Increased speed of rotation for the smallest light-driven molecular motor

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2003

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# CIF-file generated for C56H48                                    CP802
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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,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;
_publ_contact_author_email           A.Meetsma@fwn.rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'JACS'
# Publication choise FI FM FO CI CM CO
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2003-06-19  13:25:02

 Consider this CIF submission for deposition of the second
 X-ray structure of a manuscript to be submitted to : JACS
  (Our Compound_Identification_Code : CP802)
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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
;
 ?
;

# 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_name
_publ_author_footnote
_publ_author_address

   'Meetsma, Auke'
;
 ? # author related footnote
;
;
     Crystal Structure Center,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     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_refinement
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;
 Altomare, A., Burla, M.C., Camalli, M., Cascarano, G.L., Giacovazzo, C.
   Guagliardi, A., Moliterni, A.G.G., Polidori, G. & Spagna, R.
   (1999). J. Appl. Cryst. 32, 115-119.

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  Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

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   Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
   (Present distributor Kluwer Academic Publishers, Dordrecht).

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   Edited by A.J.C Wilson, Kluwer Academic Publishers,
   Dordrecht, The Netherlands.

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   Groningen University, The Netherlands. (unpublished).

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   Refinement. University of G\"ottingen, Germany, 1997.

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 Spek, A.L. (1990). Acta Cryst. A46, C-34.

 Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.
;
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_publ_section_figure_captions
;
     Fig. 1. Chemical structural diagram (scheme 1) of the title compound

     Fig. 2. Perspective PLUTO drawing of the molecule illustrating the
             configuration and the adopted numbering scheme.

     Fig. 3. Molecular packing viewed down unit cell axes.

     Fig. 4. Perspective ORTEP 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.
;

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# 5. CHEMICAL DATA

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; ?
;
_chemical_name_common                ?
_chemical_melting_point              ?
_chemical_formula_moiety
'C28 H24'
# 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
'C28 H24'
_chemical_formula_iupac              ?
_chemical_formula_weight               360.50
_chemical_compound_source           'see text'

loop_
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_atom_type_scat_dispersion_real
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_atom_type_scat_source
 H   H    0.0000    0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 '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_Hall      'P 2yb'
_symmetry_space_group_name_H-M       'P 21'
_symmetry_Int_Tables_number                 4

loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -x,1/2+y,-z

_cell_length_a                        10.144(1)
_cell_length_b                        15.382(2)
_cell_length_c                        13.469(2)
_cell_angle_alpha                      90
_cell_angle_beta                      106.173(2)
_cell_angle_gamma                      90
_cell_volume                          2018.5(4)
```

```
_cell_formula_units_Z                4

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      5912
_cell_measurement_theta_min        2.47
_cell_measurement_theta_max       27.47
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   5912 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'block'
_exptl_crystal_colour            'colorless'
_exptl_crystal_size_max           0.41
_exptl_crystal_size_mid           0.39
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_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.186
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              768
_exptl_absorpt_coefficient_mu     0.067
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min   0.963
_exptl_absorpt_correction_T_max   0.978


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

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; ?
;
_diffrn_ambient_temperature            100(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
_diffrn_measurement_method           'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean     '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number             ?
_diffrn_standards_interval_count     ?
_diffrn_standards_interval_time      ?

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?
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# number of measured reflections (redundant set)
_diffrn_reflns_number             14596
_diffrn_reflns_av_R_equivalents   0.0510
_diffrn_reflns_av_sigmaI/netI     0.0834
_diffrn_reflns_limit_h_min        -12
_diffrn_reflns_limit_h_max        12
_diffrn_reflns_limit_k_min        -18
_diffrn_reflns_limit_k_max        18
_diffrn_reflns_limit_l_min        -16
_diffrn_reflns_limit_l_max        15
_diffrn_reflns_theta_min          2.47
_diffrn_reflns_theta_max          26.02
_diffrn_measured_fraction_theta_max    0.996
_diffrn_reflns_theta_full              26.02
_diffrn_measured_fraction_theta_full   0.996

_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                 6742
_reflns_threshold_expression      I>2\s(I)


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_computing_cell_refinement          'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction           'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
 SIR-97 (Altomare et al., 1997)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 PLATON (Spek, 1994)
;
_computing_publication_material      'PLATON (Spek, 1990)'

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

# 8. REFINEMENT DATA


_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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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^)+(0.1387P)^2^+1.3217P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
```

```
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.004(2)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_abs_structure_details  ?
_refine_ls_abs_structure_Flack    2(10)
_refine_ls_number_reflns          7768
_refine_ls_number_parameters      546
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_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0923
_refine_ls_R_factor_gt            0.0824
_refine_ls_wR_factor_ref          0.2161
_refine_ls_wR_factor_gt           0.2050
_refine_ls_goodness_of_fit_ref    1.046
_refine_ls_restrained_S_all       1.046
_refine_ls_shift/su_max           0.191
_refine_ls_shift/su_mean          0.077

_refine_diff_density_max          0.861
_refine_diff_density_min         -0.303
_refine_diff_density_rms          0.101


