

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: danr119

Bond precision: C-C = 0.0035 Å

Wavelength=0.71073

Cell: a=11.226(2) b=12.167(4) c=21.415(4)
 alpha=90 beta=95.400(16) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	2912.0(12)	2912.2(12)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C25 H41 Ag F3 O4 S3 Si	?
Sum formula	C25 H41 Ag F3 O4 S3 Si	C25 H41 Ag F3 O4 S3 Si
Mr	694.75	694.72
Dx, g cm-3	1.585	1.585
Z	4	4
Mu (mm-1)	0.998	0.998
F000	1436.0	1436.0
F000'	1434.83	
h, k, lmax	15, 16, 28	14, 16, 26
Nref	7293	6393
Tmin, Tmax	0.803, 0.861	0.810, 0.865
Tmin'	0.803	

Correction method= MULTI-SCAN

Data completeness= 0.877

Theta(max)= 28.390

R(reflections)= 0.0361(5415)

wR2(reflections)= 0.0951(6393)

S = 1.033

Npar= 342

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

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full	Low	0.97
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag	-- 01 ..	6.07 su
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1C	.. S3 ..	2.91 Ang.
PLAT952_ALERT_1_C Reported and Calculated Lmax Values Differ by	..	2

● Alert level G

REFLT03_ALERT_1_G ALERT: Expected hkl max differ from CIF values
From the CIF: _diffn_reflns_theta_max 28.39
From the CIF: _reflns_number_total 6393
From the CIF: _diffn_reflns_limit_max hkl 14. 15. 26.
From the CIF: _diffn_reflns_limit_min hkl -14. -16. -24.
TEST1: Expected hkl limits for theta max
Calculated maximum hkl 15. 16. 28.
Calculated minimum hkl -15. -16. -28.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 2
PLAT793_ALERT_4_G The Model has Chirality at C16 (Verify) S
PLAT793_ALERT_4_G The Model has Chirality at C24 (Verify) R

0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
4 ALERT level C = Check and explain
4 ALERT level G = General alerts; check

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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 13/08/2009; check.def file version of 12/08/2009

