checkCIF/PLATON report

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: x1950

```
Bond precision:   C-C = 0.0134 A             Wavelength=0.71073

Cell:          a=16.2901(9)      b=17.2775(8)     c=19.5167(8)
               alpha=103.329(4)  beta=101.969(4)  gamma=118.018(5)
Temperature:   180 K

                 Calculated                 Reported
Volume           4388.4(5)                  4388.4(4)
Space group      P -1                       P-1
Hall group       -P 1                       ?
Moiety formula   C81 H108 Li N9 O9 Sn4      C81 H108 Li N9 O9 Sn4
Sum formula      C81 H108 Li N9 O9 Sn4      C81 H108 Li N9 O9 Sn4
Mr               1833.55                    1833.46
Dx,g cm-3        1.388                      1.388
Z                2                          2
Mu (mm-1)        1.181                      1.181
F000             1864.0                     1864.0
F000'            1859.36
h,k,lmax         19,20,23                   19,20,23
Nref             16076                      16052
Tmin,Tmax        0.844,0.977                0.937,1.000
Tmin'            0.661

Correction method= # Reported T Limits: Tmin=0.937 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 25.350

R(reflections)= 0.0574( 10131)    wR2(reflections)= 0.1172( 16052)

S = 1.012                    Npar= 954
```

```
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

```
PLAT213_ALERT_2_C Atom C45              has ADP max/min Ratio .....      3.3 oblate
PLAT220_ALERT_2_C Large Non-Solvent  C    Ueq(max)/Ueq(min) Range      4.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O6     -- C51     ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O9     -- C78     ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C51    -- C53     ..     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C51    -- C54     ..     0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     Li1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C42 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.01335 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn    H81B   .. H26E    ..     2.11 Ang.
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      19 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      25 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF   Please Do !
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =       8 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       9 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     381 Check
           C6F  -O1  -C6    1.555   1.555   1.555         13.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     385 Check
           C24  -O3   -C24F   1.555   1.555   1.555        5.80 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      91 Note
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```
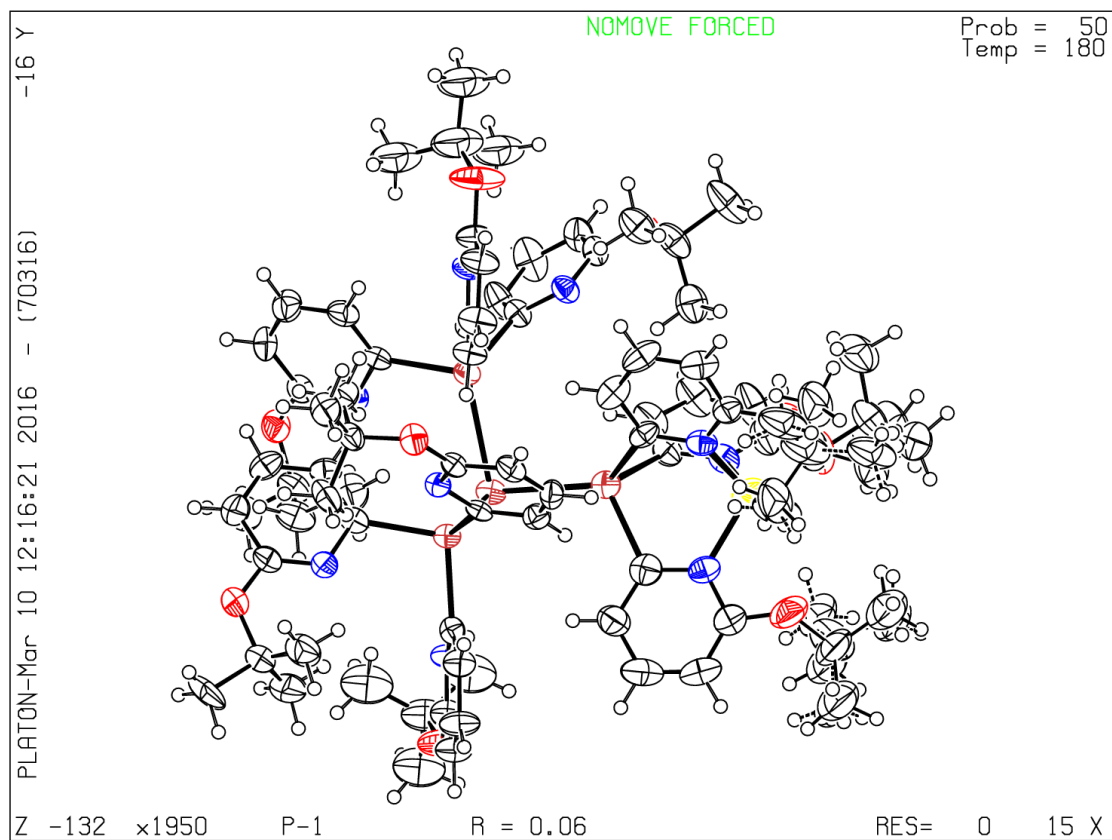
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 07/03/2016; check.def file version of 02/03/2016