_vrn_publ_code_void_volume          0.0
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_atom_site_fract_z
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_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
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C12 C Uani 0.5275(3) 0.0553(2) 0.1402(3) 1.000 0.0150(9) . .
C13 C Uani 0.4917(3) 0.0864(2) 0.0264(3) 1.000 0.0164(9) . .
C14 C Uani 0.2736(3) 0.1728(2) -0.0778(3) 1.000 0.0167(9) . .
C15 C Uani 0.1439(3) 0.2025(2) -0.0807(3) 1.000 0.0169(9) . .
C16 C Uani -0.0406(3) 0.2230(2) 0.0053(3) 1.000 0.0182(10) . .
C17 C Uani -0.0895(3) 0.2130(2) 0.0903(3) 1.000 0.0201(10) . .
C18 C Uani -0.0100(3) 0.1690(2) 0.1782(3) 1.000 0.0186(10) . .
C19 C Uani 0.1147(3) 0.1325(2) 0.1782(3) 1.000 0.0166(9) . .
C110 C Uani 0.1643(3) 0.1377(2) 0.0913(3) 1.000 0.0132(9) . .
C111 C Uani 0.0881(3) 0.1871(2) 0.0035(3) 1.000 0.0152(9) . .
C112 C Uani 0.3475(3) 0.1222(2) 0.0072(3) 1.000 0.0155(9) . .
C113 C Uani 0.2916(3) 0.0994(2) 0.0860(3) 1.000 0.0134(9) . .
C114 C Uani 0.6080(3) 0.1261(3) 0.2141(3) 1.000 0.0216(10) . .
C115 C Uani 0.3681(3) -0.0245(2) 0.2234(3) 1.000 0.0130(9) . .
C116 C Uani 0.4893(3) -0.0726(2) 0.2962(3) 1.000 0.0163(9) . .
C117 C Uani 0.4405(3) -0.0849(2) 0.3952(3) 1.000 0.0177(10) . .
C118 C Uani 0.1882(4) -0.1112(2) 0.4041(3) 1.000 0.0202(10) . .
C119 C Uani 0.0505(4) -0.1072(3) 0.3524(3) 1.000 0.0222(11) . .
C120 C Uani -0.1365(4) -0.0814(3) 0.1904(3) 1.000 0.0233(11) . .
C121 C Uani -0.1788(4) -0.0642(3) 0.0870(3) 1.000 0.0246(11) . .
```

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C122 C Uani -0.0800(4) -0.0498(2) 0.0318(3) 1.000 0.0205(10) . .
C123 C Uani 0.0580(3) -0.0481(2) 0.0834(3) 1.000 0.0165(9) . .
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C126 C Uani 0.2848(3) -0.0858(2) 0.3517(3) 1.000 0.0166(10) . .
C127 C Uani 0.2456(3) -0.0567(2) 0.2516(3) 1.000 0.0142(9) . .
C128 C Uani 0.5136(4) -0.1614(2) 0.2516(3) 1.000 0.0210(10) . .


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H13 H Uiso 0.55613 0.13208 0.01742 1.000 0.0197 . .
H13' H Uiso 0.49393 0.03747 -0.02082 1.000 0.0197 . .
H14 H Uiso 0.31264 0.18626 -0.13235 1.000 0.0200 . .
H15 H Uiso 0.09163 0.23343 -0.13951 1.000 0.0202 . .
H16 H Uiso -0.09356 0.25425 -0.05308 1.000 0.0219 . .
H17 H Uiso -0.17672 0.23590 0.08954 1.000 0.0243 . .
H18 H Uiso -0.04217 0.16431 0.23780 1.000 0.0223 . .
H19 H Uiso 0.16754 0.10333 0.23833 1.000 0.0199 . .
H114 H Uiso 0.55388 0.17974 0.20468 1.000 0.0325 . .
H114' H Uiso 0.69545 0.13715 0.19882 1.000 0.0325 . .
H114" H Uiso 0.62571 0.10619 0.28579 1.000 0.0325 . .
H116 H Uiso 0.57435 -0.03621 0.31146 1.000 0.0195 . .
H117 H Uiso 0.47465 -0.14032 0.43044 1.000 0.0213 . .
H117' H Uiso 0.47126 -0.03620 0.44427 1.000 0.0213 . .
H118 H Uiso 0.218(4) -0.131(3) 0.474(3) 1.000 0.0243 . .
H119 H Uiso -0.016(4) -0.120(3) 0.388(3) 1.000 0.0266 . .
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H121 H Uiso -0.274(5) -0.062(3) 0.052(3) 1.000 0.0295 . .
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H123 H Uiso 0.123(4) -0.038(3) 0.046(3) 1.000 0.0198 . .
H128 H Uiso 0.43016 -0.19664 0.23919 1.000 0.0315 . .
H128' H Uiso 0.58947 -0.19131 0.30092 1.000 0.0315 . .
H128" H Uiso 0.53672 -0.15268 0.18634 1.000 0.0315 . .


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C23 C Uani 0.1563(3) 0.1232(2) 0.4516(3) 1.000 0.0180(9) . .
C24 C Uani 0.4054(4) 0.1610(3) 0.4435(3) 1.000 0.0220(10) . .
C25 C Uani 0.5420(4) 0.1645(3) 0.4982(3) 1.000 0.0231(11) . .
C26 C Uani 0.7284(4) 0.1490(3) 0.6600(3) 1.000 0.0301(13) . .
C27 C Uani 0.7719(4) 0.1300(3) 0.7633(3) 1.000 0.0273(11) . .
C28 C Uani 0.6757(3) 0.1063(2) 0.8171(3) 1.000 0.0195(10) . .
C29 C Uani 0.5384(3) 0.0969(2) 0.7644(3) 1.000 0.0167(9) . .
C210 C Uani 0.4912(3) 0.1101(2) 0.6559(3) 1.000 0.0158(9) . .
C211 C Uani 0.5877(3) 0.1405(3) 0.6031(3) 1.000 0.0205(10) . .
C212 C Uani 0.3099(3) 0.1287(2) 0.4948(3) 1.000 0.0168(9) . .
C213 C Uani 0.3518(3) 0.0992(2) 0.5959(3) 1.000 0.0141(9) . .
C214 C Uani 0.0759(4) 0.1968(3) 0.5919(3) 1.000 0.0236(11) . .
C215 C Uani 0.2135(3) 0.0029(2) 0.6920(3) 1.000 0.0132(9) . .
C216 C Uani 0.0729(3) -0.0155(2) 0.7113(3) 1.000 0.0161(9) . .
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C221 C Uani 0.6955(3) -0.1645(2) 0.7662(3) 1.000 0.0192(10) . .
C222 C Uani 0.6125(3) -0.1252(2) 0.6748(3) 1.000 0.0184(10) . .
C223 C Uani 0.4886(3) -0.0899(2) 0.6726(3) 1.000 0.0158(9) . .
C224 C Uani 0.4382(3) -0.0918(2) 0.7621(3) 1.000 0.0146(9) . .
C225 C Uani 0.5171(3) -0.1371(2) 0.8513(3) 1.000 0.0156(9) . .
C226 C Uani 0.2577(3) -0.0734(2) 0.8483(3) 1.000 0.0151(9) . .
C227 C Uani 0.3109(3) -0.0540(2) 0.7660(3) 1.000 0.0141(9) . .
C228 C Uani -0.0001(4) -0.0919(3) 0.6457(3) 1.000 0.0265(11) . .


H22 H Uiso 0.02301 0.07088 0.53320 1.000 0.0204 . .
H23 H Uiso 0.12981 0.07381 0.40298 1.000 0.0216 . .
```

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H23' H Uiso 0.11860 0.17761 0.41534 1.000 0.0216 . .
H24 H Uiso 0.37560 0.17962 0.37356 1.000 0.0265 . .
H25 H Uiso 0.60717 0.18367 0.46423 1.000 0.0278 . .
H26 H Uiso 0.79312 0.16817 0.62563 1.000 0.0362 . .
H27 H Uiso 0.86685 0.13274 0.79899 1.000 0.0328 . .
H28 H Uiso 0.70551 0.09680 0.88963 1.000 0.0234 . .
H29 H Uiso 0.47467 0.08144 0.80135 1.000 0.0200 . .
H214 H Uiso 0.05399 0.18767 0.65760 1.000 0.0355 . .
H214' H Uiso -0.00227 0.22453 0.54241 1.000 0.0355 . .
H214" H Uiso 0.15673 0.23442 0.60337 1.000 0.0355 . .
H216 H Uiso 0.01388 0.03764 0.69738 1.000 0.0192 . .
H217 H Uiso 0.11339 0.01445 0.87095 1.000 0.0204 . .
H217' H Uiso 0.05203 -0.08214 0.84426 1.000 0.0204 . .
H218 H Uiso 0.300(4) -0.131(3) 0.992(3) 1.000 0.0216 . .
H219 H Uiso 0.516(4) -0.179(3) 0.996(3) 1.000 0.0202 . .
H220 H Uiso 0.701(4) -0.200(3) 0.912(3) 1.000 0.0211 . .
H221 H Uiso 0.784(4) -0.186(3) 0.768(3) 1.000 0.0231 . .
H222 H Uiso 0.644(4) -0.124(3) 0.615(3) 1.000 0.0221 . .
H223 H Uiso 0.435(4) -0.064(3) 0.611(3) 1.000 0.0190 . .
H228 H Uiso -0.01736 -0.07778 0.57225 1.000 0.0397 . .
H228' H Uiso -0.08760 -0.10305 0.66098 1.000 0.0397 . .
H228" H Uiso 0.05784 -0.14389 0.66191 1.000 0.0397 . .


