

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: Th-SINAP-100

Bond precision: C-C = 0.0196 A

Wavelength=0.71073

Cell: a=14.5147(15) b=17.2275(18) c=18.484(2)
 alpha=107.723(5) beta=99.215(5) gamma=111.643(5)
Temperature: 296 K

	Calculated	Reported
Volume	3893.7(8)	3893.6(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C132 N24 O38 Th6, 8(0)	C132 N24 O46 Th6
Sum formula	C132 N24 O46 Th6	C132 N24 O46 Th6
Mr	4049.80	4049.80
Dx, g cm-3	1.727	1.727
Z	1	1
Mu (mm-1)	5.791	5.791
F000	1868.0	1868.0
F000'	1826.00	
h, k, lmax	18, 22, 24	18, 22, 24
Nref	18081	17985
Tmin, Tmax	0.439, 0.629	0.439, 0.629
Tmin'	0.392	

Correction method= # Reported T Limits: Tmin=0.439 Tmax=0.629
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 27.615

R(reflections)= 0.0446(13184)

wR2(reflections)= 0.1287(17985)

S = 1.036

Npar= 937

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

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in Structure ! Check

Author Response: There exists a large void in the structure, which is not uncommon in this kind of metal-organic complex structure.

 Alert level B

PLAT213_ALERT_2_B Atom 016 has ADP max/min Ratio 4.1 prolat
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of 09 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of 016 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of 018 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 01W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 02W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 03W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 05W Check

 Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.32 Report
PLAT213_ALERT_2_C Atom 09 has ADP max/min Ratio 3.6 prolat
PLAT213_ALERT_2_C Atom 018 has ADP max/min Ratio 3.5 prolat
PLAT213_ALERT_2_C Atom C20 has ADP max/min Ratio 4.0 prolat
PLAT213_ALERT_2_C Atom C36 has ADP max/min Ratio 3.2 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 03 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 04 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 019 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C16 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C20 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C30 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C36 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Th1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Th2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Th3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C34 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C37 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 03W 0.128 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 05W 0.202 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01962 Ang.

 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	16.17	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.005	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	0		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	0		
PLAT794_ALERT_5_G	Tentative Bond Valency for Th1 (IV) .	4.03	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th2 (IV) .	4.20	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th3 (IV) .	4.19	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	7	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 38 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
 4 ALERT type 4 Improvement, methodology, query or suggestion
 3 ALERT type 5 Informative message, check

Datablock: Th-SINAP-100-UV

Bond precision: C-C = 0.0197 A

Wavelength=0.71073

Cell: a=14.5035(11) b=17.2237(14) c=18.4425(14)
 alpha=107.615(2) beta=99.169(3) gamma=111.597(2)
 Temperature: 296 K

	Calculated	Reported
Volume	3887.5(5)	3887.5(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C132 N24 O38 Th6, 8(0)	C132 N24 O46 Th6
Sum formula	C132 N24 O46 Th6	C132 N24 O46 Th6
Mr	4049.80	4049.80
Dx, g cm-3	1.730	1.730
Z	1	1
Mu (mm-1)	5.800	5.800
F000	1868.0	1868.0
F000'	1826.00	
h, k, lmax	18, 22, 24	18, 22, 24
Nref	18158	18027
Tmin, Tmax	0.438, 0.629	0.438, 0.629
Tmin'	0.391	

Correction method= # Reported T Limits: Tmin=0.438 Tmax=0.629
AbsCorr = MULTI-SCAN

Data completeness= 0.993

Theta(max)= 27.673

R(reflections)= 0.0423(14093)

wR2(reflections)= 0.1292(18027)

S = 1.061

Npar= 937

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

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in Structure ! Check

Author Response: There exists a large void in the structure, which is not uncommon in this kind of metal-organic complex structure.

