

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) k1892

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: k1892

Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell: a=11.339(7) b=8.255(5) c=22.051(17)
 alpha=90 beta=103.934(18) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	2003(2)	2003(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H20 F2 N4 Ni O2 S2	C20 H20 F2 N4 Ni O2 S2
Sum formula	C20 H20 F2 N4 Ni O2 S2	C20 H20 F2 N4 Ni O2 S2
Mr	509.21	509.23
Dx,g cm-3	1.689	1.689
Z	4	4
Mu (mm-1)	1.223	1.223
F000	1048.0	1048.0
F000'	1050.74	
h,k,lmax	14,10,28	14,10,29
Nref	4778	4776
Tmin,Tmax	0.568,0.976	0.597,0.976
Tmin'	0.557	

Correction method= # Reported T Limits: Tmin=0.597 Tmax=0.976
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.872

R(reflections)= 0.0554(3242) wR2(reflections)= 0.1285(4776)

S = 0.947 Npar= 284

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.127
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C5 -C10 1.37 Ang.
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C15 -C20 1.37 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 4.198 Check

● Alert level G

PLAT020_ALERT_3_G The value of Rint is greater than 0.12 0.127 Report
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-

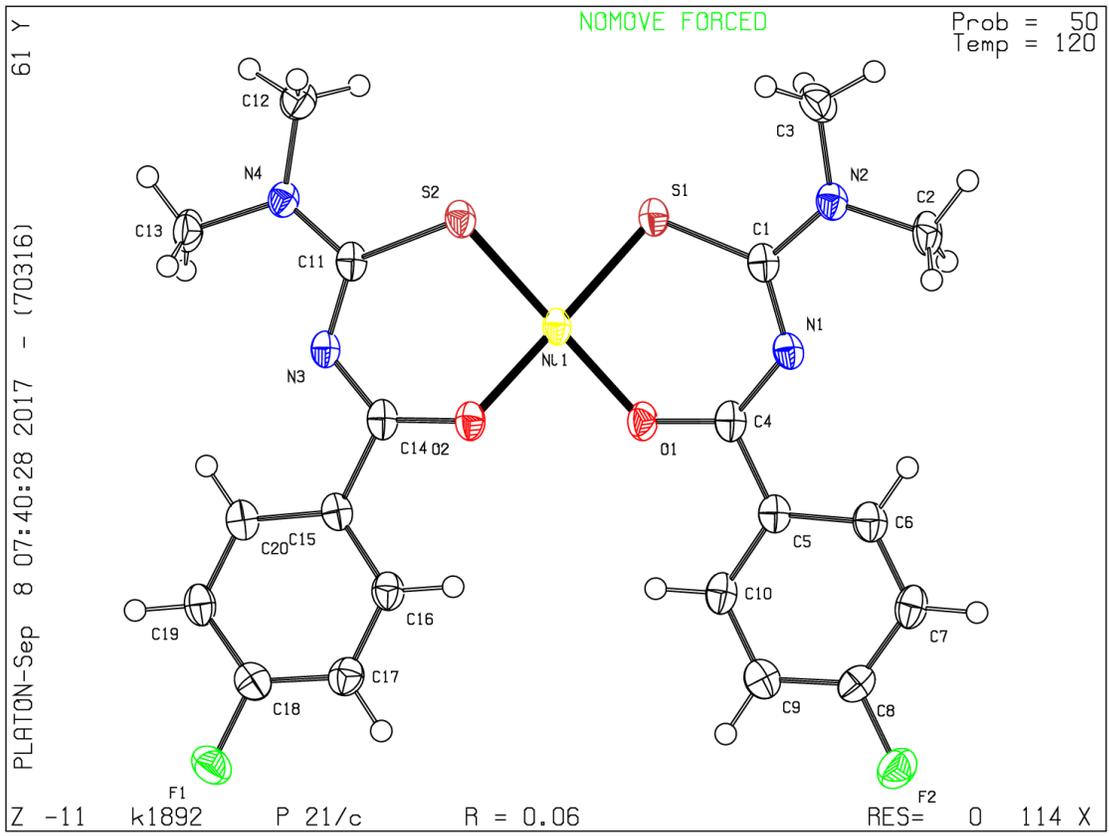
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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* 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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) k1902

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: k1902

Bond precision:	C-C = 0.0029 A	Wavelength=0.71073	
Cell:	a=11.3504(16)	b=8.5070(12)	c=22.164(3)
	alpha=90	beta=103.828(3)	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	2078.1(5)	2078.1(5)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C20 H20 Cu F2 N4 O2 S2	C20 H20 Cu F2 N4 O2 S2	
Sum formula	C20 H20 Cu F2 N4 O2 S2	C20 H20 Cu F2 N4 O2 S2	
Mr	514.07	514.06	
Dx,g cm-3	1.643	1.643	
Z	4	4	
Mu (mm-1)	1.296	1.296	
F000	1052.0	1052.0	
F000'	1054.66		
h,k,lmax	14,11,29	14,11,29	
Nref	4956	4953	
Tmin,Tmax	0.605,0.742	0.612,0.755	
Tmin'	0.574		

Correction method= # Reported T Limits: Tmin=0.612 Tmax=0.755
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.877

R(reflections)= 0.0311(4293) wR2(reflections)= 0.0829(4953)

S = 1.057 Npar= 284

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test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● **Alert level C**

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report

● **Alert level G**

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- S1 .. 5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- S2 .. 8.0 s.u.
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 13 Info

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-

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Publication of your CIF in other journals

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PLATON version of 13/08/2017; check.def file version of 27/07/2017

