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A donor–acceptor substituted molecular motor

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Beurskens, P.T., Beurskens, G., Gelder, R. de Garcia-Granda, S.
Gould, R.O. Israel, & Smits, J.M.M. (1999).
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University, The Netherlands.

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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.
All non-hydrogen atoms are represented by thermal vibrational
ellipsoids drawn to encompass 50% of the electron density.
The hydrogen atoms are drawn with an arbitrary radius.
;

#=====

5. CHEMICAL DATA

_chemical_name_systematic
;
?
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety
'C29 H24 N2 O2 S2'
_chemical_formula_structural ?
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_sum
'C29 H24 N2 O2 S2'
_chemical_formula_weight 496.64
_chemical_compound_source 'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
S S 0.1246 0.1234
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.0060
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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_cell_setting      Orthorhombic
_symmetry_space_group_name_Hall  'P 2ac 2ab'
_symmetry_space_group_name_H-M   'P 21 21 21'
```

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

```
_cell_length_a      7.7426(3)
_cell_length_b      12.4048(5)
_cell_length_c      24.867(1)
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    90
_cell_volume         2388.36(16)
_cell_formula_units_Z 4
```

```
_cell_measurement_temperature    100
_cell_measurement_reflns_used    8722
_cell_measurement_theta_min      2.32
_cell_measurement_theta_max      29.58
_cell_special_details
```

```
;
The final unit cell was obtained from the xyz centroids of
8722 reflections after integration using the SAINT software
package (Bruker, 2000).
```

```
The intensity data were corrected for decay and absorption
using SADABS (Sheldrick, 2000).
;
```

```
_exptl_crystal_description      'platelet'
_exptl_crystal_colour            'red'

_exptl_crystal_size_max          0.520
_exptl_crystal_size_mid          0.440
_exptl_crystal_size_min          0.330
_exptl_crystal_size_rad          ?
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffn     1.381
_exptl_crystal_density_method    'Not Measured'
_exptl_crystal_F_000             1040
_exptl_absorpt_coefficient_mu     0.254
_exptl_absorpt_correction_type    'Semi-empirical'
_exptl_absorpt_process_details    '(SADABS (Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min   0.8792
_exptl_absorpt_correction_T_max   0.9209
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#=====
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7. EXPERIMENTAL DATA

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_exptl_special_details
;
?
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```

;

_diffrn_ambient_temperature      100(2)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\alpha
_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
Enraf Nonius CAD-4F diffractometer
;

_diffrn_measurement_method       'phi and omega scans'
_diffrn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature
unit (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean  ' 512x512 / 62x62'

_diffrn_standards_number         ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        ?

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number            22638
_diffrn_reflns_av_R_equivalents  0.0160
_diffrn_reflns_av_sigmaI/netI   0.0170
_diffrn_reflns_limit_h_min      -9
_diffrn_reflns_limit_h_max      10
_diffrn_reflns_limit_k_min      -16
_diffrn_reflns_limit_k_max      16
_diffrn_reflns_limit_l_min      -33
_diffrn_reflns_limit_l_max      34
_diffrn_reflns_theta_min        2.32
_diffrn_reflns_theta_max        29.69
_diffrn_measured_fraction_theta_max 0.956
_diffrn_reflns_theta_full       29.69
_diffrn_measured_fraction_theta_full 0.956

_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 SABABS (Sheldrick, 2000)

Intensity data were corrected for Lorentz and polarization effects,
scale variation, for absorption and reduced to  $F_o^2$ 
;

# number of unique reflections
_reflns_number_total            6379
_reflns_number_gt               6253
_reflns_threshold_expression     >2sigma(I)

_computing_data_collection      'SMART, Bruker Version 5.168, 2000'

```

```

_computing_cell_refinement      'SAINT, Bruker Version 6.02A, 2000'
_computing_data_reduction      'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2000)
PLATON (Spek, 1994)
;
_computing_publication_material
;
PLATON (Spek, 1990)
SHELXL (Sheldrick, 1997)
;

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
'calc w=1/[\s2(Fo2)+(0.0551P)2+0.3510P] where P=(Fo2+2Fc2)/3'
_refine_ls_solution_primary        Patterson
_refine_ls_solution_secondary      direct
_refine_ls_hydrogen_treatment      difmap/geom
_refine_ls_extinction_method        none
_refine_ls_extinction_coef         ?
_refine_ls_abs_structure_details
'Flack H.D. (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack     0.59(4)
_refine_ls_number_reflns           6379
_refine_ls_number_parameters       412
_refine_ls_number_restraints        0
_refine_ls_number_constraints       ?
_refine_ls_R_factor_all             0.0291
_refine_ls_R_factor_gt              0.0285
_refine_ls_wR_factor_ref            0.0769
_refine_ls_wR_factor_gt             0.0763
_refine_ls_goodness_of_fit_ref      1.037
_refine_ls_restrained_S_all         1.037
_refine_ls_shift/su_max             0.001
_refine_ls_shift/su_mean            0.000

_refine_diff_density_max            0.389
_refine_diff_density_min            -0.236
_refine_diff_density_rms            0.051

