Supplementary Information

Effects of the Peripheral Heteroaryl Substituents on the Photochromism of New Pyridine-Containing Diarylethenes

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Supplementary data

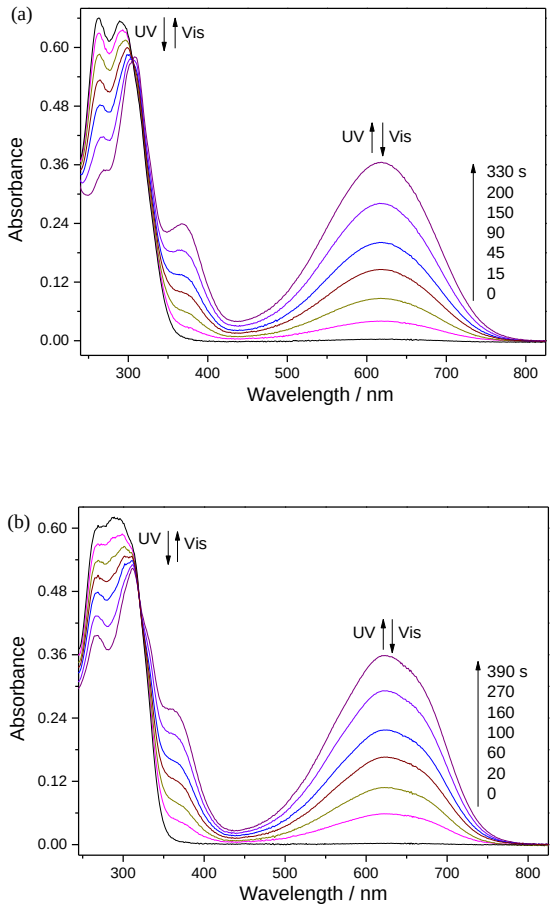

Figure S1. Absorption spectral changes of **2** and **3** induced by photoirradiation in hexane (2.0×10^{-5} mol L^{-1}): (a) **2**; and (b) **3**.

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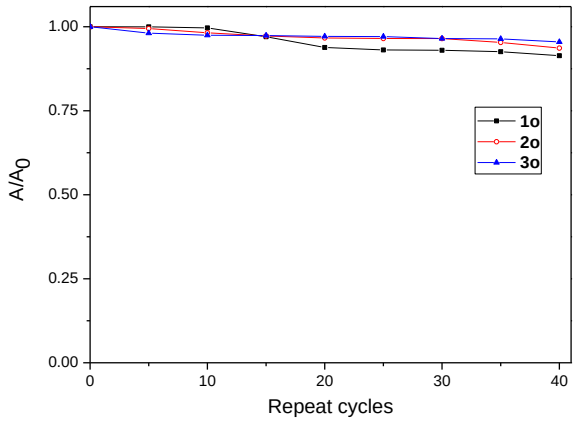

Figure S2. Fatigue resistances of diarylethenes **1**-**3** in hexane in air atmosphere at room temperature. Initial absorbance of the sample was fixed at 1.0.

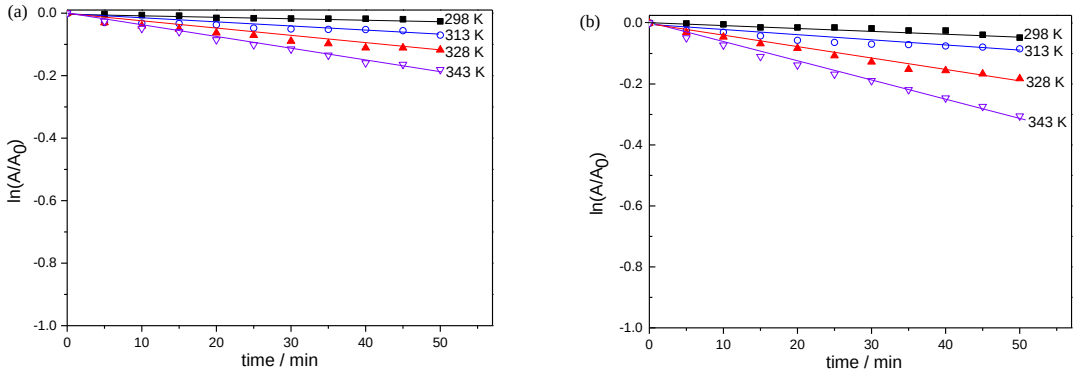

Figure S3. Thermal fading of **2c** and **3c** in hexane at various temperatures: (a) **2c**; (b) **3c**.

