checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ab_si_002_01_sq_sq_sq, jw1119_01, jw1121_01, saku001_03

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: ab_si_002_01_sq_sq_sq

Bond precision: C-C = 0.0025 A Wavelength=0.71073

Cell: a=12.1634(6) b=17.0246(10) c=11.4268(7)
alpha=90 beta=101.450(4) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	2319.1(2)	2319.1(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H17 N3 O3 Si [+ solvent]	C21 H17 N3 O3 Si, C4 H8 O
Sum formula	C21 H17 N3 O3 Si [+ solvent]	C25 H25 N3 O4 Si
Mr	387.47	459.57
Dx,g cm-3	1.110	1.316
Z	4	4
Mu (mm-1)	0.124	0.138
F000	808.0	968.0
F000'	808.65	
h,k,lmax	16,22,15	16,22,15
Nref	5596	5587
Tmin,Tmax	0.952,0.980	0.948,0.985
Tmin'	0.940	

Correction method= # Reported T Limits: Tmin=0.948 Tmax=0.985
AbsCorr = INTEGRATION

Data completeness= 0.998 Theta(max)= 27.999

R(reflections)= 0.0425(4030) wR2(reflections)= 0.1203(5587)

S = 1.072 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

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si1      --C16      .        5.9 s.u.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          5 Report
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C25 H25 N3 O4 Si1
           Atom count from the _atom_site data:  C21 H17 N3 O3 Si1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C25 H25 N3 O4 Si
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        100.00     84.00   16.00
           H        100.00     68.00   32.00
           N         12.00     12.00    0.00
           O         16.00     12.00    4.00
           Si         4.00      4.00    0.00
