Supplementary Information

Synthesis of a *cone*-conformer bimodal calix[4]arene-crown-5 which forms a sensitive cesium ion sensing layer on gold-coated microcantilevers

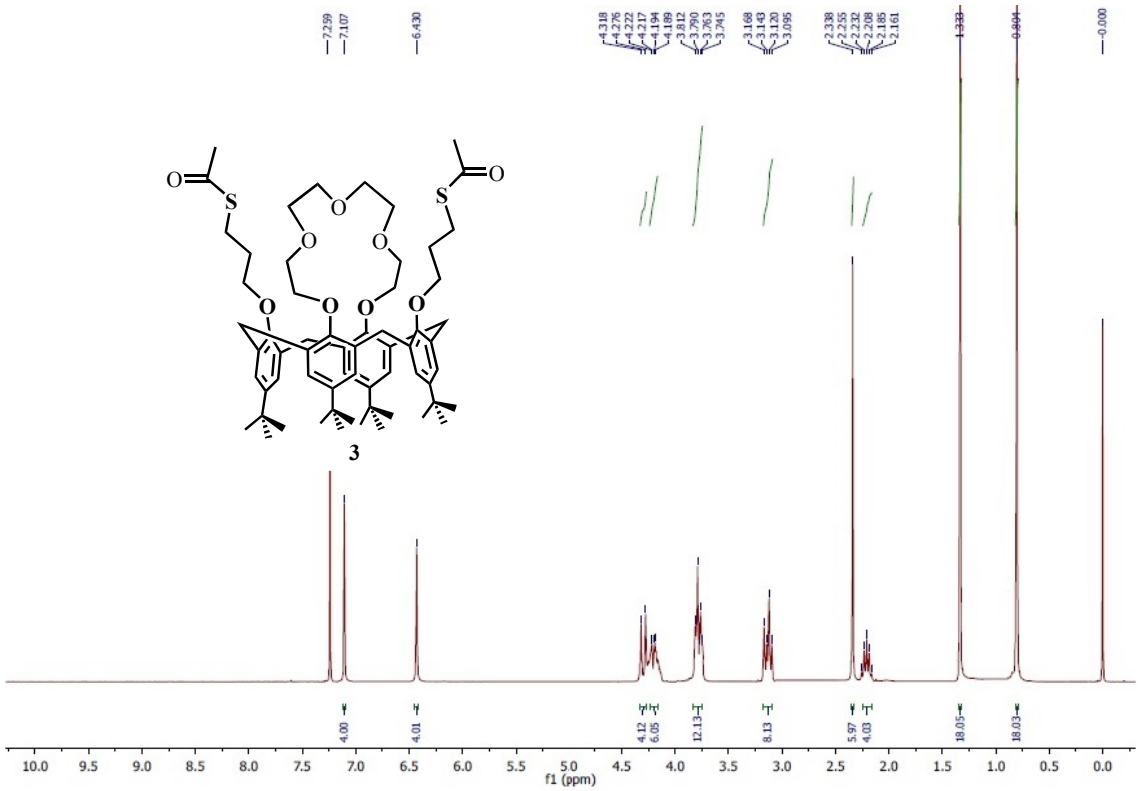
Gopikishore Valluru,[a] Shofiur Rahman,[a] Paris E. Georghiou,[a*] Louise N. Dawe,[b] Abdullah N. Alodhayb[c] and Luc Y. Beaulieu[c]

[a] Department of Chemistry, Memorial University of Newfoundland, St. John's, Newfoundland and Labrador, Canada A1B3X7. E-mail: parisg@mun.ca; Fax: +1 709 864 3702; Tel: +1 709 864 8517.

