# University of Groningen

## Ultrafast Light-Driven Nanomotors Based on an Acridane Stator

Kulago, Artem A.; Mes, Emile M.; Klok, Martin; Meetsma, Auke; Brouwer, A.M.; Feringa, B.L.

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*Document Version*
Publisher's PDF, also known as Version of record

*Publication date:*
2010

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# CIF-file generated for C66H62N2O6                        P21/c      q1141
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2009-09-14 # 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
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     Crystal Structure Center,
     Chemical Physics,
     Materials Science Center,
     University of Groningen,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
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_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              'Journal of Organic Chemistry'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
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_publ_requested_coeditor_name        ?

_publ_contact_letter                 # Include date of submission
;
 Date of submission :  2009-09-14  12:09:23

 Consider this CIF submission for deposition of the (
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     Journal of Organic Chemistry

(Our Compound_Identification_Code : Q1141)
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'?' # author name
;    # author related footnote
;
;    # Address of this author
```

```
;
    'Meetsma, Auke'
;
 ? # author related footnote
;
;
      Crystal Structure Center,
      Chemical Physics,
      Materials Science Center,
      University of Groningen,
      Nijenborgh 4,
      NL-9747 AG Groningen,
      The Netherlands.
;

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Allen, F. H. (2000). <i>Acta Cryst.</i> B<b>58</b>, 380--388.

Bondi, A. (1964). <i>J. Phys. Chem.</i> <b>68</b>, 441--451.

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Manual Bruker AXS Inc. Madison, Wisconsin, USA.

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Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). <i>SIR2004</i>. An
improved tool for crystal structure determination and refinement. J. Appl.
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Space-group symmetry, Kluwer Academic Publishers, Dordrecht, The Netherlands.

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```

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Groningen, The Netherlands. (unpublished).

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Refinement. University of G\"ottingen, Germany.

Sheldrick, G. M. (2001). <i>SADABS</i>. Version 2.03. Multi-Scan Absorption
Correction Program. University of G"\öttingenottingen, Germany.

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

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

_publ_section_figure_captions
;


Fig. 1. Perspective <i>PLUTO</i> drawing of the molecule illustrating the
configuration and the adopted numbering scheme.

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

Fig. 3. Perspective <i>ORTEP</i> drawing of the title compound. Displacement
ellipsoids for non-H are represented at the 50% probability level. The H-atoms
have been omitted to improve clarity.
;

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

# 5. CHEMICAL DATA

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;
;
_chemical_name_common                    ?
_chemical_melting_point                  ?
_chemical_formula_moiety
'C33 H31 N O3'
# 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
'C33 H31 N O3'
_chemical_formula_iupac                  ?
_chemical_formula_weight                   489.61
_chemical_compound_source          'see text'

loop_
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_atom_type_scat_source
 O    O    0.0106    0.0060
 '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 21/c'
_symmetry_Int_Tables_number                14

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

_cell_length_a                            9.020(2)
_cell_length_b                           18.831(3)
_cell_length_c                           30.265(5)
_cell_angle_alpha                        90
_cell_angle_beta                         95.108(3)
_cell_angle_gamma                        90
_cell_volume                           5120.3(16)
_cell_formula_units_Z                  8

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used       5340
_cell_measurement_theta_min         2.51
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_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
    5340 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_size_min            0.035
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_exptl_crystal_density_diffrn      1.270
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000               2080
_exptl_absorpt_coefficient_mu      0.081
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2001))'
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_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, 2000)).
;
_diffrn_detector_area_resol_mean     66.06

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_diffrn_standards_decay_%               0

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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number                   39203
_diffrn_reflns_av_R_equivalents      0.0772
_diffrn_reflns_av_sigmaI/netI        0.0834
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_diffrn_reflns_limit_h_max              10
_diffrn_reflns_limit_k_min              -23
_diffrn_reflns_limit_k_max              23
_diffrn_reflns_limit_l_min              -37
_diffrn_reflns_limit_l_max              37
_diffrn_reflns_theta_min             2.55
_diffrn_reflns_theta_max             26.02
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_diffrn_reflns_theta_full                25.00
_diffrn_measured_fraction_theta_full  0.995

_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                 6490
_reflns_threshold_expression      I>2\s(I)


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_computing_structure_solution
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 SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement     'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2006)
 PLATON (Spek, 2003)
;
_computing_publication_material     'PLATON (Spek, 2003)'

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

# 8. REFINEMENT DATA


_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 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_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0506P)^2^+0.1669P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    difmap
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_refine_ls_extinction_method      none
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_chemical_absolute_configuration  '.'

_refine_ls_abs_structure_Flack    ?
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_refine_ls_number_parameters      915
_refine_ls_number_restraints      0
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_refine_ls_goodness_of_fit_ref    1.009
_refine_ls_restrained_S_all       1.009
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_refine_ls_shift/su_mean          0.000


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O13 O Uani -0.11514(16) 0.33340(7) 0.59494(4) 1.000 0.0192(5) . .
N11 N Uani 0.18207(18) 0.13130(8) 0.50154(5) 1.000 0.0139(5) . .
C11 C Uani 0.0831(2) 0.10080(11) 0.46692(6) 1.000 0.0150(7) . .
C12 C Uani 0.0842(3) 0.02877(11) 0.45749(7) 1.000 0.0181(7) . .
C13 C Uani -0.0206(3) 0.00102(12) 0.42639(7) 1.000 0.0219(7) . .
C14 C Uani -0.1303(3) 0.04406(12) 0.40573(7) 1.000 0.0213(7) . .
C15 C Uani -0.1310(3) 0.11582(11) 0.41467(7) 1.000 0.0180(7) . .
C16 C Uani -0.0217(2) 0.14636(11) 0.44432(6) 1.000 0.0156(7) . .
C17 C Uani -0.0080(2) 0.22323(11) 0.45605(6) 1.000 0.0139(6) . .
C18 C Uani 0.0171(2) 0.23148(10) 0.50469(6) 1.000 0.0130(7) . .
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C110 C Uani -0.0331(2) 0.28392(10) 0.57430(7) 1.000 0.0151(7) . .
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C112 C Uani 0.1409(2) 0.18778(11) 0.57316(7) 1.000 0.0157(7) . .
C113 C Uani 0.1158(2) 0.18435(10) 0.52746(6) 1.000 0.0135(6) . .
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C115 C Uani 0.5622(2) 0.14242(11) 0.55206(7) 1.000 0.0173(7) . .
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C129 C Uani 0.3268(3) 0.39275(12) 0.52614(7) 1.000 0.0208(7) . .
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C132 C Uani 0.0277(2) 0.35316(10) 0.43398(6) 1.000 0.0140(6) . .
C133 C Uani 0.0683(3) 0.25028(14) 0.34974(8) 1.000 0.0239(8) . .


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H111 H Uiso 0.090(2) 0.2419(11) 0.6293(7) 1.000 0.023(6) . .
H112 H Uiso 0.206(2) 0.1557(10) 0.5888(6) 1.000 0.013(5) . .
H116 H Uiso 0.650(3) 0.0907(13) 0.4975(8) 1.000 0.034(7) . .
H116' H Uiso 0.768(3) 0.1344(11) 0.5295(7) 1.000 0.021(6) . .
H116" H Uiso 0.657(2) 0.1771(12) 0.4965(7) 1.000 0.022(6) . .
H117 H Uiso 0.491(3) 0.0823(12) 0.6033(8) 1.000 0.031(6) . .
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H118" H Uiso 0.526(3) 0.2155(12) 0.6038(8) 1.000 0.032(6) . .
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H122 H Uiso −0.102(2) 0.3577(11) 0.3347(8) 1.000 0.025(6) . .
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O21 O Uani 0.81625(16) 0.51495(7) 0.29313(5) 1.000 0.0216(5) . .
O22 O Uani 0.79031(16) 0.42704(8) 0.24187(5) 1.000 0.0232(5) . .
O23 O Uani 0.24959(17) 0.23469(8) 0.20242(4) 1.000 0.0232(5) . .
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C22 C Uani 0.5394(3) 0.55737(11) 0.32531(7) 1.000 0.0186(7) . .
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C24 C Uani 0.3873(3) 0.54440(12) 0.38565(7) 1.000 0.0198(7) . .
C25 C Uani 0.3794(2) 0.47205(11) 0.37858(7) 1.000 0.0171(7) . .
C26 C Uani 0.4558(2) 0.44023(10) 0.34556(6) 1.000 0.0146(7) . .
C27 C Uani 0.4587(2) 0.36319(10) 0.33520(6) 1.000 0.0134(6) . .
C28 C Uani 0.4408(2) 0.35177(10) 0.28681(6) 1.000 0.0143(6) . .
C29 C Uani 0.3485(2) 0.29816(11) 0.26800(7) 1.000 0.0158(7) . .
C210 C Uani 0.3324(2) 0.28856(11) 0.22288(7) 1.000 0.0174(7) . .
C211 C Uani 0.4044(3) 0.33404(12) 0.19566(7) 1.000 0.0195(7) . .
C212 C Uani 0.4920(3) 0.38872(12) 0.21365(7) 1.000 0.0196(7) . .
C213 C Uani 0.5115(2) 0.39710(10) 0.25942(6) 1.000 0.0146(7) . .
```

```
C214 C Uani 0.7433(2) 0.46927(11) 0.27354(7) 1.000 0.0176(7) . .
C215 C Uani 0.9338(3) 0.44277(12) 0.22291(7) 1.000 0.0243(8) . .
C216 C Uani 1.0633(3) 0.43578(15) 0.25794(9) 1.000 0.0316(9) . .
C217 C Uani 0.9246(3) 0.51538(14) 0.20142(9) 1.000 0.0324(9) . .
C218 C Uani 0.9385(4) 0.38475(17) 0.18830(11) 1.000 0.0419(11) . .
C219 C Uani 0.1945(3) 0.18258(13) 0.23111(8) 1.000 0.0242(8) . .
C220 C Uani 0.4783(2) 0.30884(11) 0.36469(6) 1.000 0.0132(6) . .
C221 C Uani 0.4606(2) 0.31291(11) 0.41428(6) 1.000 0.0151(7) . .
C222 C Uani 0.3994(3) 0.23875(11) 0.42453(7) 1.000 0.0172(7) . .
C223 C Uani 0.4500(2) 0.19268(11) 0.38855(7) 1.000 0.0156(6) . .
C224 C Uani 0.4458(3) 0.11804(11) 0.38643(7) 1.000 0.0201(7) . .
C225 C Uani 0.5017(3) 0.08494(12) 0.35149(7) 1.000 0.0220(7) . .
C226 C Uani 0.5733(2) 0.12308(11) 0.31891(7) 1.000 0.0173(7) . .
C227 C Uani 0.6428(3) 0.08721(12) 0.28548(7) 1.000 0.0228(7) . .
C228 C Uani 0.7211(3) 0.12305(12) 0.25614(7) 1.000 0.0238(8) . .
C229 C Uani 0.7341(2) 0.19705(12) 0.25934(7) 1.000 0.0195(7) . .
C230 C Uani 0.6654(2) 0.23372(11) 0.29076(7) 1.000 0.0158(7) . .
C231 C Uani 0.5791(2) 0.19844(11) 0.32114(6) 1.000 0.0147(6) . .
C232 C Uani 0.5045(2) 0.23278(11) 0.35522(6) 1.000 0.0142(6) . .
C233 C Uani 0.6067(3) 0.32838(13) 0.44204(7) 1.000 0.0204(7) . .