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.8 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       56.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
```

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

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

Datablock: jw1119_01

Bond precision: C-C = 0.0026 A Wavelength=0.71073

Cell: a=12.2304(4) b=16.8989(4) c=11.3681(3)
alpha=90 beta=101.160(2) gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	2305.13(11)	2305.13(11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H17 N3 O3 Si, C H Cl3	C21 H17 N3 O3 Si, C H Cl3
Sum formula	C22 H18 Cl3 N3 O3 Si	C22 H18 Cl3 N3 O3 Si
Mr	506.71	506.83
Dx,g cm-3	1.460	1.460
Z	4	4
Mu (mm-1)	0.479	0.480
F000	1039.8	1040.0
F000'	1042.22	
h,k,lmax	16,22,15	16,22,15
Nref	5568	5563
Tmin,Tmax	0.817,0.953	0.789,0.957
Tmin'	0.806	

Correction method= # Reported T Limits: Tmin=0.789 Tmax=0.957
AbsCorr = INTEGRATION

Data completeness= 0.999 Theta(max)= 28.000

R(reflections)= 0.0420(4539) wR2(reflections)= 0.1059(5563)

S = 1.053 Npar= 353

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 ..... 4.015 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        12 Note
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         2 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )      1.34 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )      1.58 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )      2.08 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        73 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.7 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......    Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      56.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         8 Info