#=====

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

```

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_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
S1 S Uani 1.20021(4) 0.22629(2) 0.02101(1) 1.000 0.0189(1) . .
S2 S Uani 0.72965(4) 0.68509(2) 0.11201(1) 1.000 0.0173(1) . .
O1 O Uani 0.67744(16) 0.15916(8) 0.15771(4) 1.000 0.0291(3) . .
O2 O Uani 0.55610(14) 0.21798(9) 0.23076(4) 1.000 0.0270(3) . .
N1 N Uani 0.62478(14) 0.23235(9) 0.18667(4) 1.000 0.0198(3) . .
N2 N Uani 0.79484(15) 0.60899(9) -0.12482(4) 1.000 0.0183(3) . .
C1 C Uani 0.78452(14) 0.46717(8) 0.10709(4) 1.000 0.0124(3) . .
C2 C Uani 0.75090(15) 0.36149(9) 0.12354(4) 1.000 0.0138(3) . .
C3 C Uani 0.64729(16) 0.34386(9) 0.16819(5) 1.000 0.0159(3) . .
C4 C Uani 0.56811(17) 0.42731(11) 0.19643(5) 1.000 0.0189(3) . .
C5 C Uani 0.59256(16) 0.53184(10) 0.17852(5) 1.000 0.0177(3) . .
C6 C Uani 0.69906(15) 0.55164(9) 0.13392(4) 1.000 0.0140(3) . .
C7 C Uani 0.75415(15) 0.66148(9) 0.04230(4) 1.000 0.0141(3) . .
C8 C Uani 0.68217(16) 0.73445(9) 0.00631(5) 1.000 0.0174(3) . .
C9 C Uani 0.69951(16) 0.72034(9) -0.04904(5) 1.000 0.0180(3) . .
C10 C Uani 0.78422(16) 0.62881(9) -0.06958(5) 1.000 0.0150(3) . .
C11 C Uani 0.85118(15) 0.55352(9) -0.03244(4) 1.000 0.0135(3) . .
C12 C Uani 0.84148(14) 0.56995(8) 0.02310(5) 1.000 0.0124(3) . .
C13 C Uani 0.90897(15) 0.49077(8) 0.06295(4) 1.000 0.0117(3) . .
C14 C Uani 1.06758(15) 0.44459(9) 0.06188(4) 1.000 0.0120(3) . .
C15 C Uani 1.12326(15) 0.36760(9) 0.10429(5) 1.000 0.0133(3) . .
C16 C Uani 1.12763(15) 0.39475(10) 0.16050(5) 1.000 0.0153(3) . .
C17 C Uani 1.10576(16) 0.50244(10) 0.17915(5) 1.000 0.0181(3) . .
C18 C Uani 1.11231(18) 0.52586(12) 0.23331(5) 1.000 0.0229(4) . .
C19 C Uani 1.13729(18) 0.44321(13) 0.27155(5) 1.000 0.0267(4) . .
C20 C Uani 1.15890(18) 0.33900(12) 0.25471(5) 1.000 0.0240(3) . .
C21 C Uani 1.15740(16) 0.31193(11) 0.19915(5) 1.000 0.0186(3) . .
C22 C Uani 1.18814(17) 0.20479(11) 0.18111(5) 1.000 0.0220(3) . .
C23 C Uani 1.20062(17) 0.18234(10) 0.12746(5) 1.000 0.0205(3) . .
C24 C Uani 1.17368(15) 0.26505(9) 0.08851(5) 1.000 0.0154(3) . .
C25 C Uani 1.19774(16) 0.35254(9) -0.01698(5) 1.000 0.0163(3) . .
C26 C Uani 1.19911(15) 0.45647(9) 0.01700(4) 1.000 0.0136(3) . .
C27 C Uani 1.37951(17) 0.48299(10) 0.03874(5) 1.000 0.0188(3) . .
C28 C Uani 0.95129(18) 0.55915(11) -0.14616(5) 1.000 0.0209(3) . .
C29 C Uani 0.7247(2) 0.69030(12) -0.16081(5) 1.000 0.0273(4) . .
H2 H Uiso 0.808(2) 0.3015(14) 0.1054(7) 1.000 0.021(4) . .
H4 H Uiso 0.501(2) 0.4099(14) 0.2264(7) 1.000 0.021(4) . .
H5 H Uiso 0.538(3) 0.5907(16) 0.1972(7) 1.000 0.027(5) . .
H8 H Uiso 0.617(2) 0.7897(14) 0.0201(7) 1.000 0.023(4) . .
H9 H Uiso 0.649(2) 0.7729(13) -0.0724(6) 1.000 0.017(4) . .
H11 H Uiso 0.902(2) 0.4877(12) -0.0437(6) 1.000 0.014(4) . .
H17 H Uiso 1.087(2) 0.5586(15) 0.1534(7) 1.000 0.021(4) . .
H18 H Uiso 1.101(3) 0.5984(16) 0.2441(8) 1.000 0.031(5) . .
H19 H Uiso 1.139(3) 0.4601(16) 0.3070(8) 1.000 0.028(5) . .
H20 H Uiso 1.178(3) 0.2815(19) 0.2780(9) 1.000 0.046(6) . .
H22 H Uiso 1.204(2) 0.1470(13) 0.2068(6) 1.000 0.015(4) . .
H23 H Uiso 1.224(3) 0.1097(16) 0.1170(8) 1.000 0.033(5) . .
H25 H Uiso 1.104(2) 0.3475(14) -0.0389(7) 1.000 0.017(4) . .
H25' H Uiso 1.295(2) 0.3512(14) -0.0384(7) 1.000 0.020(4) . .
H26 H Uiso 1.166(2) 0.5136(13) -0.0068(6) 1.000 0.015(4) . .
H27 H Uiso 1.426(2) 0.4243(14) 0.0602(7) 1.000 0.018(4) . .
H27' H Uiso 1.456(3) 0.4954(18) 0.0093(9) 1.000 0.040(6) . .
H27'' H Uiso 1.376(2) 0.5457(15) 0.0609(7) 1.000 0.025(4) . .
H28 H Uiso 0.921(3) 0.5213(16) -0.1798(8) 1.000 0.028(5) . .
H28' H Uiso 0.989(3) 0.5090(16) -0.1235(8) 1.000 0.026(5) . .
H28'' H Uiso 1.034(3) 0.6115(19) -0.1514(9) 1.000 0.044(6) . .
H29 H Uiso 0.729(3) 0.6688(16) -0.1943(8) 1.000 0.031(5) . .
H29' H Uiso 0.599(3) 0.7049(16) -0.1508(8) 1.000 0.031(5) . .

