checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: I

```
Bond precision:   C-C = 0.0187 A             Wavelength=0.71073

Cell:             a=24.5822(15)     b=13.0729(6)        c=16.1506(9)
                  alpha=90          beta=109.954(6)     gamma=90
Temperature:      293 K

                  Calculated                Reported
Volume            4878.6(5)                 4878.6(5)
Space group       C 2/c                     C2/c
Hall group        -C 2yc                    -C2yc
                  2(I3 Pb), 2(C19 H18 P), C2 2(I3 Pb), 2(C19 H18 P), C2
Moiety formula    N                         N
Sum formula       C40 H36 I6 N P2 Pb2       C40 H39 I6 N P2 Pb2
Mr                1768.44                   1771.53
Dx,g cm-3         2.408                     2.408
Z                 4                         4
Mu (mm-1)         10.782                    10.782
F000              3180.0                    3180.0
F000'             3144.78
h,k,lmax          29,15,19                  29,15,19
Nref              4306                      4241
Tmin,Tmax         0.008,0.116               0.250,1.000
Tmin'             0.003

Correction method= # Reported T Limits: Tmin=0.250 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.985          Theta(max)= 25.000

R(reflections)= 0.0344( 3876)     wR2(reflections)= 0.1188( 4241)

S = 1.120                   Npar= 242
```

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**

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as Multi-Scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   3.09 Check
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_C Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT213_ALERT_2_C Atom C5   has ADP max/min Ratio .....   3.1 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 2 C   Ueq(max)/Ueq(min) Range   3.3 Ratio
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C20 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.01867 Ang.

___

⚪ **Alert level G**

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum: C40 H39 I6 N1 P2 Pb2
            Atom count from _chemical_formula_moiety:C40 H36 I6 N1 P2 Pb2
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:C40 H39 I6 N1 P2 Pb2
            Atom count from the _atom_site data: C40 H36 I6 N1 P2 Pb2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
            From the CIF: _cell_formula_units_Z   4
            From the CIF: _chemical_formula_sum C40 H39 I6 N P2 Pb2
            TEST: Compare cell contents of formula and atom_site data

            atom   Z*formula cif sites diff
            C   160.00   160.00   0.00
            H   156.00   144.00   12.00
            I   24.00   24.00   0.00
            N   4.00   4.00   0.00
            P   8.00   8.00   0.00
            Pb   8.00   8.00   0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   1 Info
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   220.10 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group   C2/c   I2/a Note
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)   Pb1   --I3   .   6.3 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)   Pb2   --I3   .   11.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of N1   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21   Constrained at   0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3)   67% Note
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).   C21 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C10   ..C10   3.16 Ang.
                                   1/2-x,1/2-y,1-z =   7_556 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #   3 Do !
            I1 -PB1 -I1 -PB2   -98.78 0.02   2.555 1.555 1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #   10 Do !
            I1 -PB2 -I1 -PB1 -170.00 74.00   5.555 1.555 1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #   18 Do !
            I3 -PB2 -I3 -PB1 -170.00 0.01   5.555 1.555 1.555   1.555

```
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.11 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1        (II)      .      2.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2        (II)      .      2.08 Info
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/      2018 Note
```

