

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Fe-dcbdt

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: Fe-dcbdt

Bond precision:	C-C = 0.0038 A	Wavelength=1.54184	
Cell:	a=22.2191(2) alpha=90	b=22.6288(2) beta=90	c=14.4544(1) gamma=90
Temperature:	302 K		
	Calculated	Reported	
Volume	7267.55(11)	7267.55(10)	
Space group	P b c n	P b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C16 H8 Fe2 O10 S4, 2(C4 H12 N), C4 H11 N	C16 H8 Fe2 O10 S4, 2(C4 H12 N), C4 H11 N	
Sum formula	C28 H43 Fe2 N3 O10 S4	C28 H43 Fe2 N3 O10 S4	
Mr	821.59	821.59	
Dx, g cm ⁻³	1.502	1.502	
Z	8	8	
Mu (mm ⁻¹)	9.025	9.025	
F000	3424.0	3424.0	
F000'	3425.53		
h,k,lmax	28,28,18	28,28,17	
Nref	7747	7482	
Tmin,Tmax		0.525,1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.525 Tmax=1.000
AbsCorr = NONE

Data completeness= 0.966 Theta(max)= 77.571

R(reflections)= 0.0348(6112)

wR2(reflections)=
0.1093(7482)

S = 1.042

Npar= 434

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

PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N00I Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N00J Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N00Y Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	N00J 0.107 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	N00Y 0.103 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	40 Report
	0 2 0, 0 4 0, 0 6 0, 0 8 0, 7 9 0, 8 10 0,	
	0 4 1, 8 9 1, 8 10 1, 9 10 1, 8 11 1, 8 9 2,	
	9 9 2, 8 10 2, 9 10 2, 8 11 2, 7 8 3, 8 9 3,	
	9 9 3, 8 10 3, 9 10 3, 0 0 6, 1 0 6, 23 10 6,	
	22 11 6, 0 0 8, 1 0 8, 2 0 8, 3 0 8, 4 0 8,	
	5 0 8, 6 0 8, 1 1 8, 2 1 8, 3 1 8, 4 1 8,	
	5 1 8, 6 1 8, 0 2 8, 1 2 8,	



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	9 Report
	H00A H00B H00C H00D H00E H00F H00G H00H H00Y	
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00020 Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00010 Ang.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe01 --O008 .	7.4 s.u.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	90 Note
	Fe01 Fe02 Fe03 S004 S005 S006 S007 O008	
	H00A H00B O009 H00C H00D O00A O00B O00C	
	O00D O00E O00F O00G O00H N00I H00E H00F	
	N00J H00G H00H C00K C00L C00M C00N C00O	
	C00P C00Q C00R C00S C00T C00U C00V C00W	
	H00W C00X H00X N00Y H00Y C00Z H00Z C010	
	H010 C011 H01A H01B C012 H01C H01D C013	
	H01E H01F H01G C014 H01H H01I H01J C015	
	H01K H01L C016 H01U H01V C017 H01M H01N	
	C018 H01W H01X C019 H01O H01P H01Q C01A	
	H01R H01S H01T C01B H01Y Ha C01C H01Z	
	Hb Hc	
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe01 (II) .	2.02 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe02 (III) .	3.49 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe03 (III) .	3.52 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	200 Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.87 Note
	Predicted wR2: Based on SigI**2 2.83 or SHELX Weight 10.81	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	6 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	7 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully
9 **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

4 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
7 ALERT type 4 Improvement, methodology, query or suggestion
7 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.

