as rigid groups,
which were allowed to rotate freely. Assigned values of bond distances:
secondary C---H~2~ = 0.99 \%A, methyl C---H~3~ = 0.98 \%A, aromatic C---H =
0.95 \%A.

C---H distances were in the range of 0.95 -- 0.99(3) \%A.
;


_publ_section_related_literature
;
;

# Insert blank lines between references

_publ_section_references
;
Beurskens, P. T., Beurskens, G., de Gelder, R., Garc\'ia-Granda, S., Gould, R.
O., Isra\"el, R. & Smits, J. M. M. (1999). The <i>DIRDIF99</i> program system,
Technical Report of the Crystallography Laboratory, University of Nijmegen,
The Netherlands.

Brandenburg, K. (2006). <i>DIAMOND</i>. Release 3.1. Crystal Impact GbR, Bonn,
Germany

Bruker,  (2006). <i>SMART</i> (Version 5.632), <i>SAINT-Plus</i> (Version 6.45)
and <i>SADABS</i> (Version 2.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Le Page, Y. (1987). <i>J. Appl. Cryst.</i> <b>20</b>, 264--269.

Le Page, Y. (1988). <i>J. Appl. Cryst.</i> <b>21</b>, 983--984.

Meetsma, A. (2007). Extended version of the program <i>PLUTO</i>. University of
Groningen, The Netherlands. (unpublished).
```

Sheldrick, G. M. (1997). SHELXL97. Program for Crystal Structure Refinement. University of G\"ottingen, Germany.

Spek, A. L. (2003). J. Appl. Cryst. 36, 7--13.
;

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Fig. 1. Perspective PLUTO drawings of the moieties of the asymmetric unit illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the anion and cation of the title compound. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.

Fig. 4. Portion of the crystal packing, showing N---H...Cl hydrogen bonds shown as dashed lines.
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_publ_section_acknowledgements
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#==

5. CHEMICAL DATA

_chemical_name_systematic
;
;
_chemical_name_common   ?
_chemical_melting_point   ?
_chemical_formula_moiety
'2(C8 H12 N), Cl4 Cu'
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural   ?
_chemical_formula_sum
'C16 H24 Cl4 Cu N2'
_chemical_formula_iupac   ?
_chemical_formula_weight   449.74
_chemical_compound_source   'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 N   N   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cu Cu   0.3201   1.2651
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl   0.1484   0.1585
 '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'
 C   C   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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# 6. CRYSTAL DATA

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_symmetry_space_group_name_H-M       'P b c a'
_symmetry_Int_Tables_number                61

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
   1 x,y,z
   2 1/2-x,-y,1/2+z
   3 1/2+x,1/2-y,-z
   4 -x,1/2+y,1/2-z
   5 -x,-y,-z
   6 1/2+x,y,1/2-z
   7 1/2-x,1/2+y,z
   8 x,1/2-y,1/2+z

_cell_length_a                          7.2099(9)
_cell_length_b                          7.2664(9)
_cell_length_c                          38.238(5)
_cell_angle_alpha                       90
_cell_angle_beta                        90
_cell_angle_gamma                       90
_cell_volume                           2003.3(4)
_cell_formula_units_Z                  4

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      8650
_cell_measurement_theta_min        2.83
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_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   8650 reflections after integration using the SAINTPLUS
   software package (Bruker, 2000).

 Reduced cell calculations did not indicate any higher metric lattice symmetry
   and examination of the finalatomic coordinates of the structure did not
   yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

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_exptl_absorpt_coefficient_mu     1.623
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_process_details    '(SADABS, (Bruker, 2006))'
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# 7. EXPERIMENTAL DATA

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_diffrn_radiation_wavelength           0.71073
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_diffrn_radiation_monochromator        'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method             '\f and \w scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2006)).
