Table S1  Crystallographic parameters for compounds 1 - 5

<table>
<thead>
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<td><strong>Empirical formula</strong></td>
<td>C_{26}H_{62}GaLiN_{4}Si_{2}</td>
<td>C_{26}H_{62}GaLiN_{4}Si_{3}</td>
<td>C_{28}H_{63}GaLiN_{5}O_{2}Si_{3}</td>
<td>C_{28}H_{63}GaN_{4}Na_{1}Si_{2}</td>
<td>C_{25}H_{56}Ga_{1}N_{3}O_{1}Si_{3}</td>
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<td><strong>Mol. Mass</strong></td>
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<td>orthorhombic</td>
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<td>10.4261(3)</td>
<td>11.7056(6)</td>
<td>18.5579(11)</td>
<td>10.0679(4)</td>
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<tr>
<td><strong>b/ Å</strong></td>
<td>10.8705(5)</td>
<td>23.2204(7)</td>
<td>18.4572(8)</td>
<td>11.1293(5)</td>
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<td><strong>c/ Å</strong></td>
<td>16.4967(9)</td>
<td>14.7638(4)</td>
<td>18.2034(10)</td>
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<td>90</td>
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<td>90</td>
<td>90</td>
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<td>83.389(3)</td>
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<tr>
<td><strong>V/ Å³</strong></td>
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<td>3746.3(3)</td>
<td>3415.3(3)</td>
<td>1714.65(11)</td>
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<tr>
<td><strong>Z</strong></td>
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<td>0.71073</td>
<td>0.71073</td>
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<td><strong>Measured reflections</strong></td>
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<td>16366</td>
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<td><strong>Unique reflections</strong></td>
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<td><strong>R [on F, obs rflns only]</strong></td>
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<td><strong>ωR [on F^2, all data]</strong></td>
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<td>0.795 / -0.571</td>
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<td>1.006 / -0.311</td>
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</table>
GaR₃ + LiTMP + OMe

i) hexane, rt, 1h

OMe

GaR₃

Li

N

N

+ ii) PMDETA (1 eq)

3, isolated yield 55%

NMR yield 74%

NMR Characterisation of 3

Figure S1 ¹H NMR in d₈-THF
**Figure S2** $^{13}$C NMR in d$_8$-THF

**Figure S3** $^7$Li NMR in d$_8$-THF
Reaction monitoring of formation of 3 from reaction between LiTMP, GaR₃, Anisole then PMDETA. 3 forms in 74% against hexamethyldibenzene as an internal standard.

**Figure S4** ¹H NMR spectrum in C₆D₆

**Figure S5** ⁷Li NMR spectrum in C₆D₆
Figure S6 $^{13}$C NMR in C$_6$D$_6$
Iodine quench of 3

![Chemical structure](image)

6I₂, THF, -78 °C

OMe
GaR₃

3

OMe

I

ca. 1%

Labelled peaks correspond to the low yield of 4 iodo anisole ca. 1% - Calculated against hexamethylbenzene internal standard (also labelled).

Figure S7  
¹H NMR in CDCl₃
NaTMP + anisole - Iodine quench – This reaction results in only 20% of 2-I-anisole.

Figure S8  $^1$H NMR spectrum in CDCl$_3$
NMR Characterisation of isolated crystals of 5 – isolated in 17% yield

Figure S9  $^1$H NMR spectrum in C$_6$D$_6$
Figure S10 $^{13}$C NMR spectrum in C$_6$D$_6$
Changing the order of addition – Characterisation of 6 – conversion to 74% against hexamethylbenzene as an internal standard

GaR₃ + anisole then NaTMP

Figure S11 ¹H NMR spectrum in C₆D₆
GaR₃ + anisole then NaTMP followed by an iodine quench, affording 2-iodo-anisole in 63% against hexamethlbenzene as an internal standard.

**Figure S12** ¹H NMR spectrum in CDCl₃
NMR characterisation of 7

Figure S13  $^1$H NMR spectrum in CDCl$_3$
Figure S14  $^{13}$C NMR spectrum in CDCl$_3$
NMR characterisation of 8

Figure S15  $^1$H NMR spectrum in CDCl$_3$
Figure S16 $^{13}$C NMR spectrum in CDCl$_3$
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) lb-11-257c, mu547b, mu687c, mu826c, rmlb1

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: mu826c

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<tr>
<td>Data completeness= 1.74/0.90</td>
<td>Theta(max)= 29.997</td>
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<tr>
<td>R(reflections) = 0.0488( 7573)</td>
<td>wR2(reflections) = 0.1316( 8796)</td>
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</table>
The following ALERTS were generated. Each ALERT has the format
\textit{test-name_ALERT_alert-type_alert-level}.
Click on the hyperlinks for more details of the test.

