Exploring the boundaries of a light-driven molecular motor design

van Delden, Richard; ter Wiel, Matthijs; de Jong, Herman; Meetsma, Auke; Feringa, Bernard

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2004

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# 1. SUBMISSION DETAILS

_journal_coden_Cambridge        0177
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_publ_contact_author_name       # Name  of author for correspondence
'Prof Ben Feringa'
_publ_contact_author_address    # Address of author for correspondence
;
Organic and Molecular Inorganic Chemistry
University of Groningen
Nijenborgh 4
Groningen
9747 AG
NETHERLANDS
;
_publ_contact_author_email      FERINGA@CHEM.RUG.NL

_publ_section_title
;
Exploring the boundaries of a light-driven
molecular motor design: new sterically overcrowded alkenes with
preferred direction of rotation
;

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;
Altomare, A., Burla, M.C., Camalli, M., Cascarano, G.L.,
(1999) J. Appl. Cryst. 32, 115-119.

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Dordrecht, The Netherlands.

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```

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Spek, A.L. (1990). Acta Cryst. A46, C-34.
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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 are drawn with an arbitrary radius.
;
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_publ_author_name
'Ben Feringa'
'Harmen de Jong'
'Matthijs K.J. ter Wiel'
'Richard van Delden'

#===

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5. CHEMICAL DATA

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_chemical_formula_structural   ?
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C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M   'P 21/n'

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

_cell_length_a                   8.827(2)
_cell_length_b                   21.647(4)
_cell_length_c                   11.075(2)
_cell_angle_alpha                90
_cell_angle_beta                 100.493(3)
_cell_angle_gamma                90
_cell_volume                     2080.8(7)
_cell_formula_units_Z            4

_cell_measurement_temperature    293(1)
_cell_measurement_reflns_used    3334
_cell_measurement_theta_min      2.53
_cell_measurement_theta_max      21.79
_cell_special_details
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The final unit cell was obtained from the xyz centroids of
3334 reflections after integration using the SAINT software
package (Bruker, 2000).
;

_exptl_crystal_description       platelet
_exptl_crystal_colour            colorless
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_exptl_crystal_size_min          0.08
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_exptl_crystal_density_meas      ?
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_exptl_crystal_F_000             856
_exptl_absorpt_coefficient_mu    0.267
_exptl_absorpt_correction_type   Multi-Scan
_exptl_absorpt_process_details   '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min  0.8940
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;
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_diffrn_radiation_detector
;
CCD area-detector
;
_diffrn_measurement_device_type
;
Bruker Smart Apex
;
_diffrn_measurement_method       'phi and omega scans'
_diffrn_special_details          ?
_diffrn_detector_area_resol_mean '4096x4096 / 62x62 (binned 512)'
_diffrn_standards_number         ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?

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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number            14823
_diffrn_reflns_av_R_equivalents  0.0379
_diffrn_reflns_av_sigmaI/netI    0.0446
_diffrn_reflns_limit_h_min       -10
_diffrn_reflns_limit_h_max       10
_diffrn_reflns_limit_k_min       -25
_diffrn_reflns_limit_k_max       25
_diffrn_reflns_limit_l_min       -13
_diffrn_reflns_limit_l_max       12
_diffrn_reflns_theta_min         2.53
_diffrn_reflns_theta_max         25.02
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_diffrn_measured_fraction_theta_full 0.999

_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
_reflns_number_total             3673
_reflns_number_gt                2408
_reflns_threshold_expression     >2sigma(I)

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_computing_cell_refinement       'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction        'XPREP, Bruker Version 5.1/NT, 2000'
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SIR-97 (Altomare et al., 1997)
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PLUTO (Meetsma, 2001)
PLATON (Spek, 1994)
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PLATON (Spek, 1990)
SHELXL (Sheldrick, 1997)
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# 8. REFINEMENT DATA

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

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_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0598P)^2^+0.4521P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_hydrogens   difmap
_refine_ls_hydrogen_treatment    mixed
_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details ?
_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         3673
_refine_ls_number_parameters     331
_refine_ls_number_restraints     0
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          0.0834
_refine_ls_R_factor_gt           0.0498
_refine_ls_wR_factor_ref         0.1342
_refine_ls_wR_factor_gt          0.1179
_refine_ls_goodness_of_fit_ref   1.022
_refine_ls_restrained_S_all      1.022
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_refine_ls_shift/su_mean         0.000

