checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1-Ce, 1-Nd, 1-Pr

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: 1-Ce

```
Bond precision:    C-C = 0.0038 A              Wavelength=0.71075

Cell:            a=9.4469(4)        b=12.6653(9)        c=13.3774(6)
                 alpha=73.950(9)    beta=71.912(9)      gamma=71.554(9)
Temperature:     173 K

                 Calculated                    Reported
Volume           1414.83(17)                   1414.83(18)
Space group      P -1                          P -1
Hall group       -P 1                          -P 1
Moiety formula   C22 H28 Ce Cu N5 O14          C22 H28 Ce Cu N5 O14
Sum formula      C22 H28 Ce Cu N5 O14          C22 H28 Ce Cu N5 O14
Mr               790.16                        790.15
Dx,g cm-3        1.855                         1.855
Z                2                             2
Mu (mm-1)        2.418                         2.418
F000             788.0                         788.0
F000'            788.51
h,k,lmax         11,15,16                      11,15,16
Nref             5201                          5132
Tmin,Tmax        0.770,0.908                   0.857,1.000
Tmin'            0.602

Correction method= # Reported T Limits: Tmin=0.857 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.987            Theta(max)= 25.381

R(reflections)= 0.0200( 4760)                 wR2(reflections)=
                                              0.0439( 5132)
S = 1.039                    Npar= 394
```

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

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O12 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600        58 Report
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        1 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.009 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ce1      --O11      .      8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ce1      --O12      .      7.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ce1      --O21      .      7.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ce1      --O22      .      8.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ce1      --O31      .      8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ce1      --O32      .      8.3 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O33      ..C9       .     2.93 Ang.
                                            -x,-y,1-z   =     2_556 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Ce1       (III)     .     3.30 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .     2.18 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       11 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      11 Info
```

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

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

Datablock: 1-Pr

```
Bond precision:   C-C = 0.0033 A          Wavelength=0.71075

Cell:          a=9.4412(3)       b=12.6685(5)       c=13.3569(4)
               alpha=74.017(4)   beta=71.828(5)     gamma=71.364(4)
Temperature:   173 K
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	Calculated	Reported
Volume	1410.65(10)	1410.65(10)
Space group	P −1	P −1
Hall group	−P 1	−P 1
Moiety formula	C22 H28 Cu N5 O14 Pr	C22 H28 Cu N5 O14 Pr
Sum formula	C22 H28 Cu N5 O14 Pr	C22 H28 Cu N5 O14 Pr
Mr	790.95	790.94
Dx,g cm−3	1.862	1.862
Z	2	2
Mu (mm−1)	2.538	2.538
F000	790.0	790.0
F000'	790.58	
h,k,lmax	11,15,16	11,15,16
Nref	5182	5130
Tmin,Tmax	0.913,0.951	0.790,1.000
Tmin'	0.837	

Correction method= # Reported T Limits: Tmin=0.790 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.990   Theta(max)= 25.386

R(reflections)= 0.0171(4746)   wR2(reflections)= 0.0411(5130)

S = 1.043   Npar= 394

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 ....   2.56 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for   O21   --N21   .   6.5 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of   O12 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   43 Report

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⚪ **Alert level G**
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr1   --O11   .   8.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr1   --O12   .   9.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr1   --O21   .   8.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr1   --O22   .   8.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr1   --O31   .   8.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr1   --O32   .   9.3 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact O33   ..C9   .   2.93 Ang.
                                        -x,-y,1-z =   2_556 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pr1   (III)   .   3.80 Info

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PLAT794_ALERT_5_G Tentative Bond Valency for Cu1        (II)      .     2.19 Info
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      9 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........   4.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.     17 Info
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Datablock: 1-Nd

```
Bond precision:    C-C = 0.0041 A           Wavelength=0.71075

Cell:          a=8.6415(7)        b=12.9533(11)      c=13.4632(16)
               alpha=79.830(9)    beta=77.505(8)     gamma=71.963(7)
Temperature:   173 K

                  Calculated                  Reported
Volume            1389.2(2)                   1389.2(2)
Space group       P -1                        P -1
Hall group        -P 1                        -P 1
Moiety formula    C22 H28 Cu N5 Nd O14        C22 H28 Cu N5 Nd O14
Sum formula       C22 H28 Cu N5 Nd O14        C22 H28 Cu N5 Nd O14
Mr                794.28                      794.27
Dx,g cm-3         1.899                       1.899
Z                 2                           2
Mu (mm-1)         2.693                       2.693
F000              792.0                       792.0
F000'             792.63
h,k,lmax          10,15,16                    10,15,16
Nref              5131                        5062
Tmin,Tmax         0.828,0.948                 0.812,1.000
Tmin'             0.828

Correction method= # Reported T Limits: Tmin=0.812 Tmax=1.000
AbsCorr = MULTI-SCAN
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Data completeness= 0.987           Theta(max)= 25.405


R(reflections)= 0.0229( 4603)                    wR2(reflections)=
                                                 0.0570( 5062)

S = 0.971                  Npar= 394
```

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**
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   58 Report

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⚪ **Alert level G**
```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............      1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)   Nd1      --O11      .     5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)   Nd1      --O12      .     6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)   Nd1      --O21      .     6.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)   Nd1      --O22      .     7.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)   Nd1      --O31      .     5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)   Nd1      --O32      .     5.6 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Nd1      (II)       .    2.11 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1      (II)       .    2.16 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).     2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600     10 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........   3.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.     5 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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  13 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
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   1 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* 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.

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