H22 H Uiso 0.589(2) 0.5862(11) 0.3052(7) 1.000 0.016(5) . .
H23 H Uiso 0.467(2) 0.6392(12) 0.3636(7) 1.000 0.028(6) . .
H24 H Uiso 0.338(2) 0.5658(10) 0.4095(6) 1.000 0.013(5) . .
H25 H Uiso 0.319(2) 0.4446(10) 0.3967(7) 1.000 0.014(5) . .
H29 H Uiso 0.301(2) 0.2705(11) 0.2864(7) 1.000 0.020(6) . .
H211 H Uiso 0.390(2) 0.3266(10) 0.1646(7) 1.000 0.014(5) . .
H212 H Uiso 0.545(2) 0.4190(11) 0.1951(7) 1.000 0.022(6) . .
H216 H Uiso 1.066(3) 0.4730(13) 0.2815(8) 1.000 0.037(7) . .
H216' H Uiso 1.157(3) 0.4391(12) 0.2438(8) 1.000 0.035(7) . .
H216" H Uiso 1.065(3) 0.3866(15) 0.2739(9) 1.000 0.056(8) . .
H217 H Uiso 0.838(3) 0.5173(12) 0.1792(8) 1.000 0.036(7) . .
H217' H Uiso 1.016(2) 0.5242(11) 0.1866(7) 1.000 0.024(6) . .
H217" H Uiso 0.927(3) 0.5542(14) 0.2261(9) 1.000 0.054(8) . .
H218 H Uiso 0.942(3) 0.3380(14) 0.2026(8) 1.000 0.040(8) . .
H218' H Uiso 1.033(3) 0.3903(13) 0.1723(8) 1.000 0.046(7) . .
H218" H Uiso 0.853(4) 0.3859(18) 0.1671(11) 1.000 0.087(13) . .
H219 H Uiso 0.280(3) 0.1646(13) 0.2530(8) 1.000 0.040(7) . .
H219' H Uiso 0.155(2) 0.1410(12) 0.2113(7) 1.000 0.027(6) . .
H219" H Uiso 0.110(3) 0.2036(11) 0.2482(7) 1.000 0.027(6) . .
H221 H Uiso 0.388(2) 0.3485(11) 0.4204(7) 1.000 0.020(6) . .
H222 H Uiso 0.439(2) 0.2223(10) 0.4547(7) 1.000 0.015(5) . .
H222' H Uiso 0.287(2) 0.2384(10) 0.4240(6) 1.000 0.017(5) . .
H224 H Uiso 0.400(2) 0.0910(10) 0.4102(7) 1.000 0.013(5) . .
H225 H Uiso 0.497(2) 0.0325(12) 0.3501(7) 1.000 0.021(6) . .
H227 H Uiso 0.636(2) 0.0352(12) 0.2842(7) 1.000 0.028(6) . .
H228 H Uiso 0.767(2) 0.0951(12) 0.2319(7) 1.000 0.031(6) . .
H229 H Uiso 0.794(2) 0.2218(11) 0.2385(7) 1.000 0.018(5) . .
H230 H Uiso 0.676(2) 0.2847(10) 0.2934(6) 1.000 0.009(5) . .
H233 H Uiso 0.684(3) 0.2895(12) 0.4379(7) 1.000 0.031(6) . .
H233' H Uiso 0.588(2) 0.3321(11) 0.4748(7) 1.000 0.021(6) . .
H233" H Uiso 0.649(3) 0.3738(13) 0.4343(7) 1.000 0.032(7) . .


loop_
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_atom_site_aniso_U_23
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_atom_site_aniso_U_12
O11 0.0204(9) 0.0206(8) 0.0198(8) −0.0034(7) 0.0025(7) 0.0059(7)
O12 0.0122(8) 0.0173(8) 0.0174(8) −0.0008(6) −0.0002(6) 0.0009(6)
O13 0.0234(9) 0.0206(8) 0.0140(8) −0.0037(6) 0.0036(7) 0.0062(7)
N11 0.0133(10) 0.0148(9) 0.0136(9) −0.0022(7) 0.0006(8) 0.0026(7)
C11 0.0149(12) 0.0195(11) 0.0112(11) −0.0024(9) 0.0040(9) −0.0024(9)
C12 0.0216(13) 0.0176(12) 0.0157(12) −0.0008(9) 0.0049(10) 0.0007(10)
C13 0.0290(14) 0.0167(12) 0.0210(12) −0.0037(10) 0.0077(11) −0.0034(10)
C14 0.0202(13) 0.0253(13) 0.0179(12) −0.0054(10) −0.0013(10) −0.0045(10)
C15 0.0171(13) 0.0198(12) 0.0173(12) −0.0016(9) 0.0021(10) −0.0005(10)
C16 0.0158(12) 0.0201(11) 0.0115(11) −0.0005(9) 0.0044(9) −0.0004(9)
C17 0.0084(11) 0.0197(11) 0.0137(11) −0.0027(9) 0.0009(9) 0.0009(9)
C18 0.0128(12) 0.0130(11) 0.0132(11) 0.0004(8) 0.0011(9) −0.0035(9)
C19 0.0099(11) 0.0136(11) 0.0153(11) 0.0034(9) 0.0008(9) −0.0005(9)
C110 0.0166(12) 0.0115(10) 0.0177(12) −0.0020(9) 0.0038(9) −0.0011(9)
C111 0.0196(13) 0.0179(11) 0.0120(11) 0.0003(9) 0.0031(9) −0.0022(9)
C112 0.0137(12) 0.0163(11) 0.0168(12) 0.0043(9) 0.0000(9) 0.0004(9)
C113 0.0131(11) 0.0137(11) 0.0142(11) −0.0016(8) 0.0037(9) −0.0017(9)
C114 0.0182(12) 0.0143(11) 0.0105(10) 0.0022(9) 0.0004(9) 0.0002(9)
C115 0.0104(12) 0.0218(12) 0.0194(12) 0.0019(9) 0.0000(9) 0.0018(9)
C116 0.0161(14) 0.0246(14) 0.0259(13) 0.0033(11) 0.0046(11) 0.0030(10)
C117 0.0242(15) 0.0213(13) 0.0207(13) 0.0021(10) 0.0011(11) 0.0018(11)
C118 0.0190(14) 0.0204(13) 0.0271(14) −0.0028(10) 0.0015(12) −0.0021(10)
C119 0.0388(17) 0.0296(14) 0.0144(12) −0.0051(11) −0.0007(11) 0.0120(12)
C120 0.0105(11) 0.0201(11) 0.0124(11) −0.0022(9) 0.0022(9) 0.0007(9)
C121 0.0162(12) 0.0208(12) 0.0119(11) −0.0007(9) −0.0007(9) −0.0038(10)
C122 0.0171(13) 0.0247(12) 0.0127(12) 0.0012(9) 0.0015(10) −0.0005(10)
C123 0.0122(12) 0.0229(12) 0.0147(11) 0.0043(9) 0.0040(9) −0.0016(9)
C124 0.0200(13) 0.0219(12) 0.0185(12) 0.0063(10) 0.0016(10) 0.0030(10)
C125 0.0244(13) 0.0134(12) 0.0270(13) 0.0029(10) 0.0063(11) 0.0018(10)
C126 0.0166(12) 0.0197(12) 0.0156(11) 0.0003(9) 0.0063(9) −0.0008(9)
C127 0.0246(14) 0.0194(13) 0.0239(13) −0.0017(10) 0.0025(10) −0.0014(10)
C128 0.0235(14) 0.0250(13) 0.0209(13) −0.0072(10) −0.0012(11) −0.0049(10)
C129 0.0193(13) 0.0247(13) 0.0179(12) −0.0002(10) −0.0008(10) −0.0006(10)
C130 0.0180(13) 0.0193(12) 0.0143(11) −0.0010(9) 0.0060(9) −0.0014(10)
C131 0.0142(12) 0.0164(11) 0.0131(11) −0.0014(9) 0.0048(9) −0.0006(9)
C132 0.0124(11) 0.0183(11) 0.0120(11) 0.0004(9) 0.0050(9) 0.0018(9)
C133 0.0247(14) 0.0364(15) 0.0103(12) −0.0027(10) −0.0004(10) 0.0053(12)
O21 0.0217(9) 0.0200(8) 0.0233(9) 0.0010(7) 0.0032(7) −0.0023(7)
O22 0.0198(9) 0.0249(9) 0.0268(9) −0.0046(7) 0.0120(7) −0.0012(7)
O23 0.0293(10) 0.0247(9) 0.0148(8) −0.0033(7) −0.0028(7) −0.0042(7)
N21 0.0180(10) 0.0161(9) 0.0159(9) −0.0009(7) 0.0050(8) −0.0012(8)
C21 0.0140(12) 0.0205(12) 0.0131(11) −0.0001(9) 0.0009(9) 0.0038(9)
C22 0.0199(13) 0.0167(12) 0.0190(12) 0.0043(9) 0.0007(10) 0.0000(9)
C23 0.0239(13) 0.0190(13) 0.0231(13) −0.0023(10) −0.0027(10) 0.0041(10)
C24 0.0207(13) 0.0245(12) 0.0141(12) −0.0039(10) 0.0007(10) 0.0063(10)
C25 0.0163(12) 0.0194(12) 0.0151(11) 0.0021(9) −0.0005(10) 0.0038(9)
C26 0.0125(12) 0.0173(11) 0.0135(11) 0.0004(9) −0.0023(9) 0.0016(9)
C27 0.0106(11) 0.0164(11) 0.0133(11) −0.0028(9) 0.0017(9) −0.0001(9)
C28 0.0134(11) 0.0150(11) 0.0148(11) 0.0011(9) 0.0032(9) 0.0048(9)
C29 0.0148(12) 0.0182(12) 0.0148(12) 0.0029(9) 0.0031(10) 0.0044(9)
C210 0.0180(12) 0.0192(12) 0.0146(11) −0.0024(9) −0.0014(9) 0.0040(9)
C211 0.0261(13) 0.0251(12) 0.0073(11) 0.0010(9) 0.0009(10) 0.0050(10)
C212 0.0229(13) 0.0228(12) 0.0138(12) 0.0029(10) 0.0055(10) 0.0026(10)
C213 0.0164(12) 0.0133(11) 0.0141(11) −0.0004(9) 0.0008(9) 0.0031(9)
C214 0.0216(13) 0.0163(12) 0.0151(11) 0.0057(9) 0.0036(10) 0.0016(10)
C215 0.0196(13) 0.0291(13) 0.0258(13) 0.0009(10) 0.0110(10) −0.0001(10)
C216 0.0220(15) 0.0371(16) 0.0369(16) 0.0070(13) 0.0087(13) 0.0069(12)
C217 0.0274(16) 0.0401(16) 0.0312(16) 0.0109(13) 0.0107(14) 0.0017(12)
C218 0.0383(19) 0.0433(19) 0.0481(19) −0.0144(15) 0.0262(16) −0.0035(15)

```
C219 0.0290(15) 0.0212(13) 0.0215(13) -0.0031(10) -0.0030(12) -0.0043(11)
C220 0.0077(11) 0.0188(11) 0.0130(11) 0.0003(9) 0.0008(9) -0.0009(9)
C221 0.0159(12) 0.0199(12) 0.0098(11) 0.0007(9) 0.0025(9) 0.0040(10)
C222 0.0175(13) 0.0204(12) 0.0141(12) 0.0016(9) 0.0042(10) -0.0023(10)
C223 0.0106(11) 0.0206(11) 0.0147(11) 0.0023(9) -0.0043(9) -0.0003(9)
C224 0.0224(13) 0.0201(12) 0.0174(12) 0.0050(9) 0.0001(10) -0.0036(10)
C225 0.0224(13) 0.0160(12) 0.0265(13) 0.0008(10) -0.0032(10) 0.0000(10)
C226 0.0176(12) 0.0185(12) 0.0150(11) -0.0007(9) -0.0032(9) 0.0000(9)
C227 0.0268(14) 0.0192(12) 0.0218(12) -0.0049(10) -0.0018(10) 0.0012(10)
C228 0.0252(14) 0.0271(13) 0.0191(12) -0.0056(10) 0.0020(11) 0.0065(10)
C229 0.0173(12) 0.0255(13) 0.0158(12) -0.0001(10) 0.0021(10) 0.0015(10)
C230 0.0150(12) 0.0182(12) 0.0137(11) -0.0001(9) -0.0020(9) 0.0015(9)
C231 0.0111(11) 0.0190(11) 0.0131(11) -0.0012(9) -0.0037(9) 0.0020(9)
C232 0.0101(11) 0.0190(11) 0.0129(11) 0.0004(9) -0.0016(9) 0.0003(9)
C233 0.0218(13) 0.0251(13) 0.0141(12) -0.0009(10) 0.0013(10) -0.0043(11)


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

# 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
 O11    C114     1.204(2)                        .     .              yes
 O12    C114     1.344(2)                        .     .              yes
 O12    C115     1.487(2)                        .     .              yes
 O13    C110     1.374(2)                        .     .              yes
 O13    C119     1.431(3)                        .     .              yes
 O21    C214     1.206(2)                        .     .              yes
 O22    C215     1.492(3)                        .     .              yes
 O22    C214     1.343(3)                        .     .              yes
 O23    C210     1.374(3)                        .     .              yes
 O23    C219     1.429(3)                        .     .              yes
 N11    C11      1.435(2)                        .     .              yes
 N11    C114     1.386(2)                        .     .              yes
 N11    C113     1.433(2)                        .     .              yes
 N21    C213     1.436(3)                        .     .              yes
 N21    C21      1.445(2)                        .     .              yes
 N21    C214     1.387(3)                        .     .              yes
 C11    C12      1.386(3)                        .     .              no
 C11    C16      1.408(3)                        .     .              no
 C12    C13      1.376(3)                        .     .              no
 C13    C14      1.385(3)                        .     .              no
 C14    C15      1.378(3)                        .     .              no
 C15    C16      1.397(3)                        .     .              no
 C16    C17      1.493(3)                        .     .              no
 C17    C18      1.478(3)                        .     .              no
 C17    C120     1.354(3)                        .     .              no
```

