checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ao_of_tbunc_cisp2_tet_1_0m

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: ao_of_tbunc_cisp2_tet_1_0m

Bond precision: C-C = 0.0084 A Wavelength=0.71073

Cell: a=14.5642(12) b=16.7939(14) c=20.9855(18)
alpha=90 beta=90 gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	5132.8(7)	5132.8(7)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C52 H44 Au P4, F6 P, C4 H8 O	C52 H44 Au P4, F6 P, C4 H8 O
Sum formula	C56 H52 Au F6 O P5	C56 H52 Au F6 O P5
Mr	1206.80	1206.79
Dx,g cm-3	1.562	1.562
Z	4	4
Mu (mm-1)	3.084	3.084
F000	2416.0	2416.0
F000'	2411.09	
h,k,lmax	19,22,28	19,22,28
Nref	12810[7019]	12804
Tmin,Tmax	0.497,0.574	0.653,0.746
Tmin'	0.487	

Correction method= # Reported T Limits: Tmin=0.653 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.82/1.00 Theta(max)= 28.340

R(reflections)= 0.0244(11735) wR2(reflections)= 0.0546(12804)

S = 1.025 Npar= 622

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 A

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PLAT360_ALERT_2_A Short  C(sp3)-C(sp3) Bond  C5       - C6       .       1.22 Ang.
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Author Response: This is part of an ill-defined THF molecule. Treatment as a disordered solvent did not improve the solution; alternatively solvent masking yielded simi models. The main complex is not affected by this disorder.

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PLAT411_ALERT_2_A Short Inter H...H Contact  H00F     ..H5A      .       1.79 Ang.
                                                    x,y,z  =      1_555 Check
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Alert level C

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01P Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C00X Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of         O2 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of         C6 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         C3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    2)        2.4 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      P006      0.102 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O2      0.181 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00843 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C3       - C4       .       1.43 Ang.
```

Author Response: This is part of an ill-defined THF molecule. Treatment as a disordered solvent did not improve the solution; alternatively solvent masking yielded simi models. The main complex is not affected by this disorder.

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PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C4       - C5       .       1.36 Ang.
```

Author Response: This is part of an ill-defined THF molecule. Treatment as a disordered solvent did not improve the solution; alternatively solvent masking yielded simi models. The main complex is not affected by this disorder.

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PLAT411_ALERT_2_C Short Inter H...H Contact  H6A      ..H01O     .       2.02 Ang.
                                          1-x,1/2+y,3/2-z  =      3_656 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
               1  0  1,   0  6 12,
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         5 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         1 Report
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PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       P006 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O2       .       99.7 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  F00K     ..C6       .       2.94 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........       108 Note
              Au01    P002    P003    P004    P005    P006    C007    C008
              F009    F00A    C00B    H00B    C00C    H00C    F00D    C00E
              C00F    H00F    C00G    H00G    C00H    H00H    C00I    C00J
              F00K    C00L    H00L    C00M    H00M    F00N    C00O    H00O
              C00P    H00P    C00Q    H00Q    C00R    H00R    C00S    H00S
              C00T    H00T    C00U    H00U    F00V    C00W    C00X    C00Y
              H00Y    C00Z    H00Z    C010    H010    C011    H011    C012
              H012    C013    H013    C014    H014    C015    H015    C016
              H016    C017    H017    C018    H018    C019    H019    C01A
              H01A    C01B    H01B    C01D    H01D    C01E    H01E    C01F
              H01F    C01G    H01G    C01H    H01H    C01I    H01I    C01J
              H01J    C01K    C01M    H01M    C01N    H01N    C01O    H01O
              C01P    H01P    C01Q    H01Q    C01R    H01R    C01S    H01S
              C01T    H01T    C01U    H01U
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         75 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
                0  6 12,   1  0  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.44 Note
              Predicted wR2: Based on SigI**2  3.78 or SHELX Weight  5.46
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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  2 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
 14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 21 ALERT level G = General information/check it is not something unexpected

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
 12 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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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.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock ao_of_tbunc_cisp2_tet_1_0m - ellipsoid plot