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An Enantioselective Synthetic Route toward Second-Generation Light-Driven Rotary Molecular Motors

Pijper, Thomas C.; Pijper, Dirk; Pollard, Michael M.; Dumur, Frederic; Davey, Stephen G.; Meetsma, Auke; Feringa, Ben L.

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# 1. SUBMISSION DETAILS

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

_publ_requested_journal          'The Journal of Organic Chemistry'
# Publication choose FI, CI or EI for Inorganic
#                               FM, CM or EM for Metal-organic
#                               FO, CO or EO for Organic
_publ_requested_category         ?
_publ_requested_coeditor_name    ?

_publ_contact_letter             # Include date of submission
;
  Date of submission :  2008-02-13  15:59:24

  Consider this CIF submission for deposition of the (first)
  X-ray structure of a manuscript to be submitted to :
  The Journal of Organic Chemistry

  (Our Compound_Identification_Code : q1408)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_proofs_in        ?

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_journal_page_last             ?

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3. TITLE AND AUTHOR LIST

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_publ_section_title_footnote
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;

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

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_publ_author_address
'?' # author name
; # author related footnote
;
; # Address of this author
;
'Meetsma, Auke'
;
? # author related footnote

```

```

;
;
  Crystal Structure Center, Chemical Physics,
  Zernike Institute for Advanced Materials,
  University of Groningen,
  Nijenborgh 4,
  NL-9747 AG Groningen, The Netherlands.
;

#=====

# 4. TEXT

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;
_publ_section_abstract
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;

# Insert blank lines between paragraphs

_publ_section_comment
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;
_publ_section_exptl_prep
;
;
_publ_section_exptl_refinement
;

The crystal used in the experiment was a small cut fragment,
which was cleaved from large coagulated and in different directions
grown crystal chunk. This crystal diffracted weakly: so a 30.0 second
exposure time for each image was performed.

All hydrogen atoms were located in a difference Fourier map
and refined with isotropic displacement parameters.

C-H distances were in the range of 0.93 -- 1.05(3) \%.
;

_publ_section_related_literature
;
;

# Insert blank lines between references

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  Allen, F.H. (2000). Acta Cryst. B58, 380-388.

  Beurskens, P.T., Beurskens, G., Gelder, R. de, Smits, J.M.M.,
  Garc'ia-Granda, S. & Gould, R.O. (2007).
  The DIRDIF07 program system, Technical Report of the Crystallography
  Laboratory, University of Nijmegen, The Netherlands.

```

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

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Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

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

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

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

;

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

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

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

;

_publ_section_acknowledgements

;

;

#=====

5. CHEMICAL DATA

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;

;

_chemical_name_common

?

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_chemical_melting_point          ?
_chemical_formula_moiety
'C27 H20 O S'
# 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
'C27 H20 O S'
_chemical_formula_iupac           ?
_chemical_formula_weight          392.52
_chemical_compound_source         'see text'

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O      O      0.0106      0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H      H      0.0000      0.0000
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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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#=====

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6. CRYSTAL DATA

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_symmetry_Int_Tables_number       19

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loop_
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_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,-y,1/2+z
3 1/2+x,1/2-y,-z
4 -x,1/2+y,1/2-z

```

```

_cell_length_a                    7.7954(15)
_cell_length_b                    14.349(3)
_cell_length_c                    17.845(4)
_cell_angle_alpha                 90
_cell_angle_beta                  90
_cell_angle_gamma                 90
_cell_volume                      1996.1(7)
_cell_formula_units_Z             4

```

```

_cell_measurement_temperature     100(1)
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_cell_special_details

```

```

;

```

The final unit cell was obtained from the xyz centroids of 2645 reflections after integration using the SAINTPLUS software package (Bruker, 2007).