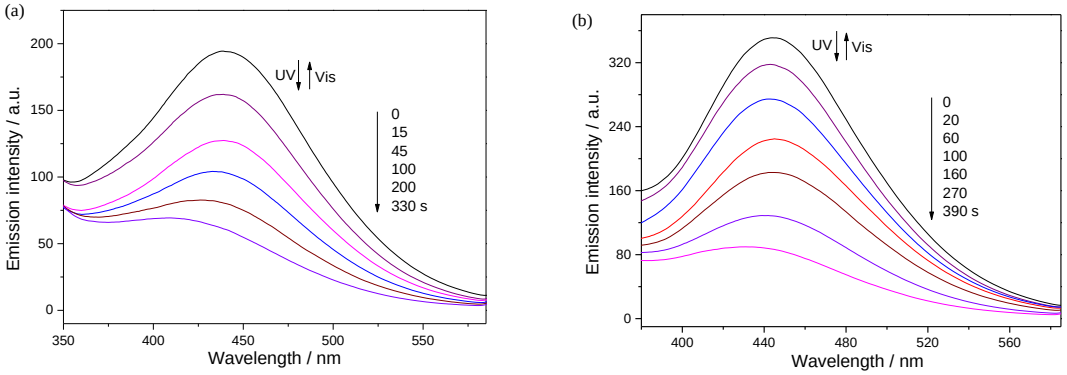

Figure S4. Fluorescence spectral changes of **2** and **3** in hexane (5.0×10^{-5} mol L^{-1}), excited at 300 nm: (a) **2**; and (b) **3**.

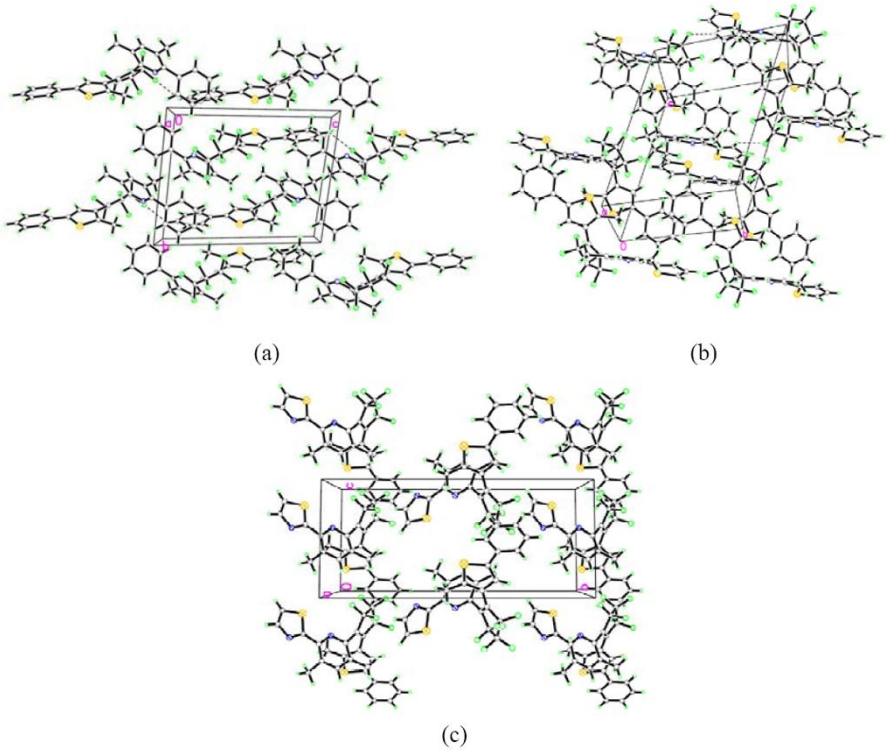

Figure S5. Packing views along the x direction: (a) **1o**; (b) **2o**; and (c) **3o**.

Table S1. Crystallographic parameters of **1o**-**3o**

Parameter	**1o**	**2o**	**3o**
Formula	$C_{29}H_{21}F_6NS$	$C_{27}H_{19}F_6NS_2$	$C_{26}H_{18}F_6N_2S_2$
Formula weight	529.53	535.55	536.54
Temperature / K	296(2)	296(2)	296(2)
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	P21/c
Unit cell dimension			
a / Å	9.4292(10)	8.6153(5)	15.0980(6)
b / Å	11.1096(13)	11.7960(8)	19.4054(8)
c / Å	13.6106(15)	13.6679(9)	8.4923(4)
α / degree	90.735(7)	73.315(3)	90.00
β / degree	106.507(6)	81.381(3)	98.468(2)
γ / degree	110.045(6)	68.866(2)	90.00
Volume / $Å^3$	1274.6(2)	1239.37(14)	2460.97(18)
Z	2	1	4
Density (calculated) / (g cm^{-3})	1.380	1.435	1.448
Goodness-of-fit on F^2	1.126	1.004	1.041
Final R index [I/2σ(I)]			
R1	0.1068	0.0678	0.0778
wR2	0.2870	0.1728	0.1886
R index (all data)			
R1	0.1068	0.0678	0.0778
wR2	0.2870	0.1728	0.1886

Z: Number of chemical formula units *per* unit cell; F: structure factor; R: discrepancy index.