\section*{Alert level B}
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... \hspace{1cm} 2 Check

\section*{Alert level C}
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range \hspace{1cm} 3.2 Ratio
PLAT241_ALERT_2_C High 'MainMo' Ueq as Compared to Neighbors of C15 Check
PLAT242_ALERT_2_C Low 'MainMo' Ueq as Compared to Neighbors of N4 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds \hspace{1cm} 0.0086 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H1A ..H23C \hspace{1cm} 1.84 Ang.
\hspace{1cm} \text{x,y,z = 1_555 Check}
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Theta(Min). \hspace{1cm} 7 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= \hspace{1cm} 0.600 2 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage \hspace{1cm} 86 %
PLAT977_ALERT_2_C Check Negative Difference Density on H14A \hspace{1cm} -0.50 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. \hspace{1cm} 0 Info

\section*{Alert level G}
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C1 Check
PLAT792_ALERT_1_G Model has Chirality at N2 (Polar SPGR) R Verify
PLAT792_ALERT_1_G Model has Chirality at N3 (Polar SPGR) S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= \hspace{1cm} 0.600 310 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... \hspace{1cm} 1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... \hspace{1cm} 3 Note

0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
10 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

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
6 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

\section*{Datablock: mu547b}

\begin{center}
\begin{tabular}{ll}
Bond precision: & C-C = 0.0035 A \\
Cell: & a=10.4261(3) \hspace{1cm} b=23.2204(7) \hspace{1cm} c=14.7638(4) \\
& alpha=90 \hspace{1cm} beta=90.048(3) \hspace{1cm} gamma=90 \\
Temperature: & 123 K \\
Volume & 3565.37(18) \\
Space group & P 21/c \\
Hall group & -P 2ybc \\
Moiety formula & C24 H64 Ga Li N4 Si3 \\
Sum formula & C24 H64 Ga Li N4 Si3 \\
Mr & 569.72 \\
\end{tabular}
\end{center}

\begin{center}
\begin{tabular}{ll}
\text{Calculated} & \text{Reported} \\
Volume & 3565.37(18) \\
Space group & P 21/c \\
Hall group & -P 2ybc \\
Moiety formula & C24 H64 Ga Li N4 Si3 \\
Sum formula & C24 H64 Ga Li N4 Si3 \\
Mr & 569.72 \\
\end{tabular}
\end{center}
Dx, g cm$^{-3}$ 1.061 1.061
Z 4 4
Mu (mm$^{-1}$) 0.889 0.889
F000 1248.0 1248.0
F000' 1250.04
h,k,l$_{\text{max}}$ 14,32,20 14,30,20
N$_{\text{ref}}$ 10382 9726
T$_{\text{min}}, T_{\text{max}}$ 0.659, 0.915 0.782, 1.000
T$_{\text{min}}'$ 0.581

Correction method: # Reported T Limits: T$_{\text{min}}$=0.782 T$_{\text{max}}$=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.937 Theta(max)= 29.977
R(reflections)= 0.0438 (6921) wR2(reflections)= 0.0934 (9726)
S = 1.034 Npar= 314

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**
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

**Alert level C**
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.5 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.7 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ...... 3.315 Check

**Alert level G**
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C17 Check
PLAT793_ALERT_4_G Model has Chirality at N1 (Centro SPGR) R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 580 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

1 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
1 ALERT type 5 Informative message, check

**Datablock: mu687c**

Bond precision: C-C = 0.0025 A
Wavelength=0.71073
Cell: a=11.7056(6) b=18.4572(8) c=18.2034(10)
alpha=90 beta=107.720(6) gamma=90
Temperature: 123 K
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<td>Moiety formula</td>
<td>C28 H63 Ga Li N3 O Si3</td>
<td>C28 H63 Ga Li N3 O Si3</td>
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<td>Sum formula</td>
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<td>Mr</td>
<td>618.74</td>
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Correction method= # Reported T Limits: Tmin=0.861
Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.952 Theta(max)= 29.997
R(reflections)= 0.0355( 8291) wR2(reflections)= 0.0837( 10393)
S = 1.049 Npar= 349

