Synthetic, Crystallographic, and Computational Study of Copper(II) Complexes of Ethylenediaminetetracarboxylate Ligands

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# CIF-file generated for C13H34BaCuN2O16              P-1           q1106
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data_global
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 First refinement :  '2006-04-21  12:23:22'
 2012-09-10     updated : H in riding mode
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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              'Inorganic Chemistry.'
# 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 :   2012-09-10   14:12:07


 Consider this CIF submission for deposition of the first
 X-ray structure of a manuscript to be submitted to : 'Inorganic Chemistry.'
  (Our Compound_Identification_Code : q1106)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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# 3. TITLE AND AUTHOR LIST

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_publ_section_title_footnote
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;

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


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_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.
;

#=============================================================================
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# 4. TEXT

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;
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;

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;
_publ_section_exptl_prep
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;
_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 methyl-groups were refined as rigid groups, which were allowed
  to rotate freely.
 Assigned values of bond distances for   secondary C-H~2~ = 0.99 \\%A,

 The hydrogen atoms of the O-H bonds were leaeve free  to a target value of
   and their isotropic displacement parameters (IDPs) were set
  to 1.5 times the U~eq~ value of their parent atom.
;


_publ_section_related_literature
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;

# Insert blank lines between references

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

Bruker,  (2001). <i>SMART</i>, SAINTPLUS and <i>XPREP</i>. Software Reference
Manual Bruker AXS Inc. Madison, Wisconsin, USA.

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

Spek, A. L. (2003). <i>J. Appl. Cryst.</i> <b>36</b>, 7--13.

;


_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.
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_publ_section_acknowledgements
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# 5. CHEMICAL DATA

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;
;
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_chemical_melting_point               ?
_chemical_formula_moiety
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# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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_chemical_formula_sum
'C13 H34 Ba Cu N2 O16'
_chemical_formula_iupac               ?
_chemical_formula_weight                 675.29
_chemical_compound_source            'see text'

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
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 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'
Ba  Ba   -0.3244    2.2819
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H    0.0000    0.0000
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 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_Int_Tables_number                2

