checkCIF/PLATON report

Structure factors have been supplied for datablock(s) magd78

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: magd78

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Bond precision:   C-C = 0.0016 A            Wavelength=1.54184

Cell:           a=9.8768(3)        b=10.2082(3)      c=11.6883(4)
                alpha=104.144(3)   beta=90.248(3)   gamma=104.209(2)
Temperature:    100 K

                   Calculated                  Reported
Volume          1105.18(6)                  1105.18(6)
Space group     P -1                        P -1
Hall group      -P 1                        ?
Moiety formula  C50 H70 Li2 N4 O2           ?
Sum formula     C50 H70 Li2 N4 O2           C50 H70 Li2 N4 O2
Mr              772.98                      772.98
Dx,g cm-3       1.161                       1.161
Z               1                           1
Mu (mm-1)       0.530                       0.530
F000            420.0                       420.0
F000'           421.06
h,k,lmax        12,12,14                    12,12,14
Nref            4665                        4628
Tmin,Tmax       0.938,0.948                 0.939,0.949
Tmin'           0.938

Correction method= MULTI-SCAN

Data completeness= 0.992          Theta(max)= 76.970

R(reflections)= 0.0392( 4442)     wR2(reflections)= 0.0974( 4628)

S = 1.027                  Npar= 262
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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 C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             CrysAlisPro,
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             Agilent
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             Technologies,
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             Version
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             1.171.36.28
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             (release
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             01
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             02
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             2013
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             CrysAlis171
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             .NET)
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             (compiled
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             Feb
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.

CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             1
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
             identifier.
             2013,16:14:44)
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical   ? Check
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .   mixed
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C1   -- C2   ..   6.7 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C3   -- C4   ..   5.5 su
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond C3   - C4   ...   1.44 Ang.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #   14 Do !
          N1 -C1 -C2 -C3   -41.10 1.30   1.555   1.555   1.555   1.555

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PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          15 Do !
          N2  -C1  -C2  -C3    136.70  1.20   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          16 Do !
          LI  -C1  -C2  -C3   -114.30  1.20   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          17 Do !
          C1  -C2  -C3  -C4     34.00  4.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          18 Do !
          C2  -C3  -C4  -C9    -94.00  4.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          19 Do !
          C2  -C3  -C4  -C5     86.00  4.00   1.555   1.555   1.555   1.555
PLAT793_ALERT_4_G The Model has Chirality at C1       .............       S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       37 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

  19 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
   0 ALERT type 3 Indicator that the structure quality may be low
   8 ALERT type 4 Improvement, methodology, query or suggestion
   1 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*, 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 24/07/2014; check.def file version of 24/07/2014

NOMOVE FORCED

Prob = 50
Temp = 100

-33 Y

PLATON-Aug 19 10:43:29 2014 — (100912)

Z -149   magd78   P -1   R = 0.04   RES=   0   -83 X