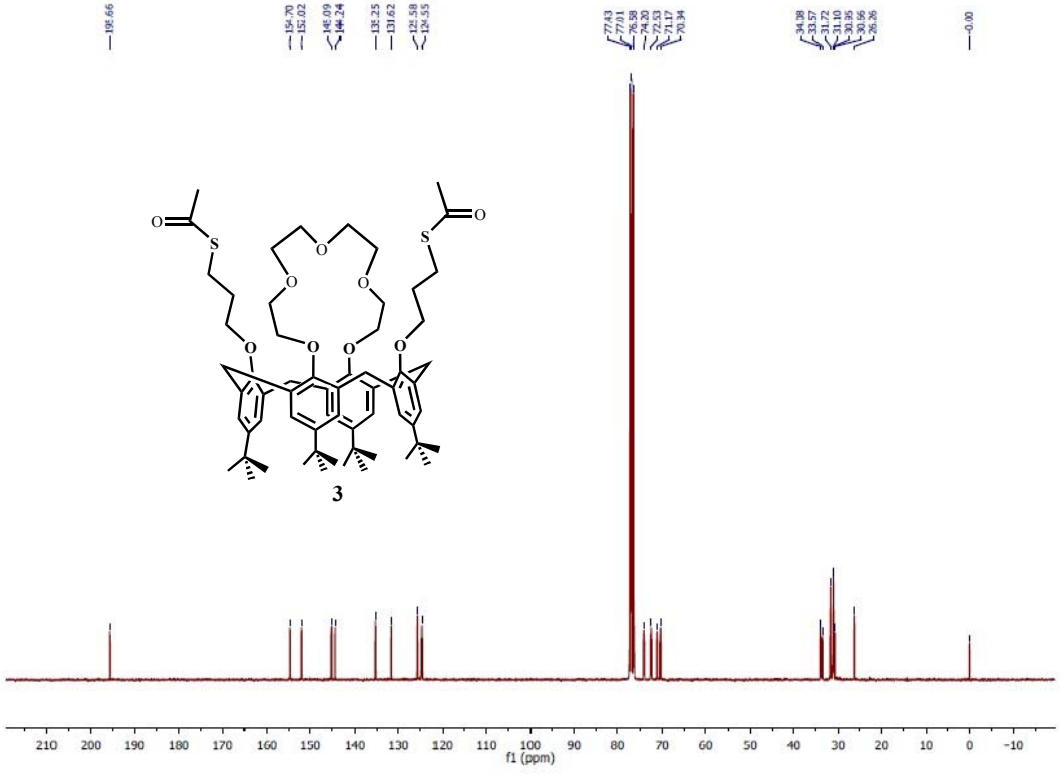
[b] Department of Chemistry and Biochemistry, Wilfrid Laurier University, Waterloo, ON, Canada N2L3C5. E-mail: ldawe@wlu.ca; Fax**:** +1 519.746.0677; Tel: +1 519.884.0710 ext.4963.

[c] Department of Physics and Physical Oceanography, Memorial University of Newfoundland, St. John's, Newfoundland and Labrador, Canada A1B3X7. E-mail: lbeaulieu@mun.ca; Fax: +1 709 864 8739; Tel: +1 709 864 6203.

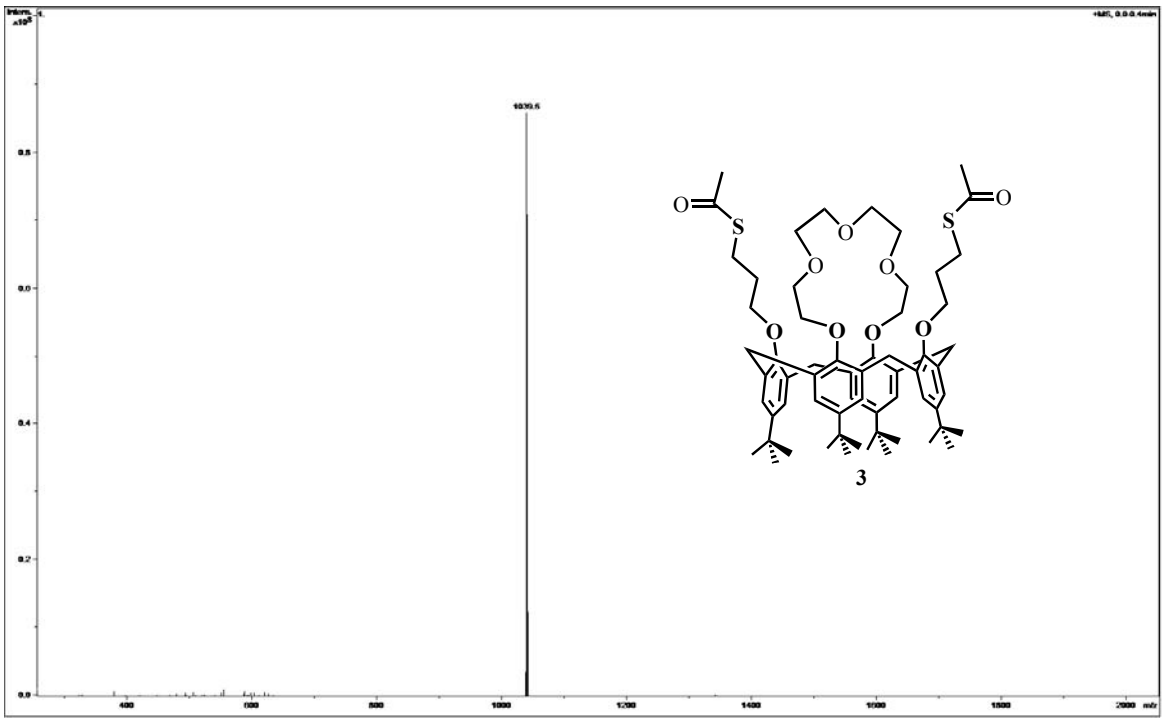
Table of Contents


7.259
7.107
6.430
4.318
4.276
4.222
4.217
4.194
4.189
3.812
3.790
3.763
3.745
3.168
3.143
3.120
3.095
2.338
2.255
2.233
2.208
2.185
2.161
1.333
0.894
-0.000
4.00
4.01
4.12
6.05
12.13
8.13
5.97
4.03
18.05
18.03
f1 (ppm)

