



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) srhfs3

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: srhfs3

Bond precision:	Hf- S = 0.0010 Å	Wavelength=0.71073	
Cell:	a=8.5041 (4)	b=3.8004 (2)	c=13.8935 (6)
	alpha=90	beta=90	gamma=90
Temperature:	300 K		
	Calculated	Reported	
Volume	449.02 (4)	449.02 (4)	
Space group	P n m a	P n m a	
Hall group	-P 2ac 2n	-P 2ac 2n	
Moiety formula	Hf2 S6, 2 (Sr)	0.5 (Hf2 S6 Sr2)	
Sum formula	Hf2 S6 Sr2	Hf S3 Sr	
Mr	724.58	362.29	
Dx, g cm-3	5.359	5.359	
Z	2	4	
Mu (mm-1)	36.164	36.164	
F000	632.0	632.0	
F000'	626.03		
h, k, lmax	12, 5, 19	12, 5, 19	
Nref	787	787	
Tmin, Tmax	0.192, 0.338	0.381, 0.746	
Tmin'	0.073		

Correction method= # Reported T Limits: Tmin=0.381 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000

Theta(max)= 30.517

R(reflections)= 0.0198(759)

wR2(reflections)=
0.0517(787)

S = 1.166

Npar= 31

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
	Calc: Hf2 S6 Sr2		
	Rep.: Hf S3 Sr		
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ	Please Check
	Calc: Hf2 S6, 2(Sr)		
	Rep.: 0.5(Hf2 S6 Sr2)		



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT013_ALERT_1_G	No _shelx_hkl_checksum Found in CIF	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	1.682 Note
	Predicted wR2: Based on SigI**2 3.07 or SHELX Weight	4.43
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction ..	! Note

- 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
6 **ALERT level G** = General information/check it is not something unexpected
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD or the ICSD.

DATABLOCK: srhfs3

- ICSD number: 154103



[Cell Parameters for 154103: 8.5254,3.8255,13.9246(90,90,90)]

Datablock srhfs3 - ellipsoid plot