loop_
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_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
C11 0.0091(14) 0.0189(16) 0.0150(16) -0.0019(13) 0.0032(12) 0.0016(13)
C12 0.0081(14) 0.0178(16) 0.0202(17) 0.0033(14) 0.0060(12) -0.0013(13)
C13 0.0138(15) 0.0206(17) 0.0178(17) 0.0002(13) 0.0094(13) 0.0010(13)
C14 0.0180(15) 0.0190(18) 0.0144(16) 0.0026(13) 0.0066(13) -0.0015(14)
C15 0.0149(16) 0.0164(17) 0.0164(16) 0.0043(13) -0.0005(13) -0.0019(13)
C16 0.0158(16) 0.0149(17) 0.0212(18) 0.0020(13) 0.0005(14) 0.0027(13)
C17 0.0100(15) 0.0178(17) 0.031(2) -0.0004(15) 0.0030(14) 0.0054(13)
C18 0.0181(16) 0.0200(18) 0.0192(18) -0.0032(14) 0.0077(14) 0.0007(14)
C19 0.0131(15) 0.0135(16) 0.0215(17) 0.0003(13) 0.0022(13) 0.0004(13)
C110 0.0099(14) 0.0125(15) 0.0154(16) -0.0026(12) 0.0006(12) -0.0007(12)
C111 0.0133(15) 0.0159(16) 0.0146(16) -0.0035(12) 0.0008(12) -0.0030(13)
C112 0.0157(16) 0.0170(17) 0.0134(16) -0.0006(13) 0.0033(12) -0.0003(13)
C113 0.0107(15) 0.0122(15) 0.0146(16) -0.0003(12) -0.0009(12) 0.0001(13)
C114 0.0144(16) 0.0258(19) 0.0223(18) 0.0026(15) 0.0012(13) -0.0030(15)
C115 0.0081(14) 0.0141(15) 0.0154(16) -0.0021(12) 0.0011(12) 0.0008(12)
C116 0.0123(15) 0.0178(17) 0.0188(17) 0.0041(13) 0.0044(13) 0.0000(13)
C117 0.0149(16) 0.0217(18) 0.0163(17) 0.0046(13) 0.0040(13) 0.0010(14)
C118 0.0201(17) 0.0167(18) 0.0252(19) 0.0024(14) 0.0087(15) -0.0039(14)
C119 0.0208(18) 0.0236(19) 0.0257(19) -0.0026(15) 0.0123(15) -0.0030(15)
C120 0.0161(17) 0.028(2) 0.028(2) -0.0027(15) 0.0096(15) -0.0035(15)
C121 0.0125(16) 0.029(2) 0.032(2) -0.0087(16) 0.0057(15) -0.0014(15)
C122 0.0163(17) 0.0236(19) 0.0207(18) -0.0049(14) 0.0035(14) -0.0021(14)
C123 0.0124(15) 0.0134(16) 0.0229(18) -0.0029(13) 0.0035(14) -0.0018(13)
C124 0.0135(16) 0.0119(16) 0.0237(18) 0.0018(13) 0.0107(14) 0.0019(12)
C125 0.0138(16) 0.0201(17) 0.0230(18) -0.0045(14) 0.0078(14) -0.0017(13)
C126 0.0161(17) 0.0140(16) 0.0209(17) -0.0019(13) 0.0072(14) 0.0000(13)
C127 0.0129(16) 0.0117(16) 0.0189(16) -0.0014(12) 0.0061(13) 0.0008(12)
C128 0.0162(16) 0.0191(18) 0.0277(19) 0.0067(15) 0.0062(14) 0.0064(14)
C21 0.0092(14) 0.0167(16) 0.0141(16) -0.0011(12) 0.0021(12) 0.0050(12)
C22 0.0096(14) 0.0198(17) 0.0199(17) 0.0022(14) 0.0014(12) 0.0026(13)
C23 0.0138(16) 0.0196(17) 0.0176(16) 0.0032(14) -0.0004(13) 0.0041(14)
C24 0.0254(18) 0.0262(19) 0.0150(17) 0.0058(14) 0.0065(14) 0.0026(15)
C25 0.0234(18) 0.026(2) 0.0221(19) 0.0007(15) 0.0102(15) -0.0031(16)
C26 0.0135(16) 0.049(3) 0.030(2) -0.0029(18) 0.0098(15) -0.0030(17)
C27 0.0119(16) 0.039(2) 0.031(2) -0.0077(17) 0.0061(14) -0.0024(16)
```

```
C28 0.0138(15) 0.0233(18) 0.0192(17) 0.0002(14) 0.0010(13) 0.0001(14)
C29 0.0135(15) 0.0180(17) 0.0195(17) -0.0014(13) 0.0061(13) 0.0013(14)
C210 0.0125(15) 0.0137(16) 0.0207(17) -0.0027(12) 0.0040(13) -0.0022(12)
C211 0.0128(16) 0.0282(19) 0.0206(18) -0.0003(14) 0.0046(13) -0.0028(14)
C212 0.0168(16) 0.0123(16) 0.0198(17) 0.0025(13) 0.0026(13) 0.0003(13)
C213 0.0111(15) 0.0122(15) 0.0193(16) 0.0009(12) 0.0045(12) 0.0019(12)
C214 0.0194(18) 0.025(2) 0.0264(19) 0.0002(15) 0.0062(15) 0.0050(15)
C215 0.0104(14) 0.0112(15) 0.0180(17) -0.0016(12) 0.0041(12) 0.0005(12)
C216 0.0100(15) 0.0209(18) 0.0176(16) 0.0000(14) 0.0043(12) 0.0024(13)
C217 0.0126(16) 0.0218(17) 0.0177(17) 0.0006(13) 0.0062(13) -0.0038(14)
C218 0.0243(18) 0.0139(17) 0.0173(17) 0.0001(13) 0.0083(14) -0.0071(14)
C219 0.0167(16) 0.0145(16) 0.0178(17) 0.0010(13) 0.0022(14) -0.0003(13)
C220 0.0115(15) 0.0153(16) 0.0245(18) 0.0016(14) 0.0024(13) 0.0001(13)
C221 0.0125(16) 0.0186(17) 0.0258(18) -0.0001(14) 0.0040(14) 0.0028(13)
C222 0.0178(17) 0.0169(17) 0.0211(18) -0.0015(14) 0.0063(14) -0.0011(14)
C223 0.0153(16) 0.0162(16) 0.0148(16) -0.0014(12) 0.0023(13) -0.0035(13)
C224 0.0087(14) 0.0130(16) 0.0207(17) 0.0009(13) 0.0017(12) -0.0009(12)
C225 0.0151(15) 0.0113(15) 0.0198(17) 0.0021(13) 0.0038(13) 0.0004(13)
C226 0.0115(15) 0.0155(16) 0.0178(17) -0.0022(13) 0.0033(13) -0.0006(13)
C227 0.0117(15) 0.0156(16) 0.0133(16) -0.0015(13) 0.0008(12) -0.0017(13)
C228 0.0195(18) 0.037(2) 0.0213(19) -0.0061(16) 0.0030(15) -0.0080(17)