```

H29" H Uiso 0.788(3) 0.7574(19) -0.1602(8) 1.000 0.043(6) . .

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_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
S1 0.0242(2) 0.0138(1) 0.0189(1) -0.0022(1) 0.0008(1) 0.0028(1)
S2 0.0234(2) 0.0131(1) 0.0154(1) -0.0027(1) 0.0012(1) 0.0029(1)
O1 0.0405(6) 0.0191(4) 0.0277(5) 0.0034(4) 0.0042(4) -0.0054(4)
O2 0.0265(5) 0.0343(5) 0.0203(4) 0.0118(4) 0.0037(4) -0.0040(4)
N1 0.0186(5) 0.0224(5) 0.0184(5) 0.0058(4) -0.0015(4) -0.0049(4)
N2 0.0199(5) 0.0213(5) 0.0138(4) 0.0030(4) -0.0009(4) 0.0023(4)
C1 0.0104(4) 0.0145(4) 0.0122(5) 0.0000(4) -0.0007(4) 0.0004(4)
C2 0.0127(5) 0.0156(5) 0.0132(5) 0.0006(4) -0.0006(4) -0.0007(4)
C3 0.0143(5) 0.0185(5) 0.0148(5) 0.0039(4) -0.0009(4) -0.0030(4)
C4 0.0161(5) 0.0272(6) 0.0134(5) 0.0005(4) 0.0018(4) -0.0009(5)
C5 0.0160(5) 0.0231(5) 0.0139(5) -0.0028(4) 0.0019(4) 0.0027(4)
C6 0.0133(5) 0.0154(4) 0.0134(5) -0.0012(4) -0.0009(4) 0.0009(4)
C7 0.0144(5) 0.0136(4) 0.0143(5) -0.0010(4) 0.0008(4) 0.0005(4)
C8 0.0183(5) 0.0139(5) 0.0201(5) 0.0004(4) 0.0005(4) 0.0045(4)
C9 0.0187(5) 0.0162(5) 0.0191(5) 0.0036(4) -0.0019(4) 0.0032(5)
C10 0.0143(5) 0.0153(5) 0.0153(5) 0.0019(4) -0.0007(4) -0.0016(4)
C11 0.0130(5) 0.0118(4) 0.0157(5) 0.0002(4) -0.0005(4) -0.0002(4)
C12 0.0105(4) 0.0117(4) 0.0149(5) 0.0010(4) -0.0008(4) -0.0001(4)
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C14 0.0129(5) 0.0112(4) 0.0118(5) -0.0009(4) -0.0009(4) -0.0001(4)
C15 0.0110(5) 0.0152(5) 0.0137(5) 0.0017(4) -0.0003(4) 0.0006(4)
C16 0.0108(5) 0.0201(5) 0.0151(5) 0.0017(4) -0.0008(4) 0.0008(4)
C17 0.0151(5) 0.0225(5) 0.0167(5) -0.0012(4) -0.0018(4) -0.0002(4)
C18 0.0189(6) 0.0302(7) 0.0195(6) -0.0062(5) -0.0003(5) -0.0002(5)
C19 0.0224(6) 0.0436(8) 0.0140(5) -0.0013(5) 0.0000(5) 0.0008(6)
C20 0.0194(6) 0.0360(7) 0.0165(5) 0.0070(5) -0.0006(5) 0.0023(5)
C21 0.0139(5) 0.0243(5) 0.0175(5) 0.0052(4) -0.0003(4) 0.0017(5)
C22 0.0188(6) 0.0239(6) 0.0232(6) 0.0091(5) 0.0007(5) 0.0030(5)
C23 0.0195(6) 0.0164(5) 0.0257(6) 0.0043(4) 0.0004(5) 0.0035(5)
C24 0.0126(5) 0.0162(5) 0.0175(5) 0.0006(4) -0.0002(4) 0.0018(4)
C25 0.0180(5) 0.0159(4) 0.0149(5) -0.0014(4) 0.0016(4) 0.0016(4)
C26 0.0119(5) 0.0149(5) 0.0139(5) -0.0006(4) 0.0010(4) 0.0006(4)
C27 0.0131(5) 0.0216(6) 0.0216(6) 0.0001(5) -0.0003(4) -0.0012(4)
C28 0.0246(6) 0.0211(6) 0.0171(6) 0.0001(4) 0.0036(5) 0.0003(5)
C29 0.0337(8) 0.0319(7) 0.0163(6) 0.0071(5) -0.0028(5) 0.0071(6)
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#=====