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
   1 x,y,z
   2 -x,-y,-z
```

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_cell_length_a                          9.0778(4)
_cell_length_b                         11.8362(5)
_cell_length_c                         11.9806(5)
_cell_angle_alpha                     101.056(1)
_cell_angle_beta                      108.737(1)
_cell_angle_gamma                      95.195(1)
_cell_volume                          1180.29(9)
_cell_formula_units_Z                  2

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      9337
_cell_measurement_theta_min        2.24
_cell_measurement_theta_max       29.65
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   9337 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_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.900
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_exptl_crystal_F_000              678
_exptl_absorpt_coefficient_mu     2.637
_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_process_details    '(SADABS, Bruker, 2001))'
_exptl_absorpt_correction_T_min    0.4069
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#===============================================================================

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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
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```
   (KRYOFLEX, (Bruker, 2000)).
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_diffrn_standards_interval_time      ?
_diffrn_standards_decay_%            0

loop_
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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              10786
_diffrn_reflns_av_R_equivalents    0.0133
_diffrn_reflns_av_sigmaI/netI      0.0213
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_diffrn_reflns_limit_k_min         -15
_diffrn_reflns_limit_k_max         15
_diffrn_reflns_limit_l_min         -15
_diffrn_reflns_limit_l_max         15
_diffrn_reflns_theta_min           2.24
_diffrn_reflns_theta_max           28.28
_diffrn_measured_fraction_theta_max    0.960
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.982

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
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_reflns_number_gt                  5496
_reflns_threshold_expression      I>2\s(I)


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_computing_cell_refinement          'SAINT-Plus, (Bruker, 2001)'
_computing_data_reduction           'SAINT-Plus, (Bruker, 2001)'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2006)
 PLATON (Spek, 2003)
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_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_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0174P)^2^+1.8242P] where P=(Fo^2^+2Fc^2^)/3'
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?
;
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_refine_ls_abs_structure_Flack    ?
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_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
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_refine_ls_R_factor_gt            0.0224
_refine_ls_wR_factor_ref          0.0529
_refine_ls_wR_factor_gt           0.0526
_refine_ls_goodness_of_fit_ref    1.118
_refine_ls_restrained_S_all       1.118
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_refine_ls_shift/su_mean          0.000
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_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags

_atom_site_disorder_assembly
_atom_site_disorder_group

Ba Ba Uani 1.23683(1) 0.04164(1) 0.47151(1) 1.0   0.0107(1) . . . .
Cu Cu Uani 0.80510(3) 0.21778(2) 0.29180(2) 1.0   0.0113(1) . . . .
```

```
O1 O Uani 0.98645(19) 0.13973(14) 0.29569(14) 1.0   0.0161(4) . . . .
O2 O Uani 1.1839(2) 0.08752(15) 0.23935(15) 1.0   0.0192(5) . . . .
O3 O Uani 0.6241(2) 0.03366(14) 0.15797(15) 1.0   0.0190(5) . . . .
O4 O Uani 0.7664(2) -0.10408(15) 0.12021(16) 1.0   0.0249(6) . . . .
O5 O Uani 0.98434(19) 0.35989(14) 0.44662(14) 1.0   0.0157(4) . . . .
O6 O Uani 1.0149(2) 0.35919(16) 0.63848(15) 1.0   0.0206(5) . . . .
O7 O Uani 0.74574(19) 0.14838(13) 0.41525(14) 1.0   0.0145(4) . . . .
O8 O Uani 0.53672(19) 0.10704(14) 0.46801(14) 1.0   0.0152(5) . . . .
O24 O Uani 1.2401(2) -0.12805(16) 0.26496(16) 1.0   0.0194(5) . . . .
O25 O Uani 1.2722(2) 0.28326(15) 0.51929(16) 1.0   0.0183(5) . . . .
O27 O Uani 1.4459(2) 0.11633(15) 0.71288(16) 1.0   0.0163(5) . . . .
O28 O Uani 1.0653(2) 0.11434(15) 0.63277(15) 1.0   0.0162(5) . . . .
N1 N Uani 0.7949(3) 0.26769(18) 0.13729(18) 1.0   0.0200(6) . . . .
N2 N Uani 0.6307(2) 0.30989(18) 0.30142(18) 1.0   0.0185(6) . . . .
C1 C Uani 1.0790(3) 0.1491(2) 0.2359(2) 1.0   0.0164(6) . . . .
C2 C Uani 1.0722(3) 0.2382(2) 0.1575(2) 1.0   0.0230(7) . . . .
C3 C Uani 0.9554(3) 0.3222(2) 0.1524(2) 1.0   0.0225(7) . . . .
C4 C Uani 0.7197(3) 0.1747(2) 0.0220(2) 1.0   0.0213(7) . . . .
C5 C Uani 0.7592(3) 0.0513(2) 0.0190(2) 1.0   0.0196(6) . . . .
C6 C Uani 0.7131(3) -0.0109(2) 0.1063(2) 1.0   0.0182(6) . . . .
C7 C Uani 0.6929(3) 0.3635(2) 0.1349(2) 1.0   0.0203(7) . . . .
C8 C Uani 0.5606(3) 0.3303(2) 0.1783(2) 1.0   0.0214(7) . . . .
C9 C Uani 0.6870(3) 0.4247(2) 0.3930(2) 1.0   0.0193(6) . . . .
C10 C Uani 0.7775(3) 0.4146(2) 0.5203(2) 1.0   0.0175(6) . . . .
C11 C Uani 0.9370(3) 0.37473(19) 0.5362(2) 1.0   0.0159(6) . . . .
C12 C Uani 0.5171(3) 0.2333(2) 0.3331(2) 1.0   0.0185(6) . . . .
C13 C Uani 0.6047(3) 0.15829(19) 0.4123(2) 1.0   0.0143(6) . . . .
O21 O Uani 0.7659(2) 0.66118(17) 0.06159(17) 1.0   0.0232(5) . . . .
O22 O Uani 0.0769(2) 0.65073(16) 0.17716(17) 1.0   0.0210(5) . . . .
O23 O Uani 0.5838(2) 0.65497(17) 0.21733(18) 1.0   0.0235(6) . . . .
O26 O Uani 0.2937(3) 0.51643(19) 0.1445(2) 1.0   0.0317(6) . . . .
H2 H Uiso 1.17865 0.28532 0.18556 1.0   0.0276 . . . .
H2' H Uiso 1.05102 0.19405 0.07340 1.0   0.0276 . . . .
H3 H Uiso 0.99552 0.38445 0.22805 1.0   0.0270 . . . .
H3' H Uiso 0.94890 0.35952 0.08411 1.0   0.0270 . . . .
H4 H Uiso 0.74767 0.20228 -0.04275 1.0   0.0257 . . . .
H4' H Uiso 0.60396 0.16887 0.00002 1.0   0.0257 . . . .
H5 H Uiso 0.70587 0.00304 -0.06441 1.0   0.0235 . . . .
H5' H Uiso 0.87417 0.05562 0.03726 1.0   0.0235 . . . .
H7 H Uiso 0.75789 0.43811 0.18776 1.0   0.0244 . . . .
H7' H Uiso 0.64913 0.37435 0.05126 1.0   0.0244 . . . .
H8 H Uiso 0.49690 0.39369 0.18078 1.0   0.0256 . . . .
H8' H Uiso 0.49103 0.25861 0.12246 1.0   0.0256 . . . .
H9 H Uiso 0.59474 0.46272 0.39452 1.0   0.0232 . . . .
H9' H Uiso 0.75558 0.47573 0.36688 1.0   0.0232 . . . .
H10 H Uiso 0.71173 0.35878 0.54374 1.0   0.0210 . . . .
H10' H Uiso 0.79480 0.49156 0.57660 1.0   0.0210 . . . .
H12 H Uiso 0.43825 0.18293 0.25799 1.0   0.0222 . . . .
H12' H Uiso 0.46044 0.28218 0.37655 1.0   0.0222 . . . .
H24 H Uiso 1.184(4) -0.200(3) 0.236(3) 1.0   0.0291 . . . .
H24' H Uiso 1.205(4) -0.084(3) 0.234(3) 1.0   0.0291 . . . .
H25 H Uiso 1.313(4) 0.306(3) 0.591(3) 1.0   0.0275 . . . .
H25' H Uiso 1.182(4) 0.308(3) 0.499(3) 1.0   0.0275 . . . .
H27 H Uiso 1.427(4) 0.079(3) 0.754(3) 1.0   0.0244 . . . .
H27' H Uiso 1.518(4) 0.121(3) 0.715(3) 1.0   0.0244 . . . .
H28 H Uiso 1.113(4) 0.112(3) 0.700(3) 1.0   0.0243 . . . .
H28' H Uiso 1.059(4) 0.179(3) 0.638(3) 1.0   0.0243 . . . .
H21 H Uiso 0.861(5) 0.659(3) 0.094(3) 1.0   0.0347 . . . .
H21' H Uiso 0.761(4) 0.727(3) 0.068(3) 1.0   0.0347 . . . .
H22 H Uiso 0.125(4) 0.615(3) 0.165(3) 1.0   0.0315 . . . .
H22' H Uiso 0.061(4) 0.639(3) 0.240(3) 1.0   0.0315 . . . .
H23 H Uiso 0.633(4) 0.646(3) 0.176(3) 1.0   0.0352 . . . .
H23' H Uiso 0.567(5) 0.708(3) 0.221(3) 1.0   0.0352 . . . .
H26 H Uiso 0.265(5) 0.467(4) 0.083(4) 1.0   0.0475 . . . .
H26' H Uiso 0.360(5) 0.552(4) 0.152(4) 1.0   0.0475 . . . .
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_atom_site_aniso_U_13
_atom_site_aniso_U_12
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Cu 0.0121(1) 0.0116(1) 0.0125(1) 0.0059(1) 0.0049(1) 0.0044(1)
O1 0.0143(8) 0.0200(8) 0.0144(7) 0.0034(6) 0.0051(6) 0.0054(7)
O2 0.0203(9) 0.0222(9) 0.0194(8) 0.0068(7) 0.0099(7) 0.0097(7)
O3 0.0215(9) 0.0168(8) 0.0175(8) 0.0040(6) 0.0057(7) 0.0011(7)
O4 0.0361(11) 0.0172(9) 0.0226(9) 0.0063(7) 0.0101(8) 0.0072(8)
O5 0.0153(8) 0.0131(7) 0.0166(8) 0.0023(6) 0.0035(6) 0.0019(6)
O6 0.0192(8) 0.0257(9) 0.0172(8) 0.0058(7) 0.0054(7) 0.0070(7)
O7 0.0156(8) 0.0126(7) 0.0172(8) 0.0028(6) 0.0092(6) 0.0006(6)
O8 0.0152(8) 0.0148(8) 0.0201(8) 0.0078(6) 0.0093(6) 0.0045(6)
O24 0.0240(9) 0.0145(8) 0.0206(8) 0.0045(7) 0.0081(7) 0.0052(7)
O25 0.0177(9) 0.0159(8) 0.0197(8) 0.0023(7) 0.0046(7) 0.0058(7)
O27 0.0153(8) 0.0170(8) 0.0186(8) 0.0057(6) 0.0077(7) 0.0027(7)
O28 0.0170(8) 0.0157(8) 0.0161(8) 0.0039(7) 0.0054(6) 0.0046(7)
N1 0.0254(11) 0.0181(10) 0.0146(9) 0.0050(8) 0.0052(8) -0.0012(8)
N2 0.0172(10) 0.0158(9) 0.0196(10) 0.0035(8) 0.0021(8) 0.0051(8)
C1 0.0180(11) 0.0167(11) 0.0129(10) 0.0021(8) 0.0037(8) 0.0040(9)
C2 0.0267(13) 0.0207(12) 0.0221(12) 0.0091(10) 0.0065(10) 0.0050(10)
C3 0.0261(13) 0.0194(12) 0.0228(12) 0.0079(10) 0.0079(10) 0.0035(10)
C4 0.0314(14) 0.0188(11) 0.0113(10) 0.0041(9) 0.0048(9) -0.0001(10)
C5 0.0258(12) 0.0179(11) 0.0131(10) 0.0029(8) 0.0053(9) 0.0009(10)
C6 0.0217(12) 0.0148(11) 0.0127(10) 0.0019(8) 0.0009(9) -0.0021(9)
C7 0.0232(12) 0.0168(11) 0.0208(11) 0.0119(9) 0.0031(9) 0.0034(9)
C8 0.0219(12) 0.0199(12) 0.0218(12) 0.0074(9) 0.0050(10) 0.0048(10)
C9 0.0184(11) 0.0132(11) 0.0222(11) 0.0014(9) 0.0020(9) 0.0066(9)
C10 0.0154(11) 0.0137(10) 0.0202(11) 0.0003(8) 0.0036(9) 0.0037(9)
C11 0.0149(11) 0.0104(10) 0.0205(11) 0.0025(8) 0.0043(9) 0.0024(8)
C12 0.0193(11) 0.0129(10) 0.0218(11) 0.0069(9) 0.0036(9) 0.0021(9)
C13 0.0185(11) 0.0088(9) 0.0143(10) 0.0008(8) 0.0054(8) 0.0011(8)
O21 0.0219(9) 0.0184(9) 0.0252(9) 0.0011(7) 0.0047(7) 0.0049(8)
O22 0.0225(9) 0.0205(9) 0.0218(9) 0.0037(7) 0.0098(7) 0.0068(7)
O23 0.0258(10) 0.0172(9) 0.0277(10) 0.0021(8) 0.0107(8) 0.0061(8)
O26 0.0264(11) 0.0249(11) 0.0343(11) -0.0079(9) 0.0068(9) 0.0031(8)

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

# 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
 Ba      O1       3.0481(17)                    .       .                 yes
 Ba      O2       2.8337(17)                    .       .                 yes
 Ba      O24      2.8828(18)                    .       .                 yes
 Ba      O25      2.7744(18)                    .       .                 yes
```