NMR spectra

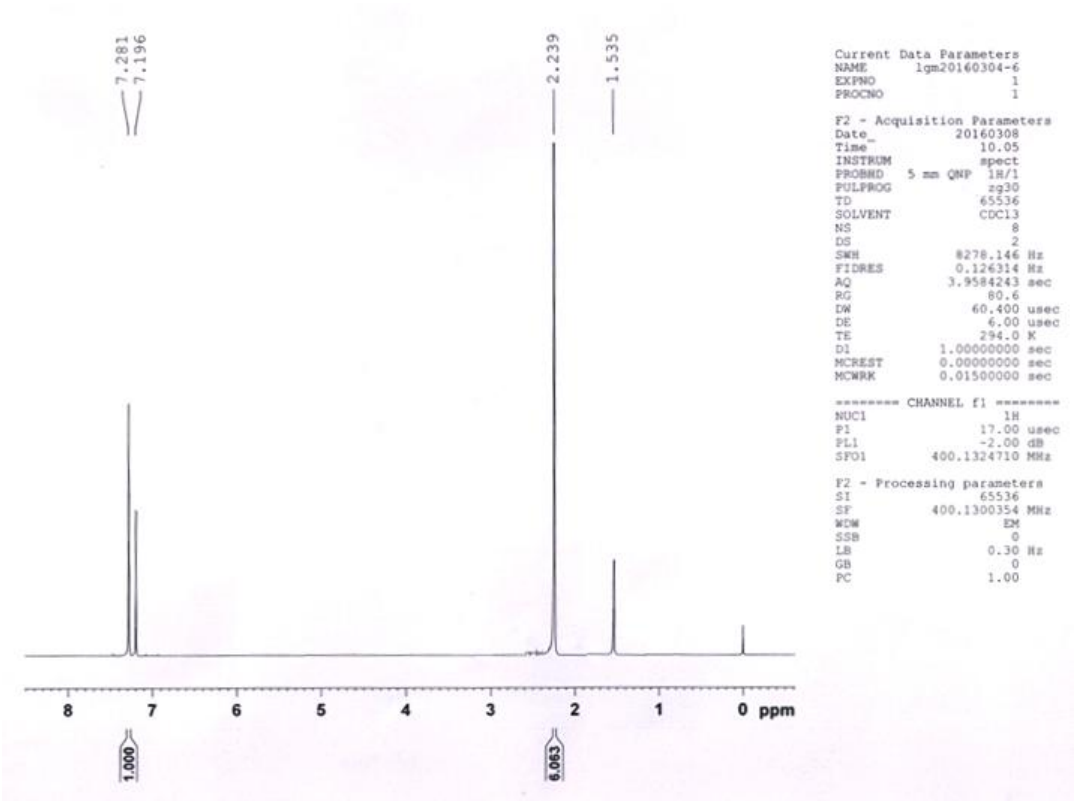

Figure S6. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4**.

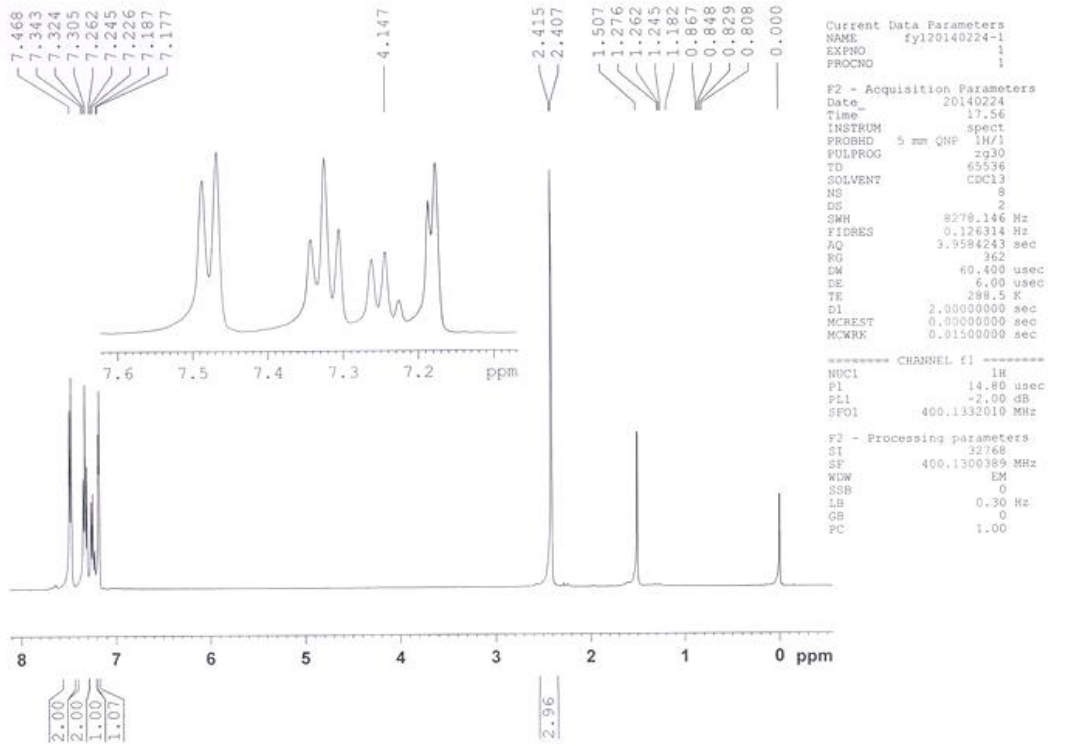

Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**.

