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: Zn_AIm

Bond precision: C-C = 0.0117 A Wavelength=1.54180

Cell: a=17.0454(11) b=17.0454(11) c=17.0454(11)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	4952.5(10)	4952.5(9)
Space group	I -4 3 m	I-43m
Hall group	: I -4 2 3	I -4 2 3
Moiety formula	C10 H6 N4 Zn	C10 H6 N4 Zn
Sum formula	C10 H6 N4 Zn	C10 H6 N4 Zn
Mr	247.58	247.56
Dx,g cm-3	0.996	0.996
Z	12	12
Mu (mm-1)	1.911	0.000
F000	1488.0	1488.0
F000’	1472.58	
h,k,lmax	12,12,12	
Nref	222[130]	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 2116 Ang**3

Author Response: This is an open, microporous metal-organic framework

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Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.9961 Check

Author Response: The low density is the consequence of structure porosity.

Alert level C

REFI015_ALERT_1_C _refine_ls_shift/su_max is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed
SHFSU_01

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01167 Ang.

Alert level G

PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 2 Note
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C1 - C3 . 1.41 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 2.00 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 41 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note

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

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

Datablock: Co_AIm

Bond precision: C-C = 0.0180 A Wavelength=1.54180

Cell:	a=16.9604(17)	b=16.9604(17)	c=16.9604(17)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	4878.8(15)	4878.8(14)
Space group	I -4 3 m	I-4 3 m
Hall group	: I -4 2 3	I -4 2 3
Moiety formula	C10 H6 Co N4	C10 H6 Co N4
Sum formula	C10 H6 Co N4	C10 H6 Co N4
Mr	241.12	241.12
Dx,g cm-3	0.985	0.985
Z	12	12
Mu (mm-1)	8.116	0.000
F000	1452.0	1452.0
F000’	1427.51	
h,k,lmax	10,10,10	
Nref	153[91]	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 2087 Ang**3

Author Response: This is an open, microporous metal-organic framework

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Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.9848 Check

Author Response: The low density is the consequence of porocity

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.018 Ang.

Author Response: The structure was solved from powder data.

Alert level C

```
REFI015_ALERT_1_C  _refine_ls_shift/su_max is missing
           Maximum shift/s.u. ratio after final refinement cycle.
           The following tests will not be performed
           SHFSU_01
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Alert level G

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PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          2 Note
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C1       - C3       .       1.42 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       1.71 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          41 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         3 Note
```

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1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: Co_VIm

Bond precision: C-C = 0.0190 A Wavelength=1.54180

Cell:	a=17.2960(14)	b=17.2960(14)	c=17.2960(14)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	5174.1(13)	5174.1(13)
Space group	I -4 3 m	I -4 3 m
Hall group	: I -4 2 3	I -4 2 3
Moiety formula	C10 H10 Co N4	C10 H10 Co N4
Sum formula	C10 H10 Co N4	C10 H10 Co N4
Mr	245.15	245.15
Dx,g cm-3	0.944	0.944
Z	12	12
Mu (mm-1)	7.653	0.000
F000	1500.0	1500.0
F000’	1475.48	
h,k,lmax	7,7,7	
Nref	58[37]	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 2297 Ang**3

Author Response: This is an open, microporous metal-organic framework

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Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.9441 Check

Author Response: .Low density is a consequence of structure porosity.

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.019 Ang.

Author Response: The structure was solved from powder data.

Alert level C

REFI015_ALERT_1_C _refine_ls_shift/su_max is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed
SHFSU_01

Alert level G

PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2	Note
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =	3	Note
PLAT300_ALERT_4_G Atom Site Occupancy of C4 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4 Constrained at	0.5	Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1)	12%	Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #	4	Check
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON	45	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	1	Note

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1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: Cd_AIm

Bond precision: C-C = 0.0123 A Wavelength=1.54180

Cell: a=17.9712(9) b=17.9712(9) c=17.9712(9)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	5804.1(9)	5804.0(9)
Space group	I -4 3 m	I -4 3 m
Hall group	: I -4 2 3	I -4 2 3
Moiety formula	C10 H6 Cd N4	C10 H6 Cd N4
Sum formula	C10 H6 Cd N4	C10 H6 Cd N4
Mr	294.60	294.60
Dx,g cm-3	1.011	1.011
Z	12	12
Mu (mm-1)	8.910	0.000
F000	1704.0	1704.0
F000’	1709.69	
h,k,lmax	7,7,7	
Nref	62[39]	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 2775 Ang**3

Author Response: This is an open, microporous metal-organic framework.

