

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: shelx

Bond precision: C-C = 0.0072 A

Wavelength=0.71073

Cell: a=9.9129(5) b=12.8302(5) c=14.0185(6)
 alpha=116.357(4) beta=103.424(4) gamma=96.119(4)
Temperature: 293 K

	Calculated	Reported
Volume	1508.31(14)	1508.31(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H16 Cl2 Co N4, C6 F4 I2	C24 H16 Cl2 Co N4, C6 F4 I2
Sum formula	C30 H16 Cl2 Co F4 I2 N4	C30 H16 Cl2 Co F4 I2 N4
Mr	892.10	892.10
Dx,g cm-3	1.964	1.964
Z	2	2
Mu (mm-1)	2.846	2.846
F000	854.0	854.0
F000'	853.72	
h,k,lmax	12,16,18	12,16,18
Nref	6931	6632
Tmin,Tmax	0.430,0.731	0.654,1.000
Tmin'	0.267	

Correction method= # Reported T Limits: Tmin=0.654 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.957

Theta(max)= 27.496

R(reflections)= 0.0294(4212)

wR2(reflections)= 0.0772(6632)

S = 0.879

Npar= 388

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

ABSTY02_ALERT_1_C An `_exptl_absorpt_correction_type` has been given without a literature citation. This should be contained in the `_exptl_absorpt_process_details` field.

Absorption correction given as multi-scan

PLAT029_ALERT_3_C	<code>_diffrn_measured_fraction_theta_full</code> value Low .	0.977	Why?
PLAT193_ALERT_1_C	Cell and Diffraction Temperatures Differ by	2	Degree
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C27	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C29	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.5	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.3	Note
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist C25 -C30	1.36	Ang.
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist C27 -C29_b	1.37	Ang.

● Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.004	Degree
PLAT200_ALERT_1_G	Reported <code>_diffrn_ambient_temperature</code> (K)	293	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I1 ..C12	3.14	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I2 ..C11	3.14	Ang.

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
4 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
0 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

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