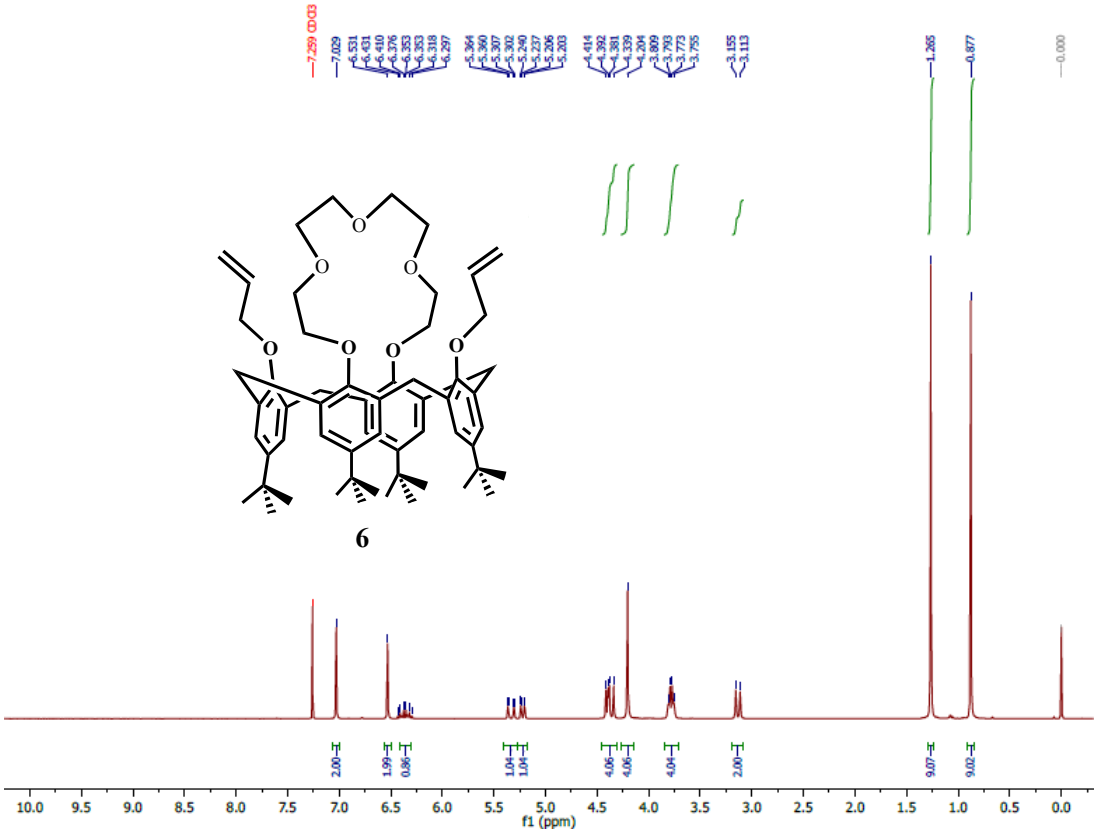
3


195.66
154.70
152.02
146.09
144.24
135.25
131.62
122.58
120.55
77.43
77.01
76.58
74.20
72.53
71.17
70.94
34.38
33.57
31.72
31.10
30.95
30.56
26.26
-0.00
f1 (ppm)