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

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
  12 ALERT type 4 Improvement, methodology, query or suggestion
   4 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
;
```
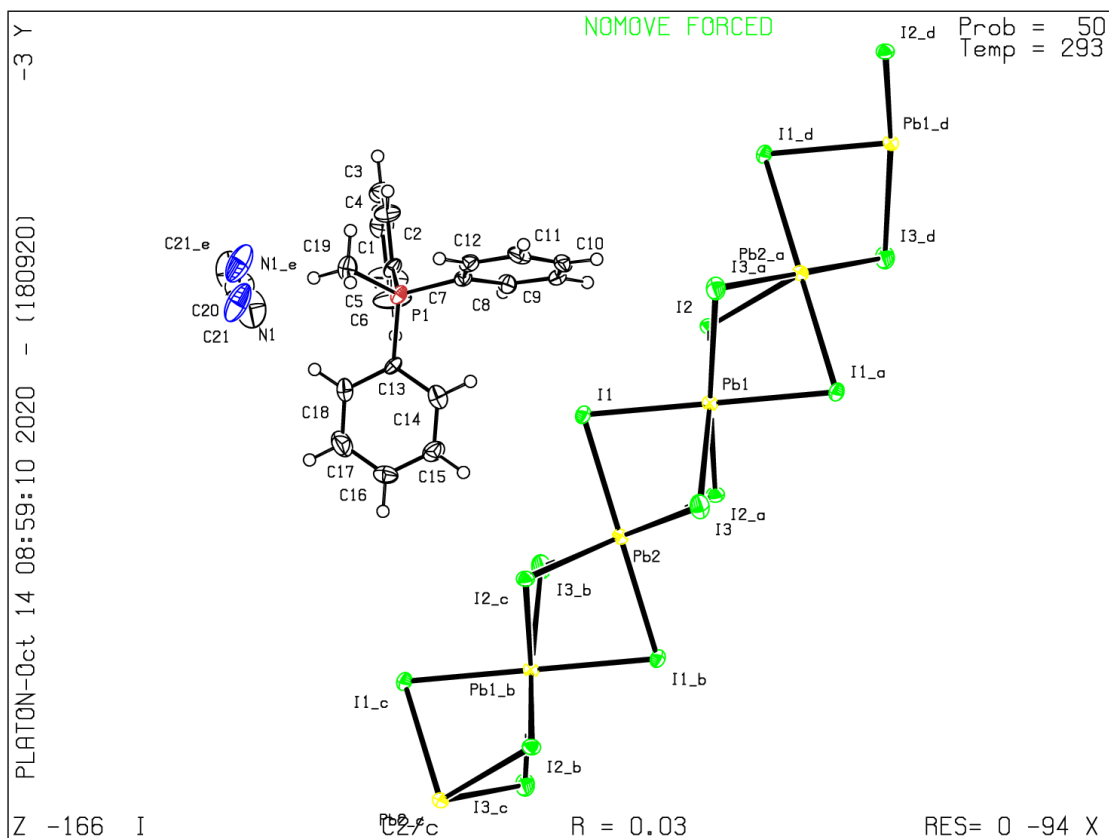
```
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

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 18/09/2020; check.def file version of 20/08/2020

Datablock I - ellipsoid plot

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: I

```
Bond precision:    C-C = 0.0141 A              Wavelength=0.71073

Cell:              a=22.636(3)      b=7.8012(12)      c=24.279(4)
                   alpha=90         beta=90           gamma=90
Temperature:       296 K

                   Calculated                  Reported
Volume             4287.4(11)                  4287.3(11)
Space group        P b c a                     Pbca
Hall group         -P 2ac 2ab                  -P2ac2ab
Moiety formula     C19 H18 P, Br3 Pb           C19 H18 P, Br3 Pb
Sum formula        C19 H18 Br3 P Pb            C19 H18 Br3 P Pb
Mr                 724.20                       724.20
Dx,g cm-3          2.244                        2.244
Z                  8                            8
Mu (mm-1)          13.535                       13.535
F000               2672.0                       2672.0
F000'              2642.26
h,k,lmax           26,9,28                      26,9,28
Nref               3777                         3770
Tmin,Tmax          0.002,0.067                  0.250,1.000
Tmin'              0.001

Correction method= # Reported T Limits: Tmin=0.250 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 24.990

R(reflections)= 0.0379( 2730)      wR2(reflections)= 0.0862( 3770)

S = 1.053                   Npar= 217
```

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

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as Multi-Scan
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.01411 Ang.
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension       1 Info
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   32.63 Why ?
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)     Pb1       --Br1     .    16.5 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)     Pb1       --Br2     .    13.4 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)     Pb1       --Br3     .    23.6 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)     Pb1       --Br2_a   .    14.6 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)     Pb1       --Br3_a   .    15.6 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)     Pb1       --Br1_b   .    21.8 s.u.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .    1.11 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1        (II)      .    2.25 Info
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checkCIF publication errors

Alert level A

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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.
```

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```
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;
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 18/09/2020; check.def file version of 20/08/2020

Datablock I - ellipsoid plot