 Alert level B

PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	03	Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	09	Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	016	Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	018	Check
PLAT306_ALERT_2_B	Isolated	Oxygen Atom (H-atoms Missing ?)		01W	Check
PLAT306_ALERT_2_B	Isolated	Oxygen Atom (H-atoms Missing ?)		02W	Check
PLAT306_ALERT_2_B	Isolated	Oxygen Atom (H-atoms Missing ?)		03W	Check
PLAT306_ALERT_2_B	Isolated	Oxygen Atom (H-atoms Missing ?)		04W	Check

 Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		3.32	Report
PLAT213_ALERT_2_C	Atom O9	has ADP max/min Ratio		3.1 prolat
PLAT213_ALERT_2_C	Atom O16	has ADP max/min Ratio		3.3 prolat
PLAT213_ALERT_2_C	Atom C18	has ADP max/min Ratio		3.4 prolat
PLAT213_ALERT_2_C	Atom C36	has ADP max/min Ratio		3.1 prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C Ueq(max)/Ueq(min) Range	5.8	Ratio
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	04	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	08	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C3	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C4	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C18	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C20	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C30	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C35	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C36	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C66	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Th1	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Th2	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Th3	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C5	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C34	Check

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C37	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	03W	0.143	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	04W	0.224	Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.0197	Ang.

● Alert level G

PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please	Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	14.05	Why ?
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # 0	2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # 0	3	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Th1 (IV) .	4.02	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th2 (IV) .	4.24	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th3 (IV) .	4.19	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check

1 **ALERT level A** = Most likely a serious problem - resolve or explain
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4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
36 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
3 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: Th-SINAP-100-beforegama

Bond precision: C-C = 0.0143 A

Wavelength=0.71073

Cell:	a=14.5258(11)	b=17.2459(16)	c=18.5038(15)
	alpha=107.681(3)	beta=99.357(3)	gamma=111.482(3)
Temperature:	293 K		

	Calculated	Reported
Volume	3908.7(6)	3908.7(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C132 H84 N24 O38 Th6, 8(0)	C132 H84 N24 O46 Th6
Sum formula	C132 H84 N24 O46 Th6	C132 H84 N24 O46 Th6
Mr	4134.48	4134.47
Dx, g cm-3	1.757	1.756
Z	1	1
Mu (mm-1)	5.770	5.770
F000	1952.0	1952.0
F000'	1909.96	
h, k, lmax	18, 22, 24	18, 22, 24
Nref	18121	18031
Tmin, Tmax	0.413, 0.500	0.439, 0.629
Tmin'	0.382	

Correction method= # Reported T Limits: Tmin=0.439 Tmax=0.629
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.594

R(reflections)= 0.0313(15721) wR2(reflections)= 0.1019(18031)

S = 1.069 Npar= 937

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

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in Structure ! Check

Author Response: There exists a large void in the structure, which is not uncommon in this kind of metal-organic complex structure.

Alert level B

PLAT241_ALERT_2_B High	'MainMol' Ueq as Compared to Neighbors of	09	Check
PLAT241_ALERT_2_B High	'MainMol' Ueq as Compared to Neighbors of	016	Check
PLAT241_ALERT_2_B High	'MainMol' Ueq as Compared to Neighbors of	018	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)		01W	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)		02W	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)		03W	Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)		04W	Check
PLAT430_ALERT_2_B Short Inter D...A Contact	01 ..02W .	2.74	Ang.
	x, y, z =	1_555	Check
PLAT430_ALERT_2_B Short Inter D...A Contact	03W ..013 .	2.73	Ang.
	x, y, z =	1_555	Check
PLAT430_ALERT_2_B Short Inter D...A Contact	04W ..05 .	2.66	Ang.

Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.28	Report
PLAT193_ALERT_1_C	Cell and Diffraction Temperatures Differ by	3	Degree
PLAT213_ALERT_2_C	Atom O9 has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom O16 has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom O18 has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C19 has ADP max/min Ratio	3.1	prolat
PLAT213_ALERT_2_C	Atom C20 has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C36 has ADP max/min Ratio	3.3	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.6	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C14 --C15 .	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C15 --C16 .	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C50 --C51 .	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C62 --C63 .	0.16	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	03	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	04	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	014	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C3	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C20	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C30	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C35	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C36	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C66	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Th1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Th2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Th3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C37	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including 03W	0.134	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including 04W	0.238	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01428	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 01 ..01W .	2.86	Ang.
	x,y,z = 1_555 Check		
PLAT430_ALERT_2_C	Short Inter D...A Contact 03W ..N10 .	2.88	Ang.
	x,y,z = 1_555 Check		

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.47	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --01 .	6.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --03 .	7.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --018 .	14.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th2 --05 .	6.8	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th2 --09 .	6.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th3 --016 .	9.5	s.u.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	0		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	0		
PLAT794_ALERT_5_G	Tentative Bond Valency for Th1 (IV) .	4.02	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th2 (IV) .	4.22	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th3 (IV) .	4.17	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !