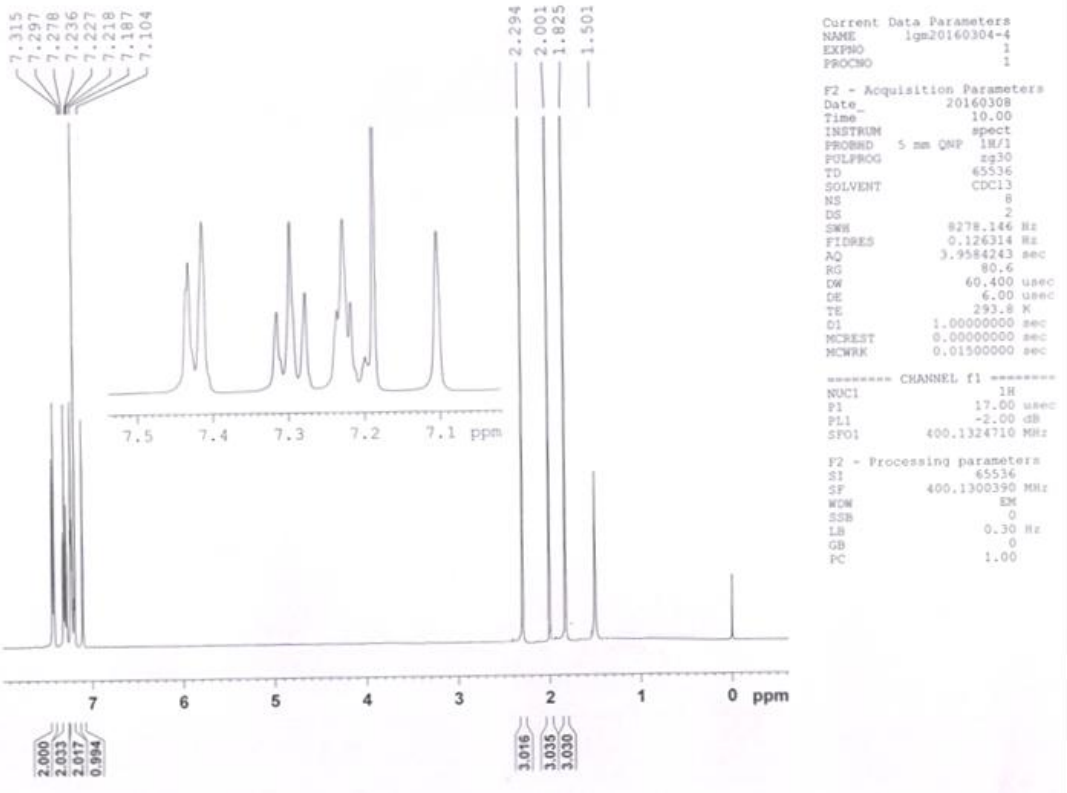

Figure S8. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6**.