checkCIF/PLATON report

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: x1964

```
Bond precision:   C-C = 0.0099 A            Wavelength=0.71073

Cell:         a=17.2766(4)       b=19.4489(6)      c=28.6285(7)
              alpha=88.874(2)   beta=85.776(2)   gamma=65.256(3)
Temperature:  130 K

                 Calculated                  Reported
Volume           8711.9(5)                   8711.9(4)
Space group      P -1                        P-1
Hall group       -P 1                        ?
Moiety formula   C81 H108 Li N9 O9 Pb Sn3    C81 H108 Li N9 O9 Pb Sn3
Sum formula      C81 H108 Li N9 O9 Pb Sn3    C81 H108 Li N9 O9 Pb Sn3
Mr               1922.04                     1921.96
Dx,g cm-3        1.465                       1.465
Z                4                           4
Mu (mm-1)        2.833                       2.833
F000             3856.0                      3856.0
F000'            3835.94
h,k,lmax         22,25,37                    22,25,37
Nref             41571                       41501
Tmin,Tmax        0.512,0.893                 0.780,1.000
Tmin'            0.319

Correction method= # Reported T Limits: Tmin=0.780 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 27.880

R(reflections)= 0.0531( 28567)     wR2(reflections)= 0.1050( 41501)

S = 1.080                   Npar= 1922
```

