

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-2Ca

Bond precision: C-C = 0.0220 Å Wavelength=1.54178

Cell: a=7.4775(10) b=7.3925(10) c=22.5829(16)
 alpha=90 beta=90 gamma=90
Temperature: 163 K

	Calculated	Reported
Volume	1248.3(3)	1248.3(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	?
Moiety formula	C5 H4 N O3 W, 0.5(Ca0.10)	C5 H4 Ca0.05 N O3 W
Sum formula	C5 H4 Ca0.05 N O3 W	C5 H4 Ca0.05 N O3 W
Mr	311.94	311.94
Dx,g cm-3	3.320	3.298
Z	8	8
Mu (mm-1)	34.224	33.861
F000	1120.0	1112.0
F000'	1079.03	
h,k,lmax	7,7,23	7,7,23
Nref	756	756
Tmin,Tmax	0.164,0.713	0.293,1.000
Tmin'	0.027	

Correction method= EMPIRICAL

Data completeness= 1.000 Theta(max)= 54.230

R(reflections)= 0.0651(693) wR2(reflections)= 0.1319(756)

S = 1.120 Npar= 104

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

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20

Absolute value of the parameter shift to su ratio given 0.340

Additional refinement cycles may be required.

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550

Calculated sin(theta_max)/wavelength = 0.5263
 PLAT080_ALERT_2_A Maximum Shift/Error 0.34

Alert level B

REFNR01_ALERT_3_B Ratio of reflections to parameters is < 8 for a centrosymmetric structure
 sine(theta)/lambda 0.5263
 Proportion of unique data used 1.0000
 Ratio reflections to parameters 7.2692
 PLAT088_ALERT_3_B Poor Data / Parameter Ratio 7.27
 PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.0220 Ang

Alert level C

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies outside the range 0.99 <> 1.01
 Calculated value of mu = 34.224
 Value of mu given = 33.861
 PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.07 Perc.
 PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
 PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. ?
 PLAT234_ALERT_4_C Large Hirshfeld Difference W1 -- O1 .. 0.16 Ang.
 PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for W1

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 9
 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. 49.06
 PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 2
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W1 -- O2 .. 6.4 su
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W1 -- O1_d .. 5.2 su
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) W1 -- O2_g .. 6.4 su
 PLAT301_ALERT_3_G Note: Main Residue Disorder 0 Perc.
 PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.64 Ratio
 PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 54

3 **ALERT level A** = Most likely a serious problem - resolve or explain
 3 **ALERT level B** = A potentially serious problem, consider carefully
 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 12 **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
 6 ALERT type 3 Indicator that the structure quality may be low
 4 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*, 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.

