

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound_2

Bond precision: C-C = 0.0049 A Wavelength=0.71073

Cell: a=11.6289(7) b=6.6998(5) c=18.6130(11)
 alpha=90 beta=90 gamma=90

Temperature: 115 K

	Calculated	Reported
Volume	1450.16(16)	1450.16(16)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C13 H10 N, C F3 O3 S, H2 O	C13 H10 N, C F3 O3 S, H2 O
Sum formula	C14 H12 F3 N O4 S	C14 H12 F3 N O4 S
Mr	347.32	347.31
Dx,g cm ⁻³	1.591	1.591
Z	4	4
Mu (mm ⁻¹)	0.277	0.277
F000	712.0	712.0
F000'	713.00	
h,k,lmax	15,8,24	14,8,24
Nref	1812	1740
Tmin,Tmax	0.984,0.986	0.870,1.107
Tmin'	0.933	

Correction method= MULTI-SCAN

Data completeness= 0.960 Theta(max)= 27.510

R(reflections)= 0.0487(1360) wR2(reflections)= 0.1013(1740)

S = 1.143 Npar= 133

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 _diffrn_measured_fraction_theta_full	Low	0.960
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds		0.0049 Ang

● **Alert level G**

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 2

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

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

Datablock: compound_3

Bond precision: C-C = 0.0022 Å Wavelength=0.71073

Cell: a=7.0899(3) b=9.6716(4) c=10.5407(4)
 alpha=74.269(2) beta=78.855(2) gamma=81.869(2)
Temperature: 115 K

	Calculated	Reported
Volume	679.55(5)	679.55(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C13 H10 N, C F3 O3 S	C13 H10 N, C F3 O3 S
Sum formula	C14 H10 F3 N O3 S	C14 H10 F3 N O3 S
Mr	329.30	329.29
Dx, g cm-3	1.609	1.609
Z	2	2
Mu (mm-1)	0.286	0.286
F000	336.0	336.0
F000'	336.48	
h,k,lmax	9,12,13	9,12,13
Nref	3109	3074
Tmin,Tmax	0.956,0.972	
Tmin'	0.939	

Correction method= Not given

Data completeness= 0.989 Theta(max)= 27.470

R(reflections)= 0.0388(2852) wR2(reflections)= 0.1018(3074)

S = 1.104 Npar= 199

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**

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3

● **Alert level G**

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 1
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00200 Deg.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1

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

1 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
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: compound_4

Bond precision: C-C = 0.0031 A

Wavelength=0.71073

Cell: a=9.0072(4) b=10.1453(4) c=11.2361(5)
alpha=69.110(2) beta=81.158(2) gamma=69.894(2)
Temperature: 115 K

	Calculated	Reported
Volume	900.24(7)	900.24(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C13 H10 N, 0.5(C14 H10), C F3 O3 S	C13 H10 N, 0.5(C14 H10), C F3 O3 S
Sum formula	C21 H15 F3 N O3 S	C21 H15 F3 N O3 S
Mr	418.41	418.40
Dx,g cm-3	1.544	1.544
Z	2	2
Mu (mm-1)	0.234	0.234
F000	430.0	430.0
F000'	430.51	
h,k,lmax	11,13,14	11,13,14
Nref	4124	4074
Tmin,Tmax	0.978,0.988	0.813,1.223
Tmin'	0.906	

Correction method= MULTI-SCAN

Data completeness= 0.988 Theta(max)= 27.480

R(reflections)= 0.0471(3466) wR2(reflections)= 0.1085(4074)

S = 1.062 Npar= 262

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 G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
 PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 1
 PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00200 Deg.

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 0 **ALERT level B** = A potentially serious problem, consider carefully
 - 0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 3 **ALERT level G** = General information/check it is not something unexpected
-
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 0 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
 - 0 ALERT type 4 Improvement, methodology, query or suggestion
 - 2 ALERT type 5 Informative message, check

checkCIF publication errors

● **Alert level G**

PUBL013_ALERT_1_G The `_publ_section_comment` (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).

PUBL017_ALERT_1_G The `_publ_section_references` section is missing or empty.

0 **ALERT level A** = Data missing that is essential or data in wrong format

2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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