Ba	O27	2.8170(18)	.	.	yes
Ba	O28	2.9044(18)	.	.	yes
Ba	O8	2.7778(18)	.	1_655	yes
Ba	O7	2.8321(16)	.	2_756	yes
Ba	O8	2.8346(18)	.	2_756	yes
Ba	O28	2.9135(19)	.	2_756	yes
Cu	O1	1.9515(18)	.	.	yes
Cu	O3	2.5177(17)	.	.	yes
Cu	O5	2.2991(17)	.	.	yes
Cu	O7	2.0126(16)	.	.	yes
Cu	N1	2.026(2)	.	.	yes
Cu	N2	2.022(2)	.	.	yes
O1	C1	1.277(3)	.	.	yes
O2	C1	1.246(3)	.	.	yes
O3	C6	1.260(3)	.	.	yes
O4	C6	1.262(3)	.	.	yes
O5	C11	1.267(3)	.	.	yes
O6	C11	1.261(3)	.	.	yes
O7	C13	1.286(3)	.	.	yes
O8	C13	1.244(3)	.	.	yes
O24	H24'	0.73(4)	.	.	no
O24	H24	0.89(4)	.	.	no
O25	H25'	0.87(4)	.	.	no
O25	H25	0.80(3)	.	.	no
O27	H27	0.77(4)	.	.	no
O27	H27'	0.64(4)	.	.	no
O28	H28	0.79(3)	.	.	no
O28	H28'	0.77(4)	.	.	no
O21	H21	0.83(4)	.	.	no
O21	H21'	0.78(4)	.	.	no
O22	H22	0.66(4)	.	.	no
O22	H22'	0.85(3)	.	.	no
O23	H23'	0.66(4)	.	.	no
O23	H23	0.77(4)	.	.	no
O26	H26'	0.67(5)	.	.	no
O26	H26	0.80(4)	.	.	no
N1	C7	1.526(4)	.	.	yes
N1	C3	1.479(4)	.	.	yes
N1	C4	1.504(3)	.	.	yes
N2	C9	1.501(3)	.	.	yes
N2	C12	1.498(3)	.	.	yes
N2	C8	1.483(3)	.	.	yes
C1	C2	1.534(3)	.	.	no
C2	C3	1.513(4)	.	.	no
C4	C5	1.532(3)	.	.	no
C5	C6	1.527(3)	.	.	no
C7	C8	1.504(4)	.	.	no
C9	C10	1.516(3)	.	.	no
C10	C11	1.529(4)	.	.	no
C12	C13	1.512(3)	.	.	no
C2	H2'	0.99	.	.	no
C2	H2	0.99	.	.	no
C3	H3	0.99	.	.	no
C3	H3'	0.99	.	.	no
C4	H4	0.99	.	.	no
C4	H4'	0.99	.	.	no
C5	H5	0.99	.	.	no
C5	H5'	0.99	.	.	no
C7	H7	0.99	.	.	no
C7	H7'	0.99	.	.	no
C8	H8'	0.99	.	.	no
C8	H8	0.99	.	.	no
C9	H9'	0.99	.	.	no
C9	H9	0.99	.	.	no
C10	H10	0.99	.	.	no
C10	H10'	0.99	.	.	no

```
 C12     H12          0.99                      .       .                 no
 C12     H12'         0.99                      .       .                 no

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
 O1      Ba      O2         43.87(5)             .       .       .          yes
 O1      Ba      O24        87.72(5)             .       .       .          yes
 O1      Ba      O25        64.79(5)             .       .       .          yes
 O1      Ba      O27       137.07(5)             .       .       .          yes
 O1      Ba      O28        82.97(5)             .       .       .          yes
 O1      Ba      O8        112.16(5)             .       .     1_655        yes
 O1      Ba      O7        138.06(5)             .       .     2_756        yes
 O1      Ba      O8        154.10(4)             .       .     2_756        yes
 O1      Ba      O28        67.53(5)             .       .     2_756        yes
 O2      Ba      O24        56.41(5)             .       .       .          yes
 O2      Ba      O25        77.09(5)             .       .       .          yes
 O2      Ba      O27       141.16(5)             .       .       .          yes
 O2      Ba      O28       126.36(5)             .       .       .          yes
 O2      Ba      O8         75.49(5)             .       .     1_655        yes
 O2      Ba      O7        140.21(5)             .       .     2_756        yes
 O2      Ba      O8        113.49(5)             .       .     2_756        yes
 O2      Ba      O28        87.59(5)             .       .     2_756        yes
 O24     Ba      O25       131.25(5)             .       .       .          yes
 O24     Ba      O27       132.80(5)             .       .       .          yes
 O24     Ba      O28       146.04(5)             .       .       .          yes
 O8      Ba      O24        78.19(5)           1_655     .       .          yes
 O7      Ba      O24        84.61(5)           2_756     .       .          yes
 O8      Ba      O24        66.55(5)           2_756     .       .          yes
 O24     Ba      O28        71.26(5)             .       .     2_756        yes
 O25     Ba      O27        75.59(5)             .       .       .          yes
 O25     Ba      O28        72.84(5)             .       .       .          yes
 O8      Ba      O25        76.66(5)           1_655     .       .          yes
 O7      Ba      O25       142.65(5)           2_756     .       .          yes
 O8      Ba      O25       130.39(5)           2_756     .       .          yes
 O25     Ba      O28       124.61(5)             .       .     2_756        yes
 O27     Ba      O28        69.74(5)             .       .       .          yes
 O8      Ba      O27        71.73(5)           1_655     .       .          yes
 O7      Ba      O27        70.58(5)           2_756     .       .          yes
 O8      Ba      O27        67.31(5)           2_756     .       .          yes
 O27     Ba      O28       130.85(5)             .       .     2_756        yes
 O8      Ba      O28       135.43(5)           1_655     .       .          yes
 O7      Ba      O28        80.91(5)           2_756     .       .          yes
 O8      Ba      O28       119.91(5)           2_756     .       .          yes
 O28     Ba      O28        75.01(5)             .       .     2_756        yes
 O7      Ba      O8        106.45(5)           2_756     .     1_655        yes
 O8      Ba      O8         61.43(5)           1_655     .     2_756        yes
 O8      Ba      O28       149.45(5)           1_655     .     2_756        yes
 O7      Ba      O8         46.29(5)           2_756     .     2_756        yes
 O7      Ba      O28        70.96(5)           2_756     .     2_756        yes
 O8      Ba      O28       104.66(5)           2_756     .     2_756        yes
 O1      Cu      O3         89.66(7)             .       .       .          yes
 O1      Cu      O5         84.82(7)             .       .       .          yes
 O1      Cu      O7         97.12(7)             .       .       .          yes
 O1      Cu      N1         93.38(9)             .       .       .          yes
 O1      Cu      N2        174.68(8)             .       .       .          yes
 O3      Cu      O5        166.67(6)             .       .       .          yes
 O3      Cu      O7         79.26(6)             .       .       .          yes
 O3      Cu      N1         86.79(7)             .       .       .          yes
 O3      Cu      N2         95.42(7)             .       .       .          yes
```