_refine_diff_density_max         0.342
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S2 S Uani 0.08229(9) 0.35570(4) 0.56883(6) 1.000 0.0832(3) . .
C1 C Uani 0.0182(3) 0.33838(14) -0.0034(2) 1.000 0.0690(10) . .
C2 C Uani 0.0279(4) 0.3816(2) -0.0955(3) 1.000 0.0887(14) . .
C3 C Uani 0.0987(5) 0.4355(2) -0.0668(3) 1.000 0.0926(16) . .
C4 C Uani 0.1717(4) 0.44998(15) 0.0551(3) 1.000 0.0763(12) . .
C5 C Uani 0.2578(5) 0.50398(19) 0.0842(5) 1.000 0.0998(19) . .
C6 C Uani 0.3316(5) 0.51568(18) 0.2001(5) 1.000 0.0977(18) . .
C7 C Uani 0.3224(4) 0.47323(17) 0.2943(4) 1.000 0.0827(16) . .
C8 C Uani 0.2386(3) 0.42051(15) 0.2700(3) 1.000 0.0651(11) . .
C9 C Uani 0.1605(3) 0.40705(12) 0.1499(2) 1.000 0.0592(9) . .
C10 C Uani 0.0759(3) 0.35128(13) 0.1191(2) 1.000 0.0564(9) . .
C11 C Uani 0.0613(3) 0.30195(11) 0.2093(2) 1.000 0.0509(8) . .
C12 C Uani 0.1211(3) 0.24143(14) 0.1709(3) 1.000 0.0605(10) . .
C13 C Uani 0.0067(4) 0.21327(16) 0.0646(3) 1.000 0.0872(12) . .
C14 C Uani 0.0730(5) 0.1597(2) 0.0078(4) 1.000 0.1394(19) . .
C15 C Uani -0.0046(3) 0.30976(11) 0.3090(2) 1.000 0.0515(8) . .
C16 C Uani -0.0097(3) 0.26206(13) 0.4038(3) 1.000 0.0606(10) . .
C17 C Uani -0.0596(3) 0.20202(16) 0.3785(4) 1.000 0.0754(11) . .
C18 C Uani -0.0560(4) 0.1593(2) 0.4730(6) 1.000 0.0979(18) . .
C19 C Uani -0.0052(5) 0.1766(3) 0.5921(5) 1.000 0.110(2) . .
C20 C Uani 0.0388(4) 0.2358(3) 0.6206(4) 1.000 0.0912(18) . .
C21 C Uani 0.0337(3) 0.27903(14) 0.5278(3) 1.000 0.0692(10) . .
C22 C Uani -0.0502(3) 0.39281(13) 0.4542(2) 1.000 0.0616(10) . .
C23 C Uani -0.1252(4) 0.44605(15) 0.4818(3) 1.000 0.0760(12) . .
C24 C Uani -0.2277(4) 0.47493(16) 0.3924(4) 1.000 0.0811(14) . .
C25 C Uani -0.2589(4) 0.45126(15) 0.2751(3) 1.000 0.0728(11) . .
C26 C Uani -0.1859(3) 0.39850(13) 0.2468(3) 1.000 0.0610(10) . .
C27 C Uani -0.0783(3) 0.36848(12) 0.3348(2) 1.000 0.0539(8) . .
H2 H Uiso -0.023(4) 0.3676(15) -0.187(3) 1.000 0.112(11) . .
H3 H Uiso 0.105(4) 0.4640(16) -0.123(3) 1.000 0.112(13) . .
H5 H Uiso 0.258(4) 0.5342(17) 0.019(4) 1.000 0.123(13) . .
H6 H Uiso 0.382(4) 0.5526(16) 0.215(3) 1.000 0.099(12) . .
H7 H Uiso 0.373(3) 0.4777(13) 0.372(3) 1.000 0.074(10) . .
H8 H Uiso 0.233(3) 0.3920(10) 0.329(2) 1.000 0.045(7) . .
H12 H Uiso 0.219(3) 0.2492(11) 0.150(2) 1.000 0.067(8) . .
H12' H Uiso 0.138(3) 0.2104(12) 0.238(2) 1.000 0.072(8) . .
H13 H Uiso -0.092(5) 0.1945(17) 0.099(4) 1.000 0.143(15) . .
H14 H Uiso 0.16414 0.17253 -0.02117 1.000 0.2089 . .
H14' H Uiso -0.00126 0.14441 -0.05987 1.000 0.2089 . .
H14" H Uiso 0.09879 0.12758 0.06782 1.000 0.2089 . .
H17 H Uiso -0.096(3) 0.1899(10) 0.300(2) 1.000 0.047(7) . .
H18 H Uiso -0.088(3) 0.1212(15) 0.447(3) 1.000 0.078(10) . .
H19 H Uiso -0.012(4) 0.1489(17) 0.657(4) 1.000 0.124(13) . .
H20 H Uiso 0.066(4) 0.2501(15) 0.712(3) 1.000 0.110(12) . .
H23 H Uiso -0.101(3) 0.4621(12) 0.565(3) 1.000 0.083(9) . .
H24 H Uiso -0.278(3) 0.5104(12) 0.409(2) 1.000 0.066(8) . .
H25 H Uiso -0.337(4) 0.4716(15) 0.218(3) 1.000 0.102(11) . .
H26 H Uiso -0.208(3) 0.3812(11) 0.167(2) 1.000 0.064(8) . .