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

S1	C24	1.7581(13)	.	.	yes
S1	C25	1.8291(12)	.	.	yes
S2	C6	1.7588(11)	.	.	yes

S2	C7	1.7683(10)	.	.	yes
O1	N1	1.2285(15)	.	.	yes
O2	N1	1.2315(14)	.	.	yes
N1	C3	1.4680(16)	.	.	yes
N2	C10	1.3979(16)	.	.	yes
N2	C28	1.4599(18)	.	.	yes
N2	C29	1.4537(18)	.	.	yes
C1	C2	1.3977(15)	.	.	no
C1	C6	1.4074(15)	.	.	no
C1	C13	1.4896(15)	.	.	no
C2	C3	1.3871(16)	.	.	no
C3	C4	1.3930(18)	.	.	no
C4	C5	1.3840(18)	.	.	no
C5	C6	1.4037(16)	.	.	no
C7	C8	1.3896(16)	.	.	no
C7	C12	1.4051(15)	.	.	no
C8	C9	1.3940(18)	.	.	no
C9	C10	1.4072(16)	.	.	no
C10	C11	1.4121(16)	.	.	no
C11	C12	1.3981(16)	.	.	no
C12	C13	1.4899(15)	.	.	no
C13	C14	1.3554(16)	.	.	no
C14	C15	1.4867(16)	.	.	no
C14	C26	1.5180(15)	.	.	no
C15	C16	1.4382(18)	.	.	no
C15	C24	1.3873(16)	.	.	no
C16	C17	1.4242(18)	.	.	no
C16	C21	1.4256(18)	.	.	no
C17	C18	1.3787(18)	.	.	no
C18	C19	1.412(2)	.	.	no
C19	C20	1.369(2)	.	.	no
C20	C21	1.4219(18)	.	.	no
C21	C22	1.4228(19)	.	.	no
C22	C23	1.3663(18)	.	.	no
C23	C24	1.4263(17)	.	.	no
C25	C26	1.5415(16)	.	.	no
C26	C27	1.5334(17)	.	.	no
C2	H2	0.976(17)	.	.	no
C4	H4	0.934(17)	.	.	no
C5	H5	0.96(2)	.	.	no
C8	H8	0.918(17)	.	.	no
C9	H9	0.957(16)	.	.	no
C11	H11	0.949(15)	.	.	no
C17	H17	0.957(18)	.	.	no
C18	H18	0.94(2)	.	.	no
C19	H19	0.91(2)	.	.	no
C20	H20	0.93(2)	.	.	no
C22	H22	0.968(16)	.	.	no
C23	H23	0.96(2)	.	.	no
C25	H25	0.910(16)	.	.	no
C25	H25'	0.923(16)	.	.	no
C26	H26	0.958(16)	.	.	no
C27	H27	0.972(17)	.	.	no
C27	H27'	0.95(2)	.	.	no
C27	H27"	0.954(18)	.	.	no
C28	H28	0.99(2)	.	.	no
C28	H28'	0.89(2)	.	.	no
C28	H28"	0.92(2)	.	.	no
C29	H29	0.88(2)	.	.	no
C29	H29'	1.02(2)	.	.	no
C29	H29"	0.97(2)	.	.	no

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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

