

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 4

Bond precision: C-C = 0.0074 Å

Wavelength=0.71073

Cell: a=12.6752(7) b=15.0112(9) c=19.2987(11)
 alpha=67.2482(9) beta=84.5581(10) gamma=68.1660(9)
Temperature: 193 K

	Calculated	Reported
Volume	3138.2(3)	3138.2(3)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C61 H57 Ir N O3 P4 Ru, B F4	C61 H57 Ir N O3 P4 Ru, B F4, C4 H10 O
Sum formula	C61 H57 B F4 Ir N O3 P4 Ru	C65 H67 B F4 Ir N O4 P4 Ru
Mr	1356.06	1430.16
Dx, g cm-3	1.435	1.514
Z	2	2
Mu (mm-1)	2.514	2.519
F000	1352.0	1436.0
F000'	1347.92	
h, k, lmax	15, 18, 24	15, 18, 24
Nref	12867	12757
Tmin, Tmax	0.662, 0.797	0.560, 0.805
Tmin'	0.514	

Correction method= INTEGRATION

Data completeness= 0.991

Theta(max)= 26.390

R(reflections)= 0.0331(10937)

wR2(reflections)= 0.0856(12757)

S = 1.045

Npar= 712

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 B

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.95 <> 1.05

From the CIF: _cell_formula_units_Z 2
 From the CIF: _chemical_formula_weight 1430.16
 TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	61.00	732.67
H	1.01	57.00	57.46
B	10.81	1.00	10.81
N	14.01	1.00	14.01
O	16.00	3.00	48.00
F	19.00	4.00	75.99
P	30.97	4.00	123.90
Ru	101.07	1.00	101.07
Ir	192.22	1.00	192.22
Calculated formula weight			1356.12

Author Response: Attempts to refine peaks of residual electron density as solvent diethyl ether oxygen or carbon atoms were unsuccessful. The data were corrected for disordered electron density through use of the SQUEEZE procedure (Sluis, P. van der; Spek, A. L. Acta Crystallogr. 1990, A46, 194-201) as implemented in PLATON (Spek, A.L. Acta Crystallogr. 1990, A46, C34. PLATON - a multipurpose crystallographic tool. Utrecht University, Utrecht, The Netherlands). A total solvent-accessible void volume of 513 cubic Angstroms with a total electron count of 103 (consistent with two molecules of solvent diethyl ether) was found in the unit cell.

PLAT043_ALERT_1_B Check Reported Molecular Weight 1430.16

Author Response: See above response to CHEMW03 alert.

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.3 Ratio



Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?

Author Response: See above response to CHEMW03 alert.

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?

Author Response: See above response to CHEMW03 alert.

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 5
 PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 4.1 Ratio
 PLAT234_ALERT_4_C Large Hirshfeld Difference C7A -- C8A .. 0.20 Ang.
 PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C45
 PLAT410_ALERT_2_C Short Intra H...H Contact H4AA .. H52 .. 1.93 Ang.



Alert level G

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: C65 H67 B1 F4 Ir1 N1 O4 P4 Ru1
 Atom count from the _atom_site data: C61 H57 B1 F4 Ir1 N1 O3 P4 Ru1

Author Response: See above response to CHEMW03 alert.

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

Author Response: See above response to CHEMW03 alert.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
 symmetry error - see SYMMG tests
 From the CIF: _cell_formula_units_Z 2
 From the CIF: _chemical_formula_sum C65 H67 B F4 Ir N O4 P4 Ru
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	130.00	122.00	8.00
H	134.00	114.00	20.00
B	2.00	2.00	0.00
F	8.00	8.00	0.00
Ir	2.00	2.00	0.00
N	2.00	2.00	0.00
O	8.00	6.00	2.00
P	8.00	8.00	0.00
Ru	2.00	2.00	0.00

Author Response: See above response to CHEMW03 alert.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	14
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru -- N ..	8.1 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru -- C2 ..	5.5 su
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1A
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1B
PLAT301_ALERT_3_G	Note: Main Residue Disorder	11 Perc.
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder	100 Perc.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!

