

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Yellow_CH3CN_120

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: Yellow_CH3CN_120

Bond precision:	C-C = 0.0052 A	Wavelength=0.71073	
Cell:	a=42.2980(16)	b=14.6224(6)	c=22.9540(9)
	alpha=90	beta=90	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	14197.0(10)	14197.0(10)	
Space group	F d d 2	F d d 2	
Hall group	F 2 -2d	F 2 -2d	
Moiety formula	C62 H58 Cl8 Fe N10, 2(B F4), 2(C2 H3 N)	C62 H58 Cl8 Fe N10, 2(B F4), 2(C2 H3 N)	
Sum formula	C66 H64 B2 Cl8 F8 Fe N12	C66 H64 B2 Cl8 F8 Fe N12	
Mr	1538.36	1538.36	
Dx,g cm-3	1.439	1.439	
Z	8	8	
Mu (mm-1)	0.585	0.585	
F000	6304.0	6304.0	
F000'	6318.66		
h,k,lmax	54,18,29	54,18,29	
Nref	7761[3979]	7759	
Tmin,Tmax	0.869,0.890	0.687,0.746	
Tmin'	0.864		

Correction method= # Reported T Limits: Tmin=0.687 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.95/1.00 Theta(max)= 26.993

R(reflections)= 0.0341(6893) wR2(reflections)= 0.0776(7759)

S = 1.024 Npar= 509

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**

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	7.82	Note
PLAT213_ALERT_2_C	Atom C26" has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C24A	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1S	Check

● **Alert level G**

PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	18.60	Why ?
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	15%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II) .	2.20	Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note
PLAT953_ALERT_1_G	Reported (CIF) and Actual (FCF) Hmax Differ by .	1	Units
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	2	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
6 **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
3 **ALERT type 4** Improvement, methodology, query or suggestion
1 **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.

PLATON version of 16/07/2020; check.def file version of 12/07/2020