;
_diffrn_detector_area_resol_mean       66.06

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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
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_diffrn_reflns_av_R_equivalents        0.0344
_diffrn_reflns_av_sigmaI/netI          0.0251
_diffrn_reflns_limit_h_min             -9
_diffrn_reflns_limit_h_max             8
_diffrn_reflns_limit_k_min             -9
_diffrn_reflns_limit_k_max             9
_diffrn_reflns_limit_l_min             -50
_diffrn_reflns_limit_l_max             50
_diffrn_reflns_theta_min               3.02
_diffrn_reflns_theta_max               28.27
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_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.976

_diffrn_reflns_reduction_process
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 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT-Plus & SADABS (Bruker, 2006).
;

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_reflns_number_gt                      2163
_reflns_threshold_expression           I>2\s(I)


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_computing_structure_solution
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 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
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 DIAMOND (Brandenburg, 2006)
 PLATON (Spek, 2003)
 PLUTO (Meetsma, 2007)
;
_computing_publication_material      'PLATON (Spek, 2003)'

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# 8. REFINEMENT DATA


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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^ > 2sigma(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_weighting_scheme      calc
_refine_ls_weighting_details
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_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    constr
_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  '.'

_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         2340
_refine_ls_number_parameters     107
_refine_ls_number_restraints     0
_refine_ls_number_constraints    ?
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_refine_ls_R_factor_gt           0.0400
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_refine_ls_wR_factor_gt          0.1106
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_refine_ls_restrained_S_all      1.329
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_refine_ls_shift/su_mean         0.000

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_refine_diff_density_min        -0.605
_refine_diff_density_rms         0.121

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_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
N N Uani 1.0138(4) 0.0064(4) 0.55580(7) 1.000 0.0165(8) . .
C1 C Uani 0.9605(6) -0.0433(5) 0.59223(9) 1.000 0.0176(10) . .
C2 C Uani 1.0436(6) 0.0920(5) 0.61820(9) 1.000 0.0212(10) . .
C3 C Uani 1.0184(6) 0.0273(5) 0.65541(9) 1.000 0.0179(10) . .
C4 C Uani 0.8791(6) 0.0978(5) 0.67676(10) 1.000 0.0219(11) . .
C5 C Uani 0.8605(6) 0.0357(6) 0.71109(10) 1.000 0.0265(11) . .
C6 C Uani 0.9804(7) -0.0957(6) 0.72429(10) 1.000 0.0265(11) . .
C7 C Uani 1.1182(7) -0.1673(6) 0.70311(11) 1.000 0.0283(14) . .
C8 C Uani 1.1375(6) -0.1052(6) 0.66918(10) 1.000 0.0241(11) . .
Cu Cu Uani 0.00000 0.00000 0.00000 1.000 0.0123(2) . .
Cl1 Cl Uani 0.03423(12) 0.01365(12) 0.05984(2) 1.000 0.0160(2) . .
Cl2 Cl Uani 0.21493(11) 0.22950(11) -0.00597(2) 1.000 0.0149(2) . .
H1 H Uiso 1.00485 -0.16910 0.59760 1.000 0.0211 . .
H1' H Uiso 0.82362 -0.04248 0.59440 1.000 0.0211 . .
H2 H Uiso 1.17755 0.10695 0.61326 1.000 0.0254 . .
H2' H Uiso 0.98343 0.21355 0.61530 1.000 0.0254 . .
H4 H Uiso 0.79652 0.18842 0.66792 1.000 0.0264 . .
H5 H Uiso 0.76482 0.08388 0.72551 1.000 0.0315 . .
H6 H Uiso 0.96822 -0.13651 0.74778 1.000 0.0315 . .
H7 H Uiso 1.19945 -0.25918 0.71191 1.000 0.0340 . .
H8 H Uiso 1.23375 -0.15377 0.65495 1.000 0.0291 . .
H9 H Uiso 0.97516 0.12294 0.55104 1.000 0.0247 . .
H9' H Uiso 0.95965 -0.07338 0.54056 1.000 0.0247 . .
