checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait **. . .**

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) FeGeTMS32THF2

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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: FeGeTMS32THF2

Bond precision: C-C = 0.0135 A Wavelength=0.71075

Cell: a=13.851(4) b=10.450(3) c=19.003(6)
alpha=90 beta=110.932(4) gamma=90

Temperature: 183 K

	Calculated	Reported
Volume	2569.0(13)	2569.1(13)
Space group	P 2/c	P 1 2/c 1
Hall group	-P 2yc	-P 2yc
Moiety formula	C26 H70 Fe Ge2 O2 Si6, 2(C4 O)	C34 H70 Fe Ge2 O4 Si6
Sum formula	C34 H70 Fe Ge2 O4 Si6	C34 H70 Fe Ge2 O4 Si6
Mr	912.51	912.46
Dx,g cm-3	1.180	1.179
Z	2	2
Mu (mm-1)	1.610	1.608
F000	960.0	960.0
F000'	962.45	
h,k,lmax	17,13,24	17,13,23
Nref	5907	5750
Tmin,Tmax	0.793,0.825	0.694,0.824
Tmin'	0.786	

Correction method= # Reported T Limits: Tmin=0.694 Tmax=0.824
AbsCorr = MULTI-SCAN

Data completeness= 0.973 Theta(max)= 27.483

R(reflections)= 0.0604(4106) wR2(reflections)= 0.1814(5750)

S = 1.055 Npar= 188

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.121
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 5 Check
O2 C14 C15 C16 C17
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of O2 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C15 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C17 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0135 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.731 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 9 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 44 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.80A From O2 -0.46 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
_publ_requested_category classification of your compound;
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
FO or CO or EO for organic.
From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or A
From the CIF: _chemical_formula_sum :C34 H70 Fe1 Ge2 O4 Si6
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.121 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT344_ALERT_2_G Unusual sp? Angle Range in Solvent/Ion for C14 Check
And 3 other PLAT344 Alerts
More ...
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C15 - C16 . 1.53 Ang.
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C16 - C17 . 1.56 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 82 Note
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 1 Check

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

2 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
7 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

