

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: 2

Bond precision: C-C = 0.0043 A

Wavelength=0.71073

Cell: a=8.5296(14) b=8.8986(14) c=10.5757(15)
alpha=71.300(4) beta=78.698(4) gamma=74.264(5)
Temperature: 298 K

	Calculated	Reported
Volume	726.6(2)	726.59(19)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H22 Mn N4 O6, 2(H2 O)	?
Sum formula	C30 H26 Mn N4 O8	C30 H26 Mn N4 O8
Mr	625.49	625.49
Dx, g cm-3	1.429	1.429
Z	1	1
Mu (mm-1)	0.512	0.512
F000	323.0	323.0
F000'	323.49	
h, k, lmax	10, 10, 12	10, 10, 12
Nref	2768	2748
Tmin, Tmax	0.912, 0.950	0.878, 0.951
Tmin'	0.875	

Correction method= # Reported T Limits: Tmin=0.878 Tmax=0.951
AbsCorr = MULTI-SCAN

Data completeness= 0.993

Theta(max)= 25.750

R(reflections)= 0.0592(2121)

wR2(reflections)= 0.1543(2748)

S = 1.023

Npar= 196

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 G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

-
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0 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
1 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
-

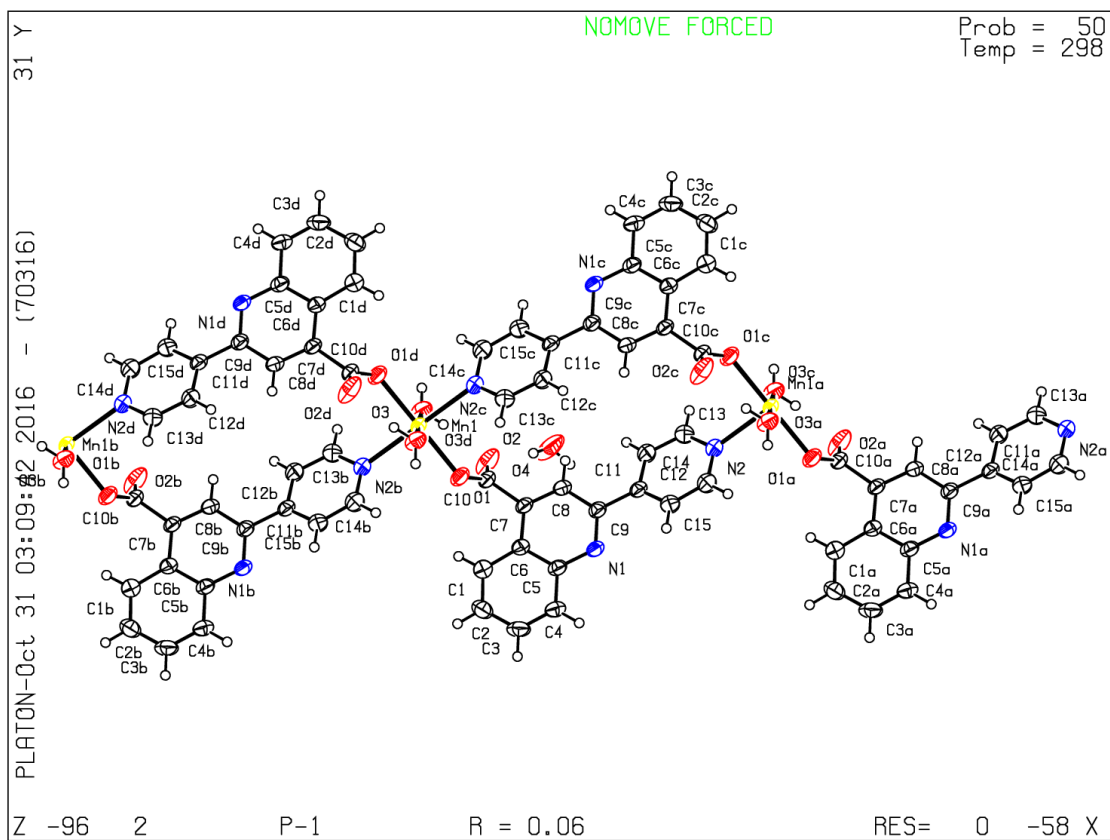
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[CIF dictionary](#)

[Interpreting this report](#)

Datablock: mo_qj_178_0m

Bond precision: C-C = 0.0022 Å

Wavelength=0.71073

Cell: a=8.5511(4) b=8.7942(5) c=10.4459(5)
alpha=70.748(2) beta=78.982(1) gamma=74.252(2)
Temperature: 298 K

	Calculated	Reported
Volume	709.29(6)	709.29(6)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H22 Co N4 O6, 2(H2 O)	?
Sum formula	C30 H26 Co N4 O8	C30 H26 Co N4 O8
Mr	629.48	629.48
Dx, g cm-3	1.474	1.474
Z	1	1
Mu (mm-1)	0.664	0.664
F000	325.0	325.0
F000'	325.50	
h, k, lmax	10, 10, 12	10, 10, 12
Nref	2643	2607
Tmin, Tmax	0.819, 0.905	0.826, 0.907
Tmin'	0.819	