| C18  | C113  | 1.395(3)   | . | . | no |
|------|-------|------------|---|---|----|
| C18  | C19   | 1.392(3)   | . | . | no |
| C19  | C110  | 1.381(3)   | . | . | no |
| C110 | C111  | 1.395(3)   | . | . | no |
| C111 | C112  | 1.386(3)   | . | . | no |
| C112 | C113  | 1.383(3)   | . | . | no |
| C12  | H12   | 0.942(19)  | . | . | no |
| C13  | H13   | 0.97(2)    | . | . | no |
| C14  | H14   | 0.98(2)    | . | . | no |
| C115 | C116  | 1.520(3)   | . | . | no |
| C115 | C118  | 1.514(3)   | . | . | no |
| C15  | H15   | 0.97(2)    | . | . | no |
| C115 | C117  | 1.514(3)   | . | . | no |
| C19  | H19   | 0.979(18)  | . | . | no |
| C120 | C132  | 1.481(3)   | . | . | no |
| C120 | C121  | 1.529(3)   | . | . | no |
| C121 | C122  | 1.537(3)   | . | . | no |
| C121 | C133  | 1.526(3)   | . | . | no |
| C122 | C123  | 1.495(3)   | . | . | no |
| C123 | C132  | 1.380(3)   | . | . | no |
| C123 | C124  | 1.399(3)   | . | . | no |
| C124 | C125  | 1.359(3)   | . | . | no |
| C125 | C126  | 1.418(3)   | . | . | no |
| C126 | C131  | 1.428(3)   | . | . | no |
| C126 | C127  | 1.412(3)   | . | . | no |
| C127 | C128  | 1.364(3)   | . | . | no |
| C128 | C129  | 1.393(3)   | . | . | no |
| C129 | C130  | 1.375(3)   | . | . | no |
| C130 | C131  | 1.414(3)   | . | . | no |
| C131 | C132  | 1.435(3)   | . | . | no |
| C111 | H111  | 0.98(2)    | . | . | no |
| C112 | H112  | 0.940(19)  | . | . | no |
| C116 | H116" | 0.99(2)    | . | . | no |
| C116 | H116  | 1.00(2)    | . | . | no |
| C116 | H116' | 0.97(3)    | . | . | no |
| C117 | H117" | 0.98(2)    | . | . | no |
| C117 | H117  | 0.97(3)    | . | . | no |
| C117 | H117' | 1.01(3)    | . | . | no |
| C118 | H118" | 1.04(3)    | . | . | no |
| C118 | H118  | 0.99(2)    | . | . | no |
| C118 | H118' | 1.01(3)    | . | . | no |
| C119 | H119' | 1.07(3)    | . | . | no |
| C119 | H119" | 1.01(3)    | . | . | no |
| C119 | H119  | 1.03(2)    | . | . | no |
| C121 | H121  | 1.027(18)  | . | . | no |
| C21  | C22   | 1.380(3)   | . | . | no |
| C21  | C26   | 1.404(3)   | . | . | no |
| C22  | C23   | 1.381(3)   | . | . | no |
| C122 | H122' | 0.994(18)  | . | . | no |
| C122 | H122  | 0.97(2)    | . | . | no |
| C23  | C24   | 1.378(3)   | . | . | no |
| C124 | H124  | 0.94(2)    | . | . | no |
| C24  | C25   | 1.380(3)   | . | . | no |
| C25  | C26   | 1.398(3)   | . | . | no |
| C125 | H125  | 0.98(2)    | . | . | no |
| C26  | C27   | 1.485(3)   | . | . | no |
| C127 | H127  | 1.03(2)    | . | . | no |
| C27  | C220  | 1.359(3)   | . | . | no |
| C27  | C28   | 1.475(3)   | . | . | no |
| C128 | H128  | 0.93(2)    | . | . | no |
| C28  | C213  | 1.384(3)   | . | . | no |

| C28 | C29 | 1.397(3) | . | . | no |
|------|-------|-----------|---|---|-----|
| C129 | H129 | 0.98(2) | . | . | no |
| C29 | C210 | 1.372(3) | . | . | no |
| C130 | H130 | 0.96(2) | . | . | no |
| C133 | H133" | 1.01(2) | . | . | no |
| C133 | H133' | 0.98(2) | . | . | no |
| C133 | H133 | 1.06(3) | . | . | no |
| C22 | H22 | 0.96(2) | . | . | no |
| C23 | H23 | 0.99(2) | . | . | no |
| C24 | H24 | 0.969(18) | . | . | no |
| C25 | H25 | 0.958(19) | . | . | no |
| C29 | H29 | 0.90(2) | . | . | no |
| C210 | C211 | 1.389(3) | . | . | no |
| C211 | C212 | 1.380(3) | . | . | no |
| C212 | C213 | 1.390(3) | . | . | no |
| C215 | C216 | 1.512(4) | . | . | no |
| C215 | C217 | 1.513(3) | . | . | no |
| C215 | C218 | 1.517(4) | . | . | no |
| C220 | C221 | 1.525(3) | . | . | no |
| C220 | C232 | 1.484(3) | . | . | no |
| C221 | C222 | 1.543(3) | . | . | no |
| C221 | C233 | 1.527(3) | . | . | no |
| C222 | C223 | 1.495(3) | . | . | no |
| C223 | C224 | 1.407(3) | . | . | no |
| C223 | C232 | 1.385(3) | . | . | no |
| C224 | C225 | 1.362(3) | . | . | no |
| C225 | C226 | 1.421(3) | . | . | no |
| C226 | C231 | 1.422(3) | . | . | no |
| C226 | C227 | 1.409(3) | . | . | no |
| C227 | C228 | 1.362(3) | . | . | no |
| C228 | C229 | 1.401(3) | . | . | no |
| C229 | C230 | 1.368(3) | . | . | no |
| C230 | C231 | 1.421(3) | . | . | no |
| C231 | C232 | 1.435(3) | . | . | no |
| C211 | H211 | 0.95(2) | . | . | no |
| C212 | H212 | 0.96(2) | . | . | no |
| C216 | H216' | 0.98(3) | . | . | no |
| C216 | H216" | 1.04(3) | . | . | no |
| C216 | H216 | 1.00(2) | . | . | no |
| C217 | H217' | 0.987(19) | . | . | no |
| C217 | H217" | 1.04(3) | . | . | no |
| C217 | H217 | 0.99(3) | . | . | no |
| C218 | H218' | 1.02(3) | . | . | no |
| C218 | H218" | 0.96(3) | . | . | no |
| C218 | H218 | 0.98(3) | . | . | no |
| C219 | H219' | 1.03(2) | . | . | no |
| C219 | H219" | 1.04(3) | . | . | no |
| C219 | H219 | 1.03(3) | . | . | no |
| C221 | H221 | 0.97(2) | . | . | no |
| C222 | H222' | 1.013(18) | . | . | no |
| C222 | H222 | 1.00(2) | . | . | no |
| C224 | H224 | 1.00(2) | . | . | no |
| C225 | H225 | 0.99(2) | . | . | no |
| C227 | H227 | 0.98(2) | . | . | no |
| C228 | H228 | 1.02(2) | . | . | no |
| C229 | H229 | 0.98(2) | . | . | no |
| C230 | H230 | 0.967(19) | . | . | no |
| C233 | H233' | 1.02(2) | . | . | no |
| C233 | H233" | 0.97(3) | . | . | no |
| C233 | H233 | 1.03(3) | . | . | no |