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

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All esds 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
 C11     C12        1.533(5)                    .       .                 no
 C11     C113       1.487(5)                    .       .                 no
 C11     C115       1.365(5)                    .       .                 no
 C12     C13        1.549(5)                    .       .                 no
 C12     C114       1.546(5)                    .       .                 no
 C13     C112       1.516(5)                    .       .                 no
 C14     C15        1.383(5)                    .       .                 no
 C14     C112       1.414(5)                    .       .                 no
 C15     C111       1.421(5)                    .       .                 no
 C16     C17        1.377(5)                    .       .                 no
 C16     C111       1.424(5)                    .       .                 no
 C17     C18        1.406(5)                    .       .                 no
 C18     C19        1.384(5)                    .       .                 no
 C19     C110       1.399(5)                    .       .                 no
 C110    C113       1.439(5)                    .       .                 no
 C110    C111       1.437(5)                    .       .                 no
 C112    C113       1.381(5)                    .       .                 no
 C12     H12          1.0006                    .       .                 no
 C13     H13'         0.9897                    .       .                 no
 C13     H13          0.9897                    .       .                 no
 C14     H14          0.9495                    .       .                 no
 C115    C116       1.533(5)                    .       .                 no
 C15     H15          0.9492                    .       .                 no
 C115    C127       1.482(5)                    .       .                 no
 C116    C117       1.558(5)                    .       .                 no
```

C116	C128	1.539(5)	.	.	no
C16	H16	0.9501	.	.	no
C17	H17	0.9497	.	.	no
C117	C126	1.524(5)	.	.	no
C18	H18	0.9498	.	.	no
C118	C119	1.378(6)	.	.	no
C118	C126	1.413(5)	.	.	no
C119	C125	1.424(5)	.	.	no
C19	H19	0.9501	.	.	no
C120	C125	1.431(5)	.	.	no
C120	C121	1.364(6)	.	.	no
C121	C122	1.422(6)	.	.	no
C122	C123	1.379(5)	.	.	no
C123	C124	1.421(5)	.	.	no
C124	C125	1.426(5)	.	.	no
C124	C127	1.440(5)	.	.	no
C126	C127	1.370(5)	.	.	no
C114	H114'	0.9797	.	.	no
C114	H114"	0.9807	.	.	no
C114	H114	0.9795	.	.	no
C116	H116	1.0006	.	.	no
C117	H117'	0.9902	.	.	no
C117	H117	0.9902	.	.	no
C118	H118	0.95(4)	.	.	no
C119	H119	0.95(4)	.	.	no
C120	H120	0.94(5)	.	.	no
C121	H121	0.95(5)	.	.	no
C21	C215	1.352(5)	.	.	no
C21	C22	1.542(5)	.	.	no
C21	C213	1.497(5)	.	.	no
C22	C23	1.550(5)	.	.	no
C122	H122	0.95(4)	.	.	no
C22	C214	1.528(6)	.	.	no
C23	C212	1.506(5)	.	.	no
C123	H123	0.95(4)	.	.	no
C24	C212	1.427(5)	.	.	no
C24	C25	1.377(6)	.	.	no
C25	C211	1.408(6)	.	.	no
C26	C27	1.369(6)	.	.	no
C26	C211	1.426(5)	.	.	no
C27	C28	1.416(5)	.	.	no
C28	C29	1.383(5)	.	.	no
C128	H128"	0.9800	.	.	no
C128	H128	0.9795	.	.	no
C128	H128'	0.9800	.	.	no
C29	C210	1.420(5)	.	.	no
C22	H22	1.0001	.	.	no
C23	H23	0.9900	.	.	no
C23	H23'	0.9905	.	.	no
C24	H24	0.9498	.	.	no
C25	H25	0.9496	.	.	no
C26	H26	0.9495	.	.	no
C27	H27	0.9501	.	.	no
C28	H28	0.9500	.	.	no
C29	H29	0.9494	.	.	no
C210	C211	1.439(5)	.	.	no
C210	C213	1.430(5)	.	.	no
C212	C213	1.385(5)	.	.	no
C215	C216	1.545(5)	.	.	no
C215	C227	1.479(5)	.	.	no
C216	C228	1.532(6)	.	.	no
C216	C217	1.558(5)	.	.	no
C217	C226	1.504(5)	.	.	no
C218	C226	1.415(5)	.	.	no
C218	C219	1.357(5)	.	.	no
C219	C225	1.422(5)	.	.	no
C220	C225	1.423(5)	.	.	no

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 C220    C221       1.375(5)                    .       .                  no
 C221    C222       1.419(5)                    .       .                  no
 C222    C223       1.362(5)                    .       .                  no
 C223    C224       1.435(5)                    .       .                  no
 C224    C225       1.426(5)                    .       .                  no
 C224    C227       1.430(5)                    .       .                  no
 C226    C227       1.394(5)                    .       .                  no
 C214    H214'        0.9801                    .       .                  no
 C214    H214"        0.9800                    .       .                  no
 C214    H214         0.9807                    .       .                  no
 C216    H216         0.9996                    .       .                  no
 C217    H217'        0.9902                    .       .                  no
 C217    H217         0.9892                    .       .                  no
 C218    H218        0.94(4)                    .       .                  no
 C219    H219        0.95(4)                    .       .                  no
 C220    H220        0.95(4)                    .       .                  no
 C221    H221        0.95(4)                    .       .                  no
 C222    H222        0.95(4)                    .       .                  no
 C223    H223        0.94(4)                    .       .                  no
 C228    H228'        0.9805                    .       .                  no
 C228    H228"        0.9804                    .       .                  no
 C228    H228         0.9798                    .       .                  no

loop_
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_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
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_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 C12     C11     C113       105.1(3)              .       .       .          no
 C12     C11     C115       121.3(3)              .       .       .          no
 C113    C11     C115       133.4(3)              .       .       .          no
 C11     C12     C13        103.5(3)              .       .       .          no
 C11     C12     C114       111.1(3)              .       .       .          no
 C13     C12     C114       110.8(3)              .       .       .          no
 C12     C13     C112       103.3(3)              .       .       .          no
 C15     C14     C112       119.4(3)              .       .       .          no
 C14     C15     C111       120.6(3)              .       .       .          no
 C17     C16     C111       121.0(3)              .       .       .          no
 C16     C17     C18        119.9(3)              .       .       .          no
 C17     C18     C19        120.3(3)              .       .       .          no
