

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 170313

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: 170313

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Bond precision:	C-C = 0.0040 A	Wavelength=1.54187
Cell:	a=21.0006(4)      b=8.10823(15)      c=7.57570(14)	alpha=90      beta=97.5156(11)      gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1278.89(4)	1278.89(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H6 N Na O6 S	C26 H16 N2 Na2 O12 S2
Sum formula	C13 H6 N Na O6 S	C26 H16 N2 Na2 O12 S2
Mr	327.24	658.52
Dx,g cm-3	1.700	1.710
Z	4	2
Mu (mm-1)	2.902	2.903
F000	664.0	672.0
F000'	668.02	
h,k,lmax	25,9,9	25,9,9
Nref	2346	2346
Tmin,Tmax	0.785,0.971	0.786,0.971
Tmin'	0.712	

Correction method= # Reported T Limits: Tmin=0.786 Tmax=0.971  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 68.232

R(reflections)= 0.0461( 1842)      wR2(reflections)= 0.1385( 2346)

S = 1.093      Npar= 199

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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.

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● **Alert level C**

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 2.02 Check  
PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for S1 --O4 . 5.3 s.u.  
PLAT790\_ALERT\_4\_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note  
C13 H6 N Na O6 S  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.95A From O6 0.57 eA-3

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● **Alert level G**

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: C26 H16 N2 Na2 O12 S2  
Atom count from the \_atom\_site data: C26 H12 N2 Na2 O12 S2  
CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?  
From the CIF: \_cell\_formula\_units\_Z 2  
From the CIF: \_chemical\_formula\_sum C26 H16 N2 Na2 O12 S2  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	52.00	52.00	0.00
H	32.00	24.00	8.00
N	4.00	4.00	0.00
Na	4.00	4.00	0.00
O	24.00	24.00	0.00
S	4.00	4.00	0.00

CHEMS02\_ALERT\_1\_G Please check that you have entered the correct  
\_publ\_requested\_category classification of your compound;  
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;  
FO or CO or EO for organic.  
From the CIF: \_publ\_requested\_category CHOOSE FI FM FO CI CM CO or  
From the CIF: \_chemical\_formula\_sum: C26 H16 N2 Na2 O12 S2  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 2.00 Check  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.43 Ratio  
PLAT779\_ALERT\_4\_G Suspect or Irrelevant (Bond) Angle in CIF .... # 12 Check  
O1 -S1 -NA1 1.555 1.555 1.555 40.42 Deg.  
PLAT793\_ALERT\_4\_G Model has Chirality at S1 (Centro SPGR) S Verify  
PLAT882\_ALERT\_1\_G No Datum for \_diffrn\_reflns\_av\_unetI/netI ..... Please Do !  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 4 Info

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

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

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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**