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loop_
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_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
C114    O12     C115    120.16(15)      .       .       .       yes
C110    O13     C119    116.40(17)      .       .       .       yes
C214    O22     C215    119.80(16)      .       .       .       yes
C210    O23     C219    115.96(16)      .       .       .       yes
C113    N11     C114    124.22(15)      .       .       .       yes
C11     N11     C113    114.59(15)      .       .       .       yes
C11     N11     C114    121.05(15)      .       .       .       yes
C21     N21     C213    114.88(15)      .       .       .       yes
C21     N21     C214    119.61(16)      .       .       .       yes
C213    N21     C214    124.58(16)      .       .       .       yes
N11     C11     C12     121.78(18)      .       .       .       yes
C12     C11     C16     120.86(18)      .       .       .       no
N11     C11     C16     117.26(17)      .       .       .       yes
C11     C12     C13     119.7(2)        .       .       .       no
C12     C13     C14     120.4(2)        .       .       .       no
C13     C14     C15     120.1(2)        .       .       .       no
C14     C15     C16     121.0(2)        .       .       .       no
C11     C16     C17     115.95(16)      .       .       .       no
C15     C16     C17     126.22(18)      .       .       .       no
C11     C16     C15     117.79(19)      .       .       .       no
C18     C17     C120    124.88(18)      .       .       .       no
C16     C17     C18     109.94(16)      .       .       .       no
C16     C17     C120    125.03(17)      .       .       .       no
C17     C18     C19     123.39(17)      .       .       .       no
C17     C18     C113    117.37(17)      .       .       .       no
C19     C18     C113    119.12(17)      .       .       .       no
C18     C19     C110    120.33(18)      .       .       .       no
C19     C110    C111    120.44(18)      .       .       .       no
O13     C110    C111    123.68(18)      .       .       .       yes
O13     C110    C19     115.86(17)      .       .       .       yes
C110    C111    C112    119.18(19)      .       .       .       no
C111    C112    C113    120.54(18)      .       .       .       no
C11     C12     H12     117.9(12)       .       .       .       no
C13     C12     H12     122.4(12)       .       .       .       no
C14     C13     H13     121.1(12)       .       .       .       no
N11     C113    C112    122.74(17)      .       .       .       yes
C18     C113    C112    120.32(17)      .       .       .       no
N11     C113    C18     116.87(16)      .       .       .       yes
C12     C13     H13     118.4(12)       .       .       .       no
O12     C114    N11     110.16(16)      .       .       .       yes
C13     C14     H14     122.5(11)       .       .       .       no
O11     C114    O12     125.86(17)      .       .       .       yes
O11     C114    N11     123.96(18)      .       .       .       yes
C15     C14     H14     117.4(11)       .       .       .       no
C14     C15     H15     117.2(12)       .       .       .       no
O12     C115    C116    111.81(17)      .       .       .       yes
O12     C115    C117    108.27(16)      .       .       .       yes
C16     C15     H15     121.7(12)       .       .       .       no
C116    C115    C118    111.01(18)      .       .       .       no
C117    C115    C118    111.52(18)      .       .       .       no
O12     C115    C118    101.74(16)      .       .       .       yes
C116    C115    C117    112.03(19)      .       .       .       no
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| | | | | | | | |
|------|------|-------|-------------|---|---|---|-----|
| C18 | C19 | H19 | 121.1(11) | . | . | . | no |
| C110 | C19 | H19 | 118.6(11) | . | . | . | no |
| C17 | C120 | C121 | 124.73(18) | . | . | . | no |
| C121 | C120 | C132 | 105.64(16) | . | . | . | no |
| C17 | C120 | C132 | 129.45(17) | . | . | . | no |
| C120 | C121 | C122 | 103.37(16) | . | . | . | no |
| C120 | C121 | C133 | 111.75(16) | . | . | . | no |
| C122 | C121 | C133 | 111.50(18) | . | . | . | no |
| C121 | C122 | C123 | 104.10(18) | . | . | . | no |
| C124 | C123 | C132 | 122.49(19) | . | . | . | no |
| C122 | C123 | C124 | 126.02(19) | . | . | . | no |
| C122 | C123 | C132 | 111.49(18) | . | . | . | no |
| C123 | C124 | C125 | 118.9(2) | . | . | . | no |
| C124 | C125 | C126 | 121.2(2) | . | . | . | no |
| C127 | C126 | C131 | 119.52(18) | . | . | . | no |
| C125 | C126 | C127 | 120.3(2) | . | . | . | no |
| C125 | C126 | C131 | 120.06(18) | . | . | . | no |
| C126 | C127 | C128 | 121.3(2) | . | . | . | no |
| C127 | C128 | C129 | 119.8(2) | . | . | . | no |
| C128 | C129 | C130 | 120.5(2) | . | . | . | no |
| C129 | C130 | C131 | 121.7(2) | . | . | . | no |
| C130 | C131 | C132 | 125.38(18) | . | . | . | no |
| C126 | C131 | C132 | 117.30(17) | . | . | . | no |
| C126 | C131 | C130 | 117.10(17) | . | . | . | no |
| C123 | C132 | C131 | 119.18(17) | . | . | . | no |
| C120 | C132 | C123 | 108.68(16) | . | . | . | no |
| C120 | C132 | C131 | 131.92(17) | . | . | . | no |
| C110 | C111 | H111 | 120.3(12) | . | . | . | no |
| C112 | C111 | H111 | 120.5(12) | . | . | . | no |
| C111 | C112 | H112 | 118.6(11) | . | . | . | no |
| C113 | C112 | H112 | 120.8(11) | . | . | . | no |
| C115 | C116 | H116 | 114.1(15) | . | . | . | no |
| H116' | C116 | H116" | 106.6(17) | . | . | . | no |
| C115 | C116 | H116' | 107.7(13) | . | . | . | no |
| C115 | C116 | H116" | 108.7(12) | . | . | . | no |
| H116' | C116 | H116 | 109(2) | . | . | . | no |
| H116" | C116 | H116 | 110.7(19) | . | . | . | no |
| H117" | C117 | H117 | 110.5(18) | . | . | . | no |
| H117' | C117 | H117" | 104.1(17) | . | . | . | no |
| H117' | C117 | H117 | 109(2) | . | . | . | no |
| C115 | C117 | H117' | 109.2(13) | . | . | . | no |
| C115 | C117 | H117" | 113.3(13) | . | . | . | no |
| C115 | C117 | H117 | 110.5(14) | . | . | . | no |
| H118" | C118 | H118 | 107.8(17) | . | . | . | no |
| C115 | C118 | H118 | 110.7(13) | . | . | . | no |
| C115 | C118 | H118' | 108.8(13) | . | . | . | no |
| C115 | C118 | H118" | 111.8(13) | . | . | . | no |
| H118' | C118 | H118" | 108.1(19) | . | . | . | no |
| H118' | C118 | H118 | 109.5(17) | . | . | . | no |
| O13 | C119 | H119' | 105.2(13) | . | . | . | no |
| H119" | C119 | H119 | 112(2) | . | . | . | no |
| O13 | C119 | H119" | 111.9(14) | . | . | . | no |
| O13 | C119 | H119 | 108.2(14) | . | . | . | no |
| H119' | C119 | H119" | 108(2) | . | . | . | no |
| H119' | C119 | H119 | 112(2) | . | . | . | no |
| C133 | C121 | H121 | 107.8(10) | . | . | . | no |
| C22 | C21 | C26 | 121.34(18) | . | . | . | no |
| C122 | C121 | H121 | 109.4(11) | . | . | . | no |
| C120 | C121 | H121 | 113.0(10) | . | . | . | no |
| N21 | C21 | C22 | 120.84(18) | . | . | . | yes |
| N21 | C21 | C26 | 117.72(17) | . | . | . | yes |