 C18     C19     C110       121.2(3)              .       .       .          no
 C19     C110    C111       118.8(3)              .       .       .          no
 C19     C110    C113       123.7(3)              .       .       .          no
 C111    C110    C113       117.4(3)              .       .       .          no
 C15     C111    C16        121.3(3)              .       .       .          no
 C15     C111    C110       120.2(3)              .       .       .          no
 C16     C111    C110       118.5(3)              .       .       .          no
 C13     C112    C14        127.3(3)              .       .       .          no
 C13     C112    C113       111.1(3)              .       .       .          no
 C14     C112    C113       121.6(3)              .       .       .          no
 C114    C12     H12          110.43              .       .       .          no
 C13     C12     H12          110.38              .       .       .          no
 C11     C12     H12          110.41              .       .       .          no
 C110    C113    C112       120.0(3)              .       .       .          no
 C11     C113    C112       109.3(3)              .       .       .          no
 C11     C113    C110       130.6(3)              .       .       .          no
 C112    C13     H13'         111.11              .       .       .          no
 H13     C13     H13'         109.10              .       .       .          no
 C112    C13     H13          111.09              .       .       .          no
 C12     C13     H13          111.06              .       .       .          no
 C12     C13     H13'         111.10              .       .       .          no
 C15     C14     H14          120.31              .       .       .          no
 C112    C14     H14          120.34              .       .       .          no
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C11	C115	C116	121.9(3)	.	.	.	no
C14	C15	H15	119.67	.	.	.	no
C111	C15	H15	119.69	.	.	.	no
C11	C115	C127	133.0(3)	.	.	.	no
C116	C115	C127	104.8(3)	.	.	.	no
C17	C16	H16	119.53	.	.	.	no
C115	C116	C117	102.5(3)	.	.	.	no
C111	C16	H16	119.46	.	.	.	no
C117	C116	C128	110.5(3)	.	.	.	no
C115	C116	C128	111.5(3)	.	.	.	no
C18	C17	H17	120.10	.	.	.	no
C16	C17	H17	119.99	.	.	.	no
C116	C117	C126	102.4(3)	.	.	.	no
C119	C118	C126	118.8(4)	.	.	.	no
C17	C18	H18	119.77	.	.	.	no
C19	C18	H18	119.90	.	.	.	no
C118	C119	C125	120.8(4)	.	.	.	no
C18	C19	H19	119.35	.	.	.	no
C110	C19	H19	119.42	.	.	.	no
C121	C120	C125	121.6(4)	.	.	.	no
C120	C121	C122	119.8(4)	.	.	.	no
C121	C122	C123	120.3(4)	.	.	.	no
C122	C123	C124	120.8(3)	.	.	.	no
C125	C124	C127	117.2(3)	.	.	.	no
C123	C124	C125	119.0(3)	.	.	.	no
C123	C124	C127	123.8(3)	.	.	.	no
C119	C125	C124	120.2(3)	.	.	.	no
C119	C125	C120	121.5(3)	.	.	.	no
C120	C125	C124	118.2(3)	.	.	.	no
C117	C126	C118	126.8(3)	.	.	.	no
C117	C126	C127	111.2(3)	.	.	.	no
C118	C126	C127	122.0(3)	.	.	.	no
C115	C127	C126	109.1(3)	.	.	.	no
C124	C127	C126	120.2(3)	.	.	.	no
C115	C127	C124	130.7(3)	.	.	.	no
C12	C114	H114'	109.49	.	.	.	no
C12	C114	H114"	109.45	.	.	.	no
C12	C114	H114	109.48	.	.	.	no
H114'	C114	H114"	109.43	.	.	.	no
H114'	C114	H114	109.53	.	.	.	no
H114"	C114	H114	109.45	.	.	.	no
C115	C116	H116	110.70	.	.	.	no
C117	C116	H116	110.70	.	.	.	no
C128	C116	H116	110.73	.	.	.	no
C116	C117	H117'	111.30	.	.	.	no
C116	C117	H117	111.27	.	.	.	no
C126	C117	H117'	111.32	.	.	.	no
C126	C117	H117	111.30	.	.	.	no
H117'	C117	H117	109.16	.	.	.	no
C119	C118	H118	121(3)	.	.	.	no
C126	C118	H118	120(3)	.	.	.	no
C118	C119	H119	120(2)	.	.	.	no
C125	C119	H119	119(2)	.	.	.	no
C121	C120	H120	119(3)	.	.	.	no
C125	C120	H120	119(3)	.	.	.	no
C120	C121	H121	120(3)	.	.	.	no
C122	C121	H121	120(3)	.	.	.	no
C22	C21	C213	104.5(3)	.	.	.	no
C22	C21	C215	121.9(3)	.	.	.	no
C213	C21	C215	133.4(3)	.	.	.	no
C121	C122	H122	120(3)	.	.	.	no
C123	C122	H122	120(3)	.	.	.	no
C23	C22	C214	110.2(3)	.	.	.	no
C21	C22	C23	102.8(3)	.	.	.	no
C21	C22	C214	110.8(3)	.	.	.	no
C122	C123	H123	120(2)	.	.	.	no
C22	C23	C212	103.4(3)	.	.	.	no

C124	C123	H123	120(2)	.	.	.	no
C25	C24	C212	118.2(4)	.	.	.	no
C24	C25	C211	121.8(4)	.	.	.	no
C27	C26	C211	121.2(4)	.	.	.	no
C26	C27	C28	120.1(4)	.	.	.	no
C116	C128	H128	109.45	.	.	.	no
H128"	C128	H128	109.51	.	.	.	no
H128'	C128	H128"	109.47	.	.	.	no
H128'	C128	H128	109.51	.	.	.	no
C116	C128	H128'	109.45	.	.	.	no
C116	C128	H128"	109.44	.	.	.	no
C27	C28	C29	120.2(4)	.	.	.	no
C28	C29	C210	121.1(3)	.	.	.	no
C23	C22	H22	110.93	.	.	.	no
C214	C22	H22	110.95	.	.	.	no
C21	C22	H22	110.95	.	.	.	no
C22	C23	H23	111.17	.	.	.	no
C212	C23	H23	111.08	.	.	.	no
C212	C23	H23'	111.03	.	.	.	no
C22	C23	H23'	111.13	.	.	.	no
H23	C23	H23'	109.02	.	.	.	no
C25	C24	H24	120.90	.	.	.	no
C212	C24	H24	120.92	.	.	.	no
C211	C25	H25	119.08	.	.	.	no
C24	C25	H25	119.08	.	.	.	no
C27	C26	H26	119.40	.	.	.	no
C211	C26	H26	119.41	.	.	.	no
C26	C27	H27	119.94	.	.	.	no
C28	C27	H27	119.91	.	.	.	no
C29	C28	H28	119.88	.	.	.	no
C27	C28	H28	119.91	.	.	.	no
C28	C29	H29	119.50	.	.	.	no
C210	C29	H29	119.45	.	.	.	no
C29	C210	C211	118.3(3)	.	.	.	no
C29	C210	C213	124.2(3)	.	.	.	no
C211	C210	C213	117.4(3)	.	.	.	no
C25	C211	C210	120.1(3)	.	.	.	no
C26	C211	C210	118.8(3)	.	.	.	no
C25	C211	C26	121.1(3)	.	.	.	no
C24	C212	C213	121.8(3)	.	.	.	no
C23	C212	C24	127.0(3)	.	.	.	no
C23	C212	C213	111.3(3)	.	.	.	no
C21	C213	C212	108.8(3)	.	.	.	no
C210	C213	C212	120.1(3)	.	.	.	no
C21	C213	C210	131.0(3)	.	.	.	no
C21	C215	C216	122.0(3)	.	.	.	no
C21	C215	C227	133.1(3)	.	.	.	no
C216	C215	C227	104.6(3)	.	.	.	no
C215	C216	C217	102.1(3)	.	.	.	no
C215	C216	C228	111.3(3)	.	.	.	no
C217	C216	C228	111.5(3)	.	.	.	no
C216	C217	C226	103.5(3)	.	.	.	no
C219	C218	C226	119.0(4)	.	.	.	no
C218	C219	C225	122.0(3)	.	.	.	no
C221	C220	C225	120.9(3)	.	.	.	no
C220	C221	C222	119.8(3)	.	.	.	no
C221	C222	C223	120.7(3)	.	.	.	no
C222	C223	C224	121.1(3)	.	.	.	no
C225	C224	C227	117.9(3)	.	.	.	no
C223	C224	C225	118.0(3)	.	.	.	no
C223	C224	C227	124.0(3)	.	.	.	no
C219	C225	C224	119.4(3)	.	.	.	no
C219	C225	C220	121.3(3)	.	.	.	no
C220	C225	C224	119.2(3)	.	.	.	no
C217	C226	C218	128.2(3)	.	.	.	no
C217	C226	C227	110.6(3)	.	.	.	no
C218	C226	C227	121.2(3)	.	.	.	no

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 C215    C227    C226       109.2(3)              .       .       .          no
 C224    C227    C226       119.7(3)              .       .       .          no
 C215    C227    C224       131.0(3)              .       .       .          no
 C22     C214    H214'        109.53              .       .       .          no
 C22     C214    H214"        109.52              .       .       .          no
 C22     C214    H214         109.50              .       .       .          no
 H214'   C214    H214"        109.46              .       .       .          no