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

;

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_exptl_crystal_size_max         0.29
_exptl_crystal_size_mid         0.15
_exptl_crystal_size_min         0.11
_exptl_crystal_size_rad         ?
_exptl_crystal_density_meas     ?
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_exptl_crystal_F_000            824
_exptl_absorpt_coefficient_mu   0.178
_exptl_absorpt_correction_type   'multi-scan'
_exptl_absorpt_process_details  '(SADABS, (Bruker, 2006))'
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#=====

7. EXPERIMENTAL DATA

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;
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_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           'MoK\alpha'
_diffn_radiation_source         'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator   'parallel mounted graphite'
_diffn_radiation_detector
;
  CCD area-detector
;
_diffn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffn_measurement_method       '\f and \w scans'
_diffn_special_details
;
  Crystal into the cold nitrogen stream of the low-temperature unit
  (KRYOFLEX, (Bruker, 2006)).
;
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_diffn_standards_number          0
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_diffn_standards_interval_time   .
_diffn_standards_decay_%         0
```

loop_

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? ? ?
```

```

# number of measured reflections (redundant set)
_diffn_reflns_number      14068
_diffn_reflns_av_R_equivalents  0.0725
_diffn_reflns_av_sigmaI/netI  0.0742
_diffn_reflns_limit_h_min   -9
_diffn_reflns_limit_h_max    9
_diffn_reflns_limit_k_min  -17
_diffn_reflns_limit_k_max   16
_diffn_reflns_limit_l_min  -21
_diffn_reflns_limit_l_max   21
_diffn_reflns_theta_min     2.69
_diffn_reflns_theta_max    25.02
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_diffn_reflns_theta_full    25.00
_diffn_measured_fraction_theta_full  0.999

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

# number of unique reflections
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_reflns_number_gt         2696
_reflns_threshold_expression   $I > 2\sigma(I)$ 

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_computing_cell_refinement  'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction   'SAINT-Plus'
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;
  DIRDIF-07 (Beurskens et al., 2007)
;
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
  PLATON (Spek, 2003)
  PLUTO (Meetsma, 2007)
;
_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
   $F^2 > 2\sigma(F^2)$  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^)+(0.0391P)^2^+0.0P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     heavy
_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   difmap
_refine_ls_hydrogen_treatment    refall
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details

```

```

;
  The absolute structure of the molecule actually chosen was
  determined by Flack's x-refinement.

```

(Flack & Bernardinelli, 1999, 2000)

```

;
_chemical_absolute_configuration 'ad'
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_refine_ls_restrained_S_all       0.971
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9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
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O O Uani 0.3057(3) 0.46794(12) 0.21041(9) 1.000 0.0261(6) . .
C1 C Uani 0.2836(4) 0.14167(17) 0.26082(14) 1.000 0.0199(9) . .
C2 C Uani 0.2914(4) 0.10989(19) 0.33479(15) 1.000 0.0236(9) . .
C3 C Uani 0.2134(4) 0.0256(2) 0.35429(16) 1.000 0.0258(10) . .
C4 C Uani 0.1274(4) -0.0259(2) 0.30111(16) 1.000 0.0280(11) . .

