checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nia026_150k

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: nia026_150k

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Bond precision:   C-C = 0.0139 A          Wavelength=1.54186

Cell:             a=8.7148(3)     b=18.4121(6)         c=18.2547(5)
                  alpha=90        beta=101.524(2)      gamma=90
Temperature:      150 K
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	Calculated	Reported
Volume	2870.06(16)	2870.06(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C68 H48 Co N10 S2	C68 H48 Co N10 S2
Sum formula	C68 H48 Co N10 S2	C68 H48 Co N10 S2
Mr	1128.21	1128.21
Dx,g cm-3	1.306	1.306
Z	2	2
Mu (mm-1)	3.430	3.430
F000	1170.0	1170.0
F000'	1169.49	
h,k,lmax	10,22,22	10,22,22
Nref	5742	5669
Tmin,Tmax	0.550,0.663	0.079,0.199
Tmin'	0.480	

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Correction method= # Reported T Limits: Tmin=0.079 Tmax=0.199
AbsCorr = MULTI-SCAN

Data completeness= 0.987           Theta(max)= 73.144

R(reflections)= 0.1458( 4410)                    wR2(reflections)=
                                                 0.3729( 5669)
S = 0.977                  Npar= 368
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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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.37 Report

Author Response: the sample was heavily twinned. A refinement with an hkl4 led to considerably lower R-factors - Rint in particular - but was presenting spurious and intense Q-peaks. The use of the hkl5 fixed this problem but led to higher R-factors.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.166

Author Response: the sample was heavily twinned. A refinement with an hkl4 led to considerably lower R-factors - Rint in particular - but was presenting spurious and intense Q-peaks. The use of the hkl5 fixed this problem but led to higher R-factors.

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.166 Report

Author Response: the sample was heavily twinned. A refinement with an hkl4 led to considerably lower R-factors - Rint in particular - but was presenting spurious and intense Q-peaks. The use of the hkl5 fixed this problem but led to higher R-factors.

PLAT082_ALERT_2_C High R1 Value ..... 0.15 Report
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C34 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01394 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 9.455 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.750 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.168 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 20 Report

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Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 30.00 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) . 1.88 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 52 Note
PLAT930_ALERT_2_G FCF-based Twin Law (0 0 1) Est.d BASF 0.38 Check

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PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF       0.38 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         10 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          3 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   9 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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   4 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* 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 18/05/2022; check.def file version of 17/05/2022

Datablock nia026_150k - ellipsoid plot