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
**PLAT910_ALERT_3_B** Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

### Alert level C
**PLAT220_ALERT_2_C** Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio
**PLAT222_ALERT_3_C** Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.2 Ratio

### Alert level G
**PLAT912_ALERT_4_G** Missing # of FCF Reflections Above Sth/L= 0.600 515 Note
**PLAT978_ALERT_2_G** Number C-C Bonds with Positive Residual Density. 4 Info

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

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
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

**Datablock: rmlb1**

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<tr>
<td></td>
<td>c=16.5363(10)</td>
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</tr>
</tbody>
</table>
alpha=90  beta=90  gamma=90

Temperature: 123 K

<table>
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<th>Calculated</th>
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<td>Hall group</td>
<td>P 2c -2n</td>
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<tr>
<td>Moiety formula</td>
<td>C26 H62 Ga N4 Na Si2</td>
<td>C26 H62 Ga N4 Na Si2</td>
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<tr>
<td>Sum formula</td>
<td>C26 H62 Ga N4 Na Si2</td>
<td>C26 H62 Ga N4 Na Si2</td>
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<td>Mr</td>
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<td>Dx, g cm-3</td>
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Correction method= # Reported T Limits: Tmin=0.185 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 1.48/0.77  Theta(max)= 73.265
R(reflections)= 0.0473(4675)  wR2(reflections)= 0.1199(5258)
S = 1.071  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**
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ... 3.23 Report
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .............. 0.0092 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H18C ..H23A . 1.85 Ang.

x,y,z = 1_555 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C26 H62 Ga N4 Na Si2
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 52 %

**Alert level G**
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for 1.11 Ratio
C23 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .
PLAT792_ALERT_1_G Model has Chirality at N1 (Polar SPGR) S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 24 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT953_ALERT_1_G Reported (CIF) and Actual (FCF) Hmax Differ by . 1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

**Datablock: lb-11-257c**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0041 A</th>
<th>Wavelength=1.54184</th>
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<tbody>
<tr>
<td>Cell:</td>
<td>a=10.0679(4) b=11.0101(4) c=15.6691(6)</td>
<td>alpha=83.626(3) beta=88.933(3) gamma=83.389(3)</td>
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<td>Temperature:</td>
<td>123 K</td>
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<tr>
<td>Volume</td>
<td>1714.65(11)</td>
<td>1714.65(11)</td>
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<tr>
<td>Space group</td>
<td>P -1</td>
<td>P -1</td>
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<tr>
<td>Hall group</td>
<td>-P 1</td>
<td>-P 1</td>
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<td>Moiety formula</td>
<td>C25 H56 Ga N2 Na O Si3</td>
<td>C25 H56 Ga N2 Na O Si3</td>
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<tr>
<td>Sum formula</td>
<td>C25 H56 Ga N2 Na O Si3</td>
<td>C25 H56 Ga N2 Na O Si3</td>
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<td>Mr</td>
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<tr>
<td>Dx, g cm-3</td>
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<tr>
<td>Z</td>
<td>2</td>
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<tr>
<td>Mu (mm-1)</td>
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<tr>
<td>F000</td>
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<tr>
<td>F000'</td>
<td>624.22</td>
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<tr>
<td>h,k,lmax</td>
<td>12,13,19</td>
<td>0,0,0</td>
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<tr>
<td>Nref</td>
<td>6910</td>
<td>6837</td>
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<tr>
<td>Tmin,Tmax</td>
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<td>0.232,1.000</td>
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<tr>
<td>Tmin'</td>
<td>0.195</td>
<td></td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.232 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 73.400
R(reflections)= 0.0751( 6270) wR2(reflections)= 0.2183( 6837)
S = 1.065 Npar= 312

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**
- PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si2 Check
- PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.96A From Ga1 1.74 eA-3
- And 3 other PLAT971 Alerts
- More ...
- PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Ga1 1.49 eA-3
- PLAT977_ALERT_2_C Check Negative Difference Density on H16A -0.54 eA-3
- PLAT977_ALERT_2_C Check Negative Difference Density on H22B -0.38 eA-3
- PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

**Alert level G**
- PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.18 Report
- PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
- PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
- PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 72 Note
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