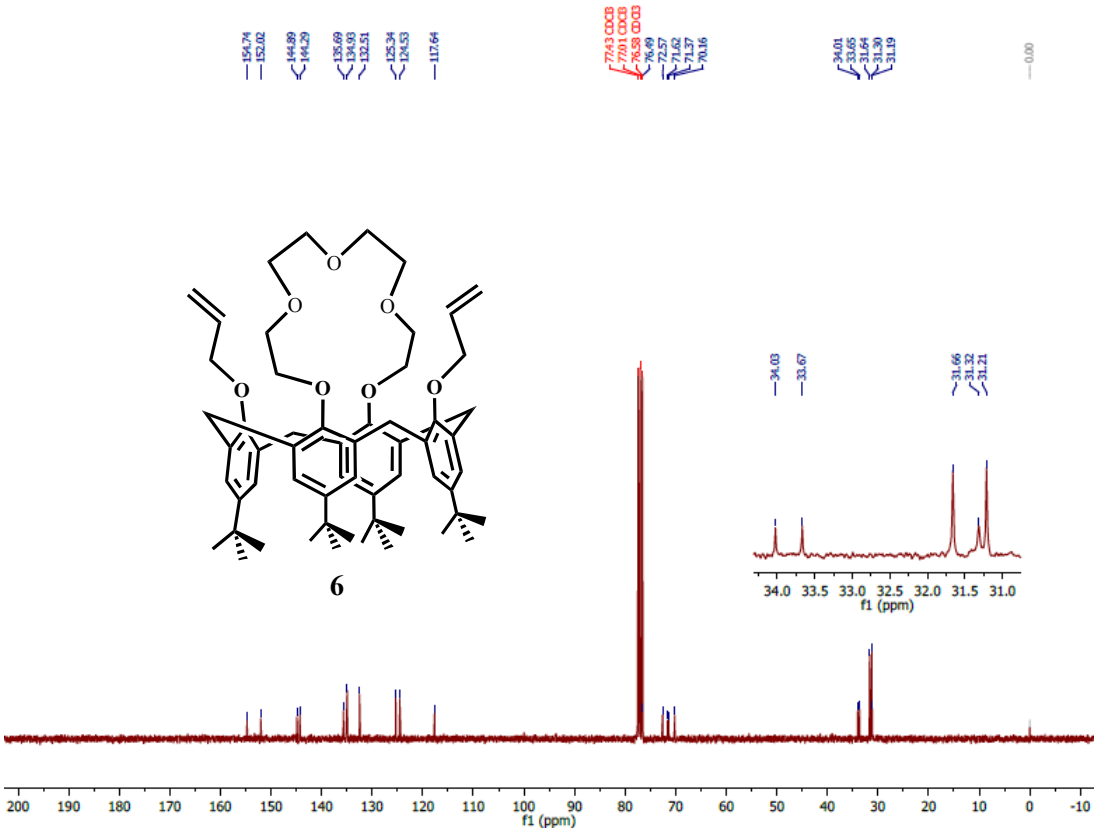
3


1039.5
0.8
0.6
0.4
0.2
0.0
400
600
800
1000
1200
1400
1600
1800
2000 m/z

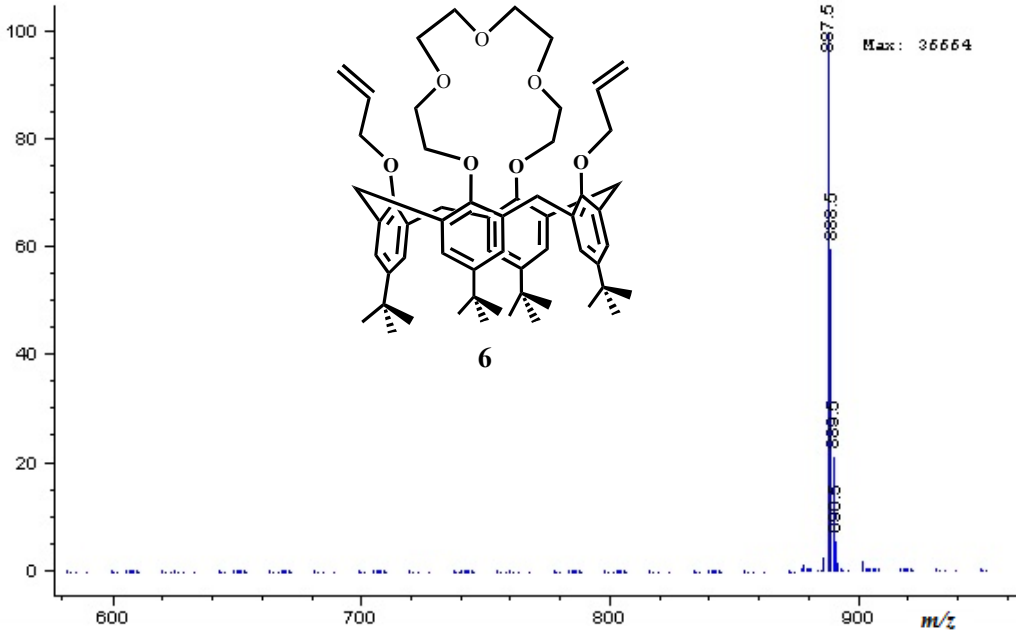
3


7.259 CDCl3
7.029
6.531
6.531
6.410
6.376
6.353
6.353
6.318
6.297
5.364
5.360
5.307
5.302
5.240
5.237
5.206
5.203
4.414
4.392
4.381
4.339
4.204
3.809
3.793
3.773
3.755
3.155
3.113
1.265
0.877
0.000
2.00
1.99
0.86
1.04
1.04
4.06
4.06
4.04
2.00
9.07
9.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

6


154.74
152.02
144.89
144.29
135.69
134.93
132.51
125.34
124.53
117.64
77.43 CDCl3
77.01 CDCl3
76.58 CDCl3
76.49
72.57
71.62
71.37
70.16
34.01
33.65
31.64
31.30
31.19
0.00
34.03
33.67
31.66
31.32
31.21
34.0 33.5 33.0 32.5 32.0 31.5 31.0
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

6



6

The structure crystallized in the monoclinic space group $P2_1/n$, with three chemically identical molecules in the asymmetric unit (Z'=3, Figure A.) The molecules pack in discrete chains perpendicular to the c-axis (Figure B), though no significant intermolecular interactions are present. Each molecule adopts a *cone*-like configuration (Figure C). The ether chains and bridge exhibited disorder in the crystal structure that was difficult to model, however, this disorder did not indicate the presence of any molecules in the *1,3-alternate* conformation.