```

C5 C Uani 0.1229(4) 0.0030(2) 0.22722(17) 1.000 0.0254(10) . .
 C6 C Uani 0.2026(4) 0.08582(18) 0.20700(14) 1.000 0.0223(9) . .
 C7 C Uani 0.4056(3) 0.17497(19) 0.10884(15) 1.000 0.0218(9) . .
 C8 C Uani 0.5038(4) 0.16430(19) 0.04393(16) 1.000 0.0256(10) . .
 C9 C Uani 0.6693(4) 0.1994(2) 0.04098(16) 1.000 0.0286(10) . .
 C10 C Uani 0.7389(4) 0.2424(2) 0.10413(17) 1.000 0.0270(10) . .
 C11 C Uani 0.6414(4) 0.25336(19) 0.16777(16) 1.000 0.0235(10) . .
 C12 C Uani 0.4708(4) 0.22287(17) 0.17094(14) 1.000 0.0201(9) . .
 C13 C Uani 0.3572(3) 0.23292(18) 0.23790(14) 1.000 0.0194(9) . .
 C14 C Uani 0.3212(4) 0.31490(18) 0.27148(13) 1.000 0.0208(9) . .
 C15 C Uani 0.2067(4) 0.33710(17) 0.33622(13) 1.000 0.0203(8) . .
 C16 C Uani 0.0448(4) 0.29968(17) 0.35951(13) 1.000 0.0194(9) . .
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 C21 C Uani -0.0345(4) 0.33923(18) 0.42484(14) 1.000 0.0214(9) . .
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 H3 H Uiso 0.217(3) 0.0061(16) 0.4037(13) 1.000 0.015(6) . .
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 H22 H Uiso -0.010(3) 0.4426(16) 0.5078(13) 1.000 0.018(7) . .
 H23 H Uiso 0.248(3) 0.5057(19) 0.4571(14) 1.000 0.032(8) . .
 H25 H Uiso 0.421(4) 0.525(2) 0.3271(15) 1.000 0.037(8) . .
 H25' H Uiso 0.540(4) 0.4339(17) 0.3555(14) 1.000 0.031(8) . .
 H26 H Uiso 0.525(3) 0.4020(16) 0.2275(13) 1.000 0.017(7) . .
 H27 H Uiso 0.237(4) 0.373(2) 0.1303(14) 1.000 0.041(9) . .
 H27' H Uiso 0.217(4) 0.484(2) 0.1076(15) 1.000 0.039(8) . .
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 O 0.0330(12) 0.0204(11) 0.0250(10) 0.0023(8) 0.0000(10) 0.0020(11)
 C1 0.0162(15) 0.0165(16) 0.0269(14) -0.0020(11) 0.0006(13) 0.0039(13)
 C2 0.0220(16) 0.0229(17) 0.0259(15) -0.0001(12) -0.0005(15) 0.0027(15)
 C3 0.0271(17) 0.0254(18) 0.0249(15) 0.0053(13) 0.0020(15) 0.0011(15)
 C4 0.0252(19) 0.0199(18) 0.0388(19) 0.0007(14) 0.0055(14) -0.0010(15)
 C5 0.0224(17) 0.0189(17) 0.0350(18) -0.0088(14) 0.0025(14) 0.0005(14)
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 C7 0.0215(16) 0.0186(16) 0.0254(15) 0.0026(13) -0.0043(14) 0.0039(13)

C8 0.035(2) 0.0190(16) 0.0229(16) 0.0018(12) -0.0032(14) 0.0041(15)
 C9 0.037(2) 0.0234(17) 0.0255(17) 0.0039(13) 0.0063(16) 0.0067(16)
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 C12 0.0214(17) 0.0152(15) 0.0237(15) 0.0012(12) -0.0010(13) 0.0034(13)
 C13 0.0223(17) 0.0174(15) 0.0186(14) 0.0019(12) -0.0028(12) -0.0019(13)
 C14 0.0233(17) 0.0177(15) 0.0214(14) 0.0000(12) -0.0036(13) 0.0006(14)
 C15 0.0248(16) 0.0175(15) 0.0186(13) 0.0013(11) -0.0021(14) 0.0006(14)
 C16 0.0216(16) 0.0148(16) 0.0218(14) 0.0035(11) 0.0003(13) -0.0013(14)
 C17 0.0257(18) 0.0184(16) 0.0252(16) 0.0025(12) -0.0011(14) 0.0010(14)
 C18 0.0258(17) 0.0219(17) 0.0282(15) -0.0002(13) -0.0022(16) -0.0031(16)
 C19 0.0230(19) 0.0342(19) 0.0288(16) 0.0088(14) -0.0022(14) -0.0056(16)
 C20 0.0277(17) 0.0292(17) 0.0237(15) 0.0048(13) 0.0035(16) 0.0007(17)
 C21 0.0227(18) 0.0203(16) 0.0213(14) 0.0027(11) -0.0011(13) 0.0016(14)
 C22 0.0309(19) 0.0222(16) 0.0216(15) -0.0002(13) 0.0023(15) 0.0021(15)
 C23 0.0359(19) 0.0180(16) 0.0225(15) -0.0009(12) 0.0005(16) -0.0042(17)
 C24 0.0275(19) 0.0179(15) 0.0220(14) 0.0015(12) -0.0020(13) -0.0013(14)
 C25 0.0258(19) 0.0196(19) 0.0268(16) 0.0010(13) -0.0015(15) -0.0030(15)
 C26 0.0222(18) 0.0192(17) 0.0262(16) 0.0031(12) -0.0011(14) -0.0008(13)
 C27 0.039(2) 0.030(2) 0.0240(16) 0.0038(13) -0.0004(17) 0.0020(19)

