checkCIF/PLATON report

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

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: 1

Bond precision: C-C = 0.0073 A Wavelength=0.71073 Cell: a=17.319(4)b=11.500(2)c=15.459(3)alpha=90 beta=99.80(3) gamma=90 Temperature: 293 K Calculated Reported Volume 3034.0(11) 3034.4(11) C 2/c C 2/c Space group Hall group -C 2yc -C 2yc Moiety formula C18 H11 Ag N2 O3 ? Sum formula C18 H11 Ag N2 O3 C18 H11 Ag N2 O3 Mr 411.16 411.16 1.800 1.800 Dx,g cm-3 Ζ 8 8 Mu (mm-1)1.348 1.347 F000 1632.0 1632.0 F000′ 1625.45 h,k,lmax 20,13,18 20,13,18 2679 2675 Nref Tmin, Tmax Tmin' Correction method= Not given Data completeness= 0.999 Theta(max) = 25.009 R(reflections) = 0.0491(1957) wR2(reflections) = 0.1203(2675) S = 1.000Npar= 217

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 Please Check PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check 02 Check PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1 1.53 Ang. Alert level G PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do ! PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check PLAT200_ALERT_1_G Reported __diffrn_ambient_temperature (K) 293 Check --02_c . PLAT232 ALERT 2 G Hirshfeld Test Diff (M-X) Aq1 8.0 s.u. PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C6 -C8 d 1.46 Ang. 0 ALERT level A = Most likely a serious problem - resolve or explain O ALERT level B = A potentially serious problem, consider carefully 5 ALERT level C = Check. Ensure it is not caused by an omission or oversight 6 ALERT level G = General information/check it is not something unexpected 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 ALERT type 2 Indicator that the structure model may be wrong or deficient

O ALERT type 3 Indicator that the structure quality may be low O 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* 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 06/01/2019; check.def file version of 19/12/2018

Datablock 1 - ellipsoid plot