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_geom_angle_site_symmetry_3							
_geom_angle_publ_flag							
C24	S1	C25	104.94(5)	.	.	.	yes
C6	S2	C7	99.34(5)	.	.	.	yes
O1	N1	O2	123.93(11)	.	.	.	yes
O1	N1	C3	118.26(10)	.	.	.	yes
O2	N1	C3	117.80(11)	.	.	.	yes
C10	N2	C28	118.72(10)	.	.	.	yes
C10	N2	C29	117.45(10)	.	.	.	yes
C28	N2	C29	112.34(10)	.	.	.	yes
C2	C1	C6	118.16(10)	.	.	.	no
C2	C1	C13	121.36(9)	.	.	.	no
C6	C1	C13	120.47(9)	.	.	.	no
C1	C2	C3	119.33(10)	.	.	.	no
N1	C3	C2	117.89(10)	.	.	.	yes
N1	C3	C4	119.35(11)	.	.	.	yes
C2	C3	C4	122.74(11)	.	.	.	no
C3	C4	C5	118.28(11)	.	.	.	no
C4	C5	C6	119.90(11)	.	.	.	no
S2	C6	C1	119.38(8)	.	.	.	yes
S2	C6	C5	119.25(9)	.	.	.	yes
C1	C6	C5	121.36(10)	.	.	.	no
S2	C7	C8	118.72(9)	.	.	.	yes
S2	C7	C12	121.24(8)	.	.	.	yes
C8	C7	C12	120.04(10)	.	.	.	no
C7	C8	C9	121.03(11)	.	.	.	no
C8	C9	C10	120.30(11)	.	.	.	no
N2	C10	C9	121.74(11)	.	.	.	yes
N2	C10	C11	120.32(10)	.	.	.	yes
C9	C10	C11	117.86(11)	.	.	.	no
C10	C11	C12	122.00(10)	.	.	.	no
C7	C12	C11	118.64(10)	.	.	.	no
C7	C12	C13	118.39(10)	.	.	.	no
C11	C12	C13	122.83(9)	.	.	.	no
C1	C13	C12	113.13(9)	.	.	.	no
C1	C13	C14	121.16(9)	.	.	.	no
C12	C13	C14	125.69(10)	.	.	.	no
C13	C14	C15	121.36(10)	.	.	.	no
C13	C14	C26	125.54(10)	.	.	.	no
C15	C14	C26	112.91(10)	.	.	.	no
C14	C15	C16	123.08(10)	.	.	.	no
C14	C15	C24	118.04(11)	.	.	.	no
C16	C15	C24	118.88(11)	.	.	.	no
C15	C16	C17	122.23(11)	.	.	.	no
C15	C16	C21	119.36(11)	.	.	.	no
C17	C16	C21	118.40(11)	.	.	.	no
C16	C17	C18	120.76(12)	.	.	.	no
C17	C18	C19	120.67(13)	.	.	.	no
C18	C19	C20	119.77(12)	.	.	.	no
C19	C20	C21	121.28(12)	.	.	.	no
C16	C21	C20	119.09(12)	.	.	.	no
C16	C21	C22	119.19(11)	.	.	.	no
C20	C21	C22	121.71(12)	.	.	.	no
C21	C22	C23	120.67(12)	.	.	.	no
C22	C23	C24	120.41(12)	.	.	.	no
S1	C24	C15	123.62(9)	.	.	.	yes
S1	C24	C23	115.76(9)	.	.	.	yes
C15	C24	C23	120.58(11)	.	.	.	no
S1	C25	C26	115.65(8)	.	.	.	yes
C14	C26	C25	108.49(9)	.	.	.	no
C14	C26	C27	111.88(9)	.	.	.	no
C25	C26	C27	112.27(10)	.	.	.	no
C1	C2	H2	119.7(10)	.	.	.	no
C3	C2	H2	120.8(10)	.	.	.	no
C3	C4	H4	118.4(11)	.	.	.	no
C5	C4	H4	123.3(11)	.	.	.	no
C4	C5	H5	119.7(12)	.	.	.	no
C6	C5	H5	120.4(12)	.	.	.	no
C7	C8	H8	117.8(11)	.	.	.	no

C9	C8	H8	121.0(11)	.	.	.	no
C8	C9	H9	118.3(9)	.	.	.	no
C10	C9	H9	121.3(9)	.	.	.	no
C10	C11	H11	121.9(9)	.	.	.	no
C12	C11	H11	116.1(9)	.	.	.	no
C16	C17	H17	118.9(11)	.	.	.	no
C18	C17	H17	120.4(11)	.	.	.	no
C17	C18	H18	118.4(12)	.	.	.	no
C19	C18	H18	120.9(12)	.	.	.	no
C18	C19	H19	119.3(13)	.	.	.	no
C20	C19	H19	120.9(13)	.	.	.	no
C19	C20	H20	123.6(14)	.	.	.	no
C21	C20	H20	115.2(14)	.	.	.	no
C21	C22	H22	120.3(9)	.	.	.	no
C23	C22	H22	119.0(9)	.	.	.	no
C22	C23	H23	118.1(12)	.	.	.	no
C24	C23	H23	121.4(12)	.	.	.	no
S1	C25	H25	105.0(11)	.	.	.	no
S1	C25	H25'	105.9(11)	.	.	.	no
C26	C25	H25	113.0(11)	.	.	.	no
C26	C25	H25'	109.0(11)	.	.	.	no
H25	C25	H25'	107.7(15)	.	.	.	no
C14	C26	H26	110.3(9)	.	.	.	no
C25	C26	H26	106.1(9)	.	.	.	no
C27	C26	H26	107.6(9)	.	.	.	no
C26	C27	H27	111.7(10)	.	.	.	no
C26	C27	H27'	109.2(14)	.	.	.	no
C26	C27	H27"	110.7(9)	.	.	.	no
H27	C27	H27'	108.2(17)	.	.	.	no
H27	C27	H27"	107.7(15)	.	.	.	no
H27'	C27	H27"	109.2(17)	.	.	.	no
N2	C28	H28	108.2(13)	.	.	.	no
N2	C28	H28'	109.8(14)	.	.	.	no
N2	C28	H28"	109.2(14)	.	.	.	no
H28	C28	H28'	106.4(18)	.	.	.	no
H28	C28	H28"	112.4(19)	.	.	.	no
H28'	C28	H28"	111(2)	.	.	.	no
N2	C29	H29	111.1(14)	.	.	.	no
N2	C29	H29'	109.2(11)	.	.	.	no
N2	C29	H29"	113.5(13)	.	.	.	no
H29	C29	H29'	108.8(19)	.	.	.	no
H29	C29	H29"	105.0(18)	.	.	.	no
H29'	C29	H29"	109.1(18)	.	.	.	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