 H214'   C214    H214         109.41              .       .       .          no
 H214"   C214    H214         109.41              .       .       .          no
 C215    C216    H216         110.57              .       .       .          no
 C217    C216    H216         110.54              .       .       .          no
 C228    C216    H216         110.56              .       .       .          no
 C216    C217    H217'        111.03              .       .       .          no
 C216    C217    H217         111.07              .       .       .          no
 C226    C217    H217'        111.00              .       .       .          no
 C226    C217    H217         111.07              .       .       .          no
 H217'   C217    H217         109.09              .       .       .          no
 C219    C218    H218         120(3)              .       .       .          no
 C226    C218    H218         121(3)              .       .       .          no
 C218    C219    H219         119(2)              .       .       .          no
 C225    C219    H219         119(2)              .       .       .          no
 C221    C220    H220         120(2)              .       .       .          no
 C225    C220    H220         119(2)              .       .       .          no
 C220    C221    H221         120(2)              .       .       .          no
 C222    C221    H221         120(2)              .       .       .          no
 C221    C222    H222         119(3)              .       .       .          no
 C223    C222    H222         120(3)              .       .       .          no
 C222    C223    H223         119(3)              .       .       .          no
 C224    C223    H223         120(3)              .       .       .          no
 C216    C228    H228'        109.49              .       .       .          no
 C216    C228    H228"        109.51              .       .       .          no
 C216    C228    H228         109.52              .       .       .          no
 H228'   C228    H228"        109.40              .       .       .          no
 H228'   C228    H228         109.46              .       .       .          no
 H228"   C228    H228         109.46              .       .       .          no

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 C115    C11     C12     C13        147.5(3)     .       .       .       .   no
 C115    C11     C12     C114       -93.5(4)     .       .       .       .   no
 C12     C11     C113    C110      -154.3(3)     .       .       .       .   no
 C12     C11     C113    C112        21.5(4)     .       .       .       .   no
 C115    C11     C113    C110        31.3(6)     .       .       .       .   no
 C115    C11     C113    C112      -152.9(4)     .       .       .       .   no
 C12     C11     C115    C116        11.0(5)     .       .       .       .   no
 C12     C11     C115    C127      -176.9(4)     .       .       .       .   no
 C113    C11     C115    C116      -175.3(4)     .       .       .       .   no
 C113    C11     C115    C127        -3.2(7)     .       .       .       .   no
 C11     C12     C13     C112        23.9(3)     .       .       .       .   no
 C114    C12     C13     C112       -95.3(3)     .       .       .       .   no
 C12     C13     C112    C14        167.9(3)     .       .       .       .   no
 C12     C13     C112    C113       -11.9(4)     .       .       .       .   no
 C15     C14     C112    C13       -177.8(3)     .       .       .       .   no
 C112    C14     C15     C111         3.8(5)     .       .       .       .   no
 C15     C14     C112    C113         2.0(5)     .       .       .       .   no
 C14     C15     C111    C110        -2.2(5)     .       .       .       .   no
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C14	C15	C111	C16	175.0(3)	.	.	.	.	no
C17	C16	C111	C110	1.9(5)	.	.	.	.	no
C111	C16	C17	C18	1.9(5)	.	.	.	.	no
C17	C16	C111	C15	-175.3(3)	.	.	.	.	no
C16	C17	C18	C19	-2.7(5)	.	.	.	.	no
C17	C18	C19	C110	-0.5(5)	.	.	.	.	no
C18	C19	C110	C111	4.3(5)	.	.	.	.	no
C18	C19	C110	C113	-178.6(3)	.	.	.	.	no
C11	C115	C116	H116	24.42	.	.	.	.	no
C127	C115	C116	H116	-149.66	.	.	.	.	no
C115	C116	C117	H117'	-91.93	.	.	.	.	no
C115	C116	C117	H117	146.08	.	.	.	.	no
C128	C116	C117	H117'	149.20	.	.	.	.	no
C128	C116	C117	H117	27.20	.	.	.	.	no
H116	C116	C117	C126	145.20	.	.	.	.	no
H116	C116	C117	H117'	26.17	.	.	.	.	no
H116	C116	C117	H117	-95.82	.	.	.	.	no
C115	C116	C128	H128'	-178.03	.	.	.	.	no
C115	C116	C128	H128"	62.01	.	.	.	.	no
C115	C116	C128	H128	-58.01	.	.	.	.	no
C117	C116	C128	H128'	-64.74	.	.	.	.	no
C117	C116	C128	H128"	175.29	.	.	.	.	no
C117	C116	C128	H128	55.28	.	.	.	.	no
H116	C116	C128	H128'	58.27	.	.	.	.	no
H116	C116	C128	H128"	-61.69	.	.	.	.	no
H116	C116	C128	H128	178.29	.	.	.	.	no
H117'	C117	C126	C118	-73.75	.	.	.	.	no
H117'	C117	C126	C127	105.32	.	.	.	.	no
H117	C117	C126	C118	48.28	.	.	.	.	no
H117	C117	C126	C127	-132.65	.	.	.	.	no
C126	C118	C119	H119	-175(3)	.	.	.	.	no
H118	C118	C119	C125	-176(3)	.	.	.	.	no
H118	C118	C119	H119	5(5)	.	.	.	.	no
H118	C118	C126	C117	-1(3)	.	.	.	.	no
H118	C118	C126	C127	-180(3)	.	.	.	.	no
H119	C119	C125	C120	-3(3)	.	.	.	.	no
H119	C119	C125	C124	178(3)	.	.	.	.	no
C125	C120	C121	H121	-179(3)	.	.	.	.	no
H120	C120	C121	C122	-179(3)	.	.	.	.	no
H120	C120	C121	H121	1(5)	.	.	.	.	no
H120	C120	C125	C119	5(3)	.	.	.	.	no
H120	C120	C125	C124	-176(3)	.	.	.	.	no
C120	C121	C122	H122	176(3)	.	.	.	.	no
H121	C121	C122	C123	176(3)	.	.	.	.	no
H121	C121	C122	H122	-3(5)	.	.	.	.	no
C213	C21	C215	C216	175.8(4)	.	.	.	.	no
C213	C21	C215	C227	1.4(7)	.	.	.	.	no
C22	C21	C213	C210	153.2(3)	.	.	.	.	no
C22	C21	C213	C212	-22.4(4)	.	.	.	.	no
C215	C21	C213	C210	-32.7(6)	.	.	.	.	no
C213	C21	C22	C23	30.2(3)	.	.	.	.	no
C213	C21	C22	C214	-87.5(3)	.	.	.	.	no
C215	C21	C22	C23	-144.9(3)	.	.	.	.	no
C215	C21	C22	C214	97.4(4)	.	.	.	.	no
C215	C21	C213	C212	151.8(4)	.	.	.	.	no
C22	C21	C215	C216	-10.9(5)	.	.	.	.	no
C22	C21	C215	C227	174.8(4)	.	.	.	.	no
H122	C122	C123	H123	0(4)	.	.	.	.	no
C214	C22	C23	C212	91.1(3)	.	.	.	.	no
C21	C22	C23	C212	-27.0(3)	.	.	.	.	no
C121	C122	C123	H123	-180(3)	.	.	.	.	no
H122	C122	C123	C124	-180(3)	.	.	.	.	no
H123	C123	C124	C127	3(3)	.	.	.	.	no
H123	C123	C124	C125	-175(3)	.	.	.	.	no
C22	C23	C212	C24	-164.2(3)	.	.	.	.	no
C22	C23	C212	C213	14.6(3)	.	.	.	.	no
C25	C24	C212	C23	176.9(4)	.	.	.	.	no

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 C212    C24     C25     C211        -2.5(7)     .       .       .       .   no
 C25     C24     C212    C213        -1.7(6)     .       .       .       .   no
 C24     C25     C211    C210         0.9(7)     .       .       .       .   no
 C24     C25     C211    C26       -176.6(4)     .       .       .       .   no