O5	Cu	O7	89.37(6)	.	.	.	yes
O5	Cu	N1	105.62(8)	.	.	.	yes
O5	Cu	N2	89.88(7)	.	.	.	yes
O7	Cu	N1	162.44(9)	.	.	.	yes
O7	Cu	N2	82.31(8)	.	.	.	yes
N1	Cu	N2	88.50(10)	.	.	.	yes
Ba	O1	Cu	139.32(7)	.	.	.	yes
Ba	O1	C1	88.71(14)	.	.	.	yes
Cu	O1	C1	128.14(16)	.	.	.	yes
Ba	O2	C1	99.50(14)	.	.	.	yes
Cu	O3	C6	100.24(15)	.	.	.	yes
Cu	O5	C11	108.27(15)	.	.	.	yes
Cu	O7	C13	113.09(14)	.	.	.	yes
Ba	O7	Cu	145.23(8)	2_756	.	.	yes
Ba	O7	C13	94.14(13)	2_756	.	.	yes
Ba	O8	C13	140.90(16)	1_455	.	.	yes
Ba	O8	C13	95.04(15)	2_756	.	.	yes
Ba	O8	Ba	118.57(6)	1_455	.	2_756	yes
Ba	O28	Ba	104.99(5)	.	.	2_756	yes
Ba	O24	H24'	81(3)	.	.	.	no
H24	O24	H24'	115(4)	.	.	.	no
Ba	O24	H24	126(2)	.	.	.	no
H25	O25	H25'	107(4)	.	.	.	no
Ba	O25	H25	106(3)	.	.	.	no
Ba	O25	H25'	112(2)	.	.	.	no
Ba	O27	H27	112(3)	.	.	.	no
H27	O27	H27'	114(4)	.	.	.	no
Ba	O27	H27'	111(3)	.	.	.	no
Ba	O28	H28	111(3)	.	.	.	no
Ba	O28	H28'	114(3)	2_756	.	.	no
Ba	O28	H28	113(3)	2_756	.	.	no
Ba	O28	H28'	110(3)	.	.	.	no
H28	O28	H28'	103(4)	.	.	.	no
H21	O21	H21'	105(4)	.	.	.	no
H22	O22	H22'	108(4)	.	.	.	no
H23	O23	H23'	108(5)	.	.	.	no
H26	O26	H26'	113(5)	.	.	.	no
Cu	N1	C4	115.60(16)	.	.	.	yes
Cu	N1	C7	103.51(15)	.	.	.	yes
C3	N1	C7	107.71(19)	.	.	.	yes
C4	N1	C7	108.3(2)	.	.	.	yes
C3	N1	C4	113.2(2)	.	.	.	yes
Cu	N1	C3	107.86(15)	.	.	.	yes
Cu	N2	C12	105.94(15)	.	.	.	yes
C8	N2	C9	109.63(19)	.	.	.	yes
C8	N2	C12	112.14(19)	.	.	.	yes
C9	N2	C12	110.32(18)	.	.	.	yes
Cu	N2	C8	104.97(15)	.	.	.	yes
Cu	N2	C9	113.75(15)	.	.	.	yes
O1	C1	O2	122.0(2)	.	.	.	yes
O2	C1	C2	115.2(2)	.	.	.	yes
O1	C1	C2	122.8(2)	.	.	.	yes
C1	C2	C3	119.7(2)	.	.	.	no
N1	C3	C2	114.3(2)	.	.	.	yes
N1	C4	C5	119.0(2)	.	.	.	yes
C4	C5	C6	115.8(2)	.	.	.	no
O3	C6	O4	125.0(2)	.	.	.	yes
O3	C6	C5	117.9(2)	.	.	.	yes
O4	C6	C5	117.1(2)	.	.	.	yes
N1	C7	C8	109.6(2)	.	.	.	yes
N2	C8	C7	108.1(2)	.	.	.	yes
N2	C9	C10	113.9(2)	.	.	.	yes
C9	C10	C11	114.8(2)	.	.	.	no
O5	C11	O6	123.6(3)	.	.	.	yes
O5	C11	C10	118.5(2)	.	.	.	yes
O6	C11	C10	117.9(2)	.	.	.	yes

```
 N2      C12     C13        110.0(2)            .       .       .          yes
 O7      C13     C12        117.4(2)            .       .       .          yes
 O8      C13     C12        119.2(2)            .       .       .          yes
 O7      C13     O8         123.4(2)            .       .       .          yes
 C3      C2      H2'          107               .       .       .          no
 C1      C2      H2           107               .       .       .          no
 C1      C2      H2'          107               .       .       .          no
 H2      C2      H2'          107               .       .       .          no
 C3      C2      H2           107               .       .       .          no
 N1      C3      H3           109               .       .       .          no
 N1      C3      H3'          109               .       .       .          no
 C2      C3      H3           109               .       .       .          no
 C2      C3      H3'          109               .       .       .          no
 H3      C3      H3'          108               .       .       .          no
 N1      C4      H4'          108               .       .       .          no
 C5      C4      H4           108               .       .       .          no
 C5      C4      H4'          108               .       .       .          no
 N1      C4      H4           108               .       .       .          no
 H4      C4      H4'          107               .       .       .          no
 C6      C5      H5'          108               .       .       .          no
 H5      C5      H5'          107               .       .       .          no
 C4      C5      H5           108               .       .       .          no
 C4      C5      H5'          108               .       .       .          no
 C6      C5      H5           108               .       .       .          no
 N1      C7      H7'          110               .       .       .          no
 C8      C7      H7           110               .       .       .          no
 N1      C7      H7           110               .       .       .          no
 C8      C7      H7'          110               .       .       .          no
 H7      C7      H7'          108               .       .       .          no
 H8      C8      H8'          108               .       .       .          no
 C7      C8      H8           110               .       .       .          no
 C7      C8      H8'          110               .       .       .          no
 N2      C8      H8           110               .       .       .          no
 N2      C8      H8'          110               .       .       .          no
 H9      C9      H9'          108               .       .       .          no
 N2      C9      H9           109               .       .       .          no
 N2      C9      H9'          109               .       .       .          no
 C10     C9      H9           109               .       .       .          no
 C10     C9      H9'          109               .       .       .          no
 C9      C10     H10'         109               .       .       .          no
 C11     C10     H10          109               .       .       .          no
 C9      C10     H10          109               .       .       .          no
 C11     C10     H10'         109               .       .       .          no
 H10     C10     H10'         108               .       .       .          no
 H12     C12     H12'         108               .       .       .          no
 C13     C12     H12          110               .       .       .          no
 C13     C12     H12'         110               .       .       .          no
 N2      C12     H12          110               .       .       .          no
 N2      C12     H12'         110               .       .       .          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
 O2      Ba      O1      Cu      -170.01(16)     .       .       .       .   no
 O2      Ba      O1      C1       -12.87(13)     .       .       .       .   no
 O24     Ba      O1      Cu       149.24(12)     .       .       .       .   no
 O24     Ba      O1      C1       -53.62(13)     .       .       .       .   no
 O25     Ba      O1      Cu       -72.34(12)     .       .       .       .   no
```

