checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1Er_auto

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: 1Er_auto

Bond precision:	C-C = 0.0038 A	Wavelength=1.54184			
Cell:		b=16.97080(9)			
Temperature:	alpha=90 100 K	beta=102.2514(6)	gamma=90		
	Calculated	Reported			
Volume	4385.09(5)	4385.09(5	5)		
Space group	P 21/c	P 1 21/c	1		
Hall group	-P 2ybc	-P 2ybc			
Moiety formula	C18 H36 K N2 O6, Ge Si2	C20 H32 ErC20 H32 E K N2 O6	Er Ge Si2, C18 H36		
Sum formula	C38 H68 Er Ge K 1	N2 O6 Si2 C38 H68 E	Er Ge K N2 O6 Si2		
Mr	984.09	984.07			
Dx,g cm-3	1.491	1.491			
Z	4	4			
Mu (mm-1)	6.008	6.008			
F000	2020.0	2020.0			
F000′	1985.42				
h,k,lmax	16,20,24	16,20,24			
Nref	8644	8561			
Tmin,Tmax	0.272,0.548	0.316,1.0	000		
Tmin'	0.143				
Correction method= # Reported T Limits: Tmin=0.316 Tmax=1.000 AbsCorr = MULTI-SCAN					
Data completeness= 0.990 Theta(max)= 72.120					
R(reflections)=	0.0283(8380)		wR2(reflections)= 0.0776(8561)		
S = 1.067	Npar=	469			

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

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT221_ALERT_2_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range	4.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	Er1 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.1 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.7 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H14 .	-0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19 .	-0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21 .	-0.43 eA-3

Alert level G

PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing	0.00009 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing	0.00013 Ang.
<pre>PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).</pre>	2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	81 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	4.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	8 Info

0 ALERT level A = Most likely a serious problem - resolve or explain 0 ALERT level B = A potentially serious problem, consider carefully 8 ALERT level C = Check. Ensure it is not caused by an omission or oversight 6 ALERT level G = General information/check it is not something unexpected 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 8 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 3 ALERT type 4 Improvement, methodology, query or suggestion 0 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 28/11/2022; check.def file version of 28/11/2022

Datablock 1Er_auto - ellipsoid plot