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

```
PLAT213_ALERT_2_C Atom O8              has ADP max/min Ratio .....      3.1 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C    Ueq(max)/Ueq(min) Range      4.4 Ratio
PLAT220_ALERT_2_C Large Non-Solvent  C    Ueq(max)/Ueq(min) Range      5.4 Ratio
PLAT222_ALERT_3_C Large Non-Solvent  H    Uiso(max)/Uiso(min) ...      4.6 Ratio
PLAT222_ALERT_3_C Large Non-Solvent  H    Uiso(max)/Uiso(min) ...      5.9 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C69   -- C71     ..      0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     O8 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C75 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C24 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C51 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C69 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C96 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C114 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C123 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00986 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #        1 Note
            C81 H108 Li N9 O9 Pb Sn3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       32 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF   Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    14.56 Why ?
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =        1 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      142 Check
            C35F -C33  -C35     1.555   1.555   1.555          12.70 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      166 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  17 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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```
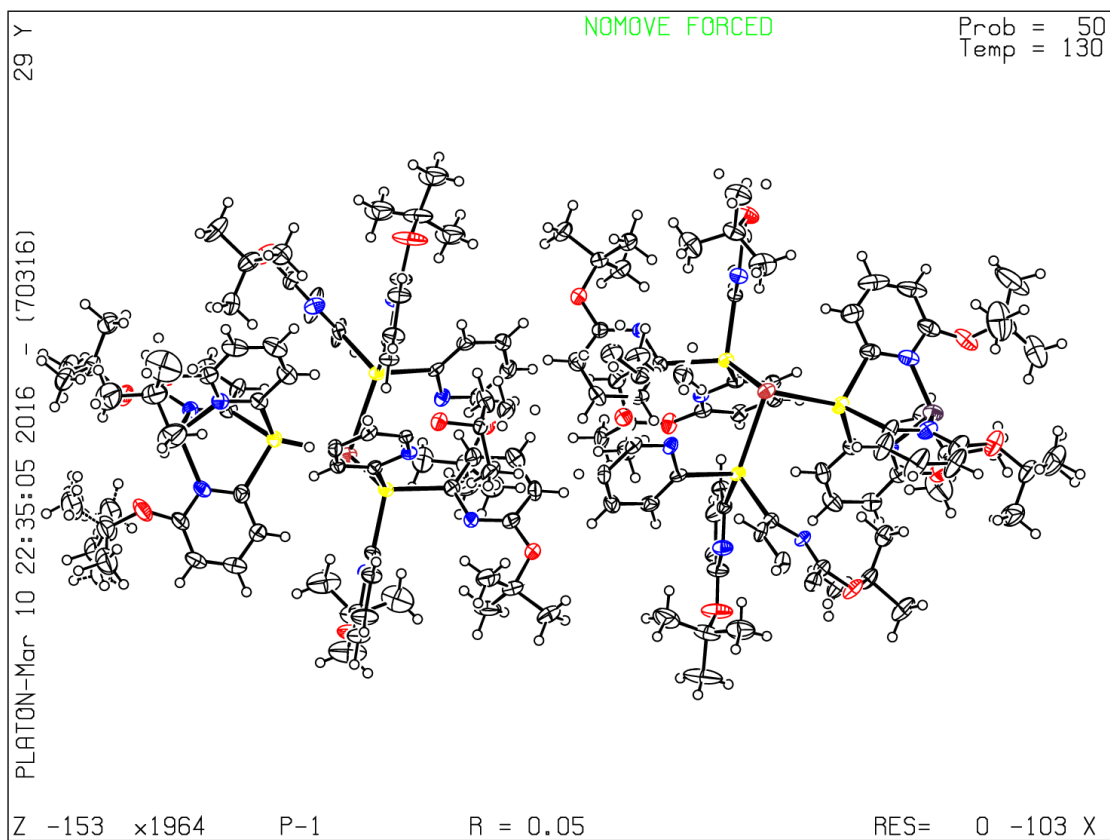
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PLATON version of 07/03/2016; check.def file version of 02/03/2016

NOMOVE FORCED

Prob = 50
Temp = 130

29 Y

PLATON-Mar 10 22:35:05 2016 - (70316)

Z -153   x1964   P-1   R = 0.05   RES=   0 -103 X

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: x2008

```
Bond precision:    C-C = 0.0046 A           Wavelength=0.71073

Cell:              a=14.4547(3)      b=14.4547(3)      c=8.7666(3)
                   alpha=90          beta=90           gamma=120
Temperature:       130 K

                   Calculated               Reported
Volume             1586.28(10)              1586.28(7)
Space group        P -3                     P-3
Hall group         -P 3                     ?
                   C54 H72 N6 O6 Sn2, 2(C6  C54 H72 N6 O6 Sn2, 2(C6
Moiety formula     H6)                      H6)
Sum formula        C66 H84 N6 O6 Sn2        C66 H84 N6 O6 Sn2
Mr                 1294.81                  1294.77
Dx,g cm-3          1.355                    1.355
Z                  1                        1
Mu (mm-1)          0.841                    0.841
F000               670.0                    670.0
F000'              668.92
h,k,lmax           18,18,10                 18,14,10
Nref               2162                     2160
Tmin,Tmax          0.904,0.992              0.978,1.000
Tmin'              0.810

Correction method= # Reported T Limits: Tmin=0.978 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 26.350

R(reflections)= 0.0321( 1868)     wR2(reflections)= 0.0621( 2160)

S = 1.056                   Npar= 124
```

```
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

```
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF      Please Do !
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...           3 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           4 Units
```

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

   1 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
```

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