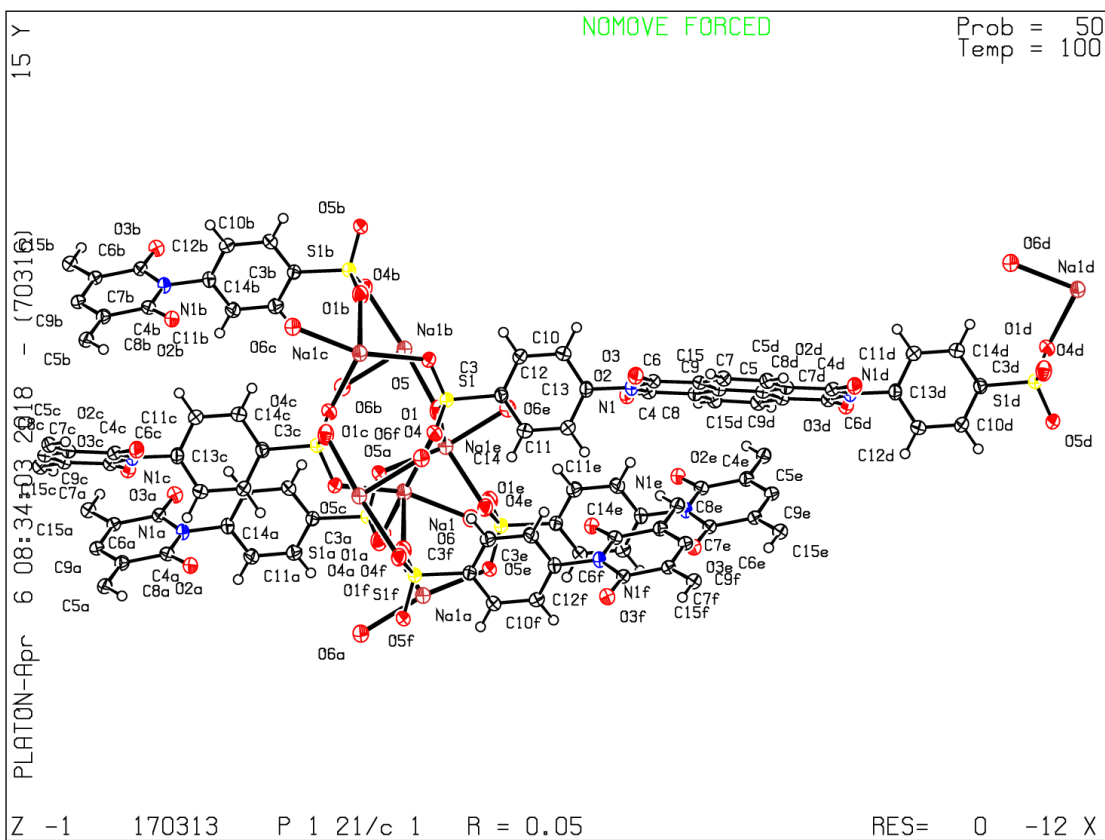
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

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**PLATON version of 30/01/2018; check.def file version of 30/01/2018**



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 171019

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No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: 171019

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Bond precision:    C-C = 0.0027 Å                      Wavelength=1.54187

Cell:                a=7.39936(19)        b=8.9486(2)            c=20.4815(6)  
                      alpha=78.417(2)    beta=77.9681(18)    gamma=76.6033(18)  
Temperature:    100 K

	Calculated	Reported
Volume	1273.60(6)	1273.60(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H12 N2 O10 S2, 2(H4 N)	C26 H20 N4 O10 S2
Sum formula	C26 H20 N4 O10 S2	C26 H20 N4 O10 S2
Mr	612.58	612.58
Dx,g cm-3	1.597	1.597
Z	2	2
Mu (mm-1)	2.516	2.518
F000	632.0	632.0
F000'	635.42	
h,k,lmax	8,10,24	8,10,24
Nref	4668	4581
Tmin,Tmax	0.860,0.882	0.756,0.882
Tmin'	0.604	

Correction method= # Reported T Limits: Tmin=0.756 Tmax=0.882  
AbsCorr = MULTI-SCAN

Data completeness= 0.981                      Theta(max)= 68.234

R(reflections)= 0.0356( 3969)              wR2(reflections)= 0.0986( 4577)

S = 1.033                                      Npar= 401

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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.

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● **Alert level C**

PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced .....	Please Do !
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent .....	2 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.353 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	79 Report

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● **Alert level G**

CHEMS02\_ALERT\_1\_G Please check that you have entered the correct  
\_publ\_requested\_category classification of your compound;  
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;  
FO or CO or EO for organic.  
From the CIF: \_publ\_requested\_category CHOOSE FI FM FO CI CM CO or  
From the CIF: \_chemical\_formula\_sum:C26 H20 N4 O10 S2

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H4 N	2 Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI .....	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	12 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7 Info

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### **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**

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**PLATON version of 30/01/2018; check.def file version of 30/01/2018**