H9" H Uiso 1.13931 -0.00002 0.55354 1.000 0.0247 . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_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
N 0.0180(15) 0.0196(14) 0.0119(13) -0.0003(12) -0.0003(12) 0.0007(13)
C1 0.0199(19) 0.0210(17) 0.0120(15) 0.0011(13) 0.0006(14) -0.0029(15)
C2 0.032(2) 0.0196(17) 0.0120(16) -0.0007(14) 0.0014(15) -0.0050(16)
C3 0.0239(19) 0.0173(17) 0.0124(15) -0.0024(13) -0.0007(14) -0.0023(15)
C4 0.024(2) 0.0201(18) 0.0217(19) -0.0007(15) 0.0007(16) 0.0026(16)
C5 0.030(2) 0.031(2) 0.0184(18) -0.0044(16) 0.0072(16) -0.0008(18)
C6 0.037(2) 0.028(2) 0.0144(17) 0.0008(15) -0.0011(17) -0.0066(19)
C7 0.035(3) 0.028(2) 0.022(2) 0.0021(16) -0.0064(18) 0.0061(19)
C8 0.026(2) 0.027(2) 0.0193(18) -0.0031(16) 0.0014(16) 0.0056(17)
Cu 0.0132(3) 0.0118(3) 0.0120(3) -0.0002(2) 0.0001(2) -0.0022(2)
Cl1 0.0183(4) 0.0171(4) 0.0126(4) -0.0003(3) 0.0000(3) -0.0003(3)
Cl2 0.0133(4) 0.0136(4) 0.0179(4) 0.0003(3) 0.0001(3) -0.0017(3)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
```

```
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

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      Cl2      2.2879(9)                    .      .                yes
 Cu      Cl2      2.8531(9)                    .     3_455             yes
 Cu      Cl1      2.3036(8)                    .     5_555             yes
 Cu      Cl2      2.2879(9)                    .     5_555             yes
 Cu      Cl2      2.8531(9)                    .     7_545             yes
 Cu      Cl1      2.3036(8)                    .      .                yes
 N       C1        1.490(4)                    .      .                yes
 N       H9"         0.9100                    .      .                no
 N       H9'         0.9100                    .      .                no
 N       H9          0.9100                    .      .                no
 C1      C2        1.520(5)                    .      .                no
 C2      C3        1.510(5)                    .      .                no
 C3      C8        1.393(6)                    .      .                no
 C3      C4        1.392(6)                    .      .                no
 C4      C5        1.395(5)                    .      .                no
 C5      C6        1.383(6)                    .      .                no
 C6      C7        1.383(7)                    .      .                no
 C7      C8        1.381(6)                    .      .                no
 C1      H1'         0.9900                    .      .                no
 C1      H1          0.9900                    .      .                no
 C2      H2          0.9900                    .      .                no
 C2      H2'         0.9900                    .      .                no
 C4      H4          0.9500                    .      .                no
 C5      H5          0.9500                    .      .                no
 C6      H6          0.9500                    .      .                no
 C7      H7          0.9500                    .      .                no
 C8      H8          0.9500                    .      .                no

loop_
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_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
 Cl2     Cu      Cl2       90.36(3)          3_455     .     5_555        yes
 Cl2     Cu      Cl2         180.00          3_455     .     7_545        yes
 Cl1     Cu      Cl2       89.72(3)          5_555     .     5_555        yes
 Cl1     Cu      Cl2       88.17(3)          5_555     .     7_545        yes
 Cl2     Cu      Cl2       89.64(3)          5_555     .     7_545        yes
 Cl1     Cu      Cl2       89.72(3)            .       .       .          yes
 Cl1     Cu      Cl2       88.17(3)            .       .     3_455        yes
 Cl1     Cu      Cl1         180.00            .       .     5_555        yes
 Cl1     Cu      Cl2       90.28(3)            .       .     5_555        yes
 Cl1     Cu      Cl2       91.83(3)            .       .     7_545        yes
 Cl2     Cu      Cl2       89.64(3)            .       .     3_455        yes
 Cl1     Cu      Cl2       90.28(3)          5_555     .       .          yes
 Cl2     Cu      Cl2         180.00            .       .     5_555        yes
 Cl2     Cu      Cl2       90.36(3)            .       .     7_545        yes
 Cl1     Cu      Cl2       91.83(3)          5_555     .     3_455        yes
 Cu      Cl2     Cu       169.15(3)            .       .     3_555        yes
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```
 H9      N       H9"          109.00            .       .       .          no
 H9'     N       H9"          109.00            .       .       .          no
 C1      N       H9"          109.00            .       .       .          no
 C1      N       H9           109.00            .       .       .          no
 C1      N       H9'          109.00            .       .       .          no
 H9      N       H9'          109.00            .       .       .          no