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  2 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
  5 ALERT type 3 Indicator that the structure quality may be low
  8 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check

Datablock: jw1121_01

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell:	a=9.7609(3)	b=9.7775(3)	c=9.8668(3)
	alpha=82.957(2)	beta=83.434(2)	gamma=86.564(2)
Temperature:	180 K		

	Calculated	Reported
Volume	927.42(5)	927.42(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H17 Ge N3 O3	C21 H17 Ge N3 O3
Sum formula	C21 H17 Ge N3 O3	C21 H17 Ge N3 O3
Mr	431.99	431.96
Dx,g cm-3	1.547	1.547
Z	2	2
Mu (mm-1)	1.680	1.680
F000	440.0	440.0
F000'	440.45	
h,k,lmax	12,12,13	12,12,13
Nref	4479	4480
Tmin,Tmax	0.817,0.845	0.737,0.938
Tmin'	0.604	

Correction method= # Reported T Limits: Tmin=0.737 Tmax=0.938
AbsCorr = INTEGRATION

Data completeness= 1.000 Theta(max)= 27.995

R(reflections)= 0.0310(4063) wR2(reflections)= 0.0708(4480)

S = 1.077 Npar= 254

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 G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	56.0 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	10 Info

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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
0 **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
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

Datablock: saku001_03

Bond precision: C-C = 0.0056 A Wavelength=0.71073

