

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ewc160008, rm634

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: ewc160008

Bond precision: C-C = 0.0040 A

Wavelength=0.68890

Cell: a=8.5700(6) b=11.6230(8) c=21.8670(15)
 alpha=104.360(3) beta=92.391(3) gamma=99.597(3)
Temperature: 100 K

	Calculated	Reported
Volume	2072.7(3)	2072.7(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C41 H54 Mg N4 O2), C7 H8	C41 H54 Mg N4 O2,0.5 C7 H8
Sum formula	C89 H116 Mg2 N8 O4	C44.5 H58 Mg N4 O2
Mr	1410.52	705.26
Dx,g cm-3	1.130	1.130
Z	1	2
Mu (mm-1)	0.076	0.078
F000	762.0	762.0
F000'	762.28	
h,k,lmax	10,14,27	10,14,27
Nref	8455	39658
Tmin,Tmax	0.994,0.998	
Tmin'	0.993	

Correction method= Not given

Data completeness= 4.690

Theta(max)= 25.458

R(reflections)= 0.0608(28963)

wR2(reflections)= 0.1770(39658)

S = 1.077

Npar= 509

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	Please Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.1 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	90 Report

● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	7 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003 Degree
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	4 Note
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C42 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C44 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C45 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C46 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C47 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C48 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H45 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48C Constrained at	0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	7.50 Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C48 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	15 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	87 Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	28 Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.37 Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 2-1) Est.d BASF	0.36 Check

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
24 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: rm634

Bond precision: C-C = 0.0019 A

Wavelength=1.54184

Cell: a=8.8953(4) b=13.2359(7) c=13.5066(8)
 alpha=87.598(5) beta=79.970(4) gamma=80.009(4)
 Temperature: 123 K

	Calculated	Reported
Volume	1542.07(14)	1542.07(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H88 Mg2 N4 O2	C60 H88 Mg2 N4 O2
Sum formula	C60 H88 Mg2 N4 O2	C60 H88 Mg2 N4 O2
Mr	945.96	945.96
Dx,g cm-3	1.019	1.019
Z	1	1
Mu (mm-1)	0.647	0.647
F000	516.0	516.0
F000'	517.55	
h,k,lmax	11,16,16	10,16,16
Nref	6164	6031
Tmin,Tmax	0.792,0.879	0.374,1.000
Tmin'	0.678	

Correction method= # Reported T Limits: Tmin=0.374 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.978

Theta(max)= 72.963

R(reflections)= 0.0462(5565)

wR2(reflections)= 0.1329(6031)


S = 1.062

Npar= 330

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 A**

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 228 Ang**3

 **Alert level C**

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 19 Report

 **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
 PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
 PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
 PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 9% Note
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note

PLAT860_ALERT_3_G	Number of Least-Squares Restraints	30	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	109	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	13	Info

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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.