C25	S1	C24	C15	12.77(12)	.	.	.	.	no
C25	S1	C24	C23	-169.70(9)	.	.	.	.	no
C24	S1	C25	C26	7.83(10)	.	.	.	.	no
C7	S2	C6	C1	33.38(10)	.	.	.	.	no
C7	S2	C6	C5	-147.90(10)	.	.	.	.	no
C6	S2	C7	C8	141.86(10)	.	.	.	.	no
C6	S2	C7	C12	-36.91(11)	.	.	.	.	no
O1	N1	C3	C4	171.19(12)	.	.	.	.	no
O1	N1	C3	C2	-10.22(17)	.	.	.	.	no
O2	N1	C3	C4	-9.77(17)	.	.	.	.	no
O2	N1	C3	C2	168.81(11)	.	.	.	.	no
C28	N2	C10	C11	-38.86(17)	.	.	.	.	no
C29	N2	C10	C9	3.94(18)	.	.	.	.	no
C28	N2	C10	C9	144.56(12)	.	.	.	.	no

C29	N2	C10	C11	-179.47(12)	.	.	.	.	no
C6	C1	C13	C12	-47.10(13)	.	.	.	.	no
C6	C1	C2	C3	-5.45(16)	.	.	.	.	no
C13	C1	C2	C3	173.70(10)	.	.	.	.	no
C2	C1	C6	S2	-176.72(8)	.	.	.	.	no
C2	C1	C6	C5	4.58(16)	.	.	.	.	no
C13	C1	C6	S2	4.12(14)	.	.	.	.	no
C13	C1	C6	C5	-174.58(10)	.	.	.	.	no
C2	C1	C13	C12	133.77(10)	.	.	.	.	no
C2	C1	C13	C14	-47.75(15)	.	.	.	.	no
C6	C1	C13	C14	131.38(11)	.	.	.	.	no
C1	C2	C3	N1	-175.69(10)	.	.	.	.	no
C1	C2	C3	C4	2.85(18)	.	.	.	.	no
C2	C3	C4	C5	0.89(19)	.	.	.	.	no
N1	C3	C4	C5	179.41(11)	.	.	.	.	no
C3	C4	C5	C6	-1.84(18)	.	.	.	.	no
C4	C5	C6	S2	-179.60(10)	.	.	.	.	no
C4	C5	C6	C1	-0.91(18)	.	.	.	.	no
C8	C7	C12	C11	-1.11(17)	.	.	.	.	no
C12	C7	C8	C9	-2.00(18)	.	.	.	.	no
C8	C7	C12	C13	-176.91(10)	.	.	.	.	no
S2	C7	C8	C9	179.21(9)	.	.	.	.	no
S2	C7	C12	C11	177.65(9)	.	.	.	.	no
S2	C7	C12	C13	1.85(15)	.	.	.	.	no
C7	C8	C9	C10	2.84(18)	.	.	.	.	no
C8	C9	C10	C11	-0.53(18)	.	.	.	.	no
C8	C9	C10	N2	176.14(11)	.	.	.	.	no
N2	C10	C11	C12	-179.35(11)	.	.	.	.	no
C9	C10	C11	C12	-2.64(17)	.	.	.	.	no
C10	C11	C12	C7	3.46(17)	.	.	.	.	no
C10	C11	C12	C13	179.06(11)	.	.	.	.	no
C11	C12	C13	C1	-132.40(11)	.	.	.	.	no
C7	C12	C13	C1	43.21(13)	.	.	.	.	no
C7	C12	C13	C14	-135.18(12)	.	.	.	.	no
C11	C12	C13	C14	49.21(16)	.	.	.	.	no
C1	C13	C14	C26	175.32(10)	.	.	.	.	no
C1	C13	C14	C15	0.71(16)	.	.	.	.	no
C12	C13	C14	C15	178.99(10)	.	.	.	.	no
C12	C13	C14	C26	-6.40(18)	.	.	.	.	no
C26	C14	C15	C16	126.91(11)	.	.	.	.	no
C13	C14	C15	C16	-57.85(16)	.	.	.	.	no
C13	C14	C15	C24	122.37(12)	.	.	.	.	no
C13	C14	C26	C25	-103.00(13)	.	.	.	.	no
C13	C14	C26	C27	132.60(12)	.	.	.	.	no
C26	C14	C15	C24	-52.87(14)	.	.	.	.	no
C15	C14	C26	C27	-52.40(13)	.	.	.	.	no
C15	C14	C26	C25	72.00(12)	.	.	.	.	no
C14	C15	C16	C21	170.60(11)	.	.	.	.	no
C14	C15	C16	C17	-10.38(18)	.	.	.	.	no
C16	C15	C24	C23	10.72(17)	.	.	.	.	no
C14	C15	C24	S1	7.94(16)	.	.	.	.	no
C24	C15	C16	C17	169.40(11)	.	.	.	.	no
C24	C15	C16	C21	-9.62(17)	.	.	.	.	no
C14	C15	C24	C23	-169.48(11)	.	.	.	.	no
C16	C15	C24	S1	-171.86(9)	.	.	.	.	no
C15	C16	C21	C20	-179.03(11)	.	.	.	.	no
C21	C16	C17	C18	-0.35(18)	.	.	.	.	no
C15	C16	C17	C18	-179.37(12)	.	.	.	.	no
C17	C16	C21	C22	-176.88(11)	.	.	.	.	no
C15	C16	C21	C22	2.18(17)	.	.	.	.	no
C17	C16	C21	C20	1.91(18)	.	.	.	.	no
C16	C17	C18	C19	-1.3(2)	.	.	.	.	no
C17	C18	C19	C20	1.4(2)	.	.	.	.	no
C18	C19	C20	C21	0.2(2)	.	.	.	.	no
C19	C20	C21	C16	-1.9(2)	.	.	.	.	no
C19	C20	C21	C22	176.87(13)	.	.	.	.	no
C20	C21	C22	C23	-174.41(13)	.	.	.	.	no
C16	C21	C22	C23	4.35(19)	.	.	.	.	no
C21	C22	C23	C24	-3.4(2)	.	.	.	.	no

