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: grot292

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Bond precision:  C-C = 0.0086 A          Wavelength=1.54178

Cell:           a=22.6979(12)    b=20.6402(10)    c=28.5118(13)
                alpha=90         beta=90          gamma=90
Temperature:    100 K
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	Calculated	Reported
Volume	13357.5(11)	13357.5(11)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	2(C23 H32 Cl Ir N3), C4 H8 F18 K O P3, C4 H8 O	2(C23 H32 Cl Ir N3), C4 H8 F18 K O P3, C4 H8 O
Sum formula	C54 H80 Cl2 F18 Ir2 K N6 O2 P3	C54 H84 Cl2 F18 Ir2 K N6 O2 P3
Mr	1774.59	1778.58
Dx,g cm-3	1.765	1.769
Z	8	8
Mu (mm-1)	10.411	10.412
F000	7008.0	7040.0
F000’	6968.29	
h,k,lmax	26,24,33	25,24,33
Nref	11401	11166
Tmin,Tmax	0.217,0.392	0.141,0.454
Tmin’	0.032	

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Correction method= # Reported T Limits: Tmin=0.141 Tmax=0.454
AbsCorr = MULTI-SCAN

Data completeness= 0.979          Theta(max)= 65.104

R(reflections)= 0.0356( 8943)     wR2(reflections)= 0.0918( 11166)

S = 1.038                 Npar= 818
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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 A

PLAT410_ALERT_2_A Short Intra H...H Contact H1SA ..H2SC . 1.56 Ang.

Author Response: These short contacts are all part of a highly disordered molecule of T

PLAT410_ALERT_2_A Short Intra H...H Contact H2SC ..H3SA . 1.67 Ang.

Author Response: These short contacts are all part of a highly disordered molecule of T

Alert level B

PLAT213_ALERT_2_B Atom C17 has ADP max/min Ratio ..... 4.7 oblate

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Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5883
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.979 Why?
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.99 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT213_ALERT_2_C Atom C19' has ADP max/min Ratio ..... 4.0 prolat
PLAT213_ALERT_2_C Atom C22' has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C23' has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 4.2 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 2 H Uiso(max)/Uiso(min) Range 5.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C2SB --C3S 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of F2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of F7 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3S Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00859 Ang.

Alert level G

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: C54 H84 Cl2 F18 Ir2 K1 N6 O
Atom count from _chemical_formula_moiety:C54 H80 Cl2 F18 Ir2 K1 N6 O
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:C54 H84 Cl2 F18 Ir2 K1 N6 O2 P
Atom count from the _atom_site data: C54 H80 Cl2 F18 Ir2 K1 N6 O2 P
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 8
From the CIF: _chemical_formula_sum C54 H84 Cl2 F18 Ir2 K N6 O2 P3
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	432.00	432.00	0.00
H	672.00	640.00	32.00

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          Cl        16.00     16.00    0.00
          F        144.00    144.00    0.00
          Ir        16.00     16.00    0.00
          K          8.00      8.00    0.00
          N         48.00     48.00    0.00
          O         16.00     16.00    0.00
          P         24.00     24.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      49.70 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         10 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C2S      --C3S       .        6.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ir1'     --C1'       .        6.5 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         P1 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         P2 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         P3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SC       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SD       Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )         4% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C3S      - C4S       .       1.59 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2S            106.9 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  F16      ..C15'             2.95 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         21 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        107 Check
              O1S  -C1S  -K1      1.555   1.555   1.555             43.20 Deg.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         22 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
31 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
23 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 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

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 13/12/2017; check.def file version of 12/12/2017

Datablock grot292 - ellipsoid plot