Author Response: See above response to CHEMW03 alert.

PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	4
	C6A -IR -RU -C2 -141.90 1.20 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	13
	C6A -IR -RU -C1 -145.20 1.20 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	21
	C6A -IR -RU -N 37.20 1.20 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	30
	C6A -IR -RU -P2 123.30 1.20 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	39
	C6A -IR -RU -P4 -51.10 1.20 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	51
	P3 -IR -P1 -C21 51.70 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	60
	P3 -IR -P1 -C11 173.80 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	69
	P3 -IR -P1 -C10 -65.10 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	75
	P4 -RU -P2 -C31 -149.70 0.30 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	80
	P4 -RU -P2 -C10 86.40 0.30 1.555 1.555 1.555	1.555

PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	85
P4 -RU -P2 -C41	-30.90 0.40	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	93
P1 -IR -P3 -C51	-175.80 0.40	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	102
P1 -IR -P3 -C20	64.50 0.40	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	111
P1 -IR -P3 -C61	-51.10 0.40	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	117
P2 -RU -P4 -C71	148.20 0.30	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	122
P2 -RU -P4 -C81	28.60 0.40	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	127
P2 -RU -P4 -C20	-87.80 0.30	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	129
C2 -RU -N -C17	-127.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	130
C1 -RU -N -C17	49.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	131
P2 -RU -N -C17	-37.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	132
P4 -RU -N -C17	144.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	133
IR -RU -N -C17	54.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	160
C1 -RU -C2 -O2	10.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	161
N -RU -C2 -O2	-172.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	162
P2 -RU -C2 -O2	102.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	163
P4 -RU -C2 -O2	-84.00 3.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	164
IR -RU -C2 -O2	7.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	165
C3B -IR -C3A -O3A	6.00 8.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	166
C4A -IR -C3A -O3A	25.00 5.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	167
C6A -IR -C3A -O3A	34.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	168
C6B -IR -C3A -O3A	30.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	169
C4B -IR -C3A -O3A	34.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	170
P1 -IR -C3A -O3A	-60.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	171
P3 -IR -C3A -O3A	118.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	172
C1 -IR -C3A -O3A	-150.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	173
RU -IR -C3A -O3A	-151.00 4.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	194
RU -IR -C6A -C7A	-42.30 1.70	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	203
RU -IR -C6A -C5A	136.90 1.10	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	208
C3A -IR -C3B -O3B	50.00 34.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	209
C4A -IR -C3B -O3B	14.00 24.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	210
C6A -IR -C3B -O3B	22.00 30.00	1.555	1.555	1.555	1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	211
C6B -IR -C3B -03B 27.00 30.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	212
C4B -IR -C3B -03B 36.00 32.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	213
P1 -IR -C3B -03B 117.00 30.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	214
P3 -IR -C3B -03B -61.00 30.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	215
C1 -IR -C3B -03B -152.00 30.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	216
RU -IR -C3B -03B -153.00 30.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	271
RU -N -C17 -C18 24.00 21.00 1.555 1.555 1.555 1.555	
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	20
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	!
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints	25
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed	!

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 3 **ALERT level B** = A potentially serious problem, consider carefully
 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 64 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 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
 55 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

Datablock: 5

Bond precision: C-C = 0.0080 A

Wavelength=0.71073

Cell: a=12.6893(11) b=14.9289(13) c=19.3173(16)
 alpha=67.1788(12) beta=84.9075(14) gamma=68.7623(12)
 Temperature: 193 K

	Calculated	Reported
Volume	3138.2(5)	3138.2(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H55 Ir N 03 P4 Ru, 0.5(B2 F8)	C60 H55 Ir N 03 P4 Ru, B F4, C4 H10 O
Sum formula	C60 H55 B F4 Ir N 03 P4 Ru	C64 H65 B F4 Ir N 04 P4 Ru
Mr	1342.03	1416.13
Dx, g cm-3	1.420	1.499
Z	2	2
Mu (mm-1)	2.513	2.519
F000	1336.0	1420.0
F000'	1331.92	
h, k, lmax	15, 18, 24	15, 18, 24
Nref	12927	12822
Tmin, Tmax	0.420, 0.575	0.343, 0.607
Tmin'	0.247	