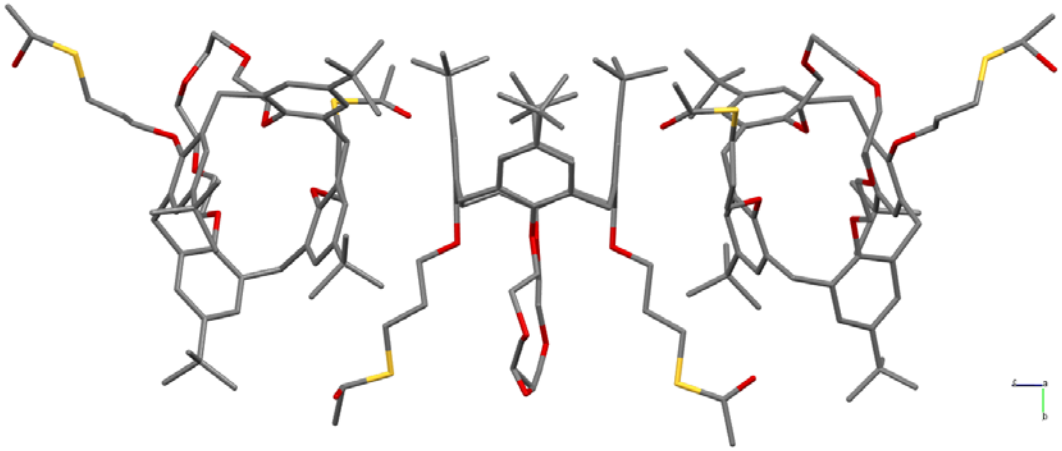


Figure A: The asymmetric unit, represented with capped sticks, containing three chemically identical, but crystallographically independent molecules (Z' = 3.) H-atoms and minor disorder component omitted for clarity.

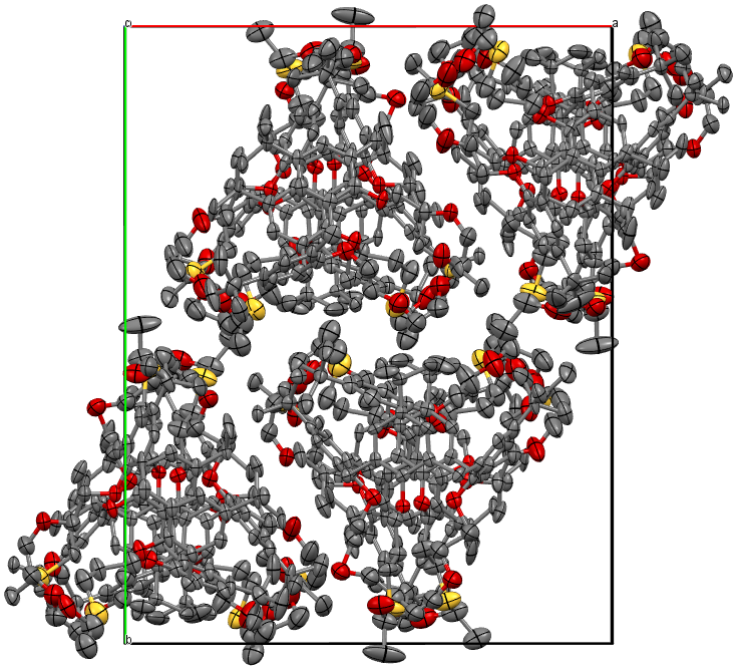


Figure B: Packed unit cell, represented with 30% displacement ellipsoids, looking down the c-axis, showing the discrete chain-like arrangement of molecules in the structure.

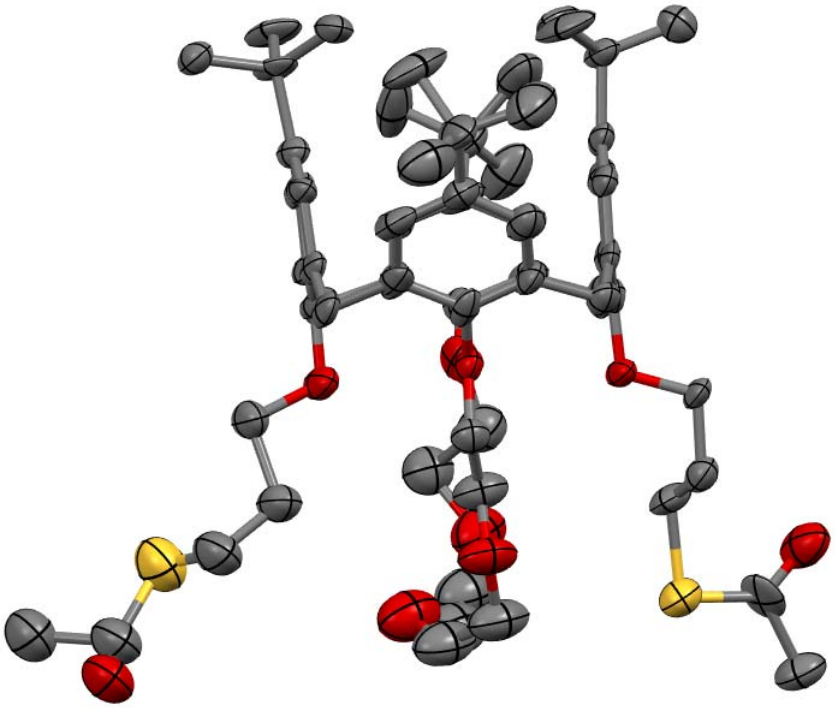


Figure C: One molecule, represented with 30% displacement ellipsoids, showing the cone conformation. H-atoms and minor disorder components omitted for clarity.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) LTS02_14