O25	Ba	O1	C1	84.81(14)	.	.	.	.	no
O27	Ba	O1	Cu	-47.88(15)	.	.	.	.	no
O27	Ba	O1	C1	109.26(14)	.	.	.	.	no
O28	Ba	O1	Cu	1.96(12)	.	.	.	.	no
O28	Ba	O1	C1	159.11(14)	.	.	.	.	no
O8	Ba	O1	Cu	-134.49(11)	1_655	.	.	.	no
O8	Ba	O1	C1	22.66(14)	1_655	.	.	.	no
O7	Ba	O1	Cu	69.91(14)	2_756	.	.	.	no
O7	Ba	O1	C1	-132.95(13)	2_756	.	.	.	no
O8	Ba	O1	Cu	155.59(10)	2_756	.	.	.	no
O8	Ba	O1	C1	-47.26(19)	2_756	.	.	.	no
O28	Ba	O1	Cu	78.60(12)	2_756	.	.	.	no
O28	Ba	O1	C1	-124.25(14)	2_756	.	.	.	no
O1	Ba	O2	C1	13.38(14)	.	.	.	.	no
O24	Ba	O2	C1	141.84(17)	.	.	.	.	no
O25	Ba	O2	C1	-53.53(15)	.	.	.	.	no
O27	Ba	O2	C1	-99.75(16)	.	.	.	.	no
O28	Ba	O2	C1	3.47(17)	.	.	.	.	no
O8	Ba	O2	C1	-132.85(16)	1_655	.	.	.	no
O7	Ba	O2	C1	128.73(15)	2_756	.	.	.	no
O8	Ba	O2	C1	177.77(14)	2_756	.	.	.	no
O28	Ba	O2	C1	72.83(15)	2_756	.	.	.	no
O1	Ba	O28	Ba	68.55(5)	.	.	.	2_756	no
O2	Ba	O28	Ba	75.45(7)	.	.	.	2_756	no
O24	Ba	O28	Ba	-6.68(12)	.	.	.	2_756	no
O25	Ba	O28	Ba	134.27(7)	.	.	.	2_756	no
O27	Ba	O28	Ba	-145.15(7)	.	.	.	2_756	no
O8	Ba	O28	Ba	-176.85(5)	1_655	.	.	2_756	no
O7	Ba	O28	Ba	-72.60(6)	2_756	.	.	2_756	no
O8	Ba	O28	Ba	-98.52(6)	2_756	.	.	2_756	no
O28	Ba	O28	Ba	0.00(4)	2_756	.	.	2_756	no
O1	Ba	O8	C13	-6.2(2)	.	.	1_655	1_655	no
O2	Ba	O8	C13	18.4(2)	.	.	1_655	1_655	no
O24	Ba	O8	C13	76.4(2)	.	.	1_655	1_655	no
O25	Ba	O8	C13	-61.5(2)	.	.	1_655	1_655	no
O27	Ba	O8	C13	-140.5(2)	.	.	1_655	1_655	no
O28	Ba	O8	C13	-109.2(2)	.	.	1_655	1_655	no
O1	Ba	O7	Cu	-68.80(15)	.	.	2_756	2_756	no
O1	Ba	O7	C13	148.67(12)	.	.	2_756	2_756	no
O2	Ba	O7	Cu	-138.37(12)	.	.	2_756	2_756	no
O2	Ba	O7	C13	79.10(15)	.	.	2_756	2_756	no
O24	Ba	O7	Cu	-149.31(14)	.	.	2_756	2_756	no
O24	Ba	O7	C13	68.16(13)	.	.	2_756	2_756	no
O25	Ba	O7	Cu	45.26(18)	.	.	2_756	2_756	no
O25	Ba	O7	C13	-97.27(14)	.	.	2_756	2_756	no
O27	Ba	O7	Cu	71.50(13)	.	.	2_756	2_756	no
O27	Ba	O7	C13	-71.04(13)	.	.	2_756	2_756	no
O28	Ba	O7	Cu	-0.12(13)	.	.	2_756	2_756	no
O28	Ba	O7	C13	-142.65(13)	.	.	2_756	2_756	no
O1	Ba	O8	C13	-118.70(15)	.	.	2_756	2_756	no
O2	Ba	O8	C13	-143.97(13)	.	.	2_756	2_756	no
O24	Ba	O8	C13	-111.77(14)	.	.	2_756	2_756	no
O25	Ba	O8	C13	123.17(13)	.	.	2_756	2_756	no
O27	Ba	O8	C13	78.40(13)	.	.	2_756	2_756	no
O28	Ba	O8	C13	30.74(15)	.	.	2_756	2_756	no
O1	Ba	O28	Ba	-88.49(6)	.	.	2_756	2_756	no
O2	Ba	O28	Ba	-128.72(6)	.	.	2_756	2_756	no
O24	Ba	O28	Ba	176.07(7)	.	.	2_756	2_756	no
O25	Ba	O28	Ba	-56.22(8)	.	.	2_756	2_756	no
O27	Ba	O28	Ba	45.13(9)	.	.	2_756	2_756	no
O28	Ba	O28	Ba	0.00(6)	.	.	2_756	2_756	no
O3	Cu	O1	Ba	-107.87(11)	.	.	.	.	no
O3	Cu	O1	C1	101.72(19)	.	.	.	.	no
O5	Cu	O1	Ba	59.98(11)	.	.	.	.	no
O5	Cu	O1	C1	-90.44(19)	.	.	.	.	no
O7	Cu	O1	Ba	-28.73(12)	.	.	.	.	no

