checkCIF/PLATON report

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

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: Compound5

```
Bond precision:   C-C = 0.0074 A            Wavelength=0.71073

Cell:          a=8.5661(3)        b=8.8903(3)        c=11.3000(5)
               alpha=90.216(1)    beta=103.867(1)    gamma=101.928(3)
Temperature:   173 K

                 Calculated                    Reported
Volume           816.15(5)                     816.15(5)
Space group      P -1                          P -1
Hall group       -P 1                          ?
Moiety formula   C15 H15 Au Cl N2 P S          C15 H15 Au1 Cl1 N2 P S
Sum formula      C15 H15 Au Cl N2 P S          C15 H15 Au1 Cl1 N2 P S
Mr               518.75                        518.74
Dx,g cm-3        2.111                         2.111
Z                2                             2
Mu (mm-1)        9.396                         9.396
F000             492.0                         492.0
F000'            489.06
h,k,lmax         11,11,14                      11,11,14
Nref             3938                          3937
Tmin,Tmax        0.406,0.391                   0.453,0.453
Tmin'            0.376

Correction method= NONE

Data completeness= 1.000           Theta(max)= 28.000

R(reflections)= 0.0309( 3368)      wR2(reflections)= 0.0652( 3937)

S = 1.031                   Npar= 194
```

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
ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.
          However values have been given for Tmin and Tmax. Remove
          these if an absorption correction has not been applied.
  From the CIF: _exptl_absorpt_correction_T_min   0.453

```
   From the CIF: _exptl_absorpt_correction_T_max   0.453
PLAT352_ALERT_3_C Short   N-H Bond (0.87A)   N2    -    H1N    ...        0.76 Ang.
```

⬭ **Alert level G**
```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   1 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
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: Compound6

```
Bond precision:   C-C = 0.0162 A          Wavelength=0.71073

Cell:          a=12.7527(6)     b=8.6138(5)          c=18.7048(8)
               alpha=90         beta=129.342(3)      gamma=90
Temperature:   173 K

               Calculated                Reported
Volume         1589.06(15)               1589.06(14)
Space group    P 21/c                    P 21/c
Hall group     -P 2ybc                   ?
Moiety formula C15 H13 Au Cl N2 P S      C15 H13 Au Cl N2 P S
Sum formula    C15 H13 Au Cl N2 P S      C15 H13 Au Cl N2 P S
Mr             516.73                    516.72
Dx,g cm-3      2.160                     2.160
Z              4                         4
Mu (mm-1)      9.651                     9.651
F000           976.0                     976.0
F000'          970.13
h,k,lmax       16,11,24                  16,11,24
Nref           3630                      3621
Tmin,Tmax      0.256,0.285               0.720,0.801
Tmin'          0.216

Correction method= MULTI-SCAN

Data completeness= 0.998       Theta(max)= 27.480

R(reflections)= 0.0408( 2578)     wR2(reflections)= 0.1282( 3621)
```

```
S = 1.078                        Npar= 190
```

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**
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0162 Ang

⚪ **Alert level G**
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....   ?

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

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

Datablock: Compound7

```
Bond precision:  C-C = 0.0104 A          Wavelength=0.71073

Cell:          a=11.9973(7)    b=10.1616(3)        c=18.9570(8)
               alpha=90        beta=125.438(3)     gamma=90
Temperature:   173 K

               Calculated              Reported
Volume         1882.94(16)             1882.94(15)
Space group    P 21/c                  P 21/c
Hall group     -P 2ybc                 ?
Moiety formula C19 H15 Au Cl N2 P S    C19 H15 Au Cl N2 P S
Sum formula    C19 H15 Au Cl N2 P S    C19 H15 Au Cl N2 P S
Mr             566.79                  566.79
Dx,g cm-3      1.999                   1.999
Z              4                       4
Mu (mm-1)      8.155                   8.155
F000           1080.0                  1080.0
F000'          1074.10
h,k,lmax       16,14,26                16,14,26
Nref           5501                    5486
Tmin,Tmax      0.561,0.613             0.720,0.801
Tmin'          0.516
```

```
Correction method= MULTI-SCAN

Data completeness= 0.997          Theta(max)= 30.020

R(reflections)= 0.0359( 3762)      wR2(reflections)= 0.1097( 5486)

S = 1.016                 Npar= 226
```

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**
```
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0104 Ang
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #        1
            C19 H15 Au Cl N2 P S
```

⚪ **Alert level G**
```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....        ?
```

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

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

Datablock: Compound8

```
Bond precision:  C-C = 0.0177 A          Wavelength=0.71073

Cell:        a=9.1049(3)      b=23.3032(8)       c=28.4310(11)
             alpha=90         beta=90            gamma=90
Temperature:  173 K
```