Alert level C

```
REFI015_ALERT_1_C  _refine_ls_shift/su_max is missing
            Maximum shift/s.u. ratio after final refinement cycle.
            The following tests will not be performed
            SHFSU_01
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01233 Ang.
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Alert level G

```
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          2 Note
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C1       - C3       .       1.41 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1       (II)      .       2.11 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON           1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         1 Note
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

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

Datablock: Cd_VIm

```
Bond precision:  C-C = 0.0200 A          Wavelength=1.54180

Cell:              a=18.234(2)      b=18.234(2)      c=18.234(2)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K
```

	Calculated	Reported
Volume	6062(2)	6062(2)
Space group	I -4 3 m	I -4 3 m
Hall group	: I -4 2 3	I -4 2 3
Moiety formula	C10 H10 Cd N4	C10 H10 Cd N4
Sum formula	C10 H10 Cd N4	C10 H10 Cd N4
Mr	298.63	298.63
Dx,g cm-3	0.982	0.982
Z	12	12
Mu (mm-1)	8.531	0.000
F000	1752.0	1752.0
F000’	1757.67	
h,k,lmax	8,8,8	
Nref	63[40]	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 2904 Ang**3

Author Response: This is an open, microporous metal-organic framework.
This is an open, microporous metal-organic framework.

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.9816 Check

Author Response: Low density is a consequence of structure porosity.
Low density is a consequence of structure porosity.

Alert level C

REFI015_ALERT_1_C _refine_ls_shift/su_max is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed

```
            SHFSU_01
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............       0.02 Ang.
```

Alert level G

```
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          2 Note
PLAT300_ALERT_4_G Atom Site Occupancy of C4         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4         Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       12% Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          4 Check
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON           1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          1 Note
```

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

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  1 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
  6 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

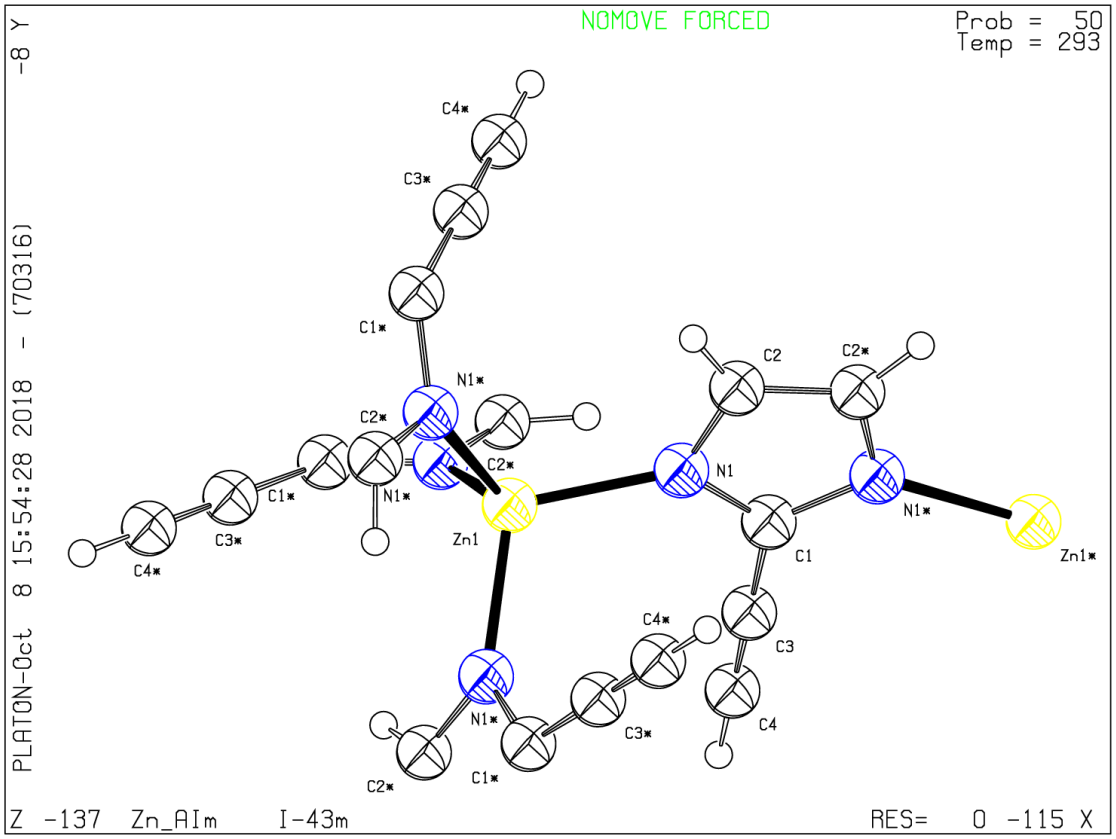
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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

