

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: naka211

Bond precision:	C-C = 0.0040 A	Wavelength=0.71073	
Cell:	a=8.3881(7)	b=12.5836(11)	c=14.1437(12)
	alpha=88.776(1)	beta=88.865(1)	gamma=89.972(1)
Temperature:	100 K		
	Calculated	Reported	
Volume	1492.3(2)	1492.3(2)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C22 H35 Cl2 Ge N2 Rh S, C6 H6	C22 H35 Cl2 Ge N2 Rh S, C6 H6	
Sum formula	C28 H41 Cl2 Ge N2 Rh S	C28 H41 Cl2 Ge N2 Rh S	
Mr	684.11	684.09	
Dx, g cm ⁻³	1.523	1.522	
Z	2	2	
Mu (mm ⁻¹)	1.829	1.829	
F000	700.0	700.0	
F000'	699.04		
h, k, lmax	10, 15, 17	10, 15, 17	
Nref	6187	5997	
Tmin, Tmax	0.880, 0.896	0.883, 0.896	
Tmin'	0.880		

Correction method= # Reported T Limits: Tmin=0.883 Tmax=0.896
AbsCorr = NUMERICAL

Data completeness= 0.969 Theta(max)= 26.499

R(reflections)= 0.0291(5267)

wR2(reflections)=
0.0739(5997)

S = 1.006

Npar= 322

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**

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.978 Why?
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C22 H35 Cl2 Ge N2 Rh S

● **Alert level G**

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
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) Rh1 --Cl2 . 6.0 s.u.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 37.64 Deg.
N2 -GE1 -S1 1_555 1_555 1_555 # 22 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 37.62 Deg.
N1 -GE1 -S1 1_555 1_555 1_555 # 23 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
-3 1 3, 1 -2 1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.3 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 53.0 Degree

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 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 13/12/2023; check.def file version of 13/12/2023

