checkCIF/PLATON report

Structure factors have been supplied for datablock(s) q

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: q

Bond precision: C-C = 0.0065 A Wavelength=0.71073

Cell: a=7.9907(12) b=12.7188(18) c=14.746(2)
alpha=114.437(4) beta=92.482(5) gamma=105.428(5)
Temperature: 110 K

	Calculated	Reported
Volume	1295.0(3)	1295.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H58 Ir2 N6 O4, 4(C H4 O), 2(Cl)	C44 H58 Ir2 N6 O4, 2(Cl), 4(C H4 O)
Sum formula	C48 H74 Cl2 Ir2 N6 O8	C48 H74 Cl2 Ir2 N6 O8
Mr	1318.47	1318.43
Dx,g cm-3	1.691	1.691
Z	1	1
Mu (mm-1)	5.292	5.292
F000	656.0	656.0
F000'	653.72	
h,k,lmax	11,17,20	11,17,20
Nref	7565	7562
Tmin,Tmax	0.484,0.571	0.455,0.648
Tmin'	0.474	

Correction method= # Reported T Limits: Tmin=0.455 Tmax=0.648
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 29.999

R(reflections)= 0.0379(6505) wR2(reflections)= 0.0823(7562)

S = 1.025 Npar= 338

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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PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C44 H58 Ir2 N6 O4, 4(C H4 O), 2(Cl)
              Rep.: C44 H58 Ir2 N6 O4, 2(Cl), 4(C H4 O)
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
               -6 -3  5,  -1  3 10,
PLAT977_ALERT_2_C Check Negative Difference Density on H19A      .      -0.35 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
              H1S   H2S
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ir1      --C17      .        5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ir1A     --C14      .        5.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ir1A     --C16      .        6.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Ir1        Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ir1A       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7AA       Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7AB       Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5         Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A        Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B        Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6C        Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BC       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BD       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6AA       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6AB       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6AC       Constrained at       0.15 Check
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PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        32% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C14      - C19      .       1.50 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C16      - C21      .       1.50 Ang.
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H2SB     ..H5A      .       1.92 Ang.
                                                1-x,1-y,1-z  =      2_666 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H2SC     ..H5A      .       1.74 Ang.
                                                1-x,1-y,1-z  =      2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1A      ..C2S      .       2.55 Ang.
                                                1-x,1-y,1-z  =      2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2S      ..C5A      .       2.92 Ang.
                                                1-x,1-y,1-z  =      2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2S      ..C1A      .       3.17 Ang.
                                                1-x,1-y,1-z  =      2_666 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         13 Note
              H7AA    H7AB    H7BC    H7BD    H1SA    H1SB    H1SC    H2SA
              H2SB    H2SC    H6AA    H6AB    H6AC
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.8 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       60.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.20 Note
              Predicted wR2: Based on SigI**2  6.86 or SHELX Weight  8.22
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
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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
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
55 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
36 ALERT type 4 Improvement, methodology, query or suggestion
4 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 06/01/2024; check.def file version of 05/01/2024

Datablock q - ellipsoid plot