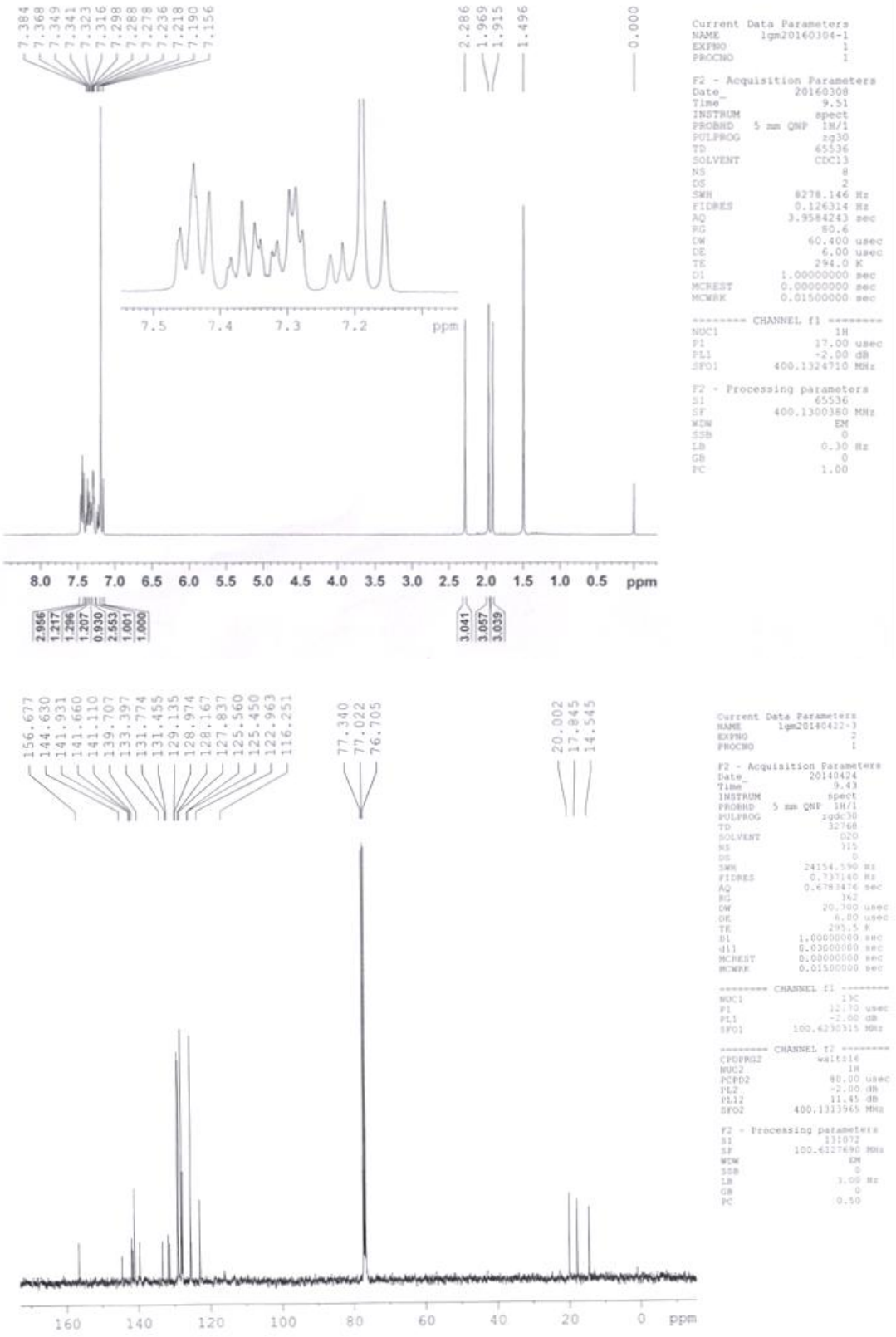

Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **1o**.

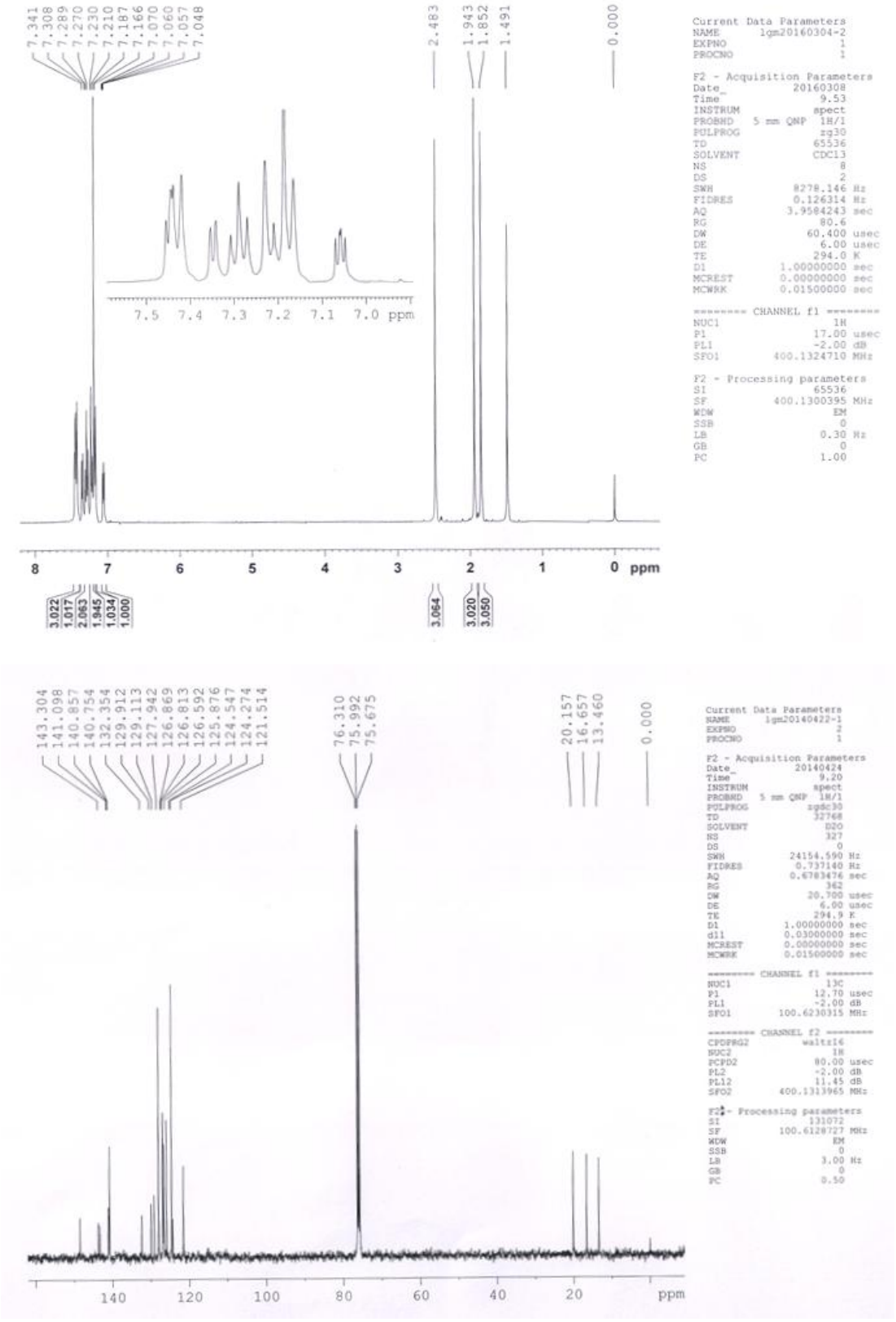

Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **2o**.