#=====

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

S	C6	1.773(3)	.	.	yes
S	C7	1.775(3)	.	.	yes
O	C26	1.440(3)	.	.	yes
O	C27	1.418(3)	.	.	yes
C1	C2	1.398(4)	.	.	no
C1	C6	1.401(4)	.	.	no
C1	C13	1.487(4)	.	.	no
C2	C3	1.398(4)	.	.	no
C3	C4	1.377(4)	.	.	no
C4	C5	1.383(4)	.	.	no
C5	C6	1.389(4)	.	.	no
C7	C8	1.397(4)	.	.	no
C7	C12	1.400(4)	.	.	no
C8	C9	1.386(4)	.	.	no
C9	C10	1.395(4)	.	.	no
C10	C11	1.376(4)	.	.	no
C11	C12	1.401(4)	.	.	no
C12	C13	1.494(4)	.	.	no
C13	C14	1.350(4)	.	.	no
C14	C15	1.494(4)	.	.	no

C14	C26	1.534(4)	.	.	no
C15	C16	1.433(4)	.	.	no
C15	C24	1.389(4)	.	.	no
C16	C17	1.418(4)	.	.	no
C16	C21	1.436(4)	.	.	no
C17	C18	1.365(4)	.	.	no
C18	C19	1.411(4)	.	.	no
C19	C20	1.365(4)	.	.	no
C20	C21	1.408(4)	.	.	no
C21	C22	1.424(4)	.	.	no
C22	C23	1.357(4)	.	.	no
C23	C24	1.396(4)	.	.	no
C24	C25	1.504(4)	.	.	no
C25	C26	1.535(4)	.	.	no
C2	H2	1.03(2)	.	.	no
C3	H3	0.93(2)	.	.	no
C4	H4	1.03(3)	.	.	no
C5	H5	0.95(3)	.	.	no
C8	H8	1.00(2)	.	.	no
C9	H9	0.94(2)	.	.	no
C10	H10	1.00(3)	.	.	no
C11	H11	0.94(3)	.	.	no
C17	H17	1.03(2)	.	.	no
C18	H18	0.99(2)	.	.	no
C19	H19	0.99(3)	.	.	no
C20	H20	1.04(3)	.	.	no
C22	H22	1.01(2)	.	.	no
C23	H23	0.95(3)	.	.	no
C25	H25	1.05(3)	.	.	no
C25	H25'	1.01(3)	.	.	no
C26	H26	1.00(2)	.	.	no
C27	H27	1.04(3)	.	.	no
C27	H27'	0.99(3)	.	.	no
C27	H27''	1.00(3)	.	.	no
loop_					
_geom_angle_atom_site_label_1					
_geom_angle_atom_site_label_2					
_geom_angle_atom_site_label_3					
_geom_angle					
_geom_angle_site_symmetry_1					
_geom_angle_site_symmetry_2					
_geom_angle_site_symmetry_3					
_geom_angle_publ_flag					
C6	S	C7	98.34(14)	.	yes
C26	O	C27	112.7(2)	.	yes
C2	C1	C6	118.7(2)	.	no
C2	C1	C13	122.0(2)	.	no
C6	C1	C13	119.3(2)	.	no
C1	C2	C3	119.9(3)	.	no
C2	C3	C4	120.3(3)	.	no
C3	C4	C5	120.6(3)	.	no
C4	C5	C6	119.5(3)	.	no
S	C6	C1	119.1(2)	.	yes
S	C6	C5	120.0(2)	.	yes
C1	C6	C5	120.9(2)	.	no
S	C7	C8	118.8(2)	.	yes
S	C7	C12	120.4(2)	.	yes
C8	C7	C12	120.8(2)	.	no
C7	C8	C9	120.1(3)	.	no
C8	C9	C10	119.5(3)	.	no

