

No syntax errors found. CIF dictionary Interpreting this report

Datablock: beta-EDT-TTF-I22Fumarate

Bond precision: C-C = 0.0038 A

Wavelength=0.71073

Cell: a=8.1576(4) b=13.1699(13) c=15.4841(9)
 alpha=78.710(7) beta=80.782(5) gamma=88.271(6)
Temperature: 293 K

	Calculated	Reported
Volume	1610.3(2)	1610.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C8 H4 I2 S6), C4 H3 O4	2(C8 H4 I2 S6), C4 H3 O4
Sum formula	C20 H11 I4 O4 S12	C20 H11 I4 O4 S12
Mr	1207.73	1207.61
Dx, g cm-3	2.491	2.491
Z	2	2
Mu (mm-1)	4.679	4.679
F000	1134.0	1134.0
F000'	1133.51	
h, k, lmax	11, 18, 21	11, 18, 21
Nref	9407	9373
Tmin, Tmax	0.576, 0.755	0.436, 0.751
Tmin'	0.388	

Correction method= MULTI-SCAN

Data completeness= 0.996

Theta(max)= 30.000

R(reflections)= 0.0270(6388)

wR2(reflections)= 0.0557(9373)

S = 1.008

Npar= 361

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

PLAT431_ALERT_2_A Short Inter HL..A Contact	I11	..	02	..	2.74 Ang.
PLAT431_ALERT_2_A Short Inter HL..A Contact	I31	..	01	..	2.90 Ang.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects Additional (Pseudo) Symm. Elem...

C

	Alert level C	# Supplementary Material (ESI) for Journal of Materials Chemistry # This journal is (C) The Royal Society of Chemistry 2010		
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor			2.05
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor			2.29
PLAT431_ALERT_2_C	Short Inter HL..A Contact I12 .. S36 ..			3.59 Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact I32 .. S16 ..			3.48 Ang.
PLAT194_ALERT_1_C	Missing _cell_measurement_reflns_used datum			?
PLAT195_ALERT_1_C	Missing _cell_measurement_theta_max datum			?
PLAT196_ALERT_1_C	Missing _cell_measurement_theta_min datum			?
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #			3
	C4 H3 O4			

	Alert level G			
PLAT432_ALERT_2_G	Short Inter X...Y Contact I11 .. C3 ..			3.43 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact I31 .. C3 ..			3.48 Ang.
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature			293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature			293 K

2 **ALERT level A** = In general: serious problem

1 **ALERT level B** = Potentially serious problem

8 **ALERT level C** = Check and explain

4 **ALERT level G** = General alerts; check

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 ALERT type 2 Indicator that the structure model may be wrong or deficient

0 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

PLATON version of 29/06/2010; check.def file version of 26/06/2010

Datablock beta-EDT-TTF-122Fumarate - ellipsoid plot