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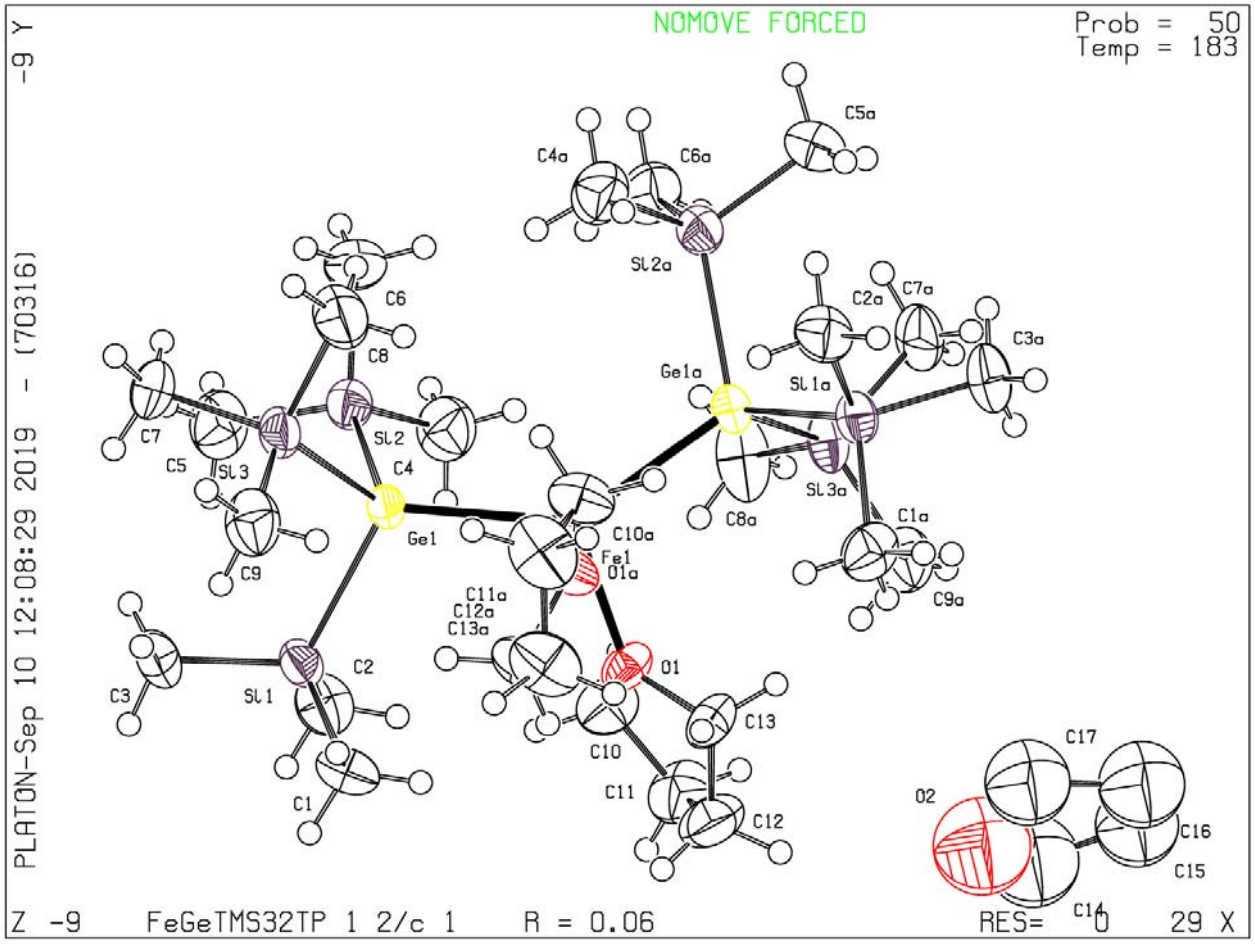
PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock FeGeTMS32THF2 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) THFMe3Si3GeFeu-OtBu2FeGeSiMe33

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: THFMe3Si3GeFeu-OtBu2FeGeSiMe33

Bond precision: C-C = 0.0060 A Wavelength=0.71075

Cell: a=15.448(2) b=16.956(2) c=19.743(3)
alpha=90 beta=102.5078(18) gamma=90

Temperature: 198 K

	Calculated	Reported
Volume	5048.7(12)	5048.6(13)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C30 H80 Fe2 Ge2 O3 Si6	C30 H80 Fe2 Ge2 O3 Si6
Sum formula	C30 H80 Fe2 Ge2 O3 Si6	C30 H80 Fe2 Ge2 O3 Si6
Mr	914.40	914.35
Dx,g cm-3	1.203	1.203
Z	4	4
Mu (mm-1)	1.909	1.908
F000	1936.0	1936.0
F000'	1942.20	
h,k,lmax	20,22,25	20,22,25
Nref	11590	11471
Tmin,Tmax	0.570,0.683	0.399,0.683
Tmin'	0.559	

Correction method= # Reported T Limits: Tmin=0.399 Tmax=0.683
AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta(max)= 27.502

R(reflections)= 0.0483(10070) wR2(reflections)= 0.1312(11471)

S = 1.047 Npar= 388

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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 21 Note

Alert level C

PLAT213_ALERT_2_C Atom C22 has ADP max/min Ratio ..... 3.6 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.4 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ge2 Check
And 5 other PLAT242 Alerts
More ...
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 66 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 11 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Fe1 1.11 eA-3

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
_publ_requested_category classification of your compound;
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
FO or CO or EO for organic.
From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or A
From the CIF: _chemical_formula_sum :C30 H80 Fe2 Ge2 O3 Si6
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 32 Note

