

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: WO3-bpy-2Na

Bond precision:	C-C = 0.0194 A	Wavelength=1.54178	
Cell:	a=7.4683(3)	b=7.3910(3)	c=22.5781(6)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1246.27(8)	1246.27(8)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	?	
Moiety formula	C5 H4 N O3 W, 0.06(Na2)	C5 H4 N1 Na0.13 O3 W1	
Sum formula	C5 H4 N Na0.13 O3 W	C5 H4 N1 Na0.13 O3 W1	
Mr	312.92	312.80	
Dx,g cm-3	3.336	3.334	
Z	8	8	
Mu (mm-1)	34.012	34.008	
F000	1123.0	1123.0	
F000'	1082.44		
h,k,lmax	9,9,27	9,8,26	
Nref	1176	1125	
Tmin,Tmax	0.125,0.712	0.008,1.000	
Tmin'	0.035		

Correction method= EMPIRICAL

Data completeness= 0.957 Theta(max)= 69.930

R(reflections)= 0.0536(1015) wR2(reflections)= 0.1279(1125)

S = 0.865 Npar= 115

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 B

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full Low	0.956
PLAT093_ALERT_1_B No su's on H-atoms, but refinement reported as .	mixed

● Alert level C

PLAT031_ALERT_4_C Refined Extinction Parameter within Range	2.667 Sigma
PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms ..	?
PLAT088_ALERT_3_C Poor Data / Parameter Ratio	9.78
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.0194 Ang
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #	1

C5 H4 N O3 W

● Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites	11
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .	3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ...	?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ	?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.	146.92
PLAT301_ALERT_3_G Note: Main Residue Disorder	20 Perc.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .	1.61 Ratio
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	!
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints	120

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
4 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
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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*, 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.