| | | | | | | | |
|------|------|-------|------------|---|---|---|-----|
| C121 | C122 | H122 | 111.3(12) | . | . | . | no |
| C123 | C122 | H122' | 110.8(11) | . | . | . | no |
| C123 | C122 | H122 | 115.0(12) | . | . | . | no |
| H122' | C122 | H122 | 105.3(15) | . | . | . | no |
| C121 | C122 | H122' | 110.3(11) | . | . | . | no |
| C21 | C22 | C23 | 119.6(2) | . | . | . | no |
| C22 | C23 | C24 | 120.2(2) | . | . | . | no |
| C123 | C124 | H124 | 118.3(13) | . | . | . | no |
| C125 | C124 | H124 | 122.8(13) | . | . | . | no |
| C23 | C24 | C25 | 120.4(2) | . | . | . | no |
| C124 | C125 | H125 | 121.3(11) | . | . | . | no |
| C24 | C25 | C26 | 120.79(19) | . | . | . | no |
| C126 | C125 | H125 | 117.5(11) | . | . | . | no |
| C21 | C26 | C27 | 116.31(16) | . | . | . | no |
| C25 | C26 | C27 | 126.06(17) | . | . | . | no |
| C21 | C26 | C25 | 117.58(18) | . | . | . | no |
| C126 | C127 | H127 | 118.7(13) | . | . | . | no |
| C128 | C127 | H127 | 120.0(14) | . | . | . | no |
| C28 | C27 | C220 | 122.59(17) | . | . | . | no |
| C26 | C27 | C28 | 110.47(16) | . | . | . | no |
| C26 | C27 | C220 | 126.92(17) | . | . | . | no |
| C129 | C128 | H128 | 119.5(14) | . | . | . | no |
| C127 | C128 | H128 | 120.7(14) | . | . | . | no |
| C29 | C28 | C213 | 119.41(17) | . | . | . | no |
| C27 | C28 | C213 | 119.29(17) | . | . | . | no |
| C27 | C28 | C29 | 121.24(17) | . | . | . | no |
| C28 | C29 | C210 | 120.47(18) | . | . | . | no |
| C130 | C129 | H129 | 118.6(12) | . | . | . | no |
| C128 | C129 | H129 | 120.9(12) | . | . | . | no |
| C129 | C130 | H130 | 119.7(12) | . | . | . | no |
| C131 | C130 | H130 | 118.6(12) | . | . | . | no |
| C121 | C133 | H133' | 109.4(11) | . | . | . | no |
| C121 | C133 | H133" | 110.5(10) | . | . | . | no |
| C121 | C133 | H133 | 111.8(13) | . | . | . | no |
| H133' | C133 | H133" | 110.4(16) | . | . | . | no |
| H133' | C133 | H133 | 108.3(16) | . | . | . | no |
| H133" | C133 | H133 | 106.6(17) | . | . | . | no |
| C21 | C22 | H22 | 118.7(12) | . | . | . | no |
| C23 | C22 | H22 | 121.6(12) | . | . | . | no |
| C24 | C23 | H23 | 119.4(12) | . | . | . | no |
| C22 | C23 | H23 | 120.2(12) | . | . | . | no |
| C25 | C24 | H24 | 120.4(11) | . | . | . | no |
| C23 | C24 | H24 | 119.3(11) | . | . | . | no |
| C24 | C25 | H25 | 117.9(12) | . | . | . | no |
| C26 | C25 | H25 | 121.3(12) | . | . | . | no |
| C28 | C29 | H29 | 117.8(13) | . | . | . | no |
| C210 | C29 | H29 | 121.8(13) | . | . | . | no |
| C29 | C210 | C211 | 119.69(19) | . | . | . | no |
| O23 | C210 | C29 | 123.42(18) | . | . | . | yes |
| O23 | C210 | C211 | 116.88(18) | . | . | . | yes |
| C210 | C211 | C212 | 120.5(2) | . | . | . | no |
| C211 | C212 | C213 | 119.7(2) | . | . | . | no |
| C28 | C213 | C212 | 120.18(18) | . | . | . | no |
| N21 | C213 | C212 | 123.69(18) | . | . | . | yes |
| N21 | C213 | C28 | 116.08(16) | . | . | . | yes |
| O21 | C214 | O22 | 125.45(17) | . | . | . | yes |
| O21 | C214 | N21 | 123.90(19) | . | . | . | yes |
| O22 | C214 | N21 | 110.65(17) | . | . | . | yes |
| O22 | C215 | C217 | 109.2(2) | . | . | . | yes |
| O22 | C215 | C218 | 101.6(2) | . | . | . | yes |
| C216 | C215 | C217 | 112.9(2) | . | . | . | no |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C216 | C215 | C218 | 110.8(2) | . | . | . | no |
| C217 | C215 | C218 | 111.0(2) | . | . | . | no |
| O22 | C215 | C216 | 110.84(18) | . | . | . | yes |
| C27 | C220 | C221 | 126.12(18) | . | . | . | no |
| C221 | C220 | C232 | 105.72(16) | . | . | . | no |
| C27 | C220 | C232 | 127.86(17) | . | . | . | no |
| C222 | C221 | C233 | 111.64(17) | . | . | . | no |
| C220 | C221 | C222 | 102.88(16) | . | . | . | no |
| C220 | C221 | C233 | 112.97(16) | . | . | . | no |
| C221 | C222 | C223 | 103.94(17) | . | . | . | no |
| C222 | C223 | C224 | 127.16(19) | . | . | . | no |
| C222 | C223 | C232 | 111.43(18) | . | . | . | no |
| C224 | C223 | C232 | 121.42(19) | . | . | . | no |
| C223 | C224 | C225 | 118.8(2) | . | . | . | no |
| C224 | C225 | C226 | 122.0(2) | . | . | . | no |
| C225 | C226 | C231 | 119.26(18) | . | . | . | no |
| C225 | C226 | C227 | 121.0(2) | . | . | . | no |
| C227 | C226 | C231 | 119.72(18) | . | . | . | no |
| C226 | C227 | C228 | 121.4(2) | . | . | . | no |
| C227 | C228 | C229 | 119.5(2) | . | . | . | no |
| C228 | C229 | C230 | 120.7(2) | . | . | . | no |
| C229 | C230 | C231 | 121.47(19) | . | . | . | no |
| C230 | C231 | C232 | 124.98(19) | . | . | . | no |
| C226 | C231 | C232 | 117.81(17) | . | . | . | no |
| C226 | C231 | C230 | 117.12(17) | . | . | . | no |
| C220 | C232 | C223 | 108.22(16) | . | . | . | no |
| C220 | C232 | C231 | 131.83(17) | . | . | . | no |
| C223 | C232 | C231 | 119.84(19) | . | . | . | no |
| C210 | C211 | H211 | 117.8(11) | . | . | . | no |
| C212 | C211 | H211 | 121.7(12) | . | . | . | no |
| C211 | C212 | H212 | 120.8(13) | . | . | . | no |
| C213 | C212 | H212 | 119.4(13) | . | . | . | no |
| C215 | C216 | H216' | 109.3(15) | . | . | . | no |
| C215 | C216 | H216" | 112.4(15) | . | . | . | no |
| C215 | C216 | H216 | 114.1(15) | . | . | . | no |
| H216' | C216 | H216" | 106(2) | . | . | . | no |
| H216' | C216 | H216 | 107(2) | . | . | . | no |
| H216" | C216 | H216 | 107(2) | . | . | . | no |
| C215 | C217 | H217' | 109.4(12) | . | . | . | no |
| C215 | C217 | H217" | 109.2(15) | . | . | . | no |
| C215 | C217 | H217 | 109.7(14) | . | . | . | no |
| H217' | C217 | H217" | 104.0(19) | . | . | . | no |
| H217' | C217 | H217 | 109.1(19) | . | . | . | no |
| H217" | C217 | H217 | 115(2) | . | . | . | no |
| C215 | C218 | H218' | 109.2(14) | . | . | . | no |
| C215 | C218 | H218" | 112(2) | . | . | . | no |
| C215 | C218 | H218 | 110.1(15) | . | . | . | no |
| H218' | C218 | H218" | 110(3) | . | . | . | no |
| H218' | C218 | H218 | 108(2) | . | . | . | no |
| H218" | C218 | H218 | 108(3) | . | . | . | no |
| O23 | C219 | H219' | 106.8(12) | . | . | . | no |
| O23 | C219 | H219" | 110.6(12) | . | . | . | no |
| O23 | C219 | H219 | 109.7(14) | . | . | . | no |
| H219' | C219 | H219" | 110.4(17) | . | . | . | no |
| H219' | C219 | H219 | 109.0(18) | . | . | . | no |
| H219" | C219 | H219 | 110.3(19) | . | . | . | no |
| C220 | C221 | H221 | 110.8(13) | . | . | . | no |
| C222 | C221 | H221 | 109.2(12) | . | . | . | no |
| C233 | C221 | H221 | 109.2(12) | . | . | . | no |
| C221 | C222 | H222' | 112.2(11) | . | . | . | no |
| C221 | C222 | H222 | 111.0(11) | . | . | . | no |

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C223      C222      H222'        110.8(11)          .       .       .             no
C223      C222      H222         112.2(11)          .       .       .             no
H222'     C222      H222         106.8(15)          .       .       .             no
C223      C224      H224         119.1(11)          .       .       .             no
C225      C224      H224         122.0(11)          .       .       .             no
C224      C225      H225         118.2(12)          .       .       .             no
C226      C225      H225         119.7(12)          .       .       .             no
C226      C227      H227         118.4(12)          .       .       .             no
C228      C227      H227         120.2(12)          .       .       .             no
C227      C228      H228         118.7(13)          .       .       .             no
C229      C228      H228         121.7(13)          .       .       .             no
C228      C229      H229         118.3(12)          .       .       .             no
C230      C229      H229         121.0(12)          .       .       .             no
C229      C230      H230         120.7(11)          .       .       .             no
C231      C230      H230         117.8(11)          .       .       .             no
C221      C233      H233'        109.7(11)          .       .       .             no
C221      C233      H233"        111.9(14)          .       .       .             no
C221      C233      H233         111.1(13)          .       .       .             no
H233'     C233      H233"        106.0(17)          .       .       .             no
H233'     C233      H233         109.9(16)          .       .       .             no
H233"     C233      H233          108(2)            .       .       .             no

