

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gvs1014c_0m

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: gvs1014c_0m

Bond precision:	C-C = 0.0192 A	Wavelength=1.54178	
Cell:	a=10.5235(15)	b=18.133(3)	c=19.488(3)
	alpha=90	beta=96.944(12)	gamma=90
Temperature:	173 K		
	Calculated	Reported	
Volume	3691.5(10)	3691.6(9)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C60 H60 N10 O26 P4 Sm2, 2(H2 O)	C60 H60 N10 O26 P4 Sm2, 2(H2 O)	
Sum formula	C60 H64 N10 O28 P4 Sm2	C60 H64 N10 O28 P4 Sm2	
Mr	1797.81	1797.79	
Dx,g cm-3	1.617	1.617	
Z	2	2	
Mu (mm-1)	13.393	13.393	
F000	1804.0	1804.0	
F000'	1791.13		
h,k,lmax	12,22,23	12,22,23	
Nref	7211	6996	
Tmin,Tmax	0.165,0.430	0.486,0.753	
Tmin'	0.024		

Correction method= # Reported T Limits: Tmin=0.486 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.970 Theta(max)= 71.720

R(reflections)= 0.0722(3911) wR2(reflections)= 0.1815(6996)

S = 1.020 Npar= 472

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

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of 09 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.146
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.146 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Sm1 --O12 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1 --C11 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11 --C12 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11 --C16 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14 --C15 . 0.21 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 05 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 06 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 012 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C9 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C18 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C28 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C30 Check

Author Response: This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Sm1	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	N3	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	N4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C25	Check
PLAT260_ALERT_2_C	Large	Average	Ueq of Residue Including	O14	0.109 Check
PLAT331_ALERT_2_C	Small	Aver	Phenyl C-C Dist	C5 -C10	1.37 Ang.
PLAT342_ALERT_3_C	Low	Bond	Precision on C-C Bonds	0.01919 Ang.
PLAT906_ALERT_3_C	Large	K	Value in the Analysis of Variance	5.488 Check
PLAT911_ALERT_3_C	Missing	FCF	Refl Between Thmin & STh/L=	0.600	91 Report
PLAT934_ALERT_3_C	Number of	(Iobs-Icalc)/Sigma(W)	> 10 Outliers	..	1 Check
PLAT975_ALERT_2_C	Check	Calcd	Resid. Dens.	0.83A From O1	0.45 eA-3
PLAT978_ALERT_2_C	Number	C-C	Bonds with Positive Residual Density.		0 Info

Alert level G

PLAT003_ALERT_2_G	Number of	Uiso or Uij	Restrained non-H Atoms	...	6 Report	
PLAT007_ALERT_5_G	Number of	Unrefined	Donor-H Atoms	4 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
PLAT232_ALERT_2_G	Hirshfeld	Test	Diff (M-X)	Sm1 --O5	.	5.6 s.u.
PLAT793_ALERT_4_G	Model	has	Chirality at	P2 (Centro	SPGR)	R Verify
PLAT794_ALERT_5_G	Tentative	Bond	Valency for	Sm1 (III)	.	3.46 Info
PLAT860_ALERT_3_G	Number of	Least-Squares	Restraints	48 Note	
PLAT912_ALERT_4_G	Missing	#	of FCF	Reflections Above	STh/L= 0.600	125 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
19 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
9 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* 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 07/08/2019; check.def file version of 30/07/2019

