

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: klat344

Bond precision: C-C = 0.0084 Å

Wavelength=0.71073

Cell: a=18.872(3) b=9.7877(15) c=29.621(5)
 alpha=90 beta=90 gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	5471.4(15)	5471.3(15)
Space group	P c a 21	Pca2(1)
Hall group	P 2c -2ac	?
Moiety formula	C24 H41 B Fe N6 S	?
Sum formula	C24 H41 B Fe N6 S	C24 H41 B Fe N6 S
Mr	512.36	512.35
Dx, g cm-3	1.244	1.244
Z	8	8
Mu (mm-1)	0.650	0.650
F000	2192.0	2192.0
F000'	2196.20	
h, k, lmax	25, 13, 39	24, 13, 39
Nref	6923[13582]	12887
Tmin, Tmax	0.918, 0.968	0.868, 0.968
Tmin'	0.867	

Correction method= MULTI-SCAN

Data completeness= 1.86/0.95 Theta(max)= 28.290

R(reflections)= 0.0732(8972) wR2(reflections)= 0.1812(12887)

S = 1.006 Npar= 626

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

STRVA01_ALERT_4_C Flack test results are ambiguous.

 From the CIF: _refine_ls_abs_structure_Flack 0.510

 From the CIF: _refine_ls_abs_structure_Flack_su 0.020

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.58

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 8

PLAT420_ALERT_2_C D-H Without Acceptor S1 - H1A ... ?

PLAT420_ALERT_2_C D-H Without Acceptor S2 - H2C ... ?
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 2
 C24 H41 B Fe N6 S

● Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffn_reflns_theta_max 28.29
From the CIF: _reflns_number_total 12887
Count of symmetry unique reflns 6923
Completeness (_total/calc) 186.15%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 5964
Fraction of Friedel pairs measured 0.861
Are heavy atom types Z>Si present yes
PLAT033_ALERT_4_G Flack x Parameter Value Deviates from Zero 0.51

0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
6 ALERT level C = Check and explain
2 ALERT level G = General alerts; check

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

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*, 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 31/03/2010; check.def file version of 22/03/2010

