

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound2a, compound2b, compound5a, compound5b

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: compound2a

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell: a=10.3039(3) b=18.5923(5) c=21.1023(6)
 alpha=90 beta=90 gamma=90
Temperature: 103 K

	Calculated	Reported
Volume	4042.6(2)	4042.6(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C20 H13 Cl Se, C6 H6	C26 H19 Cl Se
Sum formula	C26 H19 Cl Se	C26 H19 Cl Se
Mr	445.82	445.82
Dx, g cm ⁻³	1.465	1.465
Z	8	8
Mu (mm ⁻¹)	1.998	1.998
F000	1808.0	1808.0
F000'	1808.97	
h,k,lmax	12,22,26	12,22,26
Nref	3976	3943
Tmin,Tmax	0.825,0.905	0.754,0.907
Tmin'	0.741	

Correction method= # Reported T Limits: Tmin=0.754 Tmax=0.907
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 26.000

R(reflections)= 0.0279(3245) wR2(reflections)= 0.0615(3943)

S = 1.035 Npar= 253

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	3.424	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	32	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	12	Note



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	2	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	18	Info

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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
4 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: compound2b

Bond precision: C-C = 0.0050 A

Wavelength=0.78230

Cell:	a=15.3100(3)	b=8.0496(1)	c=13.8261(3)
	alpha=90	beta=115.690(3)	gamma=90

Temperature: 93 K

	Calculated	Reported
Volume	1535.49(6)	1535.49(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H13 Cl Te	C20 H13 Cl Te
Sum formula	C20 H13 Cl Te	C20 H13 Cl Te
Mr	416.35	416.35
Dx,g cm-3	1.801	1.801
Z	4	4
Mu (mm-1)	2.690	2.690
F000	808.0	808.0
F000'	807.60	
h,k,lmax	21,11,19	21,11,19
Nref	4469	4065
Tmin,Tmax	0.973,0.973	0.974,0.974
Tmin'	0.973	

Correction method= # Reported T Limits: Tmin=0.974 Tmax=0.974
AbsCorr = MULTI-SCAN

Data completeness= 0.910 Theta(max)= 33.333

R(reflections)= 0.0483(3521) wR2(reflections)= 0.1284(4065)

S = 1.084 Npar= 218

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.36	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 Cl Ueq(max)/Ueq(min) Range	5.2	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 1 Te Ueq(max)/Ueq(min) Range	3.7	Ratio
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	6	Report
PLAT926_ALERT_1_C	Reported and Calculated R1 Differ by	-0.0017	Check
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by	-0.0036	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.75A From Te1	2.21	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.71A From Te2	2.05	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.68A From Te2	2.04	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.76A From Te1	1.89	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.82A From Te1	1.67	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.84A From Te1	1.56	eA-3



Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.		
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	9%	Note
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond Cl - C2 .	1.54	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond Cl - C8 .	1.54	Ang.

PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C1 - C14 . 1.54 Ang.
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 398 Note
 PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 5 Note
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info
 PLAT984_ALERT_1_G The C-f' = -0.002 Deviates from the B&C-Value 0.004 Ch
 PLAT984_ALERT_1_G The Cl-f' = 0.143 Deviates from the B&C-Value 0.172 Ch
 PLAT984_ALERT_1_G The Te-f' = -0.734 Deviates from the B&C-Value -0.348 Ch

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

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

Datablock: compound5a

Bond precision: C-C = 0.0097 A

Wavelength=0.71075

Cell: a=9.3412(3) b=13.2993(7) c=21.3355(14)
 alpha=93.977(4) beta=101.963(4) gamma=103.821(2)

Temperature: 103 K

	Calculated	Reported
Volume	2498.1(2)	2498.1(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C58 H62 Cl2 Fe Ge Se	C58 H62 Cl2 Fe Ge Se
Sum formula	C58 H62 Cl2 Fe Ge Se	C58 H62 Cl2 Fe Ge Se
Mr	1037.40	1037.37
Dx,g cm-3	1.379	1.379
Z	2	2
Mu (mm-1)	1.765	1.765
F000	1072.0	1072.0
F000'	1073.66	
h,k,lmax	11,16,26	11,16,26
Nref	10348	10245
Tmin,Tmax	0.844,0.884	0.816,0.886
Tmin'	0.809	

Correction method= # Reported T Limits: Tmin=0.816 Tmax=0.886
 AbsCorr = MULTI-SCAN

Data completeness= 0.990

Theta(max)= 26.500

R(reflections)= 0.0736(6562) wR2(reflections)= 0.1712(10245)

S = 1.136 Npar= 596

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Gel	--Cl1	.	7.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Gel	--Cl2	.	7.6 s.u.



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.126

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.126	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C37	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C41	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00972	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	7.647	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.155	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	24	Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0	Info



Alert level G

PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		8.00	Why ?
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	5%	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1	(II)	2.09	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	78	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		5	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		64	Check

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Datablock: compound5b

Bond precision: C-C = 0.0115 A

Wavelength=0.71075

Cell: a=12.6102(6) b=15.3206(4) c=15.9034(7)
 alpha=66.692(2) beta=68.112(2) gamma=71.139(3)
 Temperature: 103 K

	Calculated	Reported
Volume	2562.02(19)	2562.03(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C58 H62 Cl2 Fe Ge Te	C58 H62 Cl2 Fe Ge Te
Sum formula	C58 H62 Cl2 Fe Ge Te	C58 H62 Cl2 Fe Ge Te
Mr	1086.04	1086.01
Dx,g cm-3	1.408	1.408
Z	2	2
Mu (mm-1)	1.568	1.568
F000	1108.0	1108.0
F000'	1108.79	
h,k,lmax	15,19,19	15,19,19
Nref	10617	10195
Tmin,Tmax	0.910,0.939	0.872,0.940
Tmin'	0.868	

Correction method= # Reported T Limits: Tmin=0.872 Tmax=0.940
 AbsCorr = MULTI-SCAN

Data completeness= 0.960 Theta(max)= 26.500

R(reflections)= 0.0680(7101) wR2(reflections)= 0.1487(10195)

S = 1.173 Npar= 632

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

PLAT213_ALERT_2_C Atom C60	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C Atom C61	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C Atom C65	has ADP max/min Ratio	3.6 prolat
PLAT213_ALERT_2_C Atom C49	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C Atom C50	has ADP max/min Ratio	3.7 prolat
PLAT213_ALERT_2_C Atom C56	has ADP max/min Ratio	3.4 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference C41	--C44	0.17 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of		C51 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds		0.01154 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance		5.494 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600		136 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers		1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H9		-0.39 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 ...	8	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	12.66	Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	11%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C23 ..C23	2.97	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II) .	2.09	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	286	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	67	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.







