

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ag_acs_s0021_0m

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: ag_acs_s0021_0m

Bond precision:	C-C = 0.0051 A		Wavelength=0.56086
Cell:	a=11.0287 (7)	b=17.3343 (10)	c=8.0027 (5)
	alpha=90	beta=101.7353 (16)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	1497.94(16)	1497.93(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C10 H13 Hg I2 N O S	C10 H13 Hg I2 N O S
Sum formula	C10 H13 Hg I2 N O S	C10 H13 Hg I2 N O S
Mr	649.66	649.66
Dx, g cm ⁻³	2.881	2.881
Z	4	4
Mu (mm ⁻¹)	7.867	7.775
F000	1160.0	1160.0
F000'	1150.08	
h, k, lmax	15, 24, 11	15, 24, 11
Nref	4605	4604
Tmin, Tmax	0.207, 0.403	0.344, 0.489
Tmin'	0.186	

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Correction method= # Reported T Limits: Tmin=0.344 Tmax=0.489
AbsCorr = MULTI-SCAN
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Data completeness= 1.000 Theta (max)= 23.659

R(reflections)= 0.0215(4136)	wR2(reflections)= 0.0493(4604)
S = 1.080	Npar= 197

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

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
outside the range 0.99 <> 1.01
Calculated value of mu = 7.867
Value of mu given = 7.775
PLAT051_ALERT_1_C Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 1.18 %
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.7 Ratio
PLAT245_ALERT_2_C U(iso) H6A Smaller than U(eq) C6 by 0.012 Ang**2
PLAT352_ALERT_3_C Short N-H (X0.87,N1.01A) N1 - H1 . 0.75 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor N1 --H1 . Please Check
PLAT977_ALERT_2_C Check Negative Difference Density on H10B . -0.37 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.21 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 12 Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Hg1 --I2 . 67.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Hg1 --I2_b . 45.2 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Hg1 (II) . 2.38 Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
-11 0 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.337 Note
Predicted wR2: Based on SigI**2 2.11 or SHELX Weight 4.56
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info
PLAT982_ALERT_1_G The Hg-f' = -0.7711 Deviates from IT-value = -0.8801 Check
PLAT982_ALERT_1_G The I-f' = -0.8561 Deviates from IT-value = -0.8919 Check
PLAT983_ALERT_1_G The Hg-f" = 6.3276 Deviates from IT-Value = 6.2989 Check
PLAT983_ALERT_1_G The I-f" = 1.1928 Deviates from IT-Value = 1.1868 Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

- 6 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
2 ALERT type 3 Indicator that the structure quality may be low
1 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* 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.