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: LTS02_14

Bond precision: C-C = 0.0191 A Wavelength=1.54178

Cell: a=21.9907(9) b=27.7429(14) c=29.1299(12)
alpha=90 beta=95.471(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17690.8(14)	17690.8(14)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C61.92 H73 O9 S2, C61.41 H71.71 O8 S2, C62 H69.37 O9 S2	0.33(C61.92 H73 O9 S2), 0.33(C62 H69.37 O9 S2), 0.33(C61.41 H71
Sum formula	C185.33 H214.08 O26 S6	C62 H88 O9 S2
Mr	3050.03	1041.44
Dx,g cm-3	1.145	1.173
Z	4	12
Mu (mm-1)	1.233	1.242
F000	6520.2	6768.0
F000’	6546.12	
h,k,lmax	21,26,28	26,33,34
Nref	16459	16373
Tmin,Tmax	0.888,0.952	
Tmin’	0.780	

Correction method= Not given

Data completeness= 0.995 Theta(max)= 47.836

R(reflections)= 0.1519(8707) wR2(reflections)= 0.4584(16373)

S = 1.595 Npar= Npar =2207

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 A

RFACR01_ALERT_3_A The value of the weighted R factor is > 0.45
Weighted R factor given 0.458

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions. The high weighted R factor results from the weak diffraction, and the inclusion of reflections that are essentially unobserved.

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4808

Author Response: Due to the weak diffraction produced by these crystals, data was truncated to include only the portion in which reflections were observed. These were still weak, despite using Cu radiation.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..... 0.46 Why ?

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions. The high R factor results from the weak diffraction, and the inclusion of reflections that are essentially unobserved.

Alert level B

REFNR01_ALERT_3_B Ratio of reflections to parameters is < 8 for a centrosymmetric structure

sine(theta)/lambda	0.4808
Proportion of unique data used	1.0000
Ratio reflections to parameters	7.4187

Author Response: There are 876 non-hydrogren atoms in the unit cell of this structure (219 in the asymmetric unit.) All non-hydrogen atoms were refined anisotropically. The reflections to parameters ratio is low due to the very large number of refined parameters and the very weakly diffracting nature of the crystals. This structure is reported in order to support the cone-conformation of the molecule, and not the anti-conformation, which can be assessed based on the available data.

RFACG01_ALERT_3_B The value of the R factor is > 0.15
R factor given   0.152

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions. The high R factor results from the weak diffraction, and the inclusion of reflections that are essentially unobserved.

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given   0.197
Crystal system given = monoclinic

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions.

PLAT019_ALERT_1_B _diffrn_measured_fraction_theta_full/_max < 1.0   0.514 Why ?

Author Response: Due to the weak diffraction produced by these crystals, data was truncated to include only the portion in which reflections were observed. These were still weak, despite using Cu radiation.

PLAT020_ALERT_3_B The value of Rint is greater than 0.12 ....   0.197

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions.

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..   74.29 Check

Author Response: Due to disorder in the ether and thioether chains many H-atoms could not be suitably AFIXed. These atoms were omitted from the model, but were included in the formula for the calculation of intensive properties.

PLAT088_ALERT_3_B Poor Data / Parameter Ratio ....   7.42 Note

Author Response: There are 876 non-hydrogren atoms in the unit cell of this structure (219 in the asymmetric unit.) All non-hydrogen atoms were refined anisotropically. The reflections to parameters ratio is low due to the very large number of refined parameters and the very weakly diffracting nature of the crystals. This structure is reported in order to support the cone-conformation of the molecule, and not the anti-conformation, which can be assessed based on the available data.

```
PLAT213_ALERT_2_B Atom C166            has ADP max/min Ratio .....        4.6 prolat
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT222_ALERT_3_B Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        7.2 Ratio
```

Author Response: H-atoms were introduced in calculated positions and refined on a riding model. Uiso(H) was calculated from U(ave) of the atom to which it was bonded.

```
PLAT222_ALERT_3_B Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        7.4 Ratio
```

Author Response: H-atoms were introduced in calculated positions and refined on a riding model. Uiso(H) was calculated from U(ave) of the atom to which it was bonded.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C53    --  C54     ..        7.4 su
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C146   --  C147    ..        8.2 su
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT234_ALERT_4_B Large Hirshfeld Difference C29    --  C31     ..       0.28 Ang.
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT234_ALERT_4_B Large Hirshfeld Difference C160   --  C163    ..       0.26 Ang.
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_B High Ueq as Compared to Neighbors for ..... S4 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_B High Ueq as Compared to Neighbors for ..... C131 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C105 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C112 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C160 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0191 Ang.

