checkCIF/PLATON report

Structure factors have been supplied for datablock(s) f2

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: f2

Bond precision: C-C = 0.0016 A Wavelength=0.82656

Cell: a=8.1200(16) b=12.280(3) c=14.770(3)
alpha=106.55(3) beta=96.00(3) gamma=93.65(3)
Temperature: 100 K

	Calculated	Reported
Volume	1397.3(6)	1397.3(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H34	;C40H34;
Sum formula	C40 H34	C40 H34
Mr	514.67	514.67
Dx,g cm-3	1.223	1.223
Z	2	2
Mu (mm-1)	0.093	0.095
F000	548.0	548.0
F000’	548.31	
h,k,lmax	10,16,19	10,16,19
Nref	7224	6363
Tmin,Tmax	0.991,0.994	
Tmin’	0.991	

Correction method= Not given

Data completeness= 0.881 Theta(max)= 33.975

R(reflections)= 0.0481(6129) wR2(reflections)= 0.1322(6363)

S = 1.042 Npar= 367

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 A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.902 Why?

Author Response: This is caused by the limited data collection strategy with the synchrotron facility.

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 494 Report

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Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT977_ALERT_2_C Check Negative Difference Density on H39A -0.33 eA-3

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C40 H34
Atom count from _chemical_formula_moiety:
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.82656 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 4 Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C12 -C19 . 1.43 Ang.
PLAT793_ALERT_4_G Model has Chirality at C1 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C10 (Centro SPGR) R Verify
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= 0.600 368 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 22 Info
PLAT984_ALERT_1_G The C-f'= 0.0037 Deviates from the B&C-Value 0.0047 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 6 Check

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

7 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
4 ALERT type 3 Indicator that the structure quality may be low
5 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 05/12/2020; check.def file version of 05/12/2020

Datablock f2 - ellipsoid plot