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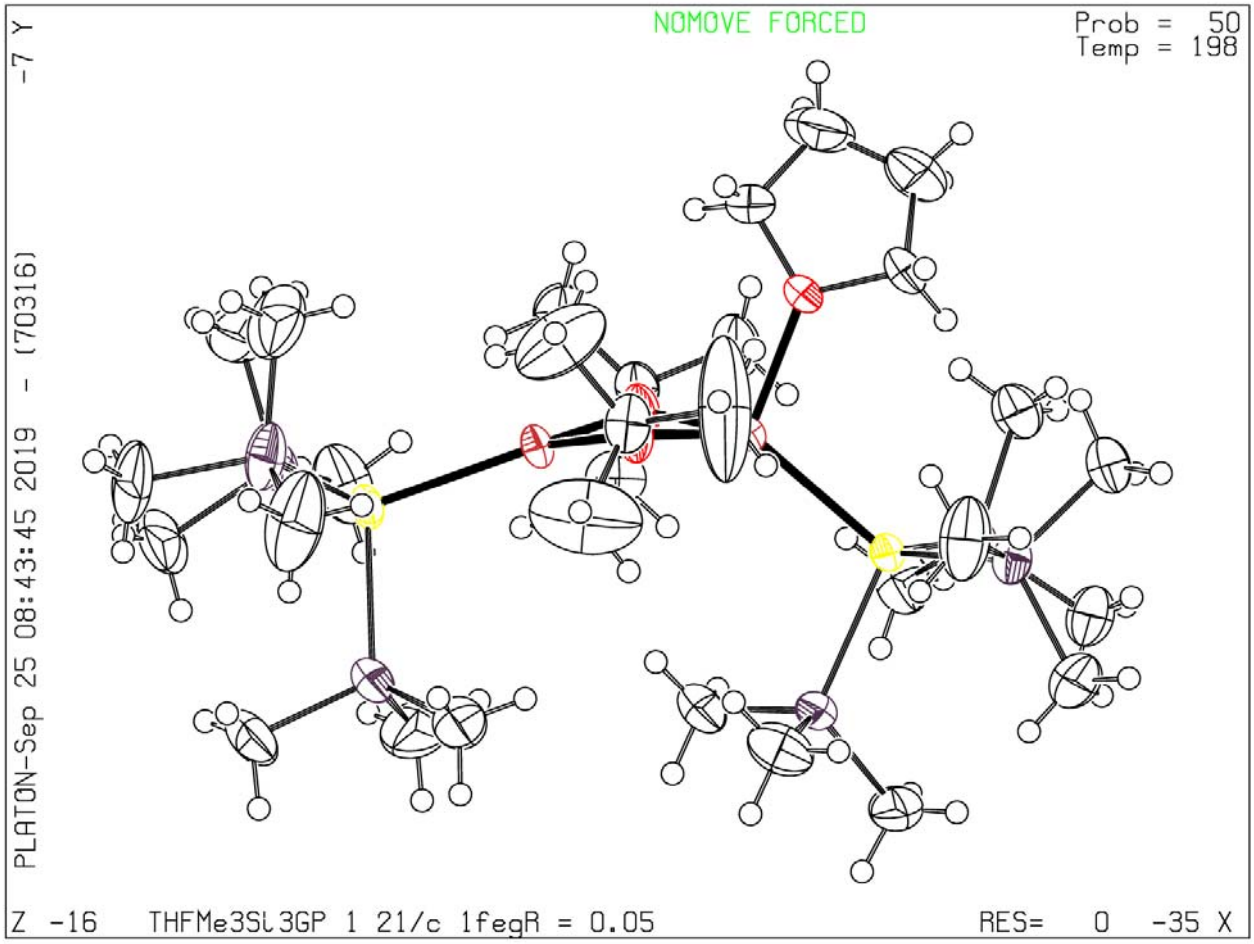
PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock THFMe3Si3GeFeu-OtBu2FeGeSiMe33 - ellipsoid plot



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