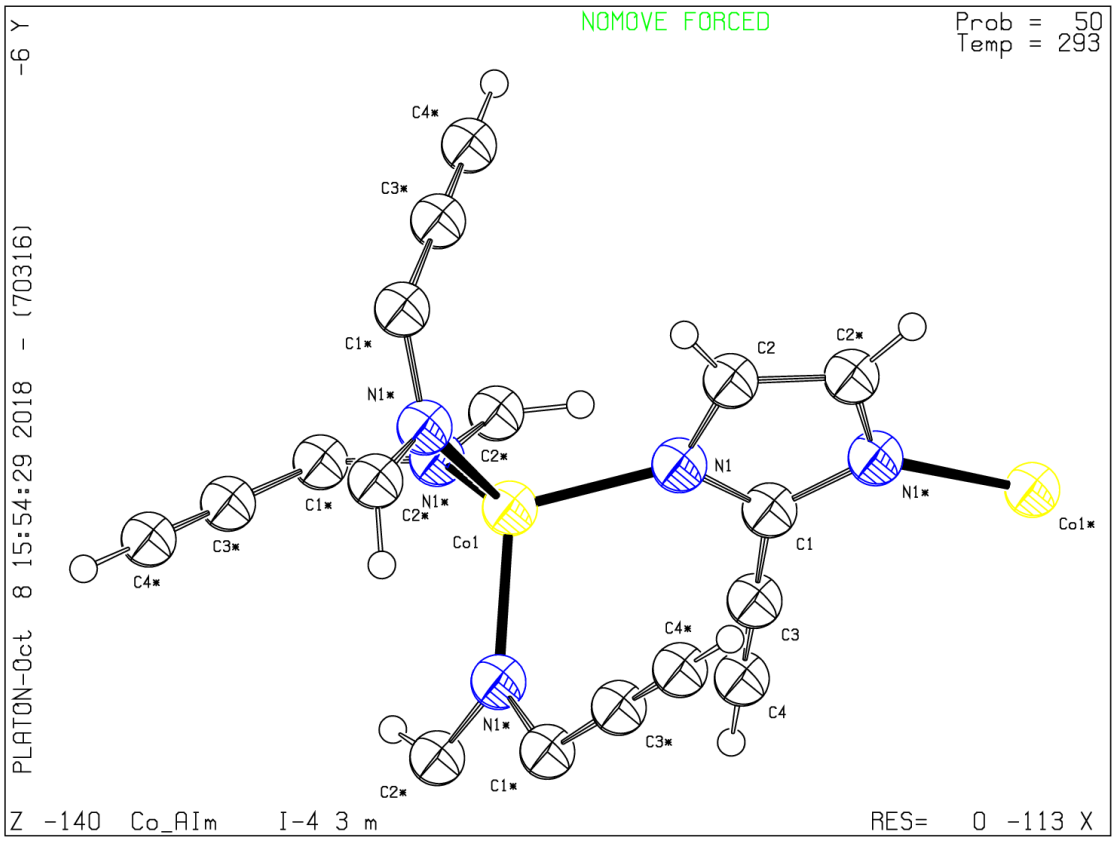
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 26/09/2018; check.def file version of 13/09/2018