Correction method= # Reported T Limits: Tmin=0.826 Tmax=0.907
AbsCorr = MULTI-SCAN

Data completeness= 0.986

Theta(max)= 25.500

R(reflections)= 0.0279(2468)

wR2(reflections)= 0.0733(2607)

S = 1.108

Npar= 196

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 G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
-

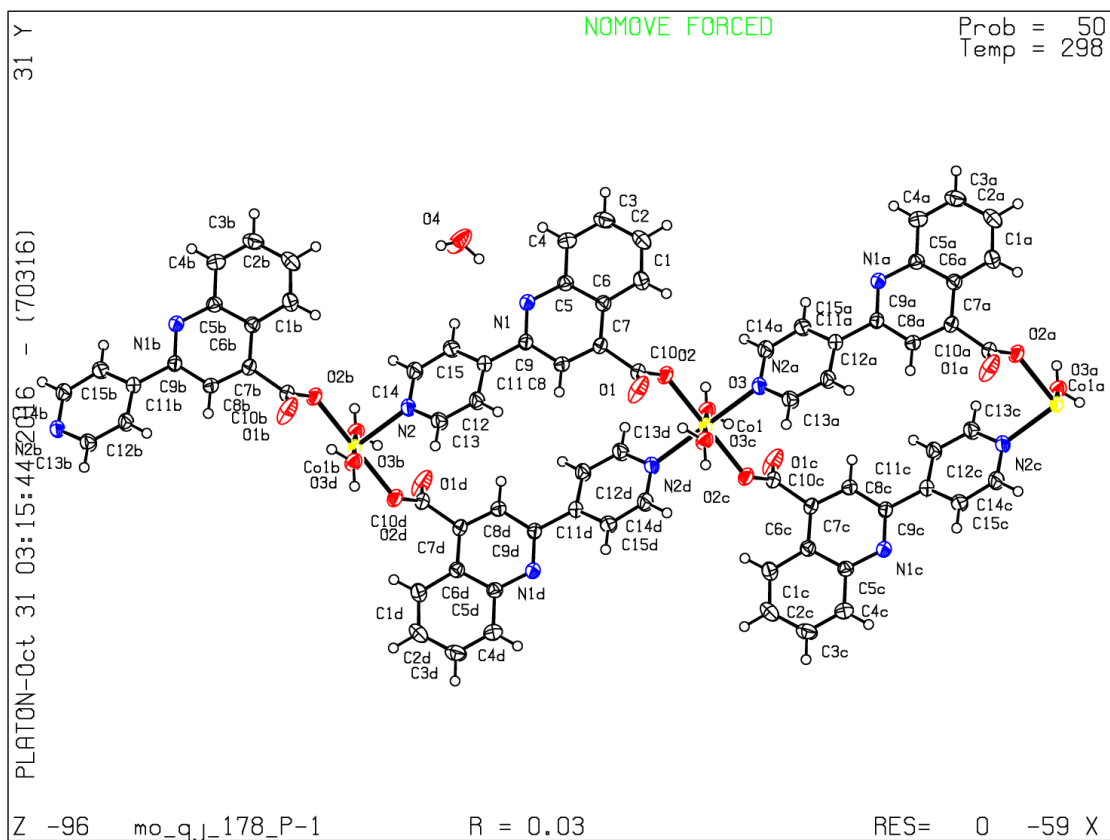
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[CIF dictionary](#)

[Interpreting this report](#)

Datablock: 3

Bond precision: C-C = 0.0028 Å

Wavelength=0.71073

Cell: a=8.6281(5) b=8.9010(5) c=10.6287(7)
alpha=72.133(2) beta=78.500(2) gamma=74.632(1)
Temperature: 298 K

	Calculated	Reported
Volume	742.90(8)	742.90(8)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H22 Cd N4 O6, 2(H2 O)	?
Sum formula	C30 H26 Cd N4 O8	C30 H26 Cd N4 O8
Mr	682.96	682.95
Dx, g cm-3	1.527	1.527
Z	1	1
Mu (mm-1)	0.791	0.791
F000	346.0	346.0
F000'	345.35	
h, k, lmax	10, 10, 13	10, 10, 13
Nref	2924	2877
Tmin, Tmax	0.827, 0.924	0.821, 0.925
Tmin'	0.814	

Correction method= # Reported T Limits: Tmin=0.821 Tmax=0.925
AbsCorr = MULTI-SCAN

Data completeness= 0.984

Theta(max)= 26.000

R(reflections)= 0.0218(2848)

wR2(reflections)= 0.0569(2877)