 C27     C26     C211    C210        -0.9(7)     .       .       .       .   no
 C211    C26     C27     C28         -3.8(7)     .       .       .       .   no
 C27     C26     C211    C25        176.6(4)     .       .       .       .   no
 C26     C27     C28     C29          4.1(6)     .       .       .       .   no
 C27     C28     C29     C210         0.4(5)     .       .       .       .   no
 C28     C29     C210    C211        -5.0(5)     .       .       .       .   no
 C28     C29     C210    C213       178.2(3)     .       .       .       .   no
 C213    C210    C211    C26       -177.7(4)     .       .       .       .   no
 C29     C210    C213    C21         -7.2(5)     .       .       .       .   no
 C211    C210    C213    C21        176.0(3)     .       .       .       .   no
 C211    C210    C213    C212        -8.8(5)     .       .       .       .   no
 C29     C210    C213    C212       168.0(3)     .       .       .       .   no
 C29     C210    C211    C25       -172.3(4)     .       .       .       .   no
 C29     C210    C211    C26          5.2(5)     .       .       .       .   no
 C213    C210    C211    C25          4.7(6)     .       .       .       .   no
 C24     C212    C213    C210         7.5(5)     .       .       .       .   no
 C24     C212    C213    C21       -176.3(3)     .       .       .       .   no
 C23     C212    C213    C21          4.8(4)     .       .       .       .   no
 C23     C212    C213    C210      -171.3(3)     .       .       .       .   no
 C21     C215    C216    C217      -144.6(3)     .       .       .       .   no
 C21     C215    C216    C228        96.3(4)     .       .       .       .   no
 C227    C215    C216    C217        31.1(3)     .       .       .       .   no
 C227    C215    C216    C228       -87.9(4)     .       .       .       .   no
 C21     C215    C227    C226       151.3(4)     .       .       .       .   no
 C216    C215    C227    C224       153.0(3)     .       .       .       .   no
 C216    C215    C227    C226       -23.8(4)     .       .       .       .   no
 C21     C215    C227    C224       -31.9(6)     .       .       .       .   no
 C228    C216    C217    C226        91.6(3)     .       .       .       .   no
 C215    C216    C217    C226       -27.3(3)     .       .       .       .   no
 C216    C217    C226    C218      -165.9(3)     .       .       .       .   no
 C216    C217    C226    C227        14.3(3)     .       .       .       .   no
 C219    C218    C226    C217       177.6(3)     .       .       .       .   no
 C219    C218    C226    C227        -2.7(5)     .       .       .       .   no
 C226    C218    C219    C225        -2.1(5)     .       .       .       .   no
 C218    C219    C225    C220      -176.9(3)     .       .       .       .   no
 C218    C219    C225    C224         0.8(5)     .       .       .       .   no
 C221    C220    C225    C219       175.7(3)     .       .       .       .   no
 C221    C220    C225    C224        -2.0(5)     .       .       .       .   no
 C225    C220    C221    C222        -2.7(5)     .       .       .       .   no
 C220    C221    C222    C223         3.9(5)     .       .       .       .   no
 C221    C222    C223    C224        -0.3(5)     .       .       .       .   no
 C222    C223    C224    C227       178.3(3)     .       .       .       .   no
 C222    C223    C224    C225        -4.3(5)     .       .       .       .   no
 C223    C224    C225    C219      -172.3(3)     .       .       .       .   no
 C223    C224    C225    C220         5.4(5)     .       .       .       .   no
 C227    C224    C225    C219         5.2(5)     .       .       .       .   no
 C227    C224    C225    C220      -177.0(3)     .       .       .       .   no
 C225    C224    C227    C226        -9.9(5)     .       .       .       .   no
 C223    C224    C227    C215        -9.1(6)     .       .       .       .   no
 C223    C224    C227    C226       167.5(3)     .       .       .       .   no
 C225    C224    C227    C215       173.5(3)     .       .       .       .   no
 C217    C226    C227    C224      -171.4(3)     .       .       .       .   no
 C218    C226    C227    C215      -173.9(3)     .       .       .       .   no
 C218    C226    C227    C224         8.8(5)     .       .       .       .   no
 C217    C226    C227    C215         5.8(4)     .       .       .       .   no

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C16	C27	3.583(6)	.	1_454	no
C17	C218	3.530(5)	.	2_556	no
C19	C123	3.045(5)	.	.	no
C19	C23	3.591(5)	.	.	no
C19	C124	2.994(4)	.	.	no
C19	C127	3.237(5)	.	.	no
C19	C115	3.455(5)	.	.	no
C21	C223	3.466(5)	.	.	no
C23	C19	3.591(5)	.	.	no
C27	C16	3.583(6)	.	1_656	no
C29	C227	3.277(4)	.	.	no
C29	C223	3.113(5)	.	.	no
C29	C224	3.073(4)	.	.	no
C29	C215	3.480(5)	.	.	no
C110	C123	3.046(4)	.	.	no
C110	C220	3.466(4)	.	2_656	no
C110	C124	3.474(5)	.	.	no
C11	H19	2.9016	.	.	no
C11	H123	2.93(4)	.	.	no
C111	C220	3.579(5)	.	2_656	no
C12	H116	2.6301	.	.	no
C13	H29	2.9887	.	1_554	no
C113	C123	3.274(5)	.	.	no
C114	C116	3.572(5)	.	.	no
C14	H217	2.9027	.	1_554	no
C14	H220	2.93(4)	.	2_656	no
C15	H220	2.81(4)	.	2_656	no
C15	H217	2.9622	.	1_554	no
C15	H27	3.0230	.	1_454	no
C115	C19	3.455(5)	.	.	no
C116	C114	3.572(5)	.	.	no
C16	H27	3.0129	.	1_454	no
C18	H23'	3.0984	.	.	no
C119	C214	3.440(6)	.	2_546	no
C19	H221	2.99(5)	.	2_656	no
C121	C220	3.576(6)	.	1_454	no
C21	H29	2.9350	.	.	no
C21	H223	2.91(4)	.	.	no
C22	H216	2.6677	.	.	no
C123	C110	3.046(4)	.	.	no
C23	H19	2.9224	.	.	no
C123	C113	3.274(5)	.	.	no
C123	C19	3.045(5)	.	.	no
C123	C11	3.475(5)	.	.	no
C23	H18	3.0848	.	.	no
C124	C19	2.994(4)	.	.	no
C124	C110	3.474(5)	.	.	no
C127	C19	3.237(5)	.	.	no
C110	H220	2.85(5)	.	2_656	no
C110	H123	2.78(5)	.	.	no
C210	C223	3.085(4)	.	.	no
C210	C224	3.523(5)	.	.	no
C111	H220	2.74(4)	.	2_656	no
C112	H220	3.03(5)	.	2_656	no
C112	H217	3.0540	.	1_554	no
C112	H114	3.0231	.	.	no
C213	C223	3.264(5)	.	.	no
C113	H114	2.9651	.	.	no
C113	H220	3.09(5)	.	2_656	no
C113	H123	2.68(4)	.	.	no
C114	H116	2.8842	.	.	no
C214	C119	3.440(6)	.	2_556	no
C115	H19	2.8764	.	.	no
C215	C29	3.480(5)	.	.	no
C115	H123	2.94(4)	.	.	no
C116	H114"	3.0993	.	.	no

C116	H12	2.6632	.	.	no
C117	H223	2.94(4)	.	.	no
C118	H23	2.9060	.	.	no
C218	C17	3.530(5)	.	2_546	no
C119	H214'	3.0549	.	2_546	no
C119	H23	2.9255	.	.	no
C120	H15	2.9939	.	2_545	no
C220	C110	3.466(4)	.	2_646	no
C120	H12	3.0286	.	1_455	no
C220	C121	3.576(6)	.	1_656	no
C220	C111	3.579(5)	.	2_646	no
C121	H12	2.9516	.	1_455	no
C223	C213	3.264(5)	.	.	no
C223	C21	3.466(5)	.	.	no
C223	C210	3.085(4)	.	.	no
C223	C29	3.113(5)	.	.	no
C224	C210	3.523(5)	.	.	no
C224	C29	3.073(4)	.	.	no
C124	H19	2.6477	.	.	no
C126	H23	3.0954	.	.	no
C126	H128	2.9364	.	.	no