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions. This structure is reported in order to support the cone-conformation of the molecule, and not the anti-conformation, which can be assessed based on the available data.

```
PLAT363_ALERT_2_B Long   C(sp3)-C(sp2) Bond  C179   -   C180   ...       1.76 Ang.
```

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions. This structure is reported in order to support the cone-conformation of the molecule, and not the anti-conformation, which can be assessed based on the available data.

Alert level C

```
CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
           calculated from the _atom_site* data lies outside
           the range 0.99 <> 1.01
          From the CIF: _cell_formula_units_Z                  12
          From the CIF: _chemical_formula_weight          1041.44
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          C        12.01   61.78  742.00
          H         1.01   71.36   71.93
          O        16.00    8.67  138.66
          S        32.07    2.00   64.13
          Calculated formula weight             1016.72
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given .     Please Do !
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT082_ALERT_2_C High R1 Value ..................................       0.15 Why ?
PLAT213_ALERT_2_C Atom C33            has ADP max/min Ratio .....        3.3 prolat
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT213_ALERT_2_C Atom C35            has ADP max/min Ratio .....        3.1 prolat
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT213_ALERT_2_C Atom C43            has ADP max/min Ratio .....        3.2 prolat
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT213_ALERT_2_C Atom C53            has ADP max/min Ratio .....        3.1 oblate
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT213_ALERT_2_C Atom C161            has ADP max/min Ratio .....        3.4 prolat
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        6.0 Ratio
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        6.0 Ratio
PLAT220_ALERT_2_C Large Non-Solvent  O     Ueq(max)/Ueq(min) Range        3.9 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O4     --  C53     ..        6.0 su
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C4     --  C29     ..        5.7 su
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    S7     --  C179    ..        5.4 su
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference S3     --  C52     ..       0.16 Ang.
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference O3     --  C27     ..       0.18 Ang.
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference O12    --  C20     ..       0.22 Ang.
```

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C15 -- C16 .. 0.20 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C16 -- C17 .. 0.25 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C18 -- C19 .. 0.18 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C21 -- C22 .. 0.18 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C29 -- C30 .. 0.22 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C33 -- C36 .. 0.20 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C37 -- C38 .. 0.24 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C37 -- C39 .. 0.24 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference S4 -- C111 .. 0.20 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference O15 -- C91 .. 0.16 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C72 -- C73 .. 0.21 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C73 -- C74 .. 0.17 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C75 -- C76 .. 0.16 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C76 -- C77 .. 0.17 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C76 -- C78 .. 0.18 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C78 -- C79 .. 0.17 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C79 -- C80 .. 0.16 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C83 -- C84 .. 0.17 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C83 -- C85 .. 0.16 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C85 -- C86 .. 0.16 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C86 -- C87 .. 0.16 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C93 -- C94 .. 0.21 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C97 -- C98 .. 0.18 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C101 -- C102 .. 0.25 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C101 -- C103 .. 0.22 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C101 -- C104 .. 0.24 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference O26 -- C158 .. 0.20 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C135 -- C136 .. 0.20 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C138 -- C139 .. 0.18 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C148 -- C149 .. 0.23 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C153 -- C154 .. 0.17 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C153 -- C158 .. 0.21 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C155 -- C156 .. 0.21 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C164 -- C165 .. 0.24 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C168 -- C170 .. 0.19 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT234_ALERT_4_C Large Hirshfeld Difference C172 -- C174 .. 0.23 Ang.

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C28 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... O29 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... O30 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C195 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C29 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C37 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C41 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... O23 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C97 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C101 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C111 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C114 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... O27 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... O32 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C164 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C168 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C172 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C193 Check

Author Response: RIGU restraints were applied to atoms in the disordered chains. Several of the atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O2 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O10 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O8 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O11 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O27 Check
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C132 -C137 1.37 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C29 - C30 ... 1.43 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C164 - C166 ... 1.41 Ang.
PLAT361_ALERT_2_C Long C(sp3)-C(sp3) Bond C168 - C170 ... 1.65 Ang.
PLAT363_ALERT_2_C Long C(sp3)-C(sp2) Bond C53 - C54 ... 1.64 Ang.

