

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 7aRu, 8bFe

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: 7aRu

Bond precision:	C-C = 0.0052 Å	Wavelength=0.71073		
Cell:	a=23.6049(17)	b=11.0767(8)	c=18.9574(14)	
	alpha=90	beta=98.353(3)	gamma=90	
Temperature:	100 K			

	Calculated	Reported
Volume	4904.1 (6)	4904.1 (6)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H24 N2 O3 Ru2, C H2 Cl2 ?	
Sum formula	C23 H26 Cl2 N2 O3 Ru2	C23 H26 Cl2 N2 O3 Ru2
Mr	651.50	651.50
Dx, g cm-3	1.765	1.765
Z	8	8
Mu (mm-1)	1.477	1.477
F000	2592.0	2592.0
F000'	2574.91	
h, k, lmax	31, 14, 25	31, 14, 25
Nref	5925	5925
Tmin, Tmax	0.741, 0.813	0.220, 0.340
Tmin'	0.726	

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Correction method= # Reported T Limits: Tmin=0.220 Tmax=0.340
AbsCorr = EMPIRICAL
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Data completeness= 1.000 Theta (max)= 27.998

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R(reflections)= 0.0353( 5242)      wR2(reflections)=
S = 1.031                          0.0962( 5925)
Npar= 300
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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

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.034	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.12Ang From Cl21	-1.58	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.19Ang From Cl11	-1.51	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.43Ang From Cl2	-1.51	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.41Ang From Cl2	-1.51	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H30A .	-0.32	eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	25.43	Why ?
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	1	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Rul --Cl .	5.4	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	4.12	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	0.88	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C3	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C4	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	10	Check
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	2	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	71	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1	Units
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	56.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.52	Note
	Predicted wR2: Based on SigI**2 3.82 or SHELX Weight	9.58	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
23 **ALERT level G** = General information/check it is not something unexpected
- 2 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
3 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

Datablock: 8bFe

Bond precision: N- C = 0.0125 Å

Wavelength=0.71073

Cell: a=7.1749(15) b=8.0419(17) c=14.623(3)
alpha=92.379(9) beta=96.023(9) gamma=106.019(9)
Temperature: 100 K

	Calculated	Reported
Volume	804.3(3)	804.3(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H16 Fe2 N2 O2, 2(H2 O)	?
Sum formula	C16 H20 Fe2 N2 O4	C16 H20 Fe2 N2 O4
Mr	416.04	416.04
Dx, g cm ⁻³	1.718	1.718
Z	2	2
Mu (mm ⁻¹)	1.827	1.827
F000	428.0	428.0
F000'	429.52	
h, k, lmax	8, 9, 17	8, 9, 17
Nref	2841	2799
Tmin, Tmax	0.786, 0.864	0.429, 0.746
Tmin'	0.760	

Correction method= # Reported T Limits: Tmin=0.429 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.985

Theta(max)= 24.993

R(reflections)= 0.0818(2190)

wR2(reflections)=
0.2047(2799)

S = 1.127

Npar= 223

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
O201

PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio 3.1 prolat

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.3 Note

PLAT415_ALERT_2_C Short Inter D-H..H-X H5C ..H231 . 2.11 Ang.

PLAT417_ALERT_2_C	Short Inter D-H..H-D	H231	x,y,z = ..H231 .	1_555 Check
			-x,-y,1-z = ..H231 .	2.11 Ang.
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H231	-x,-y,1-z = ..H232 .	2_556 Check
			-x,-y,1-z = ..H232 .	2.12 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			2_556 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			9.094 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.594		2.532 Check
				41 Report
	-6 -4 1, -4 -3 1, -6 -1 1, 6 0 1, 3 5 1, -6 -4 2,			
	-5 -4 2, -4 -3 2, 6 -1 2, -5 -5 3, -6 -4 3, -4 -3 3,			
	-6 -1 3, -6 -4 4, -5 -4 4, -6 -4 5, -6 -3 5, 4 -2 5,			
	-4 6 5, 5 0 6, 0 5 6, 5 -2 7, 5 2 7, 1 5 7,			
	5 -4 8, 5 -3 8, 4 1 8, -3 6 8, 2 -7 9, 4 -1 9,			
	-5 1 9, 0 6 9, 3 -7 10, 3 -6 10, 2 -5 10, 6 -1 10,			
	6 0 10, -3 5 10, 3 -2 11, 2 1 11, 1 1 12,			
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.19Ang From Fe1		1.88 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.10Ang From Fe2		1.79 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.74Ang From O101 .		0.59 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.70Ang From O101 .		0.54 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.61Ang From O101 .		0.51 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.89Ang From O201 .		-1.43 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.74Ang From O201 .		-0.79 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.85Ang From O201 .		-0.78 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.62Ang From O201 .		-0.77 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.79Ang From O201 .		-0.71 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.64Ang From O201 .		-0.59 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H231			-0.65 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H232			-0.63 eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	20	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.43	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.009	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	10	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	5	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
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	45%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C3	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H5A ..H215 .	2.09	Ang.
	x,y,z = ..H215 .	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H5A ..H111 .	2.08	Ang.
	x,-1+y,z = ..H111 .	1_545	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X H201 ..H231 .	2.13	Ang.
	x,y,z = ..H231 .	1_555	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X H201 ..H232 .	1.70	Ang.
	-x,-y,1-z = ..H232 .	2_556	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X H211 ..H231 .	1.96	Ang.
	x,y,z = ..H231 .	1_555	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X H211 ..H232 .	1.83	Ang.
	-x,-y,1-z = ..H232 .	2_556	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	334	Note
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	76%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
	0 0 1,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.9	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.16	Note
	Predicted wR2: Based on SigI**2 9.46 or SHELX Weight 18.93		

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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.