C127	H128	2.8880	.	.	no
C227	C29	3.277(4)	.	.	no
C127	H19	2.5767	.	.	no
C128	H12	3.0140	.	.	no
C210	H223	2.77(5)	.	.	no
C212	H214"	2.9091	.	.	no
C213	H214"	2.8919	.	.	no
C213	H223	2.64(5)	.	.	no
C214	H26	3.0585	.	1_455	no
C214	H216	2.9843	.	.	no
C214	H119	2.91(5)	.	2_556	no
C215	H29	2.9110	.	.	no
C215	H223	2.94(4)	.	.	no
C216	H22	2.6645	.	.	no
C217	H123	2.90(4)	.	1_556	no
C218	H13'	2.8764	.	1_556	no
C218	H17	2.7046	.	2_546	no
C219	H13'	2.9312	.	1_556	no
C219	H121	3.01(5)	.	1_656	no
C220	H121	3.09(4)	.	1_656	no
C220	H114	3.0148	.	2_646	no
C221	H24	3.0094	.	2_646	no
C221	H228'	3.0790	.	1_655	no
C222	H24	3.0816	.	2_646	no
C224	H29	2.7218	.	.	no
C225	H114	2.9533	.	2_646	no
C226	H13'	3.0668	.	1_556	no
C226	H228"	2.9586	.	.	no
C227	H228"	2.9090	.	.	no
C227	H29	2.6242	.	.	no
C228	H22	2.9696	.	.	no
H114'	H18	2.5992	.	1_655	no
H114'	H13	2.4596	.	.	no
H114"	C116	3.0993	.	.	no
H114"	H116	2.2998	.	.	no
H117'	H223	2.4128	.	.	no
H128'	H117	2.4793	.	.	no
H128"	H12	2.4710	.	.	no
H128"	H219	2.5457	.	1_554	no
H214'	H119	2.5564	.	2_556	no
H214'	C119	3.0549	.	2_556	no
H214'	H23'	2.4744	.	.	no
H214"	C213	2.8919	.	.	no
H214"	C212	2.9091	.	.	no
H217'	H228'	2.5012	.	.	no
H228'	H217'	2.5012	.	.	no

H228'	C221	3.0790	.	1_455	no
H228'	H221	2.5393	.	1_455	no
H228"	C227	2.9090	.	.	no
H228"	C226	2.9586	.	.	no
H12	C116	2.6632	.	.	no
H12	H128"	2.4710	.	.	no
H12	H116	2.2798	.	.	no
H12	H120	2.5681	.	1_655	no
H12	H121	2.4141	.	1_655	no
H12	C120	3.0286	.	1_655	no
H12	C121	2.9516	.	1_655	no
H12	C128	3.0140	.	.	no
H13	H114'	2.4596	.	.	no
H13'	C226	3.0668	.	1_554	no
H13'	H29	2.4437	.	1_554	no
H13'	C218	2.8764	.	1_554	no
H13'	C219	2.9312	.	1_554	no
H15	H16	2.4910	.	.	no
H15	C120	2.9939	.	2_555	no
H16	H15	2.4910	.	.	no
H17	C218	2.7046	.	2_556	no
H17	H218	2.4893	.	2_556	no
H18	H114'	2.5992	.	1_455	no
H18	C23	3.0848	.	.	no
H18	H23'	2.4995	.	.	no
H19	C11	2.9016	.	.	no
H19	C23	2.9224	.	.	no
H19	H23	2.3966	.	.	no
H19	C127	2.5767	.	.	no
H19	C115	2.8764	.	.	no
H19	C124	2.6477	.	.	no
H22	H216	2.2965	.	.	no
H22	C228	2.9696	.	.	no
H22	H228	2.4069	.	.	no
H22	C216	2.6645	.	.	no
H23	C118	2.9060	.	.	no
H23	C119	2.9255	.	.	no
H23	C126	3.0954	.	.	no
H23	H19	2.3966	.	.	no
H23'	C18	3.0984	.	.	no
H23'	H18	2.4995	.	.	no
H23'	H214'	2.4744	.	.	no
H24	C221	3.0094	.	2_656	no
H24	C222	3.0816	.	2_656	no
H25	H26	2.4610	.	.	no
H26	H214	2.5775	.	1_655	no
H26	C214	3.0585	.	1_655	no
H26	H25	2.4610	.	.	no
H27	C16	3.0129	.	1_656	no
H27	C15	3.0230	.	1_656	no
H29	C13	2.9887	.	1_556	no
H29	C21	2.9350	.	.	no
H29	C215	2.9110	.	.	no
H29	C224	2.7218	.	.	no
H29	C227	2.6242	.	.	no
H29	H13'	2.4437	.	1_556	no
H114	C113	2.9651	.	.	no
H114	C220	3.0148	.	2_656	no
H114	C112	3.0231	.	.	no
H114	C225	2.9533	.	2_656	no
H116	C12	2.6301	.	.	no
H116	C114	2.8842	.	.	no
H116	H12	2.2798	.	.	no
H116	H114"	2.2998	.	.	no
H117	H128'	2.4793	.	.	no
H119	H228	2.5690	.	.	no
H119	H120	2.50(6)	.	.	no

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 H119    C214        2.91(5)                    .      2_546                no
 H119    H214'        2.5564                    .      2_546                no
 H120    H12          2.5681                    .      1_455                no
 H120    H119        2.50(6)                    .        .                  no
 H121    C220        3.09(4)                    .      1_454                no
 H121    H12          2.4141                    .      1_455                no
 H121    C219        3.01(5)                    .      1_454                no
 H123    H218        2.55(6)                    .      1_554                no
 H123    H217         2.4681                    .      1_554                no
 H123    C113        2.68(4)                    .        .                  no
 H123    C11         2.93(4)                    .        .                  no
 H123    C110        2.78(5)                    .        .                  no
 H123    C115        2.94(4)                    .        .                  no
 H123    C217        2.90(4)                    .      1_554                no
 H128    C127         2.8880                    .        .                  no
 H128    C126         2.9364                    .        .                  no
 H214    H26          2.5775                    .      1_455                no
 H214    H216         2.4290                    .        .                  no
 H216    C22          2.6677                    .        .                  no
 H216    C214         2.9843                    .        .                  no
 H216    H22          2.2965                    .        .                  no
 H216    H214         2.4290                    .        .                  no
 H217    C14          2.9027                    .      1_556                no
 H217    C15          2.9622                    .      1_556                no
 H217    C112         3.0540                    .      1_556                no
 H217    H123         2.4681                    .      1_556                no
 H218    H123        2.55(6)                    .      1_556                no
 H218    H17          2.4893                    .      2_546                no
 H219    H128"        2.5457                    .      1_556                no
 H219    H220        2.47(6)                    .        .                  no
 H220    H219        2.47(6)                    .        .                  no
 H220    C14         2.93(4)                    .      2_646                no
 H220    C15         2.81(4)                    .      2_646                no
 H220    C110        2.85(5)                    .      2_646                no
 H220    C111        2.74(4)                    .      2_646                no
 H220    C112        3.03(5)                    .      2_646                no
 H220    C113        3.09(5)                    .      2_646                no
 H221    H228'        2.5393                    .      1_655                no
 H221    C19         2.99(5)                    .      2_646                no
 H223    C21         2.91(4)                    .        .                  no
 H223    C117        2.94(4)                    .        .                  no
 H223    C210        2.77(5)                    .        .                  no
 H223    C213        2.64(5)                    .        .                  no
 H223    C215        2.94(4)                    .        .                  no
 H223    H117'        2.4128                    .        .                  no
 H228    H22          2.4069                    .        .                  no
 H228    H119         2.5690                    .        .                  no

#===END of Crystallographic Information File
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