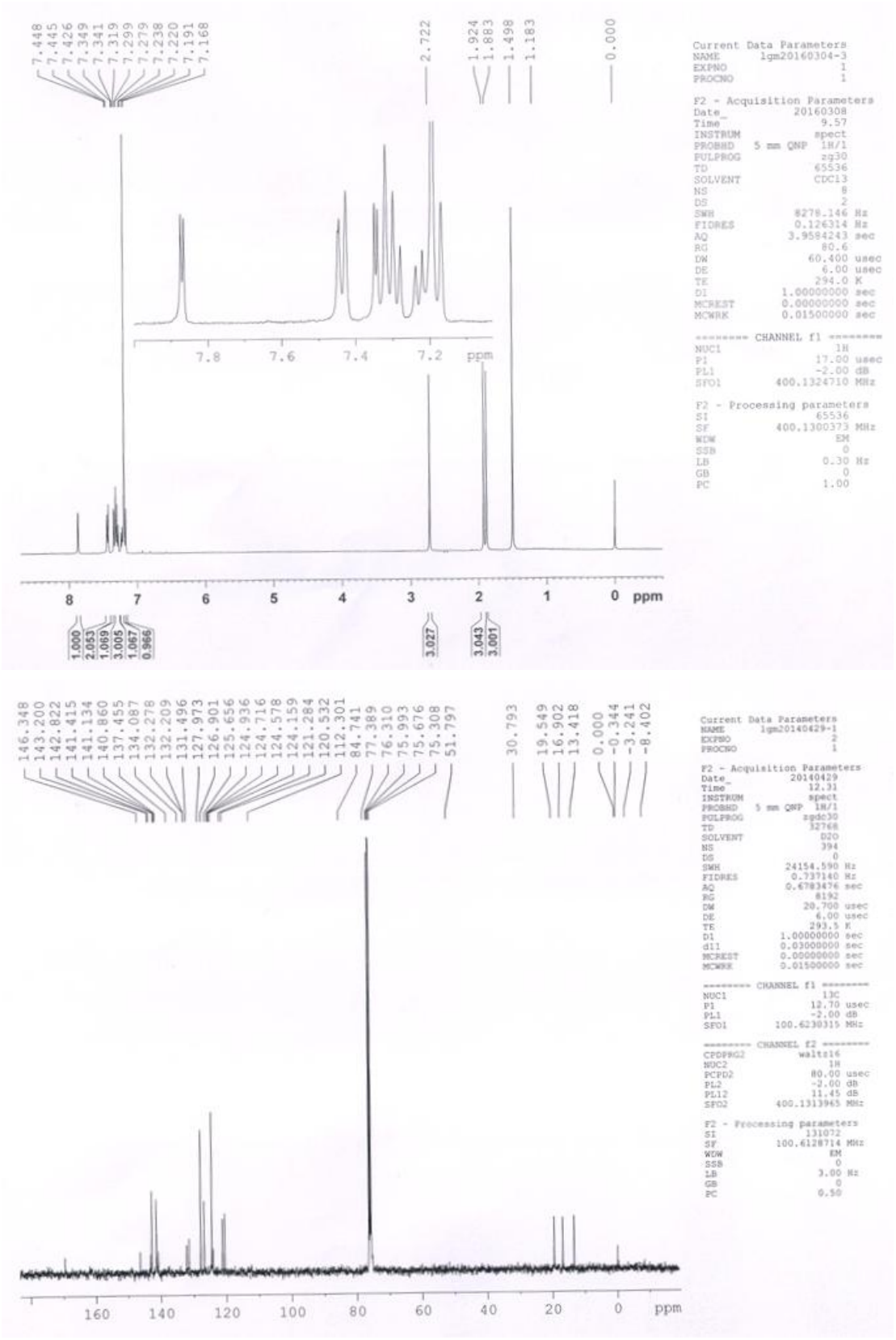

Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3o**.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 140414lgm3_0m

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Bond precision:  C-C = 0.0067 A          Wavelength=0.71073