O7	Cu	O1	C1	-179.15(19)	.	.	.	.	no
N1	Cu	O1	Ba	165.37(12)	.	.	.	.	no
N1	Cu	O1	C1	15.0(2)	.	.	.	.	no
O1	Cu	O3	C6	-27.69(14)	.	.	.	.	no
O7	Cu	O3	C6	-125.00(15)	.	.	.	.	no
N1	Cu	O3	C6	65.71(16)	.	.	.	.	no
N2	Cu	O3	C6	153.90(15)	.	.	.	.	no
O1	Cu	O5	C11	-124.50(16)	.	.	.	.	no
O7	Cu	O5	C11	-27.29(16)	.	.	.	.	no
N1	Cu	O5	C11	143.43(16)	.	.	.	.	no
N2	Cu	O5	C11	55.02(16)	.	.	.	.	no
O1	Cu	O7	C13	-162.92(15)	.	.	.	.	no
O1	Cu	O7	Ba	-24.19(14)	.	.	.	2_756	no
O3	Cu	O7	C13	-74.62(15)	.	.	.	.	no
O3	Cu	O7	Ba	64.11(13)	.	.	.	2_756	no
O5	Cu	O7	C13	112.38(15)	.	.	.	.	no
O5	Cu	O7	Ba	-108.89(13)	.	.	.	2_756	no
N2	Cu	O7	C13	22.42(15)	.	.	.	.	no
N2	Cu	O7	Ba	161.15(14)	.	.	.	2_756	no
O1	Cu	N1	C3	-49.04(16)	.	.	.	.	no
O1	Cu	N1	C4	78.7(2)	.	.	.	.	no
O1	Cu	N1	C7	-163.00(15)	.	.	.	.	no
O3	Cu	N1	C3	-138.51(16)	.	.	.	.	no
O3	Cu	N1	C4	-10.7(2)	.	.	.	.	no
O3	Cu	N1	C7	107.53(15)	.	.	.	.	no
O5	Cu	N1	C3	36.52(17)	.	.	.	.	no
O5	Cu	N1	C4	164.30(18)	.	.	.	.	no
O5	Cu	N1	C7	-77.44(16)	.	.	.	.	no
N2	Cu	N1	C3	125.97(16)	.	.	.	.	no
N2	Cu	N1	C4	-106.3(2)	.	.	.	.	no
N2	Cu	N1	C7	12.02(16)	.	.	.	.	no
O3	Cu	N2	C8	-69.85(15)	.	.	.	.	no
O3	Cu	N2	C9	170.31(15)	.	.	.	.	no
O3	Cu	N2	C12	48.96(14)	.	.	.	.	no
O5	Cu	N2	C8	122.40(15)	.	.	.	.	no
O5	Cu	N2	C9	2.56(15)	.	.	.	.	no
O5	Cu	N2	C12	-118.78(14)	.	.	.	.	no
O7	Cu	N2	C8	-148.22(15)	.	.	.	.	no
O7	Cu	N2	C9	91.94(16)	.	.	.	.	no
O7	Cu	N2	C12	-29.40(13)	.	.	.	.	no
N1	Cu	N2	C8	16.78(16)	.	.	.	.	no
N1	Cu	N2	C9	-103.06(16)	.	.	.	.	no
N1	Cu	N2	C12	135.60(15)	.	.	.	.	no
Ba	O1	C1	O2	24.4(2)	.	.	.	.	no
Ba	O1	C1	C2	-154.1(2)	.	.	.	.	no
Cu	O1	C1	O2	-174.33(16)	.	.	.	.	no
Cu	O1	C1	C2	7.2(3)	.	.	.	.	no
Ba	O2	C1	O1	-26.8(2)	.	.	.	.	no
Ba	O2	C1	C2	151.79(16)	.	.	.	.	no
Cu	O3	C6	O4	113.4(2)	.	.	.	.	no
Cu	O3	C6	C5	-67.3(2)	.	.	.	.	no
Cu	O5	C11	O6	119.8(2)	.	.	.	.	no
Cu	O5	C11	C10	-60.7(2)	.	.	.	.	no
Cu	O7	C13	O8	169.20(18)	.	.	.	.	no
Cu	O7	C13	C12	-8.7(2)	.	.	.	.	no
Ba	O7	C13	O8	11.4(2)	2_756	.	.	.	no
Ba	O7	C13	C12	-166.51(17)	2_756	.	.	.	no
Ba	O8	C13	O7	-161.79(15)	1_455	.	.	.	no
Ba	O8	C13	C12	16.1(4)	1_455	.	.	.	no
Ba	O8	C13	O7	-11.4(2)	2_756	.	.	.	no
Ba	O8	C13	C12	166.47(18)	2_756	.	.	.	no
Cu	N1	C3	C2	68.4(2)	.	.	.	.	no
C4	N1	C3	C2	-60.7(3)	.	.	.	.	no
C7	N1	C3	C2	179.55(18)	.	.	.	.	no
Cu	N1	C4	C5	-42.3(3)	.	.	.	.	no
C3	N1	C4	C5	82.8(3)	.	.	.	.	no