Correction method= INTEGRATION

Data completeness= 0.992 Theta(max)= 26.430

R(reflections)= 0.0339(11625) wR2(reflections)= 0.0931(12822)

S = 1.050 Npar= 662

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

PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) 13

Author Response: Atoms of the pent-3-ene-1,3-diyl ligand were modelled as disordered into two sets of positions with relative occupancies of 60% and 40%. These could not all be satisfactorily refined with anisotropic displacement parameters, thus were left isotropic.

Alert level B

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.95 <> 1.05

From the CIF: _cell_formula_units_Z 2

From the CIF: _chemical_formula_weight 1416.13

TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	60.00	720.66
H	1.01	55.00	55.44

B	10.81	1.00	10.81
N	14.01	1.00	14.01
O	16.00	3.00	48.00
F	19.00	4.00	75.99
P	30.97	4.00	123.90
Ru	101.07	1.00	101.07
Ir	192.22	1.00	192.22
Calculated formula weight			1342.09

Author Response: Attempts to refine peaks of residual electron density as solvent diethyl ether oxygen or carbon atoms were unsuccessful. The data were corrected for disordered electron density through use of the SQUEEZE procedure (Sluis, P. van der; Spek, A. L. Acta Crystallogr. 1990, A46, 194-201) as implemented in PLATON (Spek, A.L. Acta Crystallogr. 1990, A46, C34. PLATON - a multipurpose crystallographic tool. Utrecht University, Utrecht, The Netherlands). A total solvent-accessible void volume of 538.4 cubic Angstroms with a total electron count of 105 (consistent with two molecules of solvent diethyl ether) was found in the unit cell.

PLAT043_ALERT_1_B Check Reported Molecular Weight 1416.13

Author Response: See above response to CHEMW03 alert.

 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?

Author Response: See above response to CHEMW03 alert.

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ ?

Author Response: See above response to CHEMW03 alert.

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?

Author Response: See above response to CHEMW03 alert.

PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced ?
 PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.1 Ratio
 PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ru -- P4 .. 10.0 su

 Alert level G

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: C64 H65 B1 F4 Ir1 N1 O4 P4 Ru1
 Atom count from the _atom_site data: C60 H55 B1 F4 Ir1 N1 O3 P4 Ru1

Author Response: See above response to CHEMW03 alert.

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

Author Response: See above response to CHEMW03 alert.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C64 H65 B F4 Ir N O4 P4 Ru
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	128.00	120.00	8.00
H	130.00	110.00	20.00
B	2.00	2.00	0.00
F	8.00	8.00	0.00
Ir	2.00	2.00	0.00
N	2.00	2.00	0.00
O	8.00	6.00	2.00
P	8.00	8.00	0.00
Ru	2.00	2.00	0.00

Author Response: See above response to CHEMW03 alert.

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF	?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru -- P2 ..	9.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru -- N ..	7.9 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru -- C2 ..	8.0 su
PLAT242_ALERT_2_G Check Low Ueq as Compared to Neighbors for	B1A
PLAT242_ALERT_2_G Check Low Ueq as Compared to Neighbors for	B1B
PLAT301_ALERT_3_G Note: Main Residue Disorder	24 Perc.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure	!

Author Response: See above response to CHEMW03 alert.