```
                 Calculated                    Reported
Volume           6032.3(4)                     6032.3(4)
Space group      F 2 d d                       F 2 d d
Hall group       F -2d 2                       ?
Moiety formula   C30 H28 Au2 N4 P2 S2          C30 H28 Au2 N4 P2 S2
Sum formula      C30 H28 Au2 N4 P2 S2          C30 H28 Au2 N4 P2 S2
Mr               964.58                        964.56
Dx,g cm-3        2.124                         2.124
Z                8                             8
Mu (mm-1)        9.990                         9.990
F000             3648.0                        3648.0
F000'            3622.23
h,k,lmax         12,31,38                      12,31,38
Nref             2124[ 4008]                   3236
Tmin,Tmax        0.105,0.136                   0.133,0.159
Tmin'            0.043

Correction method= MULTI-SCAN

Data completeness= 1.52/0.81        Theta(max)= 28.990

R(reflections)= 0.0461( 2937)       wR2(reflections)= 0.1164( 3236)

S = 1.033                    Npar= 181
```

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**

```
PLAT234_ALERT_4_C Large Hirshfeld Difference C12    --  C13    ..      0.17 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0177 Ang
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #       1
              C30 H28 Au2 N4 P2 S2
```

⚪ **Alert level G**

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
          correct. If it is not, please give the correct count in the
          _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max          28.99
          From the CIF: _reflns_number_total               3236
          Count of symmetry unique reflns        2124
          Completeness (_total/calc)          152.35%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured       1112
          Fraction of Friedel pairs measured      0.524
          Are heavy atom types Z>Si present        yes
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....        ?
PLAT128_ALERT_4_G Alternate Setting of Space-group Fdd2    .......     F2dd
```

   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
 3 ALERT level G = General information/check it is not something unexpected

 0 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
 1 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
```

Datablock: Compound9

```
Bond precision:   C-C = 0.0126 A              Wavelength=0.71073

Cell:            a=16.4751(6)     b=11.3575(6)         c=18.0291(7)
                 alpha=90         beta=120.607(3)      gamma=90
Temperature:     173 K

                 Calculated                   Reported
Volume           2903.5(2)                    2903.5(2)
Space group      P 21/c                       P 21/c
Hall group       -P 2ybc                      ?
Moiety formula   C30 H24 Au2 N4 P2 S2         C30 H24 Au2 N4 P2 S2
Sum formula      C30 H24 Au2 N4 P2 S2         C30 H24 Au2 N4 P2 S2
Mr               960.55                       960.53
Dx,g cm-3        2.197                        2.197
Z                4                            4
Mu (mm-1)        10.377                       10.377
F000             1808.0                       1808.0
F000'            1795.13
h,k,lmax         21,14,23                     21,14,23
Nref             6928                         6906
Tmin,Tmax        0.384,0.436                  0.720,0.783
Tmin'            0.341

Correction method= MULTI-SCAN

Data completeness= 0.997          Theta(max)= 27.880

R(reflections)= 0.0445( 4484)     wR2(reflections)= 0.0787( 6906)

S = 0.964                Npar= 361
```

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**

```
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        3.3 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.0126 Ang
```

⬤ Alert level G
```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
```

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

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

Datablock: Compound10

```
Bond precision:  C-C = 0.0138 A          Wavelength=0.71073

Cell:         a=12.2324(4)       b=17.0012(5)       c=18.3825(5)
              alpha=77.8494(16)  beta=72.2786(15)  gamma=70.3212(15)
Temperature: 173 K

               Calculated                Reported
Volume         3403.90(18)               3403.90(18)
Space group    P -1                      P -1
Hall group     -P 1                      ?
Moiety formula C38 H28 Au2 N4 P2 S2      C38 H28 Au2 N4 P2 S2
Sum formula    C38 H28 Au2 N4 P2 S2      C38 H28 Au2 N4 P2 S2
Mr             1060.67                   1060.64
Dx,g cm-3      2.070                     2.070
Z              4                         4
Mu (mm-1)      8.862                     8.863
F000           2016.0                    2016.0
F000'          2003.06
h,k,lmax       15,22,23                  15,22,23
Nref           15564                     15530
Tmin,Tmax      0.534,0.588               0.720,0.783
Tmin'          0.487

Correction method= MULTI-SCAN

Data completeness= 0.998         Theta(max)= 27.460

R(reflections)= 0.0406( 9925)     wR2(reflections)= 0.1346( 15530)
```

```
S = 1.025                      Npar= 865
```

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**
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0138 Ang

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⚪ **Alert level G**
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....   ?

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

   0 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
   1 ALERT type 3 Indicator that the structure quality may be low
   0 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*, 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 18/07/2011; check.def file version of 04/07/2011

Datablock Compound5 - ellipsoid plot

NOMOVE FORCED

Prob = 50
Temp = 173

38 Y

PLATON-Aug 22 19:34:07 2011 - (1807711)

Z -40   Compound6 P 21/c   R = 0.04   RES=   0   147 X

Datablock Compound9 - ellipsoid plot