C7	N1	C4	C5	-157.8(2)	.	.	.	no
Cu	N1	C7	C8	-39.3(2)	.	.	.	no
C3	N1	C7	C8	-153.39(18)	.	.	.	no
C4	N1	C7	C8	83.9(2)	.	.	.	no
Cu	N2	C8	C7	-42.9(2)	.	.	.	no
C9	N2	C8	C7	79.7(2)	.	.	.	no
C12	N2	C8	C7	-157.41(19)	.	.	.	no
Cu	N2	C9	C10	-56.2(3)	.	.	.	no
C8	N2	C9	C10	-173.4(2)	.	.	.	no
C12	N2	C9	C10	62.6(3)	.	.	.	no
Cu	N2	C12	C13	32.3(2)	.	.	.	no
C8	N2	C12	C13	146.27(19)	.	.	.	no
C9	N2	C12	C13	-91.2(2)	.	.	.	no
O1	C1	C2	C3	2.0(3)	.	.	.	no
O2	C1	C2	C3	-176.6(2)	.	.	.	no
C1	C2	C3	N1	-45.1(3)	.	.	.	no
N1	C4	C5	C6	62.0(3)	.	.	.	no
C4	C5	C6	O3	11.8(3)	.	.	.	no
C4	C5	C6	O4	-168.8(2)	.	.	.	no
N1	C7	C8	N2	57.0(2)	.	.	.	no
N2	C9	C10	C11	67.5(3)	.	.	.	no
C9	C10	C11	O5	3.8(3)	.	.	.	no
C9	C10	C11	O6	-176.7(2)	.	.	.	no
N2	C12	C13	O7	-16.7(3)	.	.	.	no
N2	C12	C13	O8	165.3(2)	.	.	.	no