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	51
P3 -IR -P1 -C21 169.00 0.30 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	60
P3 -IR -P1 -C11 47.90 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	69
P3 -IR -P1 -C10 -68.70 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	75
P4 -RU -P2 -C41 -34.60 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	80
P4 -RU -P2 -C31 -154.00 0.30 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	85
P4 -RU -P2 -C10 82.50 0.30 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	90
P1 -IR -P3 -C51B -55.40 0.60 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	99
P1 -IR -P3 -C61 -172.80 0.30 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	108
P1 -IR -P3 -C20 67.00 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	114
P1 -IR -P3 -C51A -45.80 0.50 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	120
P2 -RU -P4 -C71 150.70 0.30 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	125
P2 -RU -P4 -C81 31.40 0.40 1.555 1.555 1.555	1.555

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	130
P2 -RU -P4 -C20 -84.80 0.30 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	132
C2 -RU -N -C17 -120.00 5.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	133
C1 -RU -N -C17 56.00 5.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	134
P2 -RU -N -C17 -31.00 5.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	135
P4 -RU -N -C17 151.00 5.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	136
IR -RU -N -C17 60.00 5.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	163
C1 -RU -C2 -O2 4.00 4.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	164
N -RU -C2 -O2 18.00 0.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	165
P2 -RU -C2 -O2 96.00 4.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	166
P4 -RU -C2 -O2 -90.00 4.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	167
IR -RU -C2 -O2 1.00 4.00 1.555 1.555 1.555 1.555	
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	246
RU -N -C17 -C18 58.00 20.00 1.555 1.555 1.555 1.555	
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	14
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	!
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed	!

1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
28 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: 8

Bond precision: C-C = 0.0048 A

Wavelength=0.71073

Cell: a=12.5683(8) b=12.8768(8) c=20.1977(13)
alpha=99.4872(9) beta=90.1385(9) gamma=94.0337(9)
Temperature: 193 K

	Calculated	Reported
Volume	3215.8(4)	3215.8(4)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C64 H60 Ir 03 P4 Ru, C F3 03 S	C64 H60 Ir 03 P4 Ru, C F3 03 S, 1.5(C H2 Cl2)
Sum formula	C65 H60 F3 Ir 06 P4 Ru S	C66.50 H63 Cl3 F3 Ir 06 P4 Ru S
Mr	1443.37	1570.73
Dx,g cm-3	1.491	1.622
Z	2	2
Mu (mm-1)	2.491	2.618
F000	1444.0	1570.0
F000'	1440.21	
h, k, lmax	15, 16, 25	15, 15, 25
Nref	13164	13107
Tmin, Tmax	0.179, 0.300	0.265, 0.379
Tmin'	0.151	

Correction method= INTEGRATION

Data completeness= 0.996 Theta(max)= 26.380

R(reflections)= 0.0227(12141) wR2(reflections)= 0.0611(13107)

S = 1.049 Npar= 986

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 B

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.95 <> 1.05

From the CIF: _cell_formula_units_Z 2

From the CIF: _chemical_formula_weight 1570.73

TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	65.00	780.71
H	1.01	60.00	60.48
O	16.00	6.00	95.99
F	19.00	3.00	56.99
P	30.97	4.00	123.90
S	32.07	1.00	32.07
Cl	35.45	0.00	0.00
Ru	101.07	1.00	101.07
Ir	192.22	1.00	192.22

Calculated formula weight 1443.43

Author Response: Attempts to refine peaks of residual electron density as solvent diethyl ether oxygen or carbon atoms were unsuccessful. The data were corrected for disordered electron density through use of the SQUEEZE procedure (Sluis, P. van der; Spek, A. L. Acta Crystallogr. 1990, A46, 194-201) as implemented in PLATON (Spek, A.L. Acta Crystallogr. 1990, A46, C34. PLATON - a multipurpose crystallographic tool. Utrecht University, Utrecht, The Netherlands). A total solvent-accessible void volume of 325 cubic Angstroms with a total electron count of 121 (consistent with 1.5 molecules of solvent dichloromethane per formula unit of the complex ion) was found in the unit cell.

PLAT043_ALERT_1_B Check Reported Molecular Weight 1570.73

Author Response: See above response to CHEMW03 alert.

PLAT220_ALERT_2_B Large Non-Solvent	C	Ueq(max)/Ueq(min)	...	4.2	Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for	P3	--	C71A ..	8.2	su
PLAT230_ALERT_2_B Hirshfeld Test Diff for	P4	--	C81A ..	9.2	su
PLAT230_ALERT_2_B Hirshfeld Test Diff for	P4	--	C81B ..	7.2	su

 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?