Cell:          a=9.4292(10)      b=11.1096(13)     c=13.6106(15)
               alpha=90.735(7)   beta=106.507(6)   gamma=110.045(6)
Temperature:   296 K
```

	Calculated	Reported
Volume	1274.6(3)	1274.6(2)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C29 H21 F6 N S	?
Sum formula	C29 H21 F6 N S	C29 H21 F6 N S
Mr	529.53	529.53
Dx,g cm-3	1.380	1.380
Z	2	2
Mu (mm-1)	0.189	0.189
F000	544.0	544.0
F000’	544.59	
h,k,lmax	11,13,16	11,13,16
Nref	4477	4415
Tmin,Tmax	0.959,0.967	0.960,0.967
Tmin’	0.959	

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AbsCorr = NONE

Data completeness= 0.986          Theta(max)= 25.000

R(reflections)= 0.0819( 3192)     wR2(reflections)= 0.2870( 4415)

S = 1.126                 Npar= 365
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The following ALERTS were generated. Each ALERT has the format
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Click on the hyperlinks for more details of the test.

Alert level C

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ABSTY03_ALERT_1_C  The _exptl_absorpt_correction_type has been given as none.
           However values have been given for Tmin and Tmax. Remove
           these if an absorption correction has not been applied.
  From the CIF: _exptl_absorpt_correction_T_min   0.960
  From the CIF: _exptl_absorpt_correction_T_max   0.967
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.287
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.29 Report
PLAT213_ALERT_2_C Atom F1             has ADP max/min Ratio .....        3.2 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference F3'    --  C14     ..       0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00671 Ang.
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Alert level G

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PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.16 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          8 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         62 Check
             F6'  -C15  -F6      1.555   1.555   1.555            41.60 Deg.
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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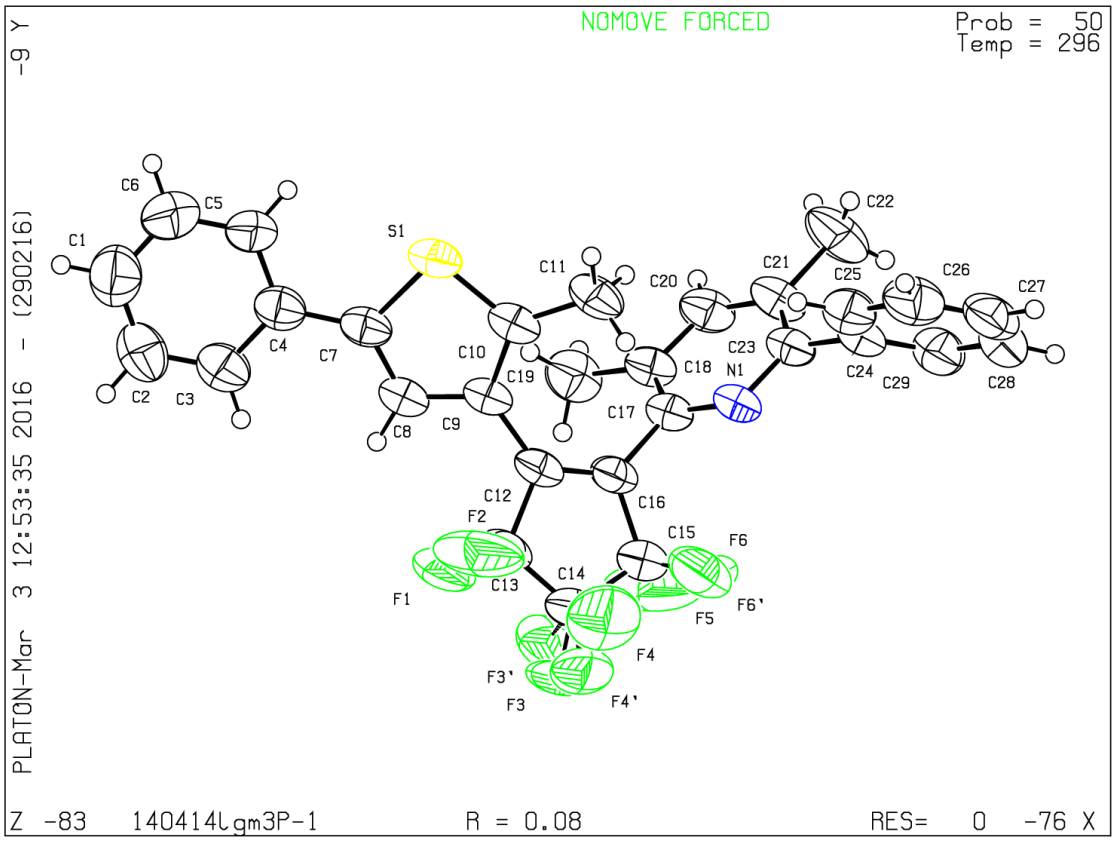
PLATON version of 29/02/2016; check.def file version of 29/02/2016

Datablock 140414lgm3_0m - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 140302lgm_0m

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               alpha=73.315(3)   beta=81.381(3)   gamma=68.866(2)
Temperature:   296 K
```

	Calculated	Reported
Volume	1239.37(14)	1239.37(14)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C27 H19 F6 N S2	?
Sum formula	C27 H19 F6 N S2	C54 H38 F12 N2 S4
Mr	535.55	1071.10
Dx,g cm-3	1.435	1.435
Z	2	1
Mu (mm-1)	0.277	0.277
F000	548.0	548.0
F000’	548.83	
h,k,lmax	10,14,16	10,14,16
Nref	4358	4280
Tmin,Tmax	0.941,0.951	0.942,0.952
Tmin’	0.941	

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R(reflections)= 0.0580( 3572)     wR2(reflections)= 0.1728( 4280)

S = 1.004                 Npar= 356
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C3 -- C4 .. 11.0 s.u.