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loop_
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_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_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)
#
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O21	H21	O22	0.83(4)	1.91(4)	2.742(3)	176(4)	1_655	yes
O21	H21'	O4	0.78(4)	1.97(4)	2.731(3)	168(3)	1_565	yes
O22	H22	O26	0.66(4)	2.06(4)	2.716(3)	173(3)	.	yes
O22	H22'	O6	0.85(3)	1.80(4)	2.618(3)	163(4)	2_666	yes
O23	H23	O21	0.77(4)	2.12(4)	2.869(3)	167(4)	.	yes
O23	H23'	O27	0.66(4)	2.11(4)	2.740(3)	163(4)	2_766	yes
O24	H24	O22	0.89(4)	1.83(4)	2.720(3)	178(4)	1_645	yes
O25	H25	O23	0.80(3)	2.12(3)	2.914(3)	173(4)	2_766	yes
O25	H25'	O5	0.87(4)	1.90(4)	2.771(3)	177(3)	.	yes
O26	H26	O21	0.80(4)	2.00(5)	2.785(3)	170(5)	2_665	yes
O26	H26'	O23	0.67(5)	2.10(5)	2.753(3)	166(5)	.	yes
O27	H27	O3	0.77(4)	1.96(4)	2.726(3)	173(4)	2_756	yes
O27	H27'	O24	0.64(4)	2.12(4)	2.765(3)	175(4)	2_856	yes
O28	H28	O4	0.79(3)	2.10(3)	2.894(2)	178(5)	2_756	yes
O28	H28'	O6	0.77(4)	2.21(4)	2.966(3)	174(4)	.	yes
C8	H8	O26	0.9900	2.4300	3.401(4)	166	.	yes
C12	H12	O2	0.9900	2.4000	3.085(3)	126	1_455	yes

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#===END of Crystallographic Information File
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