C9	C10	C11	120.2(3)	.	.	.	no
C10	C11	C12	121.5(3)	.	.	.	no
C7	C12	C11	117.8(2)	.	.	.	no
C7	C12	C13	117.7(2)	.	.	.	no
C11	C12	C13	124.4(2)	.	.	.	no
C1	C13	C12	111.3(2)	.	.	.	no
C1	C13	C14	124.4(2)	.	.	.	no
C12	C13	C14	124.2(2)	.	.	.	no
C13	C14	C15	130.8(2)	.	.	.	no
C13	C14	C26	124.4(2)	.	.	.	no
C15	C14	C26	104.5(2)	.	.	.	no
C14	C15	C16	132.1(2)	.	.	.	no
C14	C15	C24	107.9(2)	.	.	.	no
C16	C15	C24	119.7(2)	.	.	.	no
C15	C16	C17	125.1(2)	.	.	.	no
C15	C16	C21	117.8(2)	.	.	.	no
C17	C16	C21	116.9(3)	.	.	.	no
C16	C17	C18	121.9(3)	.	.	.	no
C17	C18	C19	120.6(3)	.	.	.	no
C18	C19	C20	119.5(3)	.	.	.	no
C19	C20	C21	121.4(3)	.	.	.	no
C16	C21	C20	119.7(2)	.	.	.	no
C16	C21	C22	119.3(3)	.	.	.	no
C20	C21	C22	120.8(2)	.	.	.	no
C21	C22	C23	121.3(3)	.	.	.	no
C22	C23	C24	120.0(3)	.	.	.	no
C15	C24	C23	121.6(3)	.	.	.	no
C15	C24	C25	111.3(2)	.	.	.	no
C23	C24	C25	127.0(3)	.	.	.	no
C24	C25	C26	102.9(2)	.	.	.	no
0	C26	C14	111.2(2)	.	.	.	yes
0	C26	C25	106.0(2)	.	.	.	yes
C14	C26	C25	102.6(2)	.	.	.	no
C1	C2	H2	119.8(14)	.	.	.	no
C3	C2	H2	120.2(14)	.	.	.	no
C2	C3	H3	119.1(15)	.	.	.	no
C4	C3	H3	120.6(15)	.	.	.	no
C3	C4	H4	119.6(14)	.	.	.	no
C5	C4	H4	119.7(14)	.	.	.	no
C4	C5	H5	117.4(16)	.	.	.	no
C6	C5	H5	122.9(16)	.	.	.	no
C7	C8	H8	119.7(14)	.	.	.	no
C9	C8	H8	120.2(14)	.	.	.	no
C8	C9	H9	119.9(15)	.	.	.	no
C10	C9	H9	120.5(15)	.	.	.	no
C9	C10	H10	119.8(16)	.	.	.	no
C11	C10	H10	119.8(16)	.	.	.	no
C10	C11	H11	122.2(18)	.	.	.	no
C12	C11	H11	116.2(18)	.	.	.	no
C16	C17	H17	116.6(13)	.	.	.	no
C18	C17	H17	121.4(13)	.	.	.	no
C17	C18	H18	118.1(14)	.	.	.	no
C19	C18	H18	121.4(14)	.	.	.	no
C18	C19	H19	120.7(15)	.	.	.	no
C20	C19	H19	119.8(15)	.	.	.	no
C19	C20	H20	119.2(17)	.	.	.	no
C21	C20	H20	119.4(17)	.	.	.	no
C21	C22	H22	118.8(13)	.	.	.	no
C23	C22	H22	119.9(14)	.	.	.	no
C22	C23	H23	123.5(15)	.	.	.	no
C24	C23	H23	116.4(15)	.	.	.	no

C24	C25	H25	110.8(17)	.	.	.	no
C24	C25	H25'	113.6(15)	.	.	.	no
C26	C25	H25	110.2(15)	.	.	.	no
C26	C25	H25'	109.4(14)	.	.	.	no
H25	C25	H25'	110(2)	.	.	.	no
O	C26	H26	107.1(14)	.	.	.	no
C14	C26	H26	116.3(13)	.	.	.	no
C25	C26	H26	113.4(14)	.	.	.	no
O	C27	H27	111.7(14)	.	.	.	no
O	C27	H27'	108.7(16)	.	.	.	no
O	C27	H27''	111.5(17)	.	.	.	no
H27	C27	H27'	109(2)	.	.	.	no
H27	C27	H27''	104(2)	.	.	.	no
H27'	C27	H27'''	113(2)	.	.	.	no

