

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tza-68

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: tza-68

---

Bond precision:	C-C = 0.0033 A	Wavelength=0.71073	
Cell:	a=11.5478 (4)	b=10.8419 (3)	c=27.8588 (10)
	alpha=90	beta=90.691 (1)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	3487.7 (2)	3487.7 (2)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C31 H26 N8 Ni O2, 2(C2 H6 O), 2(H2 O)	C31 H26 N8 Ni O2, 2(H2 O), 2(C2 H6 O)	
Sum formula	C35 H42 N8 Ni O6	C35 H42 N8 Ni O6	
Mr	729.46	729.47	
Dx, g cm <sup>-3</sup>	1.389	1.389	
Z	4	4	
Mu (mm <sup>-1</sup> )	0.614	0.614	
F000	1536.0	1536.0	
F000'	1537.92		
h, k, lmax	15, 14, 36	14, 14, 36	
Nref	8032	8006	
Tmin, Tmax	0.912, 0.940	0.678, 0.746	
Tmin'	0.898		

Correction method= # Reported T Limits: Tmin=0.678 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.997      Theta(max)= 27.541

R(reflections)= 0.0434 ( 6019)      wR2(reflections)=  
0.1071 ( 8006)

S = 1.033      Npar= 469

---

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**

CRYSC01\_ALERT\_1\_C The word below has not been recognised as a standard  
                  identifier.  
                  pinkish

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H32A .	-0.34 eA-3

---

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3 Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	6 Report
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	1 Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1 Report
PLAT344_ALERT_2_G	Unusual Angle Range in Solvent/Ion for	C32 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C2 H6 O	2 Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C2 H6 O	3 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni1 (II) .	2.15 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	17 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	5 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.6 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	6 Info

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
4 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 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  
2 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 06/07/2023; check.def file version of 30/06/2023**

