

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: phw1117

Bond precision: C-C = 0.0047 A Wavelength=0.71070

Cell: a=13.4860(5) b=13.4860(5) c=7.7069(7)
 alpha=90 beta=90 gamma=120

Temperature: 110 K

	Calculated	Reported
Volume	1213.88(16)	1213.87(12)
Space group	P 3 1 c	P 3 1 c
Hall group	P 3 -2c	P 3 -2c
Moiety formula	C27 H33 N3 O3	C27 H33 N3 O3
Sum formula	C27 H33 N3 O3	C27 H33 N3 O3
Mr	447.56	447.56
Dx,g cm-3	1.224	1.225
Z	2	2
Mu (mm-1)	0.080	0.080
F000	480.0	480.0
F000'	480.20	
h,k,lmax	19,19,10	17,19,10
Nref	1228[2440]	1846
Tmin,Tmax	0.993,0.996	0.996,0.998
Tmin'	0.977	

Correction method= ANALYTICAL

Data completeness= 1.50/0.76 Theta(max)= 30.390

R(reflections)= 0.0510(1453) wR2(reflections)= 0.1578(1846)

S = 1.194 Npar= 108

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 _diffn_measured_fraction_theta_full Low 0.919

 **Alert level C**
STRVA01_ALERT_4_C Flack test results are meaningless.
 From the CIF: _refine_ls_abs_structure_Flack 0.000

From the CIF: `_refine_ls_abs_structure_Flack_su` 3.000
 PLAT245_ALERT_2_C U(iso) H1A Smaller than U(eq) N1 by ... 0.014 AngSq
 PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.3
 PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0047 Ang
 PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1
 C27 H33 N3 O3

● **Alert level G**

REFLT03_ALERT_1_G ALERT: Expected hkl max differ from CIF values
 From the CIF: `_diffirn_reflms_theta_max` 30.39
 From the CIF: `_reflms_number_total` 1846
 From the CIF: `_diffirn_reflms_limit_max hkl` 17. 15. 9.
 From the CIF: `_diffirn_reflms_limit_min hkl` -6. -19. -10.
 TEST1: Expected hkl limits for theta max
 Calculated maximum hkl 19. 19. 10.
 Calculated minimum hkl -19. -19. -10.

REFLT03_ALERT_4_G ALERT: MoKa measured Friedel data cannot be used to
 determine absolute structure in a light-atom
 study EXCEPT under VERY special conditions.
 It is preferred that Friedel data is merged in such cases.
 From the CIF: `_diffirn_reflms_theta_max` 30.39
 From the CIF: `_reflms_number_total` 1846
 Count of symmetry unique reflms 1228
 Completeness (`_total/calc`) 150.33%
 TEST3: Check Friedels for noncentro structure
 Estimate of Friedel pairs measured 618
 Fraction of Friedel pairs measured 0.503
 Are heavy atom types Z>Si present no

PLAT005_ALERT_5_G No `_iucr_refine_instructions_details` in CIF ?
 PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 3.000
 PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 4 Units
 PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su .. 3.00
 PLAT950_ALERT_5_G Reported and Calculated Hmax Values Differ by .. 2

1 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 7 **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
 2 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*, 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.