loop_
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_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C115   O12    C114   O11      -14.6(3)     .    .    .    .    no
C115   O12    C114   N11      166.91(15)   .    .    .    .    no
C114   O12    C115   C116      61.6(2)     .    .    .    .    no
C114   O12    C115   C117     -62.3(2)     .    .    .    .    no
C114   O12    C115   C118    -179.91(16)   .    .    .    .    no
C119   O13    C110   C19     -166.39(18)   .    .    .    .    no
C119   O13    C110   C111      14.7(3)     .    .    .    .    no
C215   O22    C214   N21      169.67(17)   .    .    .    .    no
C214   O22    C215   C216      64.2(2)     .    .    .    .    no
C214   O22    C215   C217     -60.8(2)     .    .    .    .    no
C214   O22    C215   C218    -178.0(2)     .    .    .    .    no
C215   O22    C214   O21      -10.6(3)     .    .    .    .    no
C219   O23    C210   C29       -7.6(3)     .    .    .    .    no
C219   O23    C210   C211     171.2(2)     .    .    .    .    no
C113   N11    C11    C12     -139.35(19)   .    .    .    .    no
C113   N11    C11    C16       37.2(2)     .    .    .    .    no
C114   N11    C11    C12       44.8(3)     .    .    .    .    no
C114   N11    C11    C16     -138.69(18)   .    .    .    .    no
C11    N11    C113   C18      -39.9(2)     .    .    .    .    no
C11    N11    C113   C112     137.06(19)   .    .    .    .    no
C11    N11    C114   O11      -12.5(3)     .    .    .    .    no
C114   N11    C113   C18      135.83(19)   .    .    .    .    no
C114   N11    C113   C112     -47.2(3)     .    .    .    .    no
C113   N11    C114   O12       -9.4(2)     .    .    .    .    no
C11    N11    C114   O12      166.07(15)   .    .    .    .    no
C113   N11    C114   O11      172.06(18)   .    .    .    .    no
C213   N21    C21    C22     -139.9(2)     .    .    .    .    no
C214   N21    C213   C212     -52.5(3)     .    .    .    .    no
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| | | | | | | | | | | |
|------|------|------|------|-------------|---|---|---|---|---|----|
| C213 | N21  | C21  | C26  | 36.6(2)     | . | . | . | . | . | no |
| C214 | N21  | C21  | C22  | 50.8(3)     | . | . | . | . | . | no |
| C214 | N21  | C21  | C26  | −132.84(19) | . | . | . | . | . | no |
| C21  | N21  | C213 | C28  | −38.6(2)    | . | . | . | . | . | no |
| C21  | N21  | C213 | C212 | 138.7(2)    | . | . | . | . | . | no |
| C214 | N21  | C213 | C28  | 130.2(2)    | . | . | . | . | . | no |
| C21  | N21  | C214 | O22  | 170.81(16)  | . | . | . | . | . | no |
| C213 | N21  | C214 | O21  | −177.28(19) | . | . | . | . | . | no |
| C21  | N21  | C214 | O21  | −9.0(3)     | . | . | . | . | . | no |
| C213 | N21  | C214 | O22  | 2.5(3)      | . | . | . | . | . | no |
| N11  | C11  | C12  | C13  | 174.9(2)    | . | . | . | . | . | no |
| C16  | C11  | C12  | C13  | −1.5(3)     | . | . | . | . | . | no |
| N11  | C11  | C16  | C15  | −171.80(18) | . | . | . | . | . | no |
| N11  | C11  | C16  | C17  | 5.8(2)      | . | . | . | . | . | no |
| C12  | C11  | C16  | C15  | 4.8(3)      | . | . | . | . | . | no |
| C12  | C11  | C16  | C17  | −177.64(18) | . | . | . | . | . | no |
| C11  | C12  | C13  | C14  | −2.4(4)     | . | . | . | . | . | no |
| C12  | C13  | C14  | C15  | 3.1(4)      | . | . | . | . | . | no |
| C13  | C14  | C15  | C16  | 0.3(4)      | . | . | . | . | . | no |
| C14  | C15  | C16  | C17  | 178.5(2)    | . | . | . | . | . | no |
| C14  | C15  | C16  | C11  | −4.1(3)     | . | . | . | . | . | no |
| C11  | C16  | C17  | C120 | 131.4(2)    | . | . | . | . | . | no |
| C15  | C16  | C17  | C18  | 133.2(2)    | . | . | . | . | . | no |
| C11  | C16  | C17  | C18  | −44.2(2)    | . | . | . | . | . | no |
| C15  | C16  | C17  | C120 | −51.3(3)    | . | . | . | . | . | no |
| C18  | C17  | C120 | C121 | −169.08(17) | . | . | . | . | . | no |
| C16  | C17  | C120 | C121 | 16.0(3)     | . | . | . | . | . | no |
| C120 | C17  | C18  | C113 | −133.6(2)   | . | . | . | . | . | no |
| C16  | C17  | C18  | C19  | −133.95(19) | . | . | . | . | . | no |
| C16  | C17  | C120 | C132 | −169.60(18) | . | . | . | . | . | no |
| C18  | C17  | C120 | C132 | 5.4(3)      | . | . | . | . | . | no |
| C120 | C17  | C18  | C19  | 50.5(3)     | . | . | . | . | . | no |
| C16  | C17  | C18  | C113 | 42.0(2)     | . | . | . | . | . | no |
| C17  | C18  | C113 | C112 | −178.05(17) | . | . | . | . | . | no |
| C113 | C18  | C19  | C110 | 2.2(3)      | . | . | . | . | . | no |
| C19  | C18  | C113 | N11  | 175.09(17)  | . | . | . | . | . | no |
| C19  | C18  | C113 | C112 | −1.9(3)     | . | . | . | . | . | no |
| C17  | C18  | C19  | C110 | 178.09(18)  | . | . | . | . | . | no |
| C17  | C18  | C113 | N11  | −1.0(2)     | . | . | . | . | . | no |
| C18  | C19  | C110 | O13  | −179.19(17) | . | . | . | . | . | no |
| C18  | C19  | C110 | C111 | −0.3(3)     | . | . | . | . | . | no |
| N21  | C21  | C22  | C23  | 175.6(2)    | . | . | . | . | . | no |
| C26  | C21  | C22  | C23  | −0.6(3)     | . | . | . | . | . | no |
| N21  | C21  | C26  | C25  | −173.16(17) | . | . | . | . | . | no |
| N21  | C21  | C26  | C27  | 4.5(2)      | . | . | . | . | . | no |
| C22  | C21  | C26  | C25  | 3.2(3)      | . | . | . | . | . | no |
| C22  | C21  | C26  | C27  | −179.07(19) | . | . | . | . | . | no |
| C21  | C22  | C23  | C24  | −1.5(4)     | . | . | . | . | . | no |
| C22  | C23  | C24  | C25  | 1.0(4)      | . | . | . | . | . | no |
| C23  | C24  | C25  | C26  | 1.7(3)      | . | . | . | . | . | no |
| C24  | C25  | C26  | C21  | −3.8(3)     | . | . | . | . | . | no |
| C24  | C25  | C26  | C27  | 178.80(19)  | . | . | . | . | . | no |
| C21  | C26  | C27  | C28  | −41.0(2)    | . | . | . | . | . | no |
| C21  | C26  | C27  | C220 | 137.5(2)    | . | . | . | . | . | no |
| C25  | C26  | C27  | C28  | 136.46(19)  | . | . | . | . | . | no |
| C25  | C26  | C27  | C220 | −45.0(3)    | . | . | . | . | . | no |
| C26  | C27  | C28  | C29  | −137.39(18) | . | . | . | . | . | no |
| C26  | C27  | C28  | C213 | 39.6(2)     | . | . | . | . | . | no |
| C220 | C27  | C28  | C29  | 44.0(3)     | . | . | . | . | . | no |
| C220 | C27  | C28  | C213 | −138.94(19) | . | . | . | . | . | no |
| C26  | C27  | C220 | C232 | −169.84(18) | . | . | . | . | . | no |

| C28 | C27 | C220 | C232 | 8.5(3) | . | . | . | . | no |
|-----|-----|------|------|--------|---|---|---|---|----|
| C26 | C27 | C220 | C221 | 17.4(3) | . | . | . | . | no |
| C28 | C27 | C220 | C221 | −164.28(17) | . | . | . | . | no |
| C27 | C28 | C213 | N21 | −0.4(3) | . | . | . | . | no |
| C29 | C28 | C213 | C212 | −0.7(3) | . | . | . | . | no |
| C29 | C28 | C213 | N21 | 176.64(17) | . | . | . | . | no |
| C27 | C28 | C213 | C212 | −177.82(19) | . | . | . | . | no |
| C27 | C28 | C29 | C210 | 179.59(18) | . | . | . | . | no |
| C213 | C28 | C29 | C210 | 2.6(3) | . | . | . | . | no |
| C28 | C29 | C210 | C211 | −2.2(3) | . | . | . | . | no |
| C28 | C29 | C210 | O23 | 176.56(18) | . | . | . | . | no |
| O23 | C210 | C211 | C212 | −178.8(2) | . | . | . | . | no |
| C29 | C210 | C211 | C212 | 0.1(3) | . | . | . | . | no |
| C210 | C211 | C212 | C213 | 1.8(4) | . | . | . | . | no |
| C211 | C212 | C213 | N21 | −178.6(2) | . | . | . | . | no |
| C211 | C212 | C213 | C28 | −1.4(3) | . | . | . | . | no |
| C27 | C220 | C221 | C222 | 146.2(2) | . | . | . | . | no |
| C27 | C220 | C221 | C233 | −93.3(2) | . | . | . | . | no |
| C232 | C220 | C221 | C222 | −27.92(19) | . | . | . | . | no |
| C232 | C220 | C221 | C233 | 92.6(2) | . | . | . | . | no |
| C27 | C220 | C232 | C223 | −152.17(19) | . | . | . | . | no |
| C27 | C220 | C232 | C231 | 31.8(3) | . | . | . | . | no |
| C221 | C220 | C232 | C223 | 21.8(2) | . | . | . | . | no |
| C221 | C220 | C232 | C231 | −154.28(19) | . | . | . | . | no |
| C220 | C221 | C222 | C223 | 23.9(2) | . | . | . | . | no |
| C233 | C221 | C222 | C223 | −97.5(2) | . | . | . | . | no |
| C221 | C222 | C223 | C224 | 168.4(2) | . | . | . | . | no |
| C221 | C222 | C223 | C232 | −11.8(2) | . | . | . | . | no |
| C222 | C223 | C224 | C225 | −177.9(2) | . | . | . | . | no |
| C232 | C223 | C224 | C225 | 2.4(3) | . | . | . | . | no |
| C222 | C223 | C232 | C220 | −6.1(2) | . | . | . | . | no |
| C222 | C223 | C232 | C231 | 170.55(18) | . | . | . | . | no |
| C224 | C223 | C232 | C220 | 173.74(19) | . | . | . | . | no |
| C224 | C223 | C232 | C231 | −9.7(3) | . | . | . | . | no |
| C223 | C224 | C225 | C226 | 4.5(4) | . | . | . | . | no |
| C224 | C225 | C226 | C227 | 173.9(2) | . | . | . | . | no |
| C224 | C225 | C226 | C231 | −3.9(3) | . | . | . | . | no |
| C225 | C226 | C227 | C228 | −175.1(2) | . | . | . | . | no |
| C231 | C226 | C227 | C228 | 2.7(3) | . | . | . | . | no |
| C225 | C226 | C231 | C230 | 173.44(19) | . | . | . | . | no |
| C225 | C226 | C231 | C232 | −3.3(3) | . | . | . | . | no |
| C227 | C226 | C231 | C230 | −4.4(3) | . | . | . | . | no |
| C227 | C226 | C231 | C232 | 178.89(19) | . | . | . | . | no |
| C226 | C227 | C228 | C229 | 0.5(4) | . | . | . | . | no |
| C227 | C228 | C229 | C230 | −1.9(3) | . | . | . | . | no |
| C228 | C229 | C230 | C231 | 0.1(3) | . | . | . | . | no |
| C229 | C230 | C231 | C226 | 3.0(3) | . | . | . | . | no |
| C229 | C230 | C231 | C232 | 179.52(18) | . | . | . | . | no |
| C226 | C231 | C232 | C220 | −174.42(19) | . | . | . | . | no |
| C226 | C231 | C232 | C223 | 9.9(3) | . | . | . | . | no |
| C230 | C231 | C232 | C220 | 9.1(3) | . | . | . | . | no |
| C230 | C231 | C232 | C223 | −166.55(18) | . | . | . | . | no |