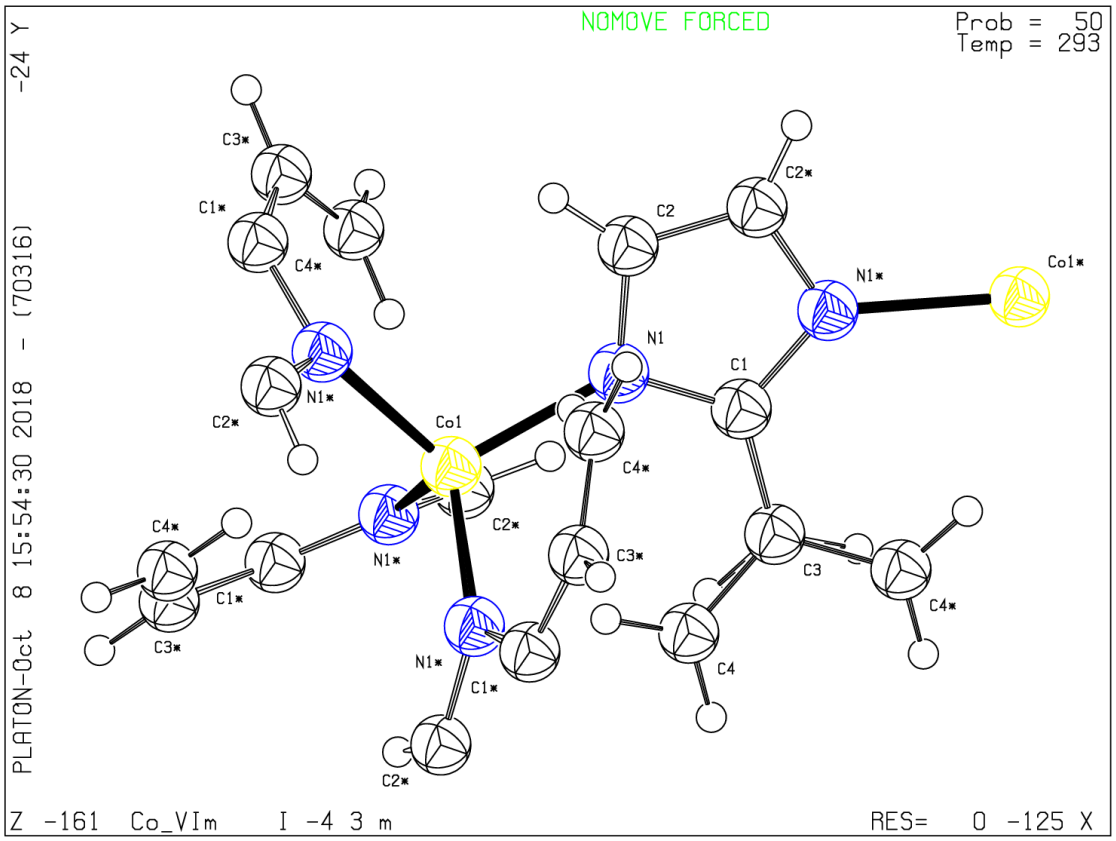
Datablock Zn_AIm - ellipsoid plot



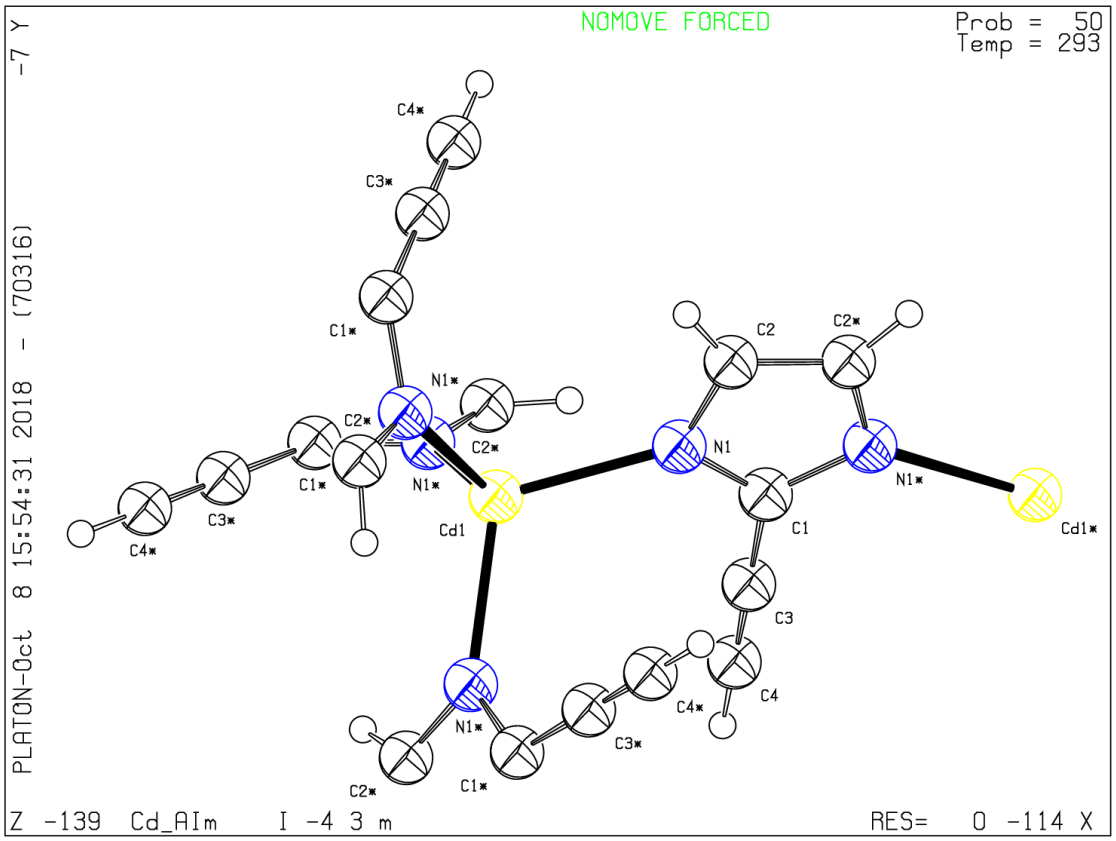
Datablock Co_AIm - ellipsoid plot



Datablock Co_VIm - ellipsoid plot



Datablock Cd_AIm - ellipsoid plot



Datablock Cd_VIm - ellipsoid plot