loop_

_geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag

C7	S	C6	C1	36.7(3)	.	.	.	.	no
C7	S	C6	C5	-144.7(3)	.	.	.	.	no
C6	S	C7	C8	141.3(2)	.	.	.	.	no
C6	S	C7	C12	-36.7(2)	.	.	.	.	no
C27	O	C26	C14	-74.1(3)	.	.	.	.	no
C27	O	C26	C25	175.2(2)	.	.	.	.	no
C6	C1	C2	C3	-2.5(4)	.	.	.	.	no
C13	C1	C2	C3	177.0(3)	.	.	.	.	no
C2	C1	C6	S	-177.8(2)	.	.	.	.	no
C2	C1	C6	C5	3.6(4)	.	.	.	.	no
C13	C1	C6	S	2.7(4)	.	.	.	.	no
C13	C1	C6	C5	-175.9(3)	.	.	.	.	no
C2	C1	C13	C12	129.8(3)	.	.	.	.	no
C2	C1	C13	C14	-52.5(4)	.	.	.	.	no
C6	C1	C13	C12	-50.8(3)	.	.	.	.	no
C6	C1	C13	C14	127.0(3)	.	.	.	.	no
C1	C2	C3	C4	-0.6(5)	.	.	.	.	no
C2	C3	C4	C5	2.7(5)	.	.	.	.	no
C3	C4	C5	C6	-1.5(5)	.	.	.	.	no
C4	C5	C6	S	179.7(2)	.	.	.	.	no
C4	C5	C6	C1	-1.7(5)	.	.	.	.	no
S	C7	C8	C9	-176.6(2)	.	.	.	.	no
C12	C7	C8	C9	1.5(4)	.	.	.	.	no
S	C7	C12	C11	173.3(2)	.	.	.	.	no
S	C7	C12	C13	-3.0(3)	.	.	.	.	no
C8	C7	C12	C11	-4.7(4)	.	.	.	.	no
C8	C7	C12	C13	179.0(2)	.	.	.	.	no
C7	C8	C9	C10	2.3(4)	.	.	.	.	no
C8	C9	C10	C11	-2.7(4)	.	.	.	.	no
C9	C10	C11	C12	-0.6(4)	.	.	.	.	no
C10	C11	C12	C7	4.3(4)	.	.	.	.	no
C10	C11	C12	C13	-179.7(3)	.	.	.	.	no
C7	C12	C13	C1	50.5(3)	.	.	.	.	no
C7	C12	C13	C14	-127.2(3)	.	.	.	.	no
C11	C12	C13	C1	-125.6(3)	.	.	.	.	no