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_geom_contact_site_symmetry_2
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 O11    C12      2.854(3)                    .      .                  no
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| | | | | | |
|---|---|---|---|---|---|
| O11 | C116 | 2.933(3) | . | . | no |
| O11 | C117 | 3.087(3) | . | . | no |
| O11 | C224 | 3.333(3) | . | . | no |
| O11 | O11 | 3.225(2) | . | 3_656 | no |
| O11 | C117 | 3.410(3) | . | 3_656 | no |
| O12 | C112 | 2.828(2) | . | . | no |
| O13 | C125 | 3.306(3) | . | 3_566 | no |
| O21 | C219 | 3.240(3) | . | 2_655 | no |
| O21 | C22 | 2.873(3) | . | . | no |
| O21 | C217 | 3.024(3) | . | . | no |
| O21 | C216 | 2.957(3) | . | . | no |
| O22 | C212 | 2.843(3) | . | . | no |
| O11 | H116 | 2.45(3) | . | . | no |
| O11 | H117" | 2.59(2) | . | . | no |
| O11 | H224 | 2.43(2) | . | . | no |
| O11 | H12 | 2.375(19) | . | . | no |
| O11 | H117" | 2.55(2) | . | 3_656 | no |
| O12 | H112 | 2.571(18) | . | . | no |
| O12 | H222 | 2.71(2) | . | . | no |
| O13 | H24 | 2.759(19) | . | 3_566 | no |
| O13 | H125 | 2.42(2) | . | 3_566 | no |
| O21 | H217" | 2.45(3) | . | . | no |
| O21 | H124 | 2.59(2) | . | 1_655 | no |
| O21 | H216 | 2.44(3) | . | . | no |
| O21 | H22 | 2.504(19) | . | . | no |
| O21 | H219' | 2.39(2) | . | 2_655 | no |
| O22 | H212 | 2.523(19) | . | . | no |
| O23 | H111 | 2.57(2) | . | 4_554 | no |
| C12 | O11 | 2.854(3) | . | . | no |
| C12 | C12 | 3.286(3) | . | 3_556 | no |
| C15 | C121 | 3.217(3) | . | . | no |
| C17 | C130 | 3.442(3) | . | . | no |
| C18 | C130 | 3.037(3) | . | . | no |
| C18 | C131 | 3.355(3) | . | . | no |
| C19 | C132 | 3.331(3) | . | . | no |
| C19 | C130 | 3.181(3) | . | . | no |
| C19 | C131 | 3.322(3) | . | . | no |
| C22 | O21 | 2.873(3) | . | . | no |
| C22 | C228 | 3.478(3) | . | 2_655 | no |
| C24 | C128 | 3.572(4) | . | 3_666 | no |
| C24 | C119 | 3.548(4) | . | 3_566 | no |
| C25 | C221 | 3.247(3) | . | . | no |
| C27 | C230 | 3.417(3) | . | . | no |
| C28 | C230 | 3.003(3) | . | . | no |
| C28 | C231 | 3.278(3) | . | . | no |
| C29 | C230 | 3.125(3) | . | . | no |
| C29 | C231 | 3.137(3) | . | . | no |
| C29 | C232 | 3.131(3) | . | . | no |
| C112 | O12 | 2.828(2) | . | . | no |
| C113 | C130 | 3.516(3) | . | . | no |
| C14 | H217' | 3.09(2) | . | 2_645 | no |
| C114 | C222 | 3.523(3) | . | . | no |
| C15 | H121 | 2.592(19) | . | . | no |
| C16 | H121 | 2.908(18) | . | . | no |
| C116 | O11 | 2.933(3) | . | . | no |
| C17 | H222' | 2.926(18) | . | . | no |
| C17 | H130 | 2.87(2) | . | . | no |
| C17 | H233 | 3.05(3) | . | 1_455 | no |
| C117 | O11 | 3.087(3) | . | . | no |
| C117 | O11 | 3.410(3) | . | 3_656 | no |
| C18 | H130 | 2.43(2) | . | . | no |

| | | | | | |
|------|--------|-----------|---|--------|-----|
| C18 | H116' | 3.04(2) | . | 1_455 | no |
| C119 | C24 | 3.548(4) | . | 3_566 | no |
| C119 | C125 | 3.598(3) | . | 3_566 | no |
| C19 | H130 | 2.938(19) | . | . | no |
| C119 | C219 | 3.511(4) | . | 4_555 | no |
| C121 | C230 | 3.509(3) | . | 1_455 | no |
| C121 | C15 | 3.217(3) | . | . | no |
| C122 | C230 | 3.529(3) | . | 1_455 | no |
| C122 | C233 | 3.562(4) | . | 1_455 | no |
| C23 | H119' | 3.06(3) | . | 3_566 | no |
| C24 | H119' | 2.71(3) | . | 3_566 | no |
| C24 | H128 | 2.85(2) | . | 3_666 | no |
| C25 | H221 | 2.65(2) | . | . | no |
| C125 | C119 | 3.598(3) | . | 3_566 | no |
| C25 | H128 | 3.04(2) | . | 3_666 | no |
| C125 | C127 | 3.360(4) | . | 3_566 | no |
| C125 | O13 | 3.306(3) | . | 3_566 | no |
| C26 | H221 | 2.96(2) | . | . | no |
| C126 | C126 | 3.520(3) | . | 3_566 | no |
| C126 | C127 | 3.563(3) | . | 3_566 | no |
| C27 | H230 | 2.841(18) | . | . | no |
| C127 | C125 | 3.360(4) | . | 3_566 | no |
| C27 | H122' | 2.903(18) | . | 1_655 | no |
| C127 | C126 | 3.563(3) | . | 3_566 | no |
| C128 | C24 | 3.572(4) | . | 3_666 | no |
| C28 | H230 | 2.462(18) | . | . | no |
| C29 | H230 | 2.996(18) | . | . | no |
| C29 | H219" | 2.82(2) | . | . | no |
| C29 | H219 | 2.62(2) | . | . | no |
| C29 | H216" | 3.07(3) | . | 1_455 | no |
| C130 | C113 | 3.516(3) | . | . | no |
| C130 | C222 | 3.541(3) | . | . | no |
| C130 | C18 | 3.037(3) | . | . | no |
| C130 | C17 | 3.442(3) | . | . | no |
| C130 | C221 | 3.489(3) | . | . | no |
| C130 | C19 | 3.181(3) | . | . | no |
| C131 | C18 | 3.355(3) | . | . | no |
| C131 | C19 | 3.322(3) | . | . | no |
| C132 | C19 | 3.331(3) | . | . | no |
| C133 | C222 | 3.590(4) | . | . | no |
| C110 | H118' | 2.98(3) | . | 1_455 | no |
| C110 | H125 | 3.07(2) | . | 3_566 | no |
| C111 | H119 | 2.77(3) | . | . | no |
| C111 | H119" | 2.76(2) | . | . | no |
| C212 | O22 | 2.843(3) | . | . | no |
| C112 | H13 | 2.83(2) | . | 3_556 | no |
| C113 | H130 | 2.69(2) | . | . | no |
| C213 | C230 | 3.472(3) | . | . | no |
| C114 | H117" | 2.81(2) | . | . | no |
| C114 | H224 | 3.06(2) | . | . | no |
| C114 | H222 | 2.81(2) | . | . | no |
| C114 | H12 | 2.78(2) | . | . | no |
| C114 | H116 | 2.94(3) | . | . | no |
| C114 | H112 | 2.938(18) | . | . | no |
| C116 | H12 | 3.00(2) | . | 3_656 | no |
| C216 | O21 | 2.957(3) | . | . | no |
| C117 | H225 | 3.01(2) | . | 3_656 | no |
| C217 | O21 | 3.024(3) | . | . | no |
| C119 | H125 | 2.924(19) | . | 3_566 | no |
| C119 | H219' | 2.81(2) | . | 4_555 | no |
| C119 | H111 | 2.50(2) | . | . | no |

| | | | | | |
|---|---|---|---|---|---|
| C219 | C119 | 3.511(4) | . | 4_554 | no |
| C219 | O21 | 3.240(3) | . | 2_645 | no |
| C120 | H130 | 2.97(2) | . | . | no |
| C120 | H233 | 2.84(3) | . | 1_455 | no |
| C120 | H222' | 2.764(18) | . | . | no |
| C120 | H19 | 3.040(18) | . | . | no |
| C221 | C130 | 3.489(3) | . | . | no |
| C121 | H15 | 2.89(2) | . | . | no |
| C221 | C25 | 3.247(3) | . | . | no |
| C122 | H230 | 2.948(18) | . | 1_455 | no |
| C222 | C130 | 3.541(3) | . | . | no |
| C222 | C114 | 3.523(3) | . | . | no |
| C222 | C133 | 3.590(4) | . | . | no |
| C123 | H133 | 3.10(2) | . | . | no |
| C123 | H233" | 3.07(3) | . | 1_455 | no |
| C224 | O11 | 3.333(3) | . | . | no |
| C125 | H24 | 3.097(18) | . | . | no |
| C125 | H25 | 3.037(19) | . | . | no |
| C126 | H25 | 2.84(2) | . | . | no |
| C228 | C22 | 3.478(3) | . | 2_645 | no |
| C230 | C27 | 3.417(3) | . | . | no |
| C230 | C121 | 3.509(3) | . | 1_655 | no |
| C230 | C28 | 3.003(3) | . | . | no |
| C130 | H221 | 2.84(2) | . | . | no |
| C230 | C213 | 3.472(3) | . | . | no |
| C230 | C122 | 3.529(3) | . | 1_655 | no |
| C230 | C29 | 3.125(3) | . | . | no |
| C131 | H25 | 3.04(2) | . | . | no |
| C131 | H221 | 2.945(19) | . | . | no |
| C231 | C29 | 3.137(3) | . | . | no |
| C231 | C28 | 3.278(3) | . | . | no |
| C132 | H133 | 3.05(2) | . | . | no |
| C132 | H19 | 3.024(18) | . | . | no |
| C232 | C29 | 3.131(3) | . | . | no |
| C233 | C122 | 3.562(4) | . | 1_655 | no |
| C133 | H29 | 2.99(2) | . | . | no |
| C133 | H222' | 2.864(18) | . | . | no |
| C212 | H227 | 2.99(2) | . | 2_655 | no |
| C213 | H230 | 2.733(19) | . | . | no |
| C214 | H212 | 3.00(2) | . | . | no |
| C214 | H217" | 2.79(3) | . | . | no |
| C214 | H216 | 2.90(3) | . | . | no |
| C214 | H122 | 3.05(2) | . | 1_655 | no |
| C214 | H22 | 2.82(2) | . | . | no |
| C219 | H29 | 2.49(2) | . | . | no |
| C219 | H22 | 2.95(2) | . | 2_645 | no |
| C219 | H119" | 2.98(2) | . | 4_554 | no |
| C219 | H217" | 3.00(3) | . | 2_645 | no |
| C220 | H133 | 2.92(3) | . | . | no |
| C220 | H122' | 2.732(18) | . | 1_655 | no |
| C220 | H230 | 2.954(18) | . | . | no |
| C220 | H29 | 2.83(2) | . | . | no |
| C221 | H25 | 2.818(19) | . | . | no |
| C222 | H130 | 3.02(2) | . | . | no |
| C222 | H133 | 3.06(2) | . | . | no |
| C223 | H233 | 3.07(2) | . | . | no |
| C225 | H15 | 3.062(19) | . | 1_655 | no |
| C225 | H14 | 2.937(19) | . | 1_655 | no |
| C226 | H15 | 3.03(2) | . | 1_655 | no |
| C230 | H121 | 2.845(18) | . | 1_655 | no |
| C231 | H29 | 2.961(19) | . | . | no |

