

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cmterpytry1

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: cmterpytry1

Bond precision: C-C = 0.0078 Å

Wavelength=0.71073

Cell: a=11.1057(2) b=15.9836(3) c=16.2475(3)
 alpha=106.305(1) beta=95.170(1) gamma=95.955(1)
Temperature: 302 K

	Calculated	Reported
Volume	2731.58(9)	2731.58(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H22 Cm N8 O6, C15 H11 Cm N7 O12, 2(C2 H3 N)	C30 H22 Cm N8 O6, C15 H11 Cm N7 O12, 2(C2 H3 N)
Sum formula	C49 H39 Cm2 N17 O18	C49 H39 Cm2 N17 O18
Mr	1642.09	1642.09
Dx, g cm ⁻³	1.997	1.996
Z	2	2
Mu (mm ⁻¹)	3.054	3.054
F000	1576.0	1576.0
F000'	1547.30	
h,k,lmax	17,24,25	17,24,24
Nref	20863	19946
Tmin,Tmax	0.505,0.697	0.619,0.747
Tmin'	0.397	

Correction method= # Reported T Limits: Tmin=0.619 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.956

Theta(max)= 33.169

R(reflections)= 0.0373(15539)

wR2(reflections)=
0.0930(19946)

S = 1.040

Npar= 772

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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N14 Check
PLAT913_ALERT_3_B Missing # of Very Strong Reflections in FCF 272 Note

5	0	0,	-4	1	0,	1	1	0,	2	1	0,	4	1	0,	-2	2	0,
5	2	0,	-2	3	0,	-1	3	0,	4	3	0,	7	3	0,	0	4	0,
1	4	0,	-6	5	0,	-3	5	0,	0	5	0,	2	5	0,	-2	6	0,
-1	7	0,	0	7	0,	-4	8	0,	1	8	0,	-1	-8	1,	2	-8	1,

Alert level C

CHEMW01_ALERT_1_C The difference between the given and expected weight for
compound is greater 1 mass unit. Check that all hydrogen
atoms have been taken into account.

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
N14

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O13 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O16 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cm2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N12 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C46 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C48 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N16 0.109 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note

1 0 0, 0 1 0, 0 -1 1, 0 0 1, 0 1 1,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 689 Report

3	0	0,	5	0	0,	8	0	0,	-6	1	0,	-4	1	0,	-3	1	0,
-2	1	0,	1	1	0,	2	1	0,	4	1	0,	6	1	0,	-5	2	0,
-2	2	0,	1	2	0,	2	2	0,	3	2	0,	5	2	0,	6	2	0,
-10	3	0,	-6	3	0,	-4	3	0,	-2	3	0,	-1	3	0,	0	3	0,
2	3	0,	4	3	0,	7	3	0,	-10	4	0,	-5	4	0,	-4	4	0,
-3	4	0,	0	4	0,	1	4	0,	3	4	0,	5	4	0,	-6	5	0,
-4	5	0,	-3	5	0,	0	5	0,	1	5	0,	2	5	0,	4	5	0,
5	5	0,	-3	6	0,	-2	6	0,	-1	6	0,	1	6	0,	3	6	0,
6	6	0,	-1	7	0,	0	7	0,	2	7	0,	-4	8	0,	1	8	0,
2	8	0,	3	8	0,	4	8	0,	-3	9	0,	5	9	0,	0	11	0,
4	12	0,	3	-11	1,	4	-10	1,	1	-9	1,	-3	-8	1,	-1	-8	1,
2	-8	1,	-2	-7	1,	0	-7	1,	3	-7	1,	4	-7	1,	-3	-6	1,
-1	-6	1,	0	-6	1,	3	-6	1,	4	-6	1,	5	-6	1,	-7	-5	1,
-4	-5	1,	-2	-5	1,	1	-5	1,	2	-5	1,	4	-5	1,	6	-5	1,
-6	-4	1,	-5	-4	1,	-3	-4	1,	-2	-4	1,	-1	-4	1,	1	-4	1,
2	-4	1,	5	-4	1,	7	-4	1,	-4	-3	1,	-1	-3	1,	0	-3	1,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.30Ang From Cm1 1.71 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.21Ang From O10 1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.36Ang From Cm2 -1.84 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.48Ang From Cm2 -1.80 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.46Ang From Cm2 -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.62Ang From Cm2 -1.64 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.53Ang From Cm2 -1.53 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.88Ang From O10 . 0.63 eA-3

PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.06Ang From O18	.	-0.51 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.81Ang From O10	.	-0.42 eA-3



Alert level G

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF		Please Check
PLAT019_ALERT_1_G	_diffrn_measured_fraction_theta_full/*_max < 1.0		0.973	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.001	Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cm1 --O2	.	5.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cm1 --O5	.	6.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cm2 --O10	.	9.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cm2 --O13	.	7.7 s.u.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		1	Note
	N013			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C2 H3 N			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		4	Note
	C2 H3 N			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	221	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		1.860	Note
	Predicted wR2: Based on SigI**2	5.00 or SHELX Weight	8.94	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info
PLAT983_ALERT_1_G	The Cm-f"=	4.8980 Deviates from IT-Value =	4.6980	Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 2 **ALERT level B** = A potentially serious problem, consider carefully
 - 23 **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
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- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 23 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 4 ALERT type 3 Indicator that the structure quality may be low
 - 6 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* 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.

