checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: 280922d_0m

Bond precision: C-C = 0.0083 A   Wavelength=0.71073

Cell: a=7.7302(12)   b=8.2404(12)   c=13.782(2)
               alpha=89.723(2)   beta=83.928(1)   gamma=62.528(2)
Temperature: 291 K

	Calculated	Reported
Volume	773.6(2)	773.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H24 Cu2 N8 O12	C32 H24 Cu2 N8 O12
Sum formula	C32 H24 Cu2 N8 O12	C32 H24 Cu2 N8 O12
Mr	839.69	839.69
Dx,g cm-3	1.802	1.802
Z	1	1
Mu (mm-1)	1.459	1.459
F000	426.0	426.0
F000'	426.82	
h,k,lmax	9,9,16	9,9,16
Nref	2728	2679
Tmin,Tmax	0.839,0.864	0.822,0.868
Tmin'	0.815	

Correction method= MULTI-SCAN

Data completeness= 0.982   Theta(max)= 25.000

R(reflections)= 0.0476(1790)   wR2(reflections)= 0.1481(2679)

S = 0.950   Npar= 245

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**
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ..   8

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   0 **ALERT level A** = In general: serious problem
   0 **ALERT level B** = Potentially serious problem
   1 **ALERT level C** = Check and explain

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  0 ALERT level G = General alerts; check

  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
  0 ALERT type 5 Informative message, check
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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 31/03/2010; check.def file version of 22/03/2010