checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound1, Compound2, Compound3, Compound4, Compound5

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: Compound1

```
Bond precision:   C-C = 0.0050 A              Wavelength=0.71069

Cell:          a=9.0847(6)        b=10.5878(8)      c=13.3058(9)
               alpha=70.313(3)    beta=82.104(3)    gamma=76.733(3)
Temperature:   150 K

                 Calculated                Reported
Volume           1170.35(14)               1170.35(14)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C13 H11 N O4 S            ?
Sum formula      C13 H11 N O4 S            C13 H11 N O4 S
Mr               277.29                    277.29
Dx,g cm-3        1.574                     1.574
Z                4                         4
Mu (mm-1)        0.286                     0.286
F000             576.0                     576.0
F000'            576.79
h,k,lmax         10,12,16                  10,12,16
Nref             4283                      4194
Tmin,Tmax        0.960,0.977               0.887,0.978
Tmin'            0.884

Correction method= # Reported T Limits: Tmin=0.887 Tmax=0.978
AbsCorr = MULTI-SCAN

Data completeness= 0.979          Theta(max)= 25.348

R(reflections)= 0.0510( 2554)     wR2(reflections)= 0.1129( 4194)

S = 0.919                    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 C

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......     0.979 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00504 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     5.834 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600        83 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       4 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical       ? Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.003 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       2 Report
PLAT432_ALERT_2_G Short Inter X...Y Contact  O13    .. C7      ..    2.93 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O21    .. C27     ..    2.81 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...       4 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       3 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......  Please Check
```

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

   2 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
   6 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: Compound2

```
Bond precision:   C-C = 0.0047 A          Wavelength=0.71073

Cell:          a=9.5036(4)     b=18.3619(8)       c=11.3390(5)
               alpha=90        beta=91.883(2)     gamma=90
Temperature:   150 K
```

```
                 Calculated              Reported
Volume           1977.63(15)             1977.63(15)
Space group      P 21/n                  P 21/n
Hall group       -P 2yn                  -P 2yn
Moiety formula   C20 H20 Cu N2 O5 S      C20 H20 Cu N2 O5 S
Sum formula      C20 H20 Cu N2 O5 S      C20 H20 Cu N2 O5 S
Mr               463.99                  463.98
Dx,g cm-3        1.558                   1.558
Z                4                       4
Mu (mm-1)        1.245                   1.245
F000             956.0                   956.0
F000'            958.14
h,k,lmax         11,22,13                11,22,13
Nref             3632                    3629
Tmin,Tmax        0.787,0.861             0.791,0.871
Tmin'            0.723

Correction method= # Reported T Limits: Tmin=0.791 Tmax=0.871
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 25.357

R(reflections)= 0.0373( 2759)     wR2(reflections)= 0.0838( 3629)

S = 1.017                   Npar= 266
```

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
```
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1    (II)   .....      2.18 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       3 Note
```

```
   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
   2 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
   0 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: Compound3

```
Bond precision:  C-C = 0.0044 A          Wavelength=0.71069
```

```
Cell:              a=8.1099(2)     b=29.4538(7)          c=10.5303(3)
                   alpha=90        beta=109.3950(9)      gamma=90
Temperature:       296 K


                   Calculated                  Reported
Volume             2372.60(11)                 2372.60(11)
Space group        P 21/n                      P 21/n
Hall group         -P 2yn                      -P 2yn
Moiety formula     C23 H17 Cu N3 O4 S, C H4 O  C23 H17 Cu N3 O4 S, C H4 O
Sum formula        C24 H21 Cu N3 O5 S          C24 H21 Cu N3 O5 S
Mr                 527.05                      527.04
Dx,g cm-3          1.475                       1.475
Z                  4                           4
Mu (mm-1)          1.049                       1.049
F000               1084.0                      1084.0
F000'              1086.18
h,k,lmax           10,36,13                    10,36,13
Nref               4835                        4826
Tmin,Tmax          0.790,0.890                 0.800,0.900
Tmin'              0.713


Correction method= # Reported T Limits: Tmin=0.800 Tmax=0.900
AbsCorr = MULTI-SCAN


Data completeness= 0.998          Theta(max)= 26.368


R(reflections)= 0.0398( 3903)     wR2(reflections)= 0.1028( 4826)