C11	C12	C13	C14	56.7(4)	.	.	.	.	no
C1	C13	C14	C15	0.1(5)	.	.	.	.	no
C1	C13	C14	C26	172.3(3)	.	.	.	.	no
C12	C13	C14	C15	177.5(3)	.	.	.	.	no
C12	C13	C14	C26	-10.3(4)	.	.	.	.	no
C13	C14	C15	C16	-36.3(5)	.	.	.	.	no
C13	C14	C15	C24	150.6(3)	.	.	.	.	no
C26	C14	C15	C16	150.3(3)	.	.	.	.	no
C26	C14	C15	C24	-22.8(3)	.	.	.	.	no
C13	C14	C26	O	105.5(3)	.	.	.	.	no
C13	C14	C26	C25	-141.6(3)	.	.	.	.	no
C15	C14	C26	O	-80.6(3)	.	.	.	.	no
C15	C14	C26	C25	32.3(3)	.	.	.	.	no
C14	C15	C16	C17	-3.7(5)	.	.	.	.	no
C14	C15	C16	C21	-178.4(3)	.	.	.	.	no
C24	C15	C16	C17	168.8(3)	.	.	.	.	no
C24	C15	C16	C21	-6.0(4)	.	.	.	.	no
C14	C15	C24	C23	-179.4(2)	.	.	.	.	no
C14	C15	C24	C25	3.5(3)	.	.	.	.	no
C16	C15	C24	C23	6.5(4)	.	.	.	.	no
C16	C15	C24	C25	-170.6(2)	.	.	.	.	no
C15	C16	C17	C18	-177.5(3)	.	.	.	.	no
C21	C16	C17	C18	-2.6(4)	.	.	.	.	no
C15	C16	C21	C20	177.8(2)	.	.	.	.	no
C15	C16	C21	C22	2.1(4)	.	.	.	.	no
C17	C16	C21	C20	2.6(4)	.	.	.	.	no
C17	C16	C21	C22	-173.1(2)	.	.	.	.	no
C16	C17	C18	C19	0.7(4)	.	.	.	.	no
C17	C18	C19	C20	1.5(4)	.	.	.	.	no
C18	C19	C20	C21	-1.5(4)	.	.	.	.	no
C19	C20	C21	C16	-0.6(4)	.	.	.	.	no
C19	C20	C21	C22	175.0(3)	.	.	.	.	no
C16	C21	C22	C23	1.5(4)	.	.	.	.	no
C20	C21	C22	C23	-174.1(3)	.	.	.	.	no
C21	C22	C23	C24	-1.3(4)	.	.	.	.	no
C22	C23	C24	C15	-2.8(4)	.	.	.	.	no
C22	C23	C24	C25	173.8(3)	.	.	.	.	no
C15	C24	C25	C26	17.1(3)	.	.	.	.	no
C23	C24	C25	C26	-159.8(3)	.	.	.	.	no
C24	C25	C26	O	87.0(3)	.	.	.	.	no
C24	C25	C26	C14	-29.7(3)	.	.	.	.	no

loop_

_geom_contact_atom_site_label_1

_geom_contact_atom_site_label_2

_geom_contact_distance

_geom_contact_site_symmetry_1

_geom_contact_site_symmetry_2

_geom_contact_publ_flag

O	C4	3.384(4)	.	4_555	no
O	H18	2.73(2)	.	4_555	no
C1	C16	3.422(4)	.	.	no
C1	C17	3.090(4)	.	.	no
C2	C17	3.196(4)	.	.	no
C2	C15	3.327(4)	.	.	no
C2	C16	3.363(4)	.	.	no
C4	C27	3.496(5)	.	4_545	no
C4	O	3.384(4)	.	4_545	no
C5	C16	3.552(4)	.	4_545	no
C6	C17	3.508(4)	.	.	no
C6	C25	3.530(4)	.	4_645	no

C8	C9	3.595(4)	.	3_455	no
C9	C8	3.595(4)	.	3_555	no
C11	C26	3.226(4)	.	.	no
C11	C18	3.440(4)	.	1_655	no
C12	C27	3.465(4)	.	.	no
C13	C17	3.498(4)	.	.	no
C13	C27	3.523(4)	.	.	no
C15	C2	3.327(4)	.	.	no
C16	C2	3.363(4)	.	.	no
C16	C1	3.422(4)	.	.	no
C16	C5	3.552(4)	.	4_555	no
C17	C2	3.196(4)	.	.	no
C17	C1	3.090(4)	.	.	no
C17	C6	3.508(4)	.	.	no
C17	C13	3.498(4)	.	.	no
C18	C11	3.440(4)	.	1_455	no
C19	C22	3.454(4)	.	3_456	no
C22	C19	3.454(4)	.	3_556	no
C25	C6	3.530(4)	.	4_655	no
C26	C11	3.226(4)	.	.	no
C27	C13	3.523(4)	.	.	no
C27	C4	3.496(5)	.	4_555	no
C27	C12	3.465(4)	.	.	no
C1	H17	2.41(2)	.	.	no
C2	H17	2.91(2)	.	.	no
C3	H26	3.07(2)	.	4_645	no
C4	H26	2.95(2)	.	4_645	no
C6	H17	2.61(2)	.	.	no
C7	H25	2.79(3)	.	4_645	no
C7	H9	3.01(2)	.	3_455	no
C8	H23	2.99(3)	.	4_645	no
C8	H10	3.07(3)	.	3_455	no
C8	H9	3.04(2)	.	3_455	no
C9	H23	2.85(3)	.	4_645	no
C10	H8	3.07(2)	.	3_555	no
C11	H26	2.55(2)	.	.	no
C11	H18	3.05(2)	.	1_655	no
C12	H27	2.91(3)	.	.	no
C12	H25	2.96(3)	.	4_645	no
C12	H26	2.79(2)	.	.	no
C13	H17	2.86(2)	.	.	no
C13	H27	2.93(3)	.	.	no
C14	H11	3.09(3)	.	.	no
C14	H17	2.93(2)	.	.	no
C14	H27	2.73(3)	.	.	no
C14	H2	3.00(2)	.	.	no
C15	H5	2.83(3)	.	4_555	no
C15	H2	2.97(2)	.	.	no
C16	H5	2.69(3)	.	4_555	no
C17	H11	2.88(3)	.	1_455	no
C18	H11	2.72(3)	.	1_455	no
C21	H5	2.79(3)	.	4_555	no
C21	H19	2.98(3)	.	3_556	no
C22	H5	2.98(3)	.	4_555	no
C22	H19	2.79(3)	.	3_556	no
C23	H5	3.04(3)	.	4_555	no
C24	H5	2.93(3)	.	4_555	no
C26	H11	2.92(3)	.	.	no
C27	H9	3.04(2)	.	3_455	no
C27	H4	2.87(3)	.	4_555	no
H2	C14	3.00(2)	.	.	no