1 **ALERT level A** = Most likely a serious problem - resolve or explain
10 **ALERT level B** = A potentially serious problem, consider carefully
34 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
45 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
6 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: Th-SINAP-100-gama

Bond precision: C-C = 0.0164 Å

Wavelength=0.71073

Cell: a=14.500(6) b=17.173(7) c=18.368(9)
alpha=106.984(15) beta=99.480(16) gamma=111.525(16)
Temperature: 296 K

	Calculated	Reported
Volume	3875(3)	3875(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C132 H84 N24 O38 Th6, 8(0)	C132 H84 N24 O46 Th6
Sum formula	C132 H84 N24 O46 Th6	C132 H84 N24 O46 Th6
Mr	4134.48	4134.47
Dx, g cm ⁻³	1.772	1.772
Z	1	1
Mu (mm ⁻¹)	5.820	5.821
F000	1952.0	1952.0
F000'	1909.96	
h, k, lmax	18, 22, 23	18, 22, 23
Nref	17957	17815
Tmin, Tmax	0.410, 0.497	0.410, 0.497
Tmin'	0.379	

Correction method= # Reported T Limits: Tmin=0.410 Tmax=0.497
AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta(max)= 27.587

R(reflections)= 0.0374(14466)

wR2(reflections)= 0.1096(17815)

S = 1.052

Npar= 925

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

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in Structure ! Check

Author Response: There exists a large void in the structure, which is not uncommon in this kind of metal-organic complex structure.

Alert level B

PLAT220_ALERT_2_B	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	6.5	Ratio	
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C15	--C16	.	0.28	Ang.	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		03	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		09	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		016	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		018	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		C19	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		C35	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of		Th2	Check	
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including		05W		0.340	Check	
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)					01W	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)					02W	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)					03W	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)					05W	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	01	..02W	.	2.74	Ang.	
			x,y,z =	1_555	Check		
PLAT430_ALERT_2_B	Short Inter D...A Contact	03W	..013	.	2.70	Ang.	
			x,y,z =	1_555	Check		
PLAT430_ALERT_2_B	Short Inter D...A Contact	05	..05W	.	2.69	Ang.	
			x,y,z =	1_555	Check		

Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.80	Report
PLAT193_ALERT_1_C	Cell and Diffraction Temperatures Differ by		3	Degree
PLAT213_ALERT_2_C	Atom 09	has ADP max/min Ratio		3.2
PLAT213_ALERT_2_C	Atom 016	has ADP max/min Ratio		3.6
PLAT213_ALERT_2_C	Atom C3	has ADP max/min Ratio		3.2
PLAT213_ALERT_2_C	Atom C19	has ADP max/min Ratio		3.6
PLAT213_ALERT_2_C	Atom C20	has ADP max/min Ratio		3.4
PLAT213_ALERT_2_C	Atom C35	has ADP max/min Ratio		3.7
PLAT213_ALERT_2_C	Atom C36	has ADP max/min Ratio		3.4
PLAT220_ALERT_2_C	NonSolvent	Resd 1	0	Ueq(max)/Ueq(min) Range
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N3	--C12	.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N6	--C32	.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C11	--C12	.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C50	--C51	.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	04
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	08
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	010
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	019
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C3
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C10
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C14
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C30

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C66	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Th1	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Th3	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C13	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C34	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C37	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	03W		0.134	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds			0.01645	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C24 - C25	.	1.53	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact	01 ..01W	.	2.88	Ang.
		x,y,z =		1_555	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	02W ..N12	.	2.89	Ang.
		-x,-y,1-z =		2_556	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	03W ..N10	.	2.88	Ang.
		x,y,z =		1_555	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	05W ..N7	.	2.88	Ang.
		x,y,z =		1_555	Check

● Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ			Please	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical			?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large			14.68	Why ?
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)			293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Th1 --03	.	6.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Th1 --018	.	7.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Th2 --03	.	5.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Th2 --05	.	8.4	s.u.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	05 ..C14		3.00	Ang.
		-x,-y,2-z =		2_557	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	0		2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	0		3	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Th1	(IV)	.	3.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th2	(IV)	.	4.25	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Th3	(IV)	.	4.14	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please	Do !
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged			Please	Check

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 54 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
 7 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.