Author Response: See above response to CHEMW03 alert.

PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 4.87 Perc.

Author Response: See above response to CHEMW03 alert.

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?

Author Response: See above response to CHEMW03 alert.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density		2.48
PLAT215_ALERT_3_C Disordered C82A	has ADP max/min Ratio	3.1
PLAT215_ALERT_3_C Disordered C82B	has ADP max/min Ratio	3.5
PLAT234_ALERT_4_C Large Hirshfeld Difference P3	-- C71B ..	0.16 Ang.
PLAT241_ALERT_2_C Check High	Ueq as Compared to Neighbors for C30	
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of	S	
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of	C99	
PLAT245_ALERT_2_C U(iso) H85A	Smaller than U(eq) C85B by ...	0.012 AngSq
PLAT410_ALERT_2_C Short Intra H...H Contact H20B	.. H56B ..	1.98 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H30A	.. H86B ..	1.99 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H14D	.. H44 ..	2.12 Ang.

 Alert level G

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: C66.5 H63 Cl3 F3 Ir1 O6 P4 Ru1
 Atom count from the _atom_site data: C65 H60 F3 Ir1 O6 P4 Ru1 S1

Author Response: See above response to CHEMW03 alert.

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

Author Response: See above response to CHEMW03 alert.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C66.50 H63 Cl3 F3 Ir 06 P4 Ru S
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	133.00	130.00	3.00
H	126.00	120.00	6.00
Cl	6.00	0.00	6.00
F	6.00	6.00	0.00
Ir	2.00	2.00	0.00
O	12.00	12.00	0.00
P	8.00	8.00	0.00
Ru	2.00	2.00	0.00
S	2.00	2.00	0.00

Author Response: See above response to CHEMW03 alert.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.69 mm
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.00090 Deg.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ir -- C1 ..	5.5 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ir -- C10 ..	6.2 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru -- P2 ..	6.5 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru -- P4 ..	6.0 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru -- C2 ..	5.8 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru -- C3 ..	6.6 su
PLAT301_ALERT_3_G	Note: Main Residue Disorder	38 Perc.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C54B .. C85B ..	2.89 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C55B .. C85B ..	2.74 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C56B .. C85B ..	3.09 Ang.
PLAT605_ALERT_4_G	Structure Contains Solvent Accessible VOIDS of .	118 A**3

Author Response: See above response to CHEMW03 alert.

PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	6
	C1 -IR -RU -C3 144.00 3.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	7
	C10 -IR -RU -C3 -36.00 3.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	8
	C4 -IR -RU -C3 -39.00 3.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	9
	P3 -IR -RU -C3 -126.00 3.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	10
	P1 -IR -RU -C3 53.00 3.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	38
	P3 -IR -P1 -C20 78.20 1.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	43
	P3 -IR -P1 -C31 -164.10 1.00 1.555 1.555 1.555	1.555

PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	48
P3 -IR -P1 -C21	-39.90	1.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	79
P1 -IR -P3 -C71B	167.30	1.20	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	84
P1 -IR -P3 -C30	-77.30	1.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	89
P1 -IR -P3 -C61	41.80	1.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	94
P1 -IR -P3 -C71A	159.80	1.10	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	127
C10 -IR -C1 -01	0.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	128
C4 -IR -C1 -01	18.00	0.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	129
P3 -IR -C1 -01	-89.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	130
P1 -IR -C1 -01	92.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	131
RU -IR -C1 -01	1.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	132
C3 -RU -C2 -02	-1.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	133
C10 -RU -C2 -02	18.00	0.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	134
C11B-RU -C2 -02	162.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	135
C11A-RU -C2 -02	-166.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	136
P2 -RU -C2 -02	88.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	137
P4 -RU -C2 -02	-91.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	138
IR -RU -C2 -02	18.00	0.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	139
C2 -RU -C3 -03	8.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	140
C10 -RU -C3 -03	-170.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	141
C11B-RU -C3 -03	-165.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	142
C11A-RU -C3 -03	18.00	0.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	143
P2 -RU -C3 -03	-87.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	144
P4 -RU -C3 -03	103.00	3.00	1.555	1.555 1.555	1.555
PLAT710_ALERT_4_G Delete	1-2-3 or 2-3-4	Linear	Torsion	Angle ... #	145
IR -RU -C3 -03	-135.00	2.00	1.555	1.555 1.555	1.555
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms					!
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints					2
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed					!