| | | | | | |
|---|---|---|---|---|---|
| C231 | H121 | 2.884(18) | . | 1_655 | no |
| C231 | H15 | 3.10(2) | . | 1_655 | no |
| C232 | H29 | 2.74(2) | . | . | no |
| C232 | H233 | 3.05(2) | . | . | no |
| C233 | H19 | 3.068(18) | . | 1_655 | no |
| C233 | H122' | 2.869(18) | . | 1_655 | no |
| H116' | C18 | 3.04(2) | . | 1_655 | no |
| H116' | H118' | 2.49(3) | . | . | no |
| H116" | H222 | 2.40(3) | . | . | no |
| H116" | H118 | 2.49(3) | . | . | no |
| H117' | H118' | 2.56(3) | . | . | no |
| H117" | C114 | 2.81(2) | . | . | no |
| H117" | O11 | 2.59(2) | . | . | no |
| H117" | O11 | 2.55(2) | . | 3_656 | no |
| H117" | H224 | 2.54(3) | . | 3_656 | no |
| H117" | H116 | 2.57(3) | . | . | no |
| H118' | C110 | 2.98(3) | . | 1_655 | no |
| H118' | H117' | 2.56(3) | . | . | no |
| H118' | H116' | 2.49(3) | . | . | no |
| H118" | H117 | 2.53(3) | . | . | no |
| H118" | H211 | 2.43(3) | . | 4_555 | no |
| H119' | C24 | 2.71(3) | . | 3_566 | no |
| H119' | H24 | 2.56(3) | . | 3_566 | no |
| H119' | C23 | 3.06(3) | . | 3_566 | no |
| H119" | H111 | 2.36(3) | . | . | no |
| H119" | C111 | 2.76(2) | . | . | no |
| H119" | C219 | 2.98(2) | . | 4_555 | no |
| H119" | H219' | 2.19(3) | . | 4_555 | no |
| H122' | C27 | 2.903(18) | . | 1_455 | no |
| H122' | C220 | 2.732(18) | . | 1_455 | no |
| H122' | C233 | 2.869(18) | . | 1_455 | no |
| H122' | H233" | 2.48(3) | . | 1_455 | no |
| H122' | H230 | 2.57(3) | . | 1_455 | no |
| H133' | H219" | 2.45(3) | . | . | no |
| H133' | H122 | 2.45(3) | . | . | no |
| H133" | H222' | 2.50(3) | . | . | no |
| H12 | C114 | 2.78(2) | . | . | no |
| H12 | C116 | 3.00(2) | . | 3_656 | no |
| H12 | H116 | 2.55(3) | . | 3_656 | no |
| H12 | O11 | 2.375(19) | . | . | no |
| H216' | H218' | 2.52(3) | . | . | no |
| H13 | C112 | 2.83(2) | . | 3_556 | no |
| H216" | C29 | 3.07(3) | . | 1_655 | no |
| H216" | H218 | 2.51(4) | . | . | no |
| H216" | H122 | 2.54(3) | . | 1_655 | no |
| H14 | C225 | 2.937(19) | . | 1_455 | no |
| H217' | H218' | 2.57(3) | . | . | no |
| H217' | C14 | 3.09(2) | . | 2_655 | no |
| H15 | C225 | 3.062(19) | . | 1_455 | no |
| H15 | C121 | 2.89(2) | . | . | no |
| H15 | H121 | 2.06(3) | . | . | no |
| H15 | C226 | 3.03(2) | . | 1_455 | no |
| H15 | C231 | 3.10(2) | . | 1_455 | no |
| H217" | O21 | 2.45(3) | . | . | no |
| H217" | C219 | 3.00(3) | . | 2_655 | no |
| H217" | H216 | 2.52(4) | . | . | no |
| H217" | C214 | 2.79(3) | . | . | no |
| H218' | H217' | 2.57(3) | . | . | no |
| H218' | H216' | 2.52(3) | . | . | no |
| H218" | H217 | 2.51(4) | . | . | no |
| H219' | C119 | 2.81(2) | . | 4_554 | no |

| | | | | | |
|---|---|---|---|---|---|
| H219' | O21 | 2.39(2) | . | 2_645 | no |
| H219' | H119" | 2.19(3) | . | 4_554 | no |
| H19 | C120 | 3.040(18) | . | . | no |
| H19 | C132 | 3.024(18) | . | . | no |
| H19 | C233 | 3.068(18) | . | 1_455 | no |
| H219" | C29 | 2.82(2) | . | . | no |
| H219" | H133' | 2.45(3) | . | . | no |
| H219" | H29 | 2.35(3) | . | . | no |
| H222' | C120 | 2.764(18) | . | . | no |
| H222' | C133 | 2.864(18) | . | . | no |
| H222' | C17 | 2.926(18) | . | . | no |
| H222' | H133" | 2.50(3) | . | . | no |
| H222' | H133 | 2.51(3) | . | . | no |
| H233' | H222 | 2.51(3) | . | . | no |
| H22 | C219 | 2.95(2) | . | 2_655 | no |
| H22 | C214 | 2.82(2) | . | . | no |
| H22 | O21 | 2.504(19) | . | . | no |
| H233" | C123 | 3.07(3) | . | 1_655 | no |
| H233" | H122' | 2.48(3) | . | 1_655 | no |
| H24 | C125 | 3.097(18) | . | . | no |
| H24 | O13 | 2.759(19) | . | 3_566 | no |
| H24 | H119' | 2.56(3) | . | 3_566 | no |
| H25 | H221 | 2.02(3) | . | . | no |
| H25 | C125 | 3.037(19) | . | . | no |
| H25 | C126 | 2.84(2) | . | . | no |
| H25 | C131 | 3.04(2) | . | . | no |
| H25 | C221 | 2.818(19) | . | . | no |
| H29 | C231 | 2.961(19) | . | . | no |
| H29 | C232 | 2.74(2) | . | . | no |
| H29 | H219" | 2.35(3) | . | . | no |
| H29 | H133 | 2.53(3) | . | . | no |
| H29 | H219 | 2.24(3) | . | . | no |
| H29 | C133 | 2.99(2) | . | . | no |
| H29 | C219 | 2.49(2) | . | . | no |
| H29 | C220 | 2.83(2) | . | . | no |
| H111 | C119 | 2.50(2) | . | . | no |
| H111 | H119" | 2.36(3) | . | . | no |
| H111 | H119 | 2.26(3) | . | . | no |
| H111 | O23 | 2.57(2) | . | 4_555 | no |
| H112 | C114 | 2.938(18) | . | . | no |
| H112 | O12 | 2.571(18) | . | . | no |
| H116 | C114 | 2.94(3) | . | . | no |
| H116 | H117" | 2.57(3) | . | . | no |
| H116 | O11 | 2.45(3) | . | . | no |
| H116 | H12 | 2.55(3) | . | 3_656 | no |
| H117 | H118" | 2.53(3) | . | . | no |
| H117 | H225 | 2.58(3) | . | 3_656 | no |
| H118 | H116" | 2.49(3) | . | . | no |
| H119 | H111 | 2.26(3) | . | . | no |
| H119 | C111 | 2.77(3) | . | . | no |
| H121 | H15 | 2.06(3) | . | . | no |
| H121 | C15 | 2.592(19) | . | . | no |
| H121 | C16 | 2.908(18) | . | . | no |
| H121 | C230 | 2.845(18) | . | 1_455 | no |
| H121 | C231 | 2.884(18) | . | 1_455 | no |
| H122 | H133' | 2.45(3) | . | . | no |
| H122 | H216" | 2.54(3) | . | 1_455 | no |
| H122 | C214 | 3.05(2) | . | 1_455 | no |
| H124 | O21 | 2.59(2) | . | 1_455 | no |
| H125 | H127 | 2.40(3) | . | . | no |
| H125 | C110 | 3.07(2) | . | 3_566 | no |

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H125      C119      2.924(19)              .      3_566          no
H125      O13       2.42(2)                .      3_566          no
H127      H125      2.40(3)                .      .              no
H128      C24       2.85(2)                .      3_666          no
H128      C25       3.04(2)                .      3_666          no
H130      C17       2.87(2)                .      .              no
H130      C18       2.43(2)                .      .              no
H130      C19       2.938(19)              .      .              no
H130      C113      2.69(2)                .      .              no
H130      C222      3.02(2)                .      .              no
H130      C120      2.97(2)                .      .              no
H133      C132      3.05(2)                .      .              no
H133      C220      2.92(3)                .      .              no
H133      C123      3.10(2)                .      .              no
H133      H222'     2.51(3)                .      .              no
H133      H29       2.53(3)                .      .              no
H133      C222      3.06(2)                .      .              no
H211      H118"     2.43(3)                .      4_554          no
H212      O22       2.523(19)              .      .              no
H212      C214      3.00(2)                .      .              no
H212      H225      2.55(3)                .      2_655          no
H216      O21       2.44(3)                .      .              no
H216      C214      2.90(3)                .      .              no
H216      H217"     2.52(4)                .      .              no
H217      H218"     2.51(4)                .      .              no
H218      H216"     2.51(4)                .      .              no
H219      C29       2.62(2)                .      .              no
H219      H29       2.24(3)                .      .              no
H221      C25       2.65(2)                .      .              no
H221      C26       2.96(2)                .      .              no
H221      C130      2.84(2)                .      .              no
H221      C131      2.945(19)              .      .              no
H221      H25       2.02(3)                .      .              no
H222      O12       2.71(2)                .      .              no
H222      C114      2.81(2)                .      .              no
H222      H116"     2.40(3)                .      .              no
H222      H233'     2.51(3)                .      .              no
H224      O11       2.43(2)                .      .              no
H224      C114      3.06(2)                .      .              no
H224      H117"     2.54(3)                .      3_656          no
H225      H227      2.45(3)                .      .              no
H225      H212      2.55(3)                .      2_645          no
H225      C117      3.01(2)                .      3_656          no
H225      H117      2.58(3)                .      3_656          no
H227      H225      2.45(3)                .      .              no
H227      C212      2.99(2)                .      2_645          no
H230      C27       2.841(18)              .      .              no
H230      C28       2.462(18)              .      .              no
H230      C29       2.996(18)              .      .              no
H230      C122      2.948(18)              .      1_655          no
H230      C213      2.733(19)              .      .              no
H230      C220      2.954(18)              .      .              no
H230      H122'     2.57(3)                .      1_655          no
H233      C17       3.05(3)                .      1_655          no
H233      C120      2.84(3)                .      1_655          no
H233      C223      3.07(2)                .      .              no
H233      C232      3.05(2)                .      .              no

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
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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)
#
C117    H117"   O11      0.98(2)    2.59(2)   3.087(3)   111.7(15)     .    yes
C117    H117"   O11      0.98(2)    2.55(2)   3.410(3)   147.5(15)   3_656  yes
C12     H12     O11      0.942(19)  2.375(19) 2.854(3)   111.1(15)     .    yes
C217    H217"   O21      1.04(3)    2.45(3)   3.024(3)   113.4(18)     .    yes
C219    H219'   O21      1.03(2)    2.39(2)   3.240(3)   138.8(16)   2_645  yes
C22     H22     O21      0.96(2)    2.504(19) 2.873(3)   103.0(14)     .    yes
C111    H111    O23      0.98(2)    2.57(2)   3.491(3)   156.0(14)   4_555  yes
C116    H116    O11      1.00(2)    2.45(3)   2.933(3)   109.5(18)     .    yes
C124    H124    O21      0.94(2)    2.59(2)   3.473(3)   155.6(17)   1_455  yes
C125    H125    O13      0.98(2)    2.42(2)   3.306(3)   150.4(15)   3_566  yes
C216    H216    O21      1.00(2)    2.44(3)   2.957(3)   111.5(19)     .    yes
C224    H224    O11      1.00(2)    2.43(2)   3.333(3)   150.5(15)     .    yes

#===END of Crystallographic Information File
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