checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2a-revised

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: 2a-revised

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Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:           a=16.4306(6)    b=7.5182(2)         c=21.6031(7)
                alpha=90        beta=103.395(7)     gamma=90
Temperature:    150 K

                Calculated                Reported
Volume          2596.00(16)               2596.01(16)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C40 H26                   C40 H26
Sum formula     C40 H26                   C40 H26
Mr              506.61                    506.61
Dx,g cm-3       1.296                     1.296
Z               4                         4
Mu (mm-1)       0.073                     0.073
F000            1064.0                    1064.0
F000'           1064.39
h,k,lmax        21,9,28                   21,9,28
Nref            5943                      5928
Tmin,Tmax       0.991,0.996
Tmin'           0.982

Correction method= Not given

Data completeness= 0.997          Theta(max)= 27.461

R(reflections)= 0.0434( 4560)     wR2(reflections)= 0.1004( 5928)

S = 1.039                 Npar= 465
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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

PLAT410_ALERT_2_B Short Intra H...H Contact H2 ..H26 . 1.83 Ang.
x,y,z = 1_555 Check

Author Response: The short intramolecular contacts, which were pointed out at 'Alart B level' were found between sterically crowded fluorenylidene and two fluorenyl groups bonded to the central carbon atom, C40. 'H2' and 'H11' are the hydrogen atoms at 1- and 8-positions (C2 and C11, respectively) of the fluorenylidene group, respectively, and 'H26' and 'H27' are those at 9-position of each of two fluorenyl groups (C26 and C27, respectively). The hydrogen atoms were located on the difference Fourier maps and refined their positions and isotropic temperature factors.

PLAT410_ALERT_2_B Short Intra H...H Contact H11 ..H27 . 1.85 Ang.
x,y,z = 1_555 Check

Author Response: The short intramolecular contacts, which were pointed out at 'Alart B level' were found between sterically crowded fluorenylidene and two fluorenyl groups bonded to the central carbon atom, C40. 'H2' and 'H11' are the hydrogen atoms at 1- and 8-positions (C2 and C11, respectively) of the fluorenylidene group, respectively, and 'H26' and 'H27' are those at 9-position of each of two fluorenyl groups (C26 and C27, respectively). The hydrogen atoms were located on the difference Fourier maps and refined their positions and isotropic temperature factors.

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.890 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

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Alert level G

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 10 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 18 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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 04/06/2020; check.def file version of 02/06/2020

Datablock 2a-revised - ellipsoid plot