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7 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

22 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
37 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: 10

Bond precision: C-C = 0.0071 A Wavelength=0.71073

Cell: a=12.4286(6) b=15.0216(7) c=18.6676(8)
 alpha=95.2809(5) beta=100.1560(5) gamma=112.2561(5)

Temperature: 173 K

	Calculated	Reported
Volume	3126.4(2)	3126.4(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H58 Ir 03 P4 Ru, 2(C H2 Cl2), B F4	C62 H58 Ir 03 P4 Ru, 2(C H2 Cl2), B F4
Sum formula	C64 H62 B Cl4 F4 Ir 03 P4 Ru	C64 H62 B Cl4 F4 Ir 03 P4 Ru
Mr	1524.92	1524.90
Dx, g cm-3	1.620	1.620
Z	2	2
Mu (mm-1)	2.698	2.698
F000	1520.0	1520.0
F000'	1517.13	
h, k, lmax	16, 19, 24	16, 19, 24
Nref	14455	14387
Tmin, Tmax	0.381, 0.433	0.374, 0.492
Tmin'	0.286	

Correction method= NUMERICAL

Data completeness= 0.995 Theta(max)= 27.560

R(reflections)= 0.0345(13492) wR2(reflections)= 0.0964(14387)

S = 1.047 Npar= 742

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 B

PLAT366_ALERT_2_B Short? C(sp?)-C(sp?) Bond C17 - C18 ... 1.25 Ang.

● Alert level C

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of

B

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	9.00
PLAT343_ALERT_2_G	Check Angle Range in Main Residue for ..	C17
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	6
C1	-IR -RU -C3 -170.00 4.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	7
C17	-IR -RU -C3 9.00 4.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	8
C6	-IR -RU -C3 18.00 4.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	9
P3	-IR -RU -C3 99.00 4.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	10
P1	-IR -RU -C3 -76.00 4.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	33
P3	-IR -P1 -C11 160.30 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	38
P3	-IR -P1 -C10 -81.10 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	43
P3	-IR -P1 -C21 35.90 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	66
P1	-IR -P3 -C20 72.90 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	71
P1	-IR -P3 -C61 -44.90 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	76
P1	-IR -P3 -C51 -166.60 0.40 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	96
C17	-IR -C1 -O1 7.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	97
C6	-IR -C1 -O1 -175.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	98
P3	-IR -C1 -O1 99.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	99
P1	-IR -C1 -O1 -84.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	100
RU	-IR -C1 -O1 9.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	101
C3	-RU -C2 -O2 5.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	102
C17	-RU -C2 -O2 -175.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	103
C18	-RU -C2 -O2 -175.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	104
P2	-RU -C2 -O2 -84.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	105
P4	-RU -C2 -O2 95.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	106
IR	-RU -C2 -O2 -175.00 5.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	107
C2	-RU -C3 -O3 -10.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	108
C17	-RU -C3 -O3 170.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	109
C18	-RU -C3 -O3 170.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	110
P2	-RU -C3 -O3 84.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	111

P4	-RU	-C3	-O3	-106.00	6.00	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete	1-2-3	or 2-3-4	Linear	Torsion	Angle	...	#	112
IR	-RU	-C3	-O3	161.00	4.00	1.555	1.555	1.555	1.555
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels								4

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 32 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 3 ALERT type 2 Indicator that the structure model may be wrong or deficient
 0 ALERT type 3 Indicator that the structure quality may be low
 30 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*, 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.