Author Response: Crystals diffracted extremely weakly. Multiple attempts were made to grow better diffracting crystals. Data was collected at three diffrent facilities with radiation sources of Mo, Cu and synchrotron. All results were consistent with the model in this report (from the Cu data collection), however, all yielded serious problems due to weak diffraction and disorder in the atom positions. This structure is reported in order to support the cone-conformation of the molecule, and not the anti-conformation, which can be assessed based on the available data.

```
PLAT367_ALERT_2_C Long?  C(sp?)-C(sp?) Bond  C193   -   C194   ...       1.62 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H16K   ..  H11N    ..       2.06 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H17M   ..  H47B    ..       2.08 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H11E   ..  H16A    ..       2.11 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C61.92 H73 O9 S2
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      7.921 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.481         85 Why ?
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) .          2 Check
PLAT953_ALERT_1_C Reported and Actual Hmax Values in FCF Differ by          5 Check
PLAT954_ALERT_1_C Reported and Actual Kmax Values in FCF Differ by          7 Check
PLAT955_ALERT_1_C Reported and Actual Lmax Values in FCF Differ by          6 Check
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C62 H88 O9 S2
           Atom count from _chemical_formula_moiety:C61.15890 H70.64639 O8.58 S
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C62 H88 O9 S2
           Atom count from the _atom_site data:  C61.77666 H71.36066 O8.666666
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z   12
          From the CIF: _chemical_formula_sum  C62 H88 O9 S2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        744.00    741.32    2.68
          H       1056.00    856.33  199.67
          O        108.00    104.00    4.00
          S         24.00     24.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         16 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          1 Why ?
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Why ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............       0.33 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.20 Why ?
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =         11 Note
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C190
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C191
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C192
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C195
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C196
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C45    --  C46A    .       1.74 Ang.
```

```
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C48    --  C49A    .       1.73 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C55    --  C57     .       1.71 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C179   --  C180    .       1.76 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C184   --  C185    .       1.78 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C185   --  C187    .       1.82 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C1A    --  C121    .       1.90 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C123   --  C124    .       2.04 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C129   --  C131    .       1.92 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          9 Check
             C48A -S1   -C48     1.555   1.555   1.555             39.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         16 Check
             C48  -S2   -O1A     1.555   1.555   1.555             29.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         24 Check
             C48  -O2   -C48A    1.555   1.555   1.555             39.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         27 Check
             C57  -O6   -C56     1.555   1.555   1.555             27.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         30 Check
             C56  -O7   -C57     1.555   1.555   1.555             30.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        135 Check
             C46  -C45  -C46A    1.555   1.555   1.555             42.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        153 Check
             C48  -C48A -O2      1.555   1.555   1.555             44.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        172 Check
             C48A -C49A -C48     1.555   1.555   1.555             39.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        181 Check
             C56  -C55  -C57     1.555   1.555   1.555             21.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        193 Check
             C56  -C57  -C55     1.555   1.555   1.555             35.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        213 Check
             O11  -C62  -O10     1.555   1.555   1.555             27.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        215 Check
             O10  -C63  -O11     1.555   1.555   1.555             27.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        222 Check
             C184 -S8   -C182    1.555   1.555   1.555             35.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        230 Check
             C184 -S9   -S8      1.555   1.555   1.555             37.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        232 Check
             C185 -S9   -S8      1.555   1.555   1.555             35.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        336 Check
             C183 -C181 -C182    1.555   1.555   1.555             20.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        341 Check
             C184 -C182 -S8      1.555   1.555   1.555             39.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        352 Check
             C182 -C184 -C183    1.555   1.555   1.555             23.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        371 Check
             C185 -C186 -S8      1.555   1.555   1.555             39.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        388 Check
             S6   -S5   -C117    1.555   1.555   1.555             41.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        390 Check
             C117 -S5   -C116    1.555   1.555   1.555             22.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        397 Check
             C117 -S6   -C116    1.555   1.555   1.555             20.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        401 Check
             C118 -O16  -O17     1.555   1.555   1.555             41.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        406 Check
             C1A  -O19  -C124    1.555   1.555   1.555             28.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        412 Check
             C1A  -O20  -C124    1.555   1.555   1.555             28.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        413 Check
             C120 -O20  -C121    1.555   1.555   1.555             37.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        421 Check
             C127 -O21  -C126    1.555   1.555   1.555             39.00 Deg.
```

```
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        534 Check
             C116 -C115 -C117    1.555   1.555   1.555             27.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        535 Check
             S6   -C116 -S5      1.555   1.555   1.555             33.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        539 Check
             C117 -C116 -S6      1.555   1.555   1.555             32.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        541 Check
             S6   -C117 -S5      1.555   1.555   1.555             39.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        547 Check
             S5   -C118 -S6      1.555   1.555   1.555             37.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        561 Check
             O19  -C121 -C1A     1.555   1.555   1.555             44.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        568 Check
             C1A  -C123 -C124    1.555   1.555   1.555             20.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        582 Check
             C125 -C124 -O21     1.555   1.555   1.555             34.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        588 Check
             C1A  -C125 -C124    1.555   1.555   1.555             29.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        593 Check
             C126 -C125 -C127    1.555   1.555   1.555             33.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        594 Check
             C125 -C126 -O21     1.555   1.555   1.555             43.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        600 Check
             O21  -C127 -C125    1.555   1.555   1.555             37.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        604 Check
             C126 -C127 -C128    1.555   1.555   1.555             41.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        608 Check
             C126 -C128 -C127    1.555   1.555   1.555             34.00 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        621 Note
PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) .....          1 Why ?
PLAT950_ALERT_5_G Reported and Calculated Hmax Values Differ by ..         -5
PLAT951_ALERT_5_G Reported and Calculated Kmax Values Differ by ..         -7
PLAT952_ALERT_5_G Reported and Calculated Lmax Values Differ by ..         -6 Check
```

---

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

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock LTS02_14 - ellipsoid plot