Cell: a=8.4129(3) b=10.9605(2) c=10.8580(3)
alpha=90 beta=98.385(2) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	990.51(5)	990.51(5)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C21 H17 N3 O3 Sn	C21 H17 N3 O3 Sn
Sum formula	C21 H17 N3 O3 Sn	C21 H17 N3 O3 Sn
Mr	478.09	478.07
Dx,g cm-3	1.603	1.603
Z	2	2
Mu (mm-1)	1.316	1.316
F000	476.0	476.0
F000'	474.86	
h,k,lmax	11,14,14	11,14,14
Nref	5262[2764]	5258
Tmin,Tmax	0.736,0.877	0.782,0.875
Tmin'	0.667	

Correction method= # Reported T Limits: Tmin=0.782 Tmax=0.875
AbsCorr = INTEGRATION

Data completeness= 1.90/1.00 Theta(max)= 28.999

R(reflections)= 0.0184(5083) wR2(reflections)= 0.0433(5258)

S = 1.256 Npar= 254

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 G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Sn1 --O2 .	5.7 s.u.
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	58.0 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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0 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
1 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

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

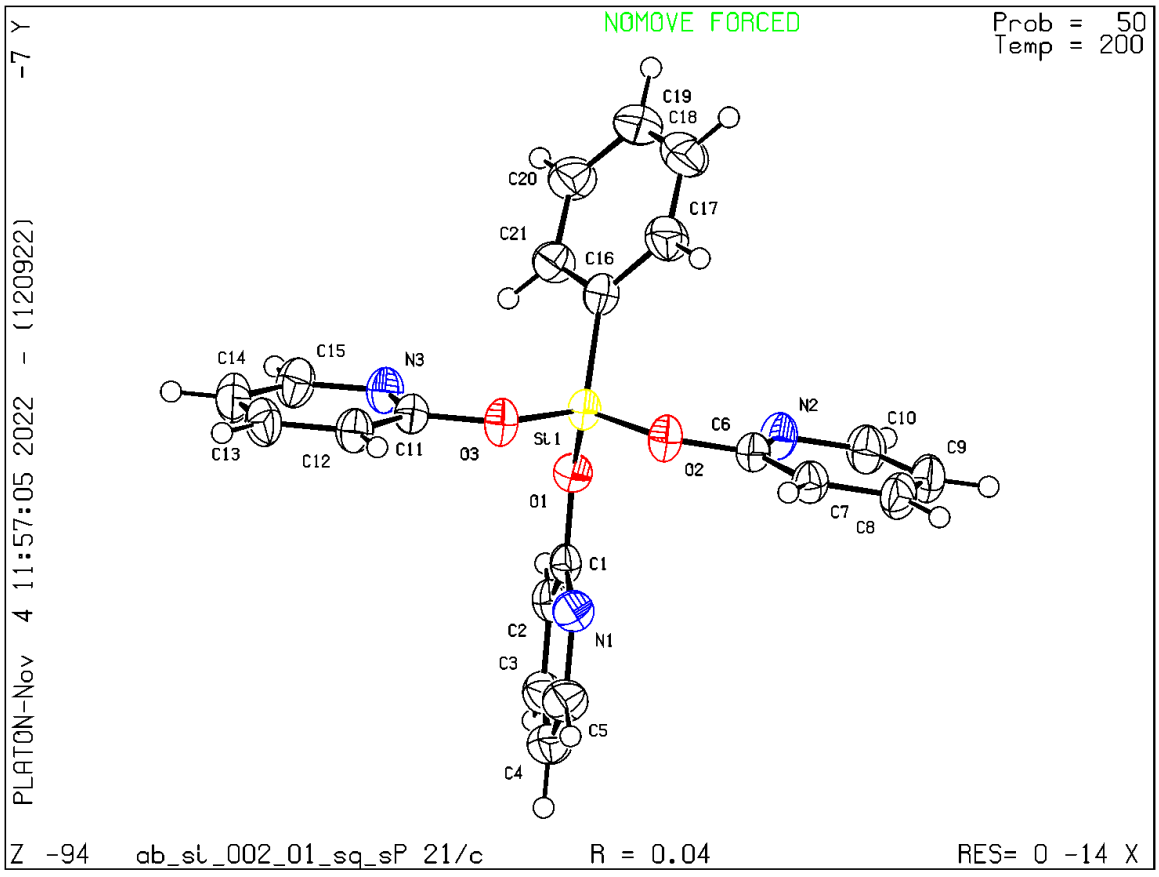
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
```

```
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

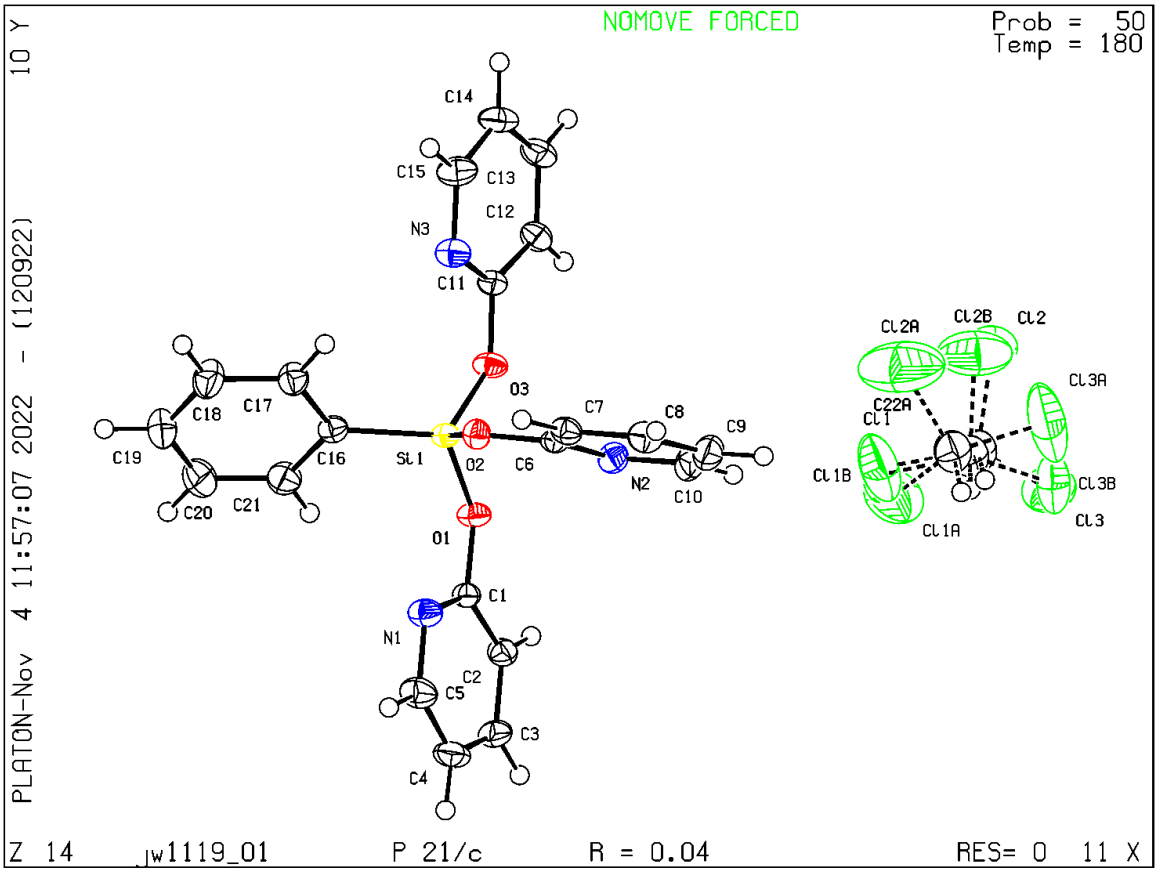
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

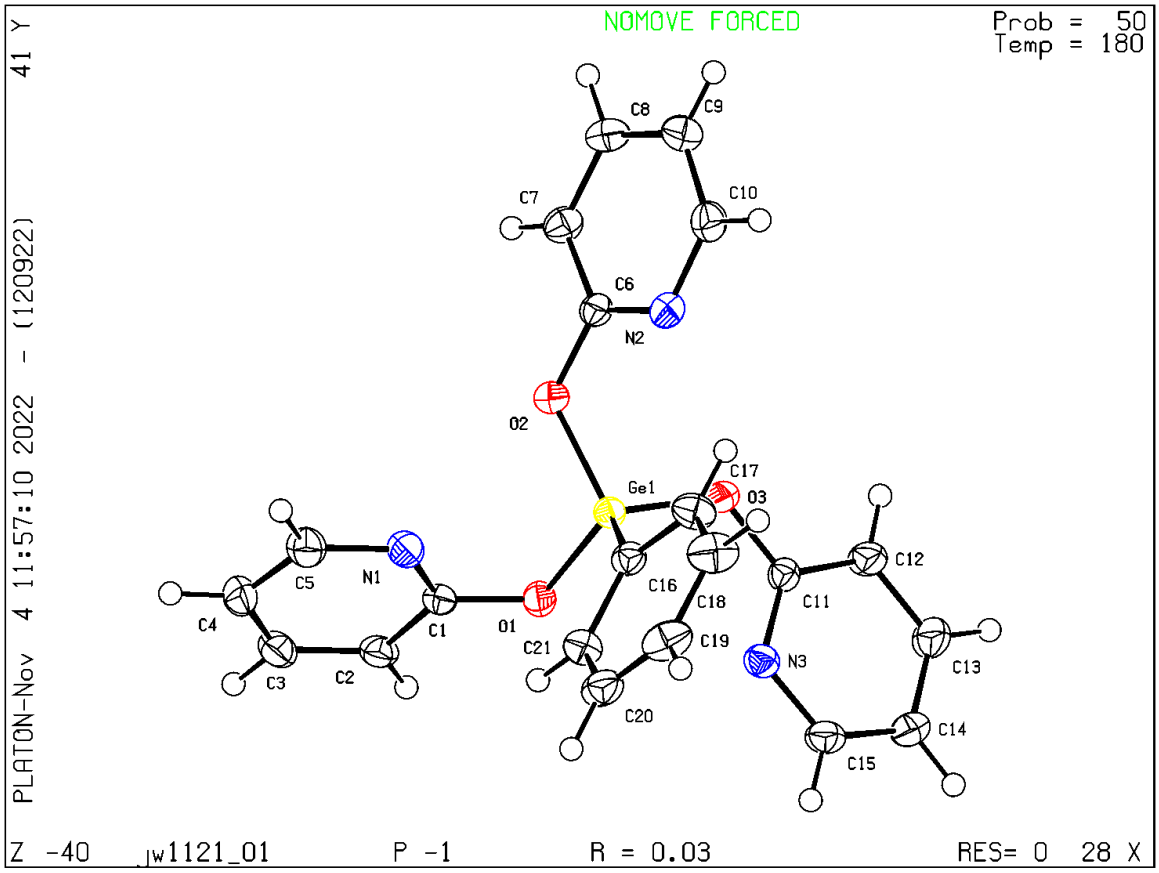
Datablock ab_si_002_01_sq_sq_sq - ellipsoid plot



Datablock jw1119_01 - ellipsoid plot



Datablock jw1121_01 - ellipsoid plot



Datablock saku001_03 - ellipsoid plot