S = 1.007                    Npar= 309
```

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**
PLAT147_ALERT_1_C s.u. on Symmetry Constrained Cell Angle(s) .....   Please Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......   5.804 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   1 Check

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⚪ **Alert level G**
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in Structure ...   63 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1   (II)   .....   2.17 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed   ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...   2 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   6 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ....   Please Check

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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
      7 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
      3 ALERT type 3 Indicator that the structure quality may be low
      3 ALERT type 4 Improvement, methodology, query or suggestion
      3 ALERT type 5 Informative message, check
```

Datablock: Compound4

```
Bond precision:   C-C = 0.0034 A            Wavelength=0.71069

Cell:          a=7.4426(4)        b=10.2904(6)      c=11.4557(7)
               alpha=75.615(2)    beta=71.959(3)    gamma=85.198(2)
Temperature:   296 K

                  Calculated                 Reported
Volume            808.05(8)                  808.05(8)
Space group       P -1                       P -1
Hall group        -P 1                       -P 1
Moiety formula    C32 H30 Cu2 N4 O10 S2      C32 H30 Cu2 N4 O10 S2
Sum formula       C32 H30 Cu2 N4 O10 S2      C32 H30 Cu2 N4 O10 S2
Mr                821.82                     821.80
Dx,g cm-3         1.689                      1.689
Z                 1                          1
Mu (mm-1)         1.512                      1.512
F000              420.0                      420.0
F000'             421.05
h,k,lmax          9,12,14                    9,12,14
Nref              3332                       3327
Tmin,Tmax         0.704,0.782                0.800,0.900
Tmin'             0.548

Correction method= # Reported T Limits: Tmin=0.800 Tmax=0.900
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.410

R(reflections)= 0.0349( 3120)      wR2(reflections)= 0.0952( 3327)

S = 1.098                   Npar= 229
```

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 ....      3.37 Report
PLAT480_ALERT_4_C Long H...A H-Bond Reported H10     .. S2       ..     2.92 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          3 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1     (II)    .....       2.15 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         1 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...         2 Report
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......   Please Check
```

```
  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
  6 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
  3 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: Compound5

```
Bond precision:   C-C = 0.0059 A          Wavelength=0.71069

Cell:          a=6.9512(9)    b=18.534(2)          c=13.4906(15)
               alpha=90       beta=100.283(3)      gamma=90
Temperature:   150 K

               Calculated              Reported
Volume         1710.1(3)               1710.1(4)
Space group    P 21/n                  P 21/n
Hall group     -P 2yn                  -P 2yn
Moiety formula C32 H36 Cu2 N4 O10 S2   C32 H36 Cu2 N4 O10 S2
Sum formula    C32 H36 Cu2 N4 O10 S2   C32 H36 Cu2 N4 O10 S2
Mr             827.87                  827.85
Dx,g cm-3      1.608                   1.608
Z              2                       2
Mu (mm-1)      1.429                   1.429
F000           852.0                   852.0
F000'          854.10
h,k,lmax       8,23,16                 8,23,16
Nref           3513                    3506
Tmin,Tmax      0.747,0.918             0.627,0.919
Tmin'          0.598
```

```
Correction method= # Reported T Limits: Tmin=0.627 Tmax=0.919
AbsCorr = MULTI-SCAN


Data completeness= 0.998          Theta(max)= 26.418


R(reflections)= 0.0526( 2114)      wR2(reflections)= 0.1035( 3506)


S = 0.920                 Npar= 229
```

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
```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.129
PLAT420_ALERT_2_C D-H Without Acceptor        N12    -- H12    ...    Please Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......    6.996 Check
```

⚪ Alert level G
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       2 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1     (II)    .....    2.19 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       8 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......    Please Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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   7 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
   3 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 19/11/2015; check.def file version of 17/11/2015

NOMOVE FORCED

Prob = 50
Temp = 296

PLATON-Feb 7 22:40:04 2016 - (191115)

40 Y

Z -12   Compound3 P 21/n   R = 0.04   RES=   0   157 X

NOMOVE FORCED

Prob = 50
Temp = 296

60 Y

PLATON-Feb 7 22:40:07 2016 - (191115)

Z -168 Compound4 P -1   R = 0.03   RES= 0 -154 X