checkCIF/PLATON report

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

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: fpycnm

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

Cell:           a=23.9090(12)    b=13.5257(7)       c=20.3311(10)
                alpha=90         beta=111.916(1)    gamma=90
Temperature:    297 K
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	Calculated	Reported
Volume	6099.7(5)	6099.6(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	?
Moiety formula	C32 H16 Cl F4 Ir N4 O2, 0.85(O)	4(C32 H16 Cl F4 Ir N4 O2), 1.2(O), 1.2(O), O
Sum formula	C32 H16 Cl F4 Ir N4 O2.85	C128 H70.80 Cl4 F16 Ir4 N16 O11.40
Mr	805.76	3229.81
Dx,g cm-3	1.755	1.759
Z	8	2
Mu (mm-1)	4.529	4.529
F000	3110.4	3124.0
F000’	3101.77	
h,k,lmax	29,16,25	29,16,25
Nref	12023	11970
Tmin,Tmax	0.131,0.386	0.487,1.000
Tmin’	0.099	

```
Correction method= # Reported T Limits: Tmin=0.487 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.996          Theta(max)= 26.030

R(reflections)= 0.0319( 9598)     wR2(reflections)= 0.0899( 11970)

S = 1.070                 Npar= 829
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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

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as empirical
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       1.69 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT213_ALERT_2_C Atom F5              has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom N8'             has ADP max/min Ratio .....        3.6 prolat
PLAT214_ALERT_2_C Atom O5      (Anion/Solvent) ADP max/min Ratio          4.4 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   N   Ueq(max)/Ueq(min) Range        4.1 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C61 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C64 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C29 Check
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C33    -C38          1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00844 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         36 Ang3
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C128 H70.8 Cl4 F16 Ir4 N16
           Atom count from _chemical_formula_moiety:C128 H64 Cl4 F16 Ir4 N16 O1
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C128 H70.8 Cl4 F16 Ir4 N16 O11
           Atom count from the _atom_site data:  C128 H64 Cl4 F16 Ir4 N16 O11.4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C128 H70.80 Cl4 F16 Ir4 N16 O11.
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        256.00    256.00    0.00
          H        141.60    128.00   13.60
          Cl         8.00      8.00    0.00
          F         32.00     32.00    0.00
          Ir         8.00      8.00    0.00
          N         32.00     32.00    0.00
          O         22.80     22.80    0.00
HYDTR01_ALERT_1_G  Extra text has been found in the _refine_ls_hydrogen_treatment fi
           Explanatory text should be in the _publ_section_refinement field.
           Hydrogen treatment given as constro
           Hydrogen treatment identified as  constr
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       4.00 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >N8     is Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <N8'    is Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O5     is Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O6     is Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O7     is Constrained at        0.5 Check
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PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          1 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =        100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.60) in Resd. #          3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.60) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #          5 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         O5 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         O6 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         O7 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        242 Check
              N8'  -C64  -N8      1.555   1.555   1.555             27.00 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
              O
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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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
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  25 ALERT level G = General information/check it is not something unexpected

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
  13 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 11/08/2016; check.def file version of 04/08/2016

Datablock fpycnm - ellipsoid plot