Alert level C

ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.
However values have been given for Tmin and Tmax. Remove
these if an absorption correction has not been applied.
From the CIF: _exptl_absorpt_correction_T_min 0.942
From the CIF: _exptl_absorpt_correction_T_max 0.952

PLAT213_ALERT_2_C Atom F6 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom F5' has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00521 Ang.

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for F4 -- C14 .. 13.5 s.u.
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C14 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 8 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 62 Check
F5' -C15 -F5 1.555 1.555 1.555 30.80 Deg.
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
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4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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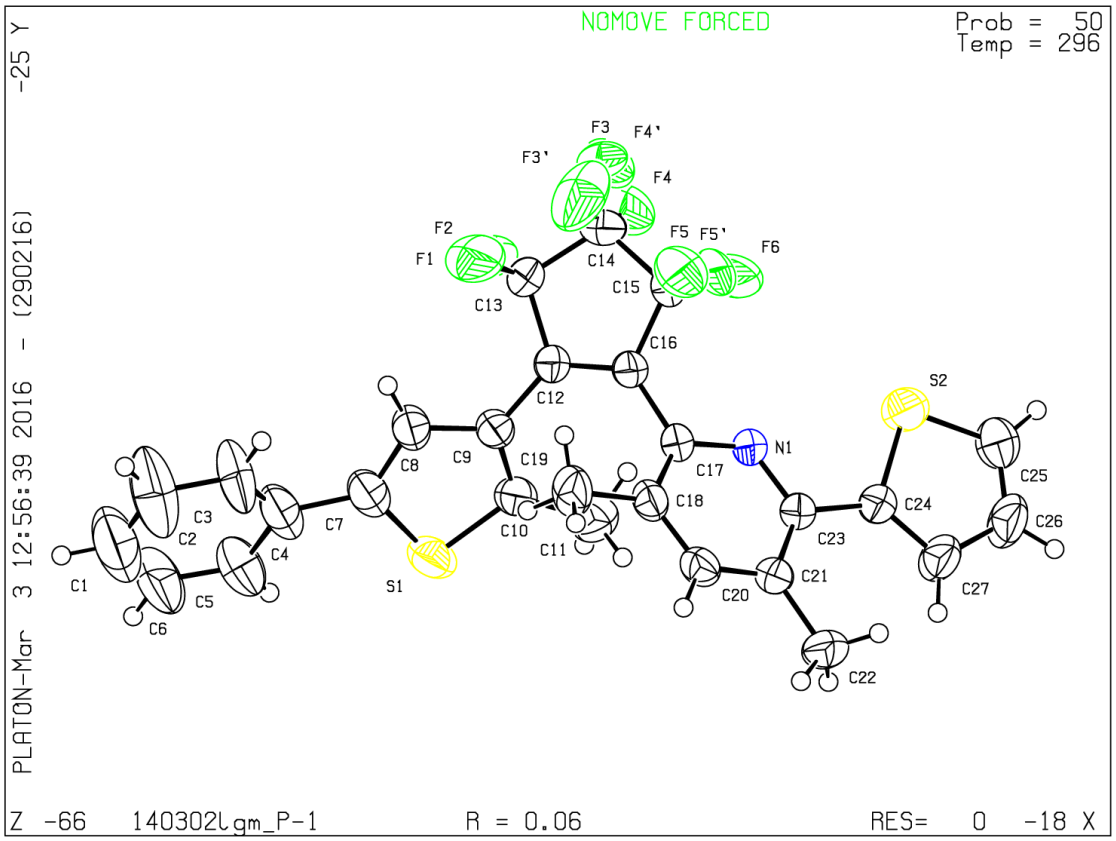
Datablock 140302lgm_0m - ellipsoid plot



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You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 140301lgm_0m

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Cell:            a=15.0980(6)     b=19.4054(8)       c=8.4923(4)
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Temperature:     296 K

                Calculated                Reported
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Space group     P 21/c                    P21/c
Hall group      -P 2ybc                   ?
Moiety formula  C26 H18 F6 N2 S2          ?
Sum formula     C26 H18 F6 N2 S2          C26 H18 F6 N2 S2
Mr              536.54                    536.54
Dx,g cm-3       1.448                     1.448
Z               4                         4
Mu (mm-1)       0.280                     0.280
F000            1096.0                    1096.0
F000'           1097.65
h,k,lmax        19,25,11                  19,25,11
Nref            5716                      5695
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Tmin'           0.914

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S = 1.041                 Npar= 328
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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ABSTY03_ALERT_1_C  The _exptl_absorpt_correction_type has been given as none.
           However values have been given for Tmin and Tmax. Remove
           these if an absorption correction has not been applied.
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  From the CIF: _exptl_absorpt_correction_T_max   0.931
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C3     --  C4      ..        6.5 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         S2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00423 Ang.
```

Alert level G

```
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PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.10 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F2     ..  F4      ..       2.82 Ang.
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

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A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 29/02/2016; check.def file version of 29/02/2016

Datablock 140301lgm_0m - ellipsoid plot