 N       C1      C2         110.6(3)            .       .       .          yes
 C1      C2      C3         111.5(3)            .       .       .          no
 C2      C3      C8         119.8(4)            .       .       .          no
 C4      C3      C8         118.5(3)            .       .       .          no
 C2      C3      C4         121.7(3)            .       .       .          no
 C3      C4      C5         120.2(4)            .       .       .          no
 C4      C5      C6         120.4(4)            .       .       .          no
 C5      C6      C7         119.7(4)            .       .       .          no
 C6      C7      C8         120.0(4)            .       .       .          no
 C3      C8      C7         121.3(4)            .       .       .          no
 N       C1      H1           110.00            .       .       .          no
 N       C1      H1'          110.00            .       .       .          no
 C2      C1      H1           110.00            .       .       .          no
 C2      C1      H1'          110.00            .       .       .          no
 H1      C1      H1'          108.00            .       .       .          no
 C1      C2      H2'          109.00            .       .       .          no
 C3      C2      H2           109.00            .       .       .          no
 C3      C2      H2'          109.00            .       .       .          no
 H2      C2      H2'          108.00            .       .       .          no
 C1      C2      H2           109.00            .       .       .          no
 C5      C4      H4           120.00            .       .       .          no
 C3      C4      H4           120.00            .       .       .          no
 C4      C5      H5           120.00            .       .       .          no
 C6      C5      H5           120.00            .       .       .          no
 C7      C6      H6           120.00            .       .       .          no
 C5      C6      H6           120.00            .       .       .          no
 C6      C7      H7           120.00            .       .       .          no
 C8      C7      H7           120.00            .       .       .          no
 C3      C8      H8           119.00            .       .       .          no
 C7      C8      H8           119.00            .       .       .          no

loop_
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_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 N       C1      C2      C3        -170.6(3)     .       .       .       .   no
 C1      C2      C3      C4        -100.5(4)     .       .       .       .   no
 C1      C2      C3      C8          80.0(5)     .       .       .       .   no
 C2      C3      C4      C5        -179.6(4)     .       .       .       .   no
 C8      C3      C4      C5          -0.1(6)     .       .       .       .   no
 C2      C3      C8      C7         180.0(4)     .       .       .       .   no
 C4      C3      C8      C7           0.5(6)     .       .       .       .   no
 C3      C4      C5      C6           0.3(6)     .       .       .       .   no
 C4      C5      C6      C7          -0.8(7)     .       .       .       .   no
 C5      C6      C7      C8           1.1(7)     .       .       .       .   no
 C6      C7      C8      C3          -1.0(7)     .       .       .       .   no

loop_
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_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
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_geom_contact_publ_flag
 Cu      H9'          3.7000                .     2_554                no
 Cu      H9"          3.3100                .     2_654                no
 Cu      H9           3.3700                .     4_645                no
 Cu      H9'          3.4800                .     4_655                no
 Cu      H9'          3.7000                .     6_455                no
 Cu      H9"          3.3100                .     6_355                no
 Cu      H9           3.3700                .     8_454                no
 Cl1     Cl2      3.2388(12)                .       .                  no
 Cl1     N          3.266(3)                .     2_654                no
 Cl1     Cl2      3.6092(12)                .     3_455                no
 Cl1     Cl2      3.2545(12)                .     5_555                no
 Cl1     N          3.494(3)                .     8_454                no
 Cl1     C2         3.633(4)                .     8_454                no
 Cl2     Cl1      3.2388(12)                .       .                  no
 Cl2     Cl1      3.6092(12)                .     3_555                no
 Cl2     N          3.302(3)                .     6_455                no
 Cl2     Cl2      3.6459(12)                .     3_455                no
 Cl2     Cl2      3.6459(12)                .     3_555                no
 Cl2     N          3.225(3)                .     4_655                no
 Cl2     N          3.371(3)                .     8_454                no
 Cl2     Cl1      3.2545(12)                .     5_555                no
