

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxl

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: shelxl

Bond precision: C-C = 0.0093 A Wavelength=0.71073

Cell: a=8.7527(1) b=30.9753(5) c=13.0054(2)
 alpha=90 beta=90 gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	3525.99(9)	3525.99(9)
Space group	P n m a	Pnma
Hall group	-P 2ac 2n	?
Moiety formula	C15 H26 Ce2 O16, 2(H2 O), 6.22(O0.50), 2.28(O)	?
Sum formula	C15 H30 Ce2 O26	C15 H46 Ce2 O26
Mr	906.63	922.76
Dx,g cm-3	1.708	1.738
Z	4	4
Mu (mm-1)	2.636	2.637
F000	1776.0	1840.0
F000'	1775.18	
h,k,lmax	10,36,15	10,36,15
Nref	3174	3171
Tmin,Tmax	0.458,0.590	0.581,0.679
Tmin'	0.449	

Correction method= # Reported T Limits: Tmin=0.581 Tmax=0.679
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0446(2873) wR2(reflections)= 0.1068(3171)

S = 1.258 Npar= 246

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

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 16.13 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 010 Check
PLAT430_ALERT_2_B Short Inter D...A Contact O2 .. O13' .. 2.84 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact O10 .. O11 .. 2.75 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact O10 .. O11' .. 2.80 Ang.
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

● Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.99 <> 1.01
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 922.76
TEST: Calculate formula weight from _atom_site_*
atom mass num sum
C 12.01 15.00 180.16
H 1.01 30.00 30.24
O 16.00 26.00 415.97
Ce 140.12 2.00 280.24
Calculated formula weight 906.62
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ce1 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00929 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact O2 .. O13 .. 2.89 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 4.784 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
PLAT972_ALERT_2_C Check Calcd Residual Density 1.27A From O1 -1.92 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.67A From O12 -1.74 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.90A From O10 1.26 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.56A From O10 0.94 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.96A From O11' 0.48 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 1.00A From O1 -0.72 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.41A From O11' -0.70 eA-3

● Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C15 H46 Ce2 O26
Atom count from the _atom_site data: C15 H30 Ce2 O26
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C15 H46 Ce2 O26
TEST: Compare cell contents of formula and atom_site data
atom Z*formula cif sites diff
C 60.00 60.00 0.00
H 184.00 120.00 64.00
Ce 8.00 8.00 0.00
O 104.00 104.00 0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 7 Report

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	22.58	Why ?
PLAT302_ALERT_4_G	Anion/Solvent Disorder Percentage =	62	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	011	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	012	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	012'	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	013	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	011'	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	013'	Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	4	Do !
	C1 -C2 -C3 -CE1 3.00 6.00 1.555 1.555 1.555	6.556	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	7	Do !
	CE1 -C4 -C5 -C6 72.00 10.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	12	Do !
	C6 -C7 -C8 -CE1 85.00 4.00 1.555 1.555 1.555	5.666	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	75	Do !
	C5 -C4 -CE1 -O1 14.00 9.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	78	Do !
	C5 -C4 -CE1 -O5 -166.00 9.00 1.555 1.555 1.555	2.664	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	81	Do !
	C5 -C4 -CE1 -O2 84.00 9.00 1.555 1.555 1.555	6.656	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	84	Do !
	C5 -C4 -CE1 -O8 101.00 9.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	86	Do !
	C5 -C4 -CE1 -O3 -3.00 9.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	89	Do !
	C5 -C4 -CE1 -O6 -97.00 9.00 1.555 1.555 1.555	5.666	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	92	Do !
	C5 -C4 -CE1 -O7 -73.00 9.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	94	Do !
	C5 -C4 -CE1 -O4 18.00 0.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	97	Do !
	C5 -C4 -CE1 -O1 133.00 9.00 1.555 1.555 1.555	6.656	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	100	Do !
	C5 -C4 -CE1 -O5 -48.00 9.00 1.555 1.555 1.555	5.666	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	103	Do !
	C5 -C4 -CE1 -C3 109.00 9.00 1.555 1.555 1.555	6.656	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.39	Ratio
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	72	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note
PLAT909_ALERT_3_G	Percentage of Observed Data at Theta(Max) Still	86	%
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min) ...	2	Report

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 24 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 17 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*, 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 19/11/2015; check.def file version of 15/11/2017