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C1 0.0671(17) 0.097(2) 0.0434(15) 0.0077(15) 0.0114(12) 0.0224(15)
C2 0.088(2) 0.123(3) 0.057(2) 0.018(2) 0.0186(17) 0.030(2)
C3 0.100(3) 0.115(3) 0.069(2) 0.043(2) 0.032(2) 0.039(2)
C4 0.076(2) 0.072(2) 0.089(2) 0.0224(18) 0.0369(18) 0.0209(17)
C5 0.108(3) 0.082(3) 0.121(4) 0.031(3) 0.052(3) 0.020(2)
C6 0.096(3) 0.064(2) 0.146(4) 0.004(3) 0.056(3) -0.002(2)
C7 0.072(2) 0.085(3) 0.097(3) -0.015(2) 0.031(2) -0.0036(18)
C8 0.0592(17) 0.074(2) 0.0675(19) 0.0002(17) 0.0258(14) -0.0036(15)
C9 0.0561(15) 0.0692(18) 0.0579(16) 0.0086(14) 0.0256(13) 0.0141(14)
C10 0.0492(14) 0.0766(18) 0.0454(14) 0.0067(13) 0.0139(11) 0.0119(13)
C11 0.0473(13) 0.0636(16) 0.0403(13) -0.0029(12) 0.0039(10) 0.0009(12)
C12 0.0521(16) 0.0735(19) 0.0555(16) -0.0078(15) 0.0091(13) -0.0003(14)
C13 0.084(2) 0.095(2) 0.077(2) -0.0250(18) -0.0004(18) 0.0015(19)
C14 0.128(3) 0.139(3) 0.138(4) -0.075(3) -0.011(3) 0.033(3)
C15 0.0465(13) 0.0617(16) 0.0453(14) 0.0021(12) 0.0060(11) -0.0005(12)
C16 0.0492(14) 0.0726(19) 0.0627(17) 0.0130(14) 0.0174(12) 0.0051(13)
C17 0.0632(19) 0.079(2) 0.088(2) 0.012(2) 0.0244(18) -0.0028(16)
C18 0.072(2) 0.077(3) 0.154(4) 0.036(3) 0.045(2) 0.005(2)
C19 0.076(2) 0.148(5) 0.116(4) 0.075(4) 0.043(2) 0.029(3)
C20 0.069(2) 0.134(4) 0.076(3) 0.038(3) 0.0272(18) 0.023(2)
C21 0.0554(16) 0.102(2) 0.0544(16) 0.0211(16) 0.0212(13) 0.0130(15)
C22 0.0560(16) 0.0746(19) 0.0575(17) -0.0074(14) 0.0189(13) -0.0080(14)
C23 0.074(2) 0.083(2) 0.077(2) -0.0240(19) 0.0300(17) -0.0136(18)
C24 0.079(2) 0.063(2) 0.110(3) -0.008(2) 0.040(2) 0.0018(17)
C25 0.0631(19) 0.073(2) 0.087(2) 0.0079(18) 0.0261(17) 0.0046(16)
C26 0.0551(16) 0.0690(19) 0.0609(18) 0.0016(15) 0.0161(14) 0.0020(14)
C27 0.0512(14) 0.0640(16) 0.0496(14) 0.0012(12) 0.0175(11) -0.0040(12)

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

# 10. MOLECULAR GEOMETRY

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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
;

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S1 C1 1.754(3) . . yes
S1 C13 1.790(4) . . yes
S2 C21 1.753(3) . . yes
S2 C22 1.756(3) . . yes
C1 C2 1.398(5) . . no
C1 C10 1.388(3) . . no
C2 C3 1.334(6) . . no
C3 C4 1.421(5) . . no
C4 C5 1.400(5) . . no
C4 C9 1.419(4) . . no
C5 C6 1.353(8) . . no
C6 C7 1.404(6) . . no
C7 C8 1.360(5) . . no
C8 C9 1.413(4) . . no
C9 C10 1.428(4) . . no
C10 C11 1.484(3) . . no
```

```
C11 C12 1.503(4) . . no
C11 C15 1.349(3) . . no
C12 C13 1.531(5) . . no
C13 C14 1.489(6) . . no
C15 C16 1.479(4) . . no
C15 C27 1.479(4) . . no
C16 C17 1.384(4) . . no
C16 C21 1.406(5) . . no
C17 C18 1.393(7) . . no
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C19 C20 1.359(9) . . no
C20 C21 1.385(6) . . no
C22 C23 1.391(4) . . no
C22 C27 1.403(3) . . no
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C7 H7 0.90(3) . . no
C8 H8 0.91(2) . . no
C12 H12 0.95(3) . . no
C12 H12' 0.99(2) . . no
C13 H13 1.09(4) . . no
C14 H14 0.9598 . . no
C14 H14' 0.9602 . . no
C14 H14" 0.9602 . . no
C17 H17 0.91(2) . . no
C18 H18 0.90(3) . . no
C19 H19 0.95(4) . . no
C20 H20 1.04(3) . . no
C23 H23 0.97(3) . . no
C24 H24 0.92(3) . . no
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