C22	C23	C24	C15	-4.30(19)	.	.	.	.	no
C22	C23	C24	S1	178.09(10)	.	.	.	.	no
S1	C25	C26	C27	78.10(11)	.	.	.	.	no
S1	C25	C26	C14	-46.07(12)	.	.	.	.	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									
S1	C11	3.6735(12)	.	3_555					no
S1	H27	3.168(17)	.	.					no
S1	H11	3.131(15)	.	3_555					no
S2	H28"	3.10(2)	.	3_465					no
S2	H20	3.07(2)	.	4_755					no
O1	C28	3.2376(17)	.	3_455					no
O2	C21	3.3920(17)	.	1_455					no
O2	C29	3.3831(17)	.	2_665					no
O2	C22	3.1093(17)	.	1_455					no
O1	H28'	2.68(2)	.	3_455					no
O1	H2	2.415(17)	.	.					no
O2	H4	2.421(17)	.	.					no
O2	H29	2.87(2)	.	2_665					no
O2	H5	2.497(19)	.	4_645					no
N1	C22	3.4008(17)	.	1_455					no
N2	H23	2.77(2)	.	3_455					no
C1	C16	3.1030(16)	.	.					no
C1	C17	3.0966(16)	.	.					no
C1	C27	3.5722(17)	.	1_455					no
C2	C16	3.0859(16)	.	.					no
C2	C17	3.5381(17)	.	.					no
C2	C15	2.9235(16)	.	.					no
C2	C24	3.5924(16)	.	.					no
C4	C16	3.5486(18)	.	1_455					no
C4	C21	3.4879(18)	.	1_455					no
C6	C17	3.3990(17)	.	.					no
C6	C27	3.5283(17)	.	1_455					no
C11	C26	3.1965(16)	.	.					no
C11	S1	3.6735(12)	.	3_455					no
C13	C17	3.2699(16)	.	.					no
C15	C2	2.9235(16)	.	.					no
C16	C4	3.5486(18)	.	1_655					no
C16	C1	3.1030(16)	.	.					no
C16	C2	3.0859(16)	.	.					no
C17	C13	3.2699(16)	.	.					no
C17	C2	3.5381(17)	.	.					no
C17	C1	3.0966(16)	.	.					no
C17	C6	3.3990(17)	.	.					no
C21	C4	3.4879(18)	.	1_655					no
C21	O2	3.3920(17)	.	1_655					no
C22	O2	3.1093(17)	.	1_655					no
C22	N1	3.4008(17)	.	1_655					no
C23	C28	3.5996(19)	.	3_555					no
C24	C27	3.3735(17)	.	.					no
C24	C2	3.5924(16)	.	.					no
C26	C11	3.1965(16)	.	.					no
C27	C6	3.5283(17)	.	1_655					no
C27	C24	3.3735(17)	.	.					no
C27	C1	3.5722(17)	.	1_655					no
C28	C23	3.5996(19)	.	3_455					no
C28	O1	3.2376(17)	.	3_555					no
C29	O2	3.3831(17)	.	2_664					no
C1	H17	2.846(16)	.	.					no
C1	H27	3.057(16)	.	1_455					no
C2	H27	3.069(16)	.	1_455					no
C6	H27"	3.092(16)	.	1_455					no
C6	H17	3.044(16)	.	.					no