H2	C15	2.97(2)	.	.	no
H2	H19	2.41(4)	.	1_655	no
H2	H20	2.42(4)	.	3_556	no
H4	C27	2.87(3)	.	4_545	no
H4	H27	2.56(4)	.	4_545	no
H5	C15	2.83(3)	.	4_545	no
H5	C16	2.69(3)	.	4_545	no
H5	C21	2.79(3)	.	4_545	no
H5	C22	2.98(3)	.	4_545	no
H5	C23	3.04(3)	.	4_545	no
H5	C24	2.93(3)	.	4_545	no
H8	C10	3.07(2)	.	3_455	no
H8	H10	2.51(4)	.	3_455	no
H9	C7	3.01(2)	.	3_555	no
H9	C8	3.04(2)	.	3_555	no
H9	C27	3.04(2)	.	3_555	no
H9	H27	2.46(3)	.	3_555	no
H10	C8	3.07(3)	.	3_555	no
H10	H8	2.51(4)	.	3_555	no
H11	C14	3.09(3)	.	.	no
H11	C17	2.88(3)	.	1_655	no
H11	C18	2.72(3)	.	1_655	no
H11	C26	2.92(3)	.	.	no
H11	H18	2.55(3)	.	1_655	no
H11	H26	2.20(3)	.	.	no
H17	C1	2.41(2)	.	.	no
H17	C2	2.91(2)	.	.	no
H17	C6	2.61(2)	.	.	no
H17	C13	2.86(2)	.	.	no
H17	C14	2.93(2)	.	.	no
H18	C11	3.05(2)	.	1_455	no
H18	H11	2.55(3)	.	1_455	no
H18	O	2.73(2)	.	4_545	no
H19	H2	2.41(4)	.	1_455	no
H19	C21	2.98(3)	.	3_456	no
H19	C22	2.79(3)	.	3_456	no
H20	H22	2.45(4)	.	.	no
H20	H2	2.42(4)	.	3_456	no
H22	H20	2.45(4)	.	.	no
H23	C8	2.99(3)	.	4_655	no
H23	C9	2.85(3)	.	4_655	no
H25	C7	2.79(3)	.	4_655	no
H25	C12	2.96(3)	.	4_655	no
H26	C11	2.55(2)	.	.	no
H26	C12	2.79(2)	.	.	no
H26	H11	2.20(3)	.	.	no
H26	H27"	2.32(4)	.	.	no
H26	C3	3.07(2)	.	4_655	no
H26	C4	2.95(2)	.	4_655	no
H27	C12	2.91(3)	.	.	no
H27	C13	2.93(3)	.	.	no
H27	C14	2.73(3)	.	.	no
H27	H9	2.46(3)	.	3_455	no
H27	H4	2.56(4)	.	4_555	no
H27"	H26	2.32(4)	.	.	no

#===END of Crystallographic Information File