S = 1.131

Npar= 196

The following ALERTS were generated. Each ALERT has the format

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PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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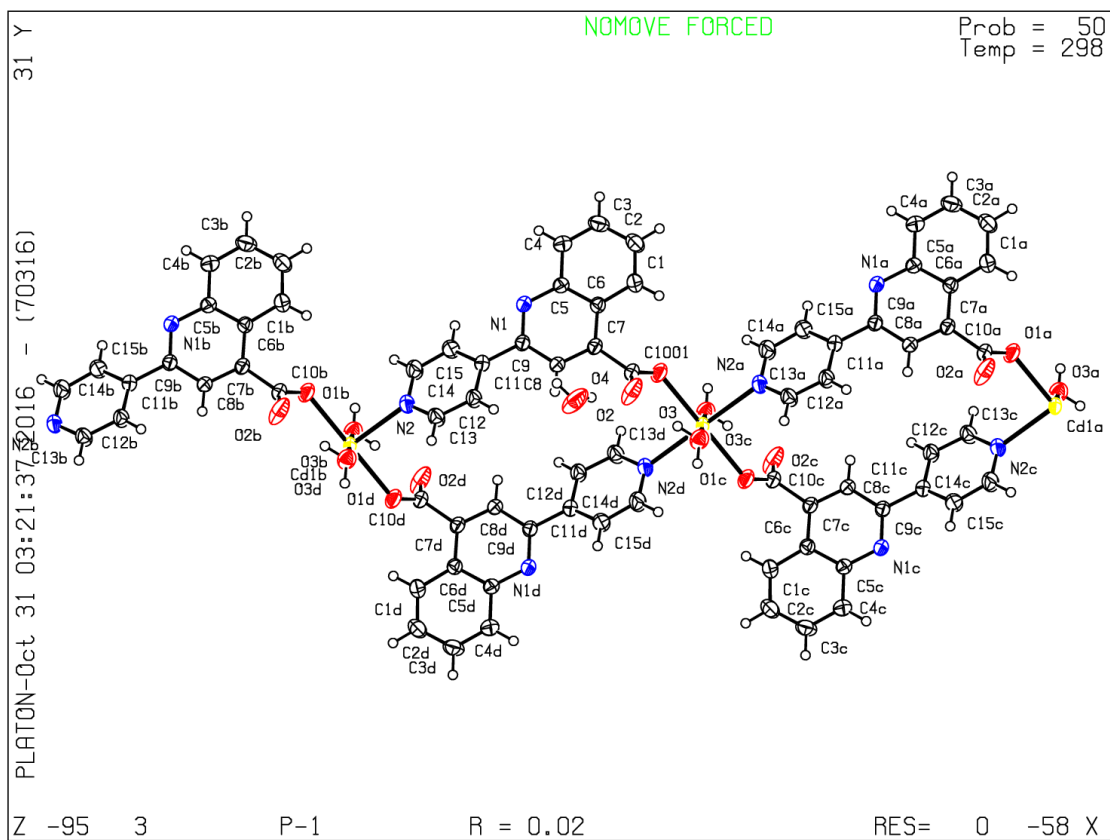
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[CIF dictionary](#)

[Interpreting this report](#)

Datablock: mm2

Bond precision: C-C = 0.0063 Å

Wavelength=0.71073

Cell: a=14.2981(7) b=17.5489(8) c=13.4398(7)
alpha=90 beta=114.657(1) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	3064.8(3)	3064.8(3)
Space group	C c	Cc
Hall group	C -2yc	?
Moiety formula	C30 H22 Ag2 N4 O6, 2(H 00.50), H 00.50, H2 O	?
Sum formula	C30 H28 Ag2 N4 O9	C30 H28 Ag2 N4 O9
Mr	804.30	804.30
Dx, g cm-3	1.743	1.743
Z	4	4
Mu (mm-1)	1.338	1.338
F000	1608.0	1608.0
F000'	1601.51	
h, k, lmax	18, 22, 17	18, 22, 17
Nref	7071[3541]	6509
Tmin, Tmax	0.733, 0.875	0.732, 0.874
Tmin'	0.709	

Correction method= # Reported T Limits: Tmin=0.732 Tmax=0.874

AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.92

Theta(max)= 27.540

R(reflections)= 0.0361(6051)

wR2(reflections)= 0.0939(6509)

S = 1.065

Npar= 410

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

PLAT420_ALERT_2_B	D-H Without Acceptor	*08	-- *H8A	...	Please Check
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 Alert level C

PLAT165_ALERT_3_C	Nr. of Status R Flagged Non-Hydrogen Atoms	2	Note
PLAT222_ALERT_3_C	Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C10	Check
PLAT314_ALERT_2_C	Check Small Angle for H2O: Metal-O6 -H6B	83.17	Degree
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C7 - C10 ..	1.53	Ang.

 Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	12	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 -- O5 ..	12.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 -- N1 ..	16.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 -- N3 ..	8.3	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of *O8 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H8A is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H8B is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O9 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H9A is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H9B is Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder Percentage =	33	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

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16 **ALERT level G** = General information/check it is not something unexpected

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

7 **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

8 **ALERT type 4** Improvement, methodology, query or suggestion

3 **ALERT type 5** Informative message, check

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