

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cemnt_020521_0m

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: cemnt_020521_0m

Bond precision:	C-C = 0.0036 Å	Wavelength=0.71073
Cell:	a=36.555 (3) b=13.7610 (11) c=19.5407 (15)	
	alpha=90 beta=109.116 (2) gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	9287.6 (13)	9287.6 (13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C64 Ce4 N32 S32, 20 (C2 N), 4 (C1.50 N0.50), 4 (C0.50 N0.50), 20 (N	C27 Ce N13.5 Na5 S8, 0.5 (C2 N)
Sum formula	C112 Ce4 N56 Na20 S32	C28 Ce N14 Na5 S8
Mr	4175.88	1043.97
Dx, g cm ⁻³	1.493	1.493
Z	2	8
Mu (mm ⁻¹)	1.424	1.424
F000	4056.0	4056.0
F000'	4063.72	
h, k, lmax	60, 22, 32	59, 22, 32
Nref	21518	21446
Tmin, Tmax	0.760, 0.867	0.643, 0.747
Tmin'	0.745	

Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.997

Theta (max)= 35.694

R(reflections)= 0.0360(17433)

wR2(reflections)=
0.0865(21446)

S = 1.043

Npar= 598

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

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C64 Ce4 N32 S32, 20(C2 N), 4(C1.50 N0.50), 4(C0.50 N0.50), 2
Rep.: C27 Ce N13.5 Na5 S8, 0.5(C2 N)

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of N55 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C47 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C53 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N46 0.155 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N41A 0.112 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 14 Report
3 1 0, 4 0 0, -3 1 1, 1 1 1, 3 1 1, 4 2 1,
-4 0 2, -2 0 2, 0 0 2, 2 0 2, -4 2 3, -3 1 3,
-4 0 4, -4 0 6,

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
3 3 1,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From Na2 1.86 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.26Ang From Na2 1.82 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.71Ang From Na2 -1.72 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.25Ang From Na2 -1.62 eA-3



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 23.38 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check
C5A C17 C23 C28 N40 C44 C19 C20
C50 C50A C18 C21 C22 C56 N41 C43
N41A C43A

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 67% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 67% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 67% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 67% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 50% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15) 100% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact N41A ..C45 . 2.97 Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact	C43A	x,y,z =	1_555 Check
		..C45	1.76 Ang.
		x,y,z =	1_555 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C50		--C19	1.84 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C45		--C43A	1.76 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #			6 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cel	(III)		3.57 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers			5 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints			42 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).			2 Note
	1 1 0, 2 0 0,		
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600		55 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File			8 Note
	1 1 1, -4 0 2, -4 0 6, 3 1 1, -4 0 4, -3 1 3,		
	4 2 1, -4 2 3,		
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value			3.018 Note
	Predicted wR2: Based on SigI**2 2.87 or SHELX Weight		8.29

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

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