C9	H29"	2.88(2)	.	.	no
C9	H29'	2.65(2)	.	.	no
C10	H8	3.029(16)	.	3_565	no
C11	H8	2.848(16)	.	3_565	no
C11	H26	2.568(16)	.	.	no
C11	H28'	2.56(2)	.	.	no
C11	H23	3.08(2)	.	3_455	no
C12	H8	2.956(16)	.	3_565	no
C12	H26	2.712(16)	.	.	no
C13	H17	2.769(17)	.	.	no
C14	H11	2.970(15)	.	.	no
C14	H17	2.684(18)	.	.	no
C14	H2	2.892(17)	.	.	no
C15	H27	2.682(16)	.	.	no
C15	H2	2.575(16)	.	.	no
C16	H2	3.056(16)	.	.	no
C19	H4	3.060(16)	.	1_655	no
C20	H4	2.878(16)	.	1_655	no
C21	H4	3.002(16)	.	1_655	no
C24	H27	2.866(17)	.	.	no
C24	H2	2.898(16)	.	.	no
C25	H2	3.036(17)	.	3_555	no
C25	H11	2.915(15)	.	.	no
C26	H11	2.779(15)	.	.	no
C28	H11	2.724(15)	.	.	no
C28	H23	2.83(2)	.	3_455	no
C29	H9	2.495(15)	.	.	no
H2	O1	2.415(17)	.	.	no
H2	C14	2.892(17)	.	.	no
H2	C15	2.575(16)	.	.	no
H2	C16	3.056(16)	.	.	no
H2	C24	2.898(16)	.	.	no
H2	C25	3.036(17)	.	3_455	no
H2	H25'	2.52(2)	.	3_455	no
H4	O2	2.421(17)	.	.	no
H4	C19	3.060(16)	.	1_455	no
H4	C20	2.878(16)	.	1_455	no
H4	C21	3.002(16)	.	1_455	no
H4	H28	2.56(3)	.	2_665	no
H5	O2	2.497(19)	.	4_655	no
H8	C10	3.029(16)	.	3_465	no
H8	C11	2.848(16)	.	3_465	no
H8	C12	2.956(16)	.	3_465	no
H8	H26	2.49(2)	.	3_465	no
H9	C29	2.495(15)	.	.	no
H9	H29'	2.16(3)	.	.	no
H9	H29"	2.44(3)	.	.	no
H11	C14	2.970(15)	.	.	no
H11	C25	2.915(15)	.	.	no
H11	C26	2.779(15)	.	.	no
H11	C28	2.724(15)	.	.	no
H11	H25	2.34(2)	.	.	no
H11	H26	2.26(2)	.	.	no
H11	H28'	2.11(3)	.	.	no
H11	S1	3.131(15)	.	3_455	no
H11	H23	2.58(3)	.	3_455	no
H17	C1	2.846(16)	.	.	no
H17	C6	3.044(16)	.	.	no
H17	C13	2.769(17)	.	.	no
H17	C14	2.684(18)	.	.	no
H20	H22	2.44(3)	.	.	no
H20	S2	3.07(2)	.	4_745	no
H22	H20	2.44(3)	.	.	no
H23	N2	2.77(2)	.	3_555	no
H23	C11	3.08(2)	.	3_555	no
H23	C28	2.83(2)	.	3_555	no
H23	H11	2.58(3)	.	3_555	no
H23	H28'	2.53(3)	.	3_555	no
H25	H11	2.34(2)	.	.	no

H25'	H27'	2.48(3)	.	.	no
H25'	H2	2.52(2)	.	3_555	no
H26	C11	2.568(16)	.	.	no
H26	C12	2.712(16)	.	.	no
H26	H11	2.26(2)	.	.	no
H26	H8	2.49(2)	.	3_565	no
H27	S1	3.168(17)	.	.	no
H27	C1	3.057(16)	.	1_655	no
H27	C2	3.069(16)	.	1_655	no
H27	C15	2.682(16)	.	.	no
H27	C24	2.866(17)	.	.	no
H27'	H25'	2.48(3)	.	.	no
H27"	C6	3.092(16)	.	1_655	no
H28	H29	2.38(3)	.	.	no
H28	H4	2.56(3)	.	2_664	no
H28'	C11	2.56(2)	.	.	no
H28'	H11	2.11(3)	.	.	no
H28'	O1	2.68(2)	.	3_555	no
H28'	H23	2.53(3)	.	3_455	no
H28"	S2	3.10(2)	.	3_565	no
H29	H28	2.38(3)	.	.	no
H29	O2	2.87(2)	.	2_664	no
H29'	C9	2.65(2)	.	.	no
H29'	H9	2.16(3)	.	.	no
H29"	C9	2.88(2)	.	.	no
H29"	H9	2.44(3)	.	.	no

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loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H   H...A   D...A   D - H...A   symm(A)
#
C5      H5      O2      0.96(2)  2.497(19) 3.4272(16) 162.5(15)  4_655 yes

# End of Crystallographic Information File

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