 Cl2     Cl2      3.6682(12)                .     7_545                no
 Cl2     Cl2      3.6682(12)                .     7_555                no
 Cl1     H1'          2.9100                .     2_554                no
 Cl1     H9"          2.3700                .     2_654                no
 Cl1     H2           3.0400                .     2_654                no
 Cl1     H2'          2.9300                .     8_454                no
 Cl1     H9           2.7000                .     8_454                no
 Cl2     H9'          3.1200                .     6_455                no
 Cl2     H9           2.6600                .     6_455                no
 Cl2     H9'          2.3200                .     4_655                no
 Cl2     H9"          3.0100                .     2_654                no
 Cl2     H9"          3.0600                .     8_454                no
 Cl2     H9           2.9800                .     8_454                no
 N       Cl2        3.302(3)                .     6_555                no
 N       Cl1        3.494(3)                .     8_655                no
 N       Cl2        3.225(3)                .     4_645                no
 N       Cl1        3.266(3)                .     2_655                no
 N       Cl2        3.371(3)                .     8_655                no
 C2      Cl1        3.633(4)                .     8_655                no
 C2      H8           2.8200                .     7_755                no
 C3      H8           2.9300                .     7_755                no
 C6      H5           2.9200                .     7_645                no
 C6      H5           3.1000                .     6_556                no
 C8      H1           2.9400                .       .                  no
 H1      C8           2.9400                .       .                  no
 H1      Cl1          2.9000                .     8_645                no
 H1'     Cl1          2.9100                .     2_555                no
 H2      H8           2.4400                .     7_755                no
 H2      Cl1          3.0400                .     2_655                no
 H2      H9"          2.4300                .       .                  no
 H2      H8           2.5100                .       .                  no
 H2'     Cl1          2.9300                .     8_655                no
 H2'     H9           2.5400                .       .                  no
 H2'     H4           2.4300                .       .                  no
 H4      H2'          2.4300                .       .                  no
 H5      C6           3.1000                .     6_456                no
 H5      C6           2.9200                .     7_655                no
 H8      H2           2.4400                .     7_745                no
 H8      H2           2.5100                .       .                  no
 H8      C2           2.8200                .     7_745                no
 H8      C3           2.9300                .     7_745                no
 H9      H2'          2.5400                .       .                  no
 H9      Cu           3.3700                .     4_655                no
 H9      Cl2          2.6600                .     6_555                no
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 H9      Cl2          2.9800                    .     8_655                no
 H9      Cu           3.3700                    .     8_655                no
 H9      Cl1          2.7000                    .     8_655                no
 H9'     Cu           3.4800                    .     4_645                no
 H9'     Cl2          3.1200                    .     6_555                no
 H9'     Cl2          2.3200                    .     4_645                no
 H9'     Cu           3.7000                    .     6_555                no
 H9'     Cu           3.7000                    .     2_555                no
 H9'     Cu           3.4800                    .     8_645                no
 H9"     Cl1          2.3700                    .     2_655                no
 H9"     Cu           3.3100                    .     6_655                no
 H9"     Cl2          3.0600                    .     8_655                no
 H9"     Cl2          3.0100                    .     2_655                no
 H9"     H2           2.4300                    .       .                  no
 H9"     Cu           3.3100                    .     2_655                no

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_geom_hbond_atom_site_label_A
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_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
N       H9      Cl2         0.9100     2.6600   3.302(3)     128.00   6_555 yes
N       H9      Cl1         0.9100     2.7000   3.494(3)     147.00   8_655 yes
N       H9'     Cl2         0.9100     2.3200   3.225(3)     172.00   4_645 yes
N       H9"     Cl1         0.9100     2.3700   3.266(3)     169.00   2_655 yes

#===END of Crystallographic Information File
```