checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Li8-MOF

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: Li8-MOF

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=9.8956(6) b=13.8451(9) c=14.4170(9)
alpha=95.736(2) beta=94.844(2) gamma=102.727(2)
Temperature: 200 K

	Calculated	Reported
Volume	1905.5(2)	1905.5(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C37 H27 Li4 N3 O9), C3 H7 N O [+ solvent]	C77 H61 Li8 N7 O19
Sum formula	C77 H61 Li8 N7 O19 [+ solvent]	C77 H61 Li8 N7 O19
Mr	1443.85	1443.84
Dx,g cm-3	1.258	1.258
Z	1	1
Mu (mm-1)	0.089	0.089
F000	748.0	748.0
F000'	748.38	
h,k,lmax	11,16,16	11,16,16
Nref	6285	6261
Tmin,Tmax	0.981,0.982	0.981,0.982
Tmin'	0.981	

Correction method= # Reported T Limits: Tmin=0.981 Tmax=0.982
AbsCorr = NONE

Data completeness= 0.996 Theta(max)= 24.420

R(reflections)= 0.0664(4709)

wR2(reflections)= 0.2200(6261)

S = 1.045 Npar= 556

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

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.02 eA-3

Author Response: The residual Q peak is situated near the coordinated DMF, which appears to be somewhat disordered.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5817
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.64 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 Li Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C15 -C17 . 1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00435 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.582 21 Report
-2 0 3, -9 -2 7, -6 1 7, -7 2 7, -4 -1 8, -10 4 8,
-7 11 9, -5 -3 10, -9 3 10, -8 4 10, 0-13 11, -5 -3 11,
3-12 12, -5 -3 12, -8 1 12, -4 -9 13, -8 1 13, -6 -3 14,
-5 -3 14, -7 -1 14, -5 4 15,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 4 Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 2(C37 H27 Li4 N3 O9), C3 H7 N O
Rep.: C77 H61 Li8 N7 O19
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N4 Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of C35       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C36       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C37       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H36A      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H36B      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H36C      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37A      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37B      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37C      Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         6% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O9       .       60.3 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        45 A**3
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.11 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      40.96 Deg.
             O6   -C25  -LI4     1_555   1_555   2_567 ......     #  124 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        63 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        48% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
               0  1  0,   0  0  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       4.23 Note
             Predicted wR2: Based on SigI**2  5.20 or SHELX Weight 22.06
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         2 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
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
20 ALERT type 4 Improvement, methodology, query or suggestion
3 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 06/01/2024; check.def file version of 05/01/2024

Datablock Li8-MOF - ellipsoid plot