
SUPPORTING INFORMATION

Synthesis, Molecular, and Supramolecular Structures of Two Azide-Bridged Cd(II) and Cu(II) Coordination Polymers

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Chemicals and Physicochemical characterizations

All chemicals were obtained from Sigma-Aldrich Company. Perkin Elmer 2400 Elemental Analyzer was used for the CHN analysis. The metal content was measured using a Shimadzu atomic absorption spectrophotometer (AA-7000 series, Shimadzu, Ltd., Japan).

Hirshfeld calculations

The Crystal Explorer Ver. 3.1 [61] program was used to construct the Hirshfeld surfaces and draw the 2D fingerprint plots. It is worth to mention that the C-H and O-H distances from SHELX in the CIF data are shorter than actual values, and Crystal Explorer corrects this automatically to 1.083 Å and 0.98 Å, respectively.

Crystal structure analysis

A Bruker APEX II diffractometer with graphite monochromated MoK α radiation was used to determine the crystal structures of the investigated complexes. **Table 1** contains all information pertaining to the crystallographic measurements. SADABS was used for absorption corrections [62] and all calculations were carried out using SHELXTL program package [63].

DFT calculations

All DFT computations were performed using Gaussian 09 software [62]. Natural charge calculations [63] were performed at MPW1PW91 [64] level combined with cc-PVTZ and cc-PVTZ-PP basis sets for nonmetal and metal atoms, respectively [65, 66]. Atoms in molecules (AIM) parameters were calculated [67] using Multiwfn program [68].

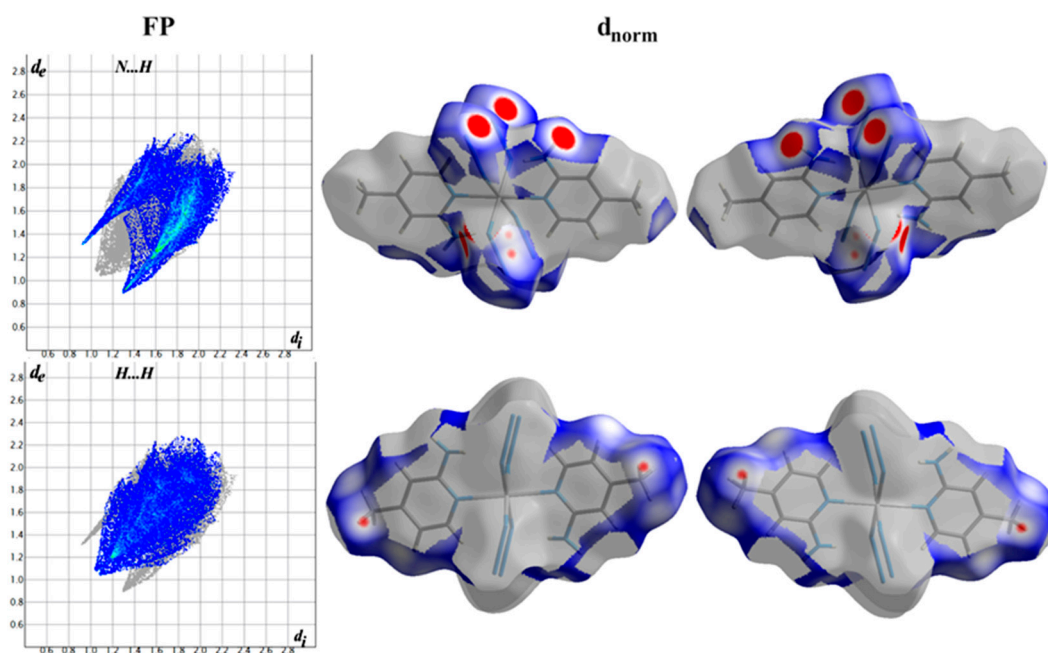


Figure S1. The FP plots and d_{norm} surface maps for the N...H and H...H contacts in complex 1.

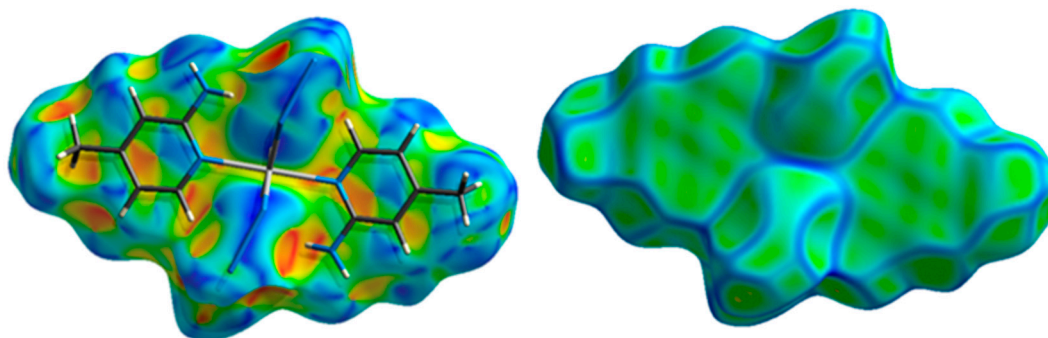


Figure S2. Shape index (SI; left) and curvedness (right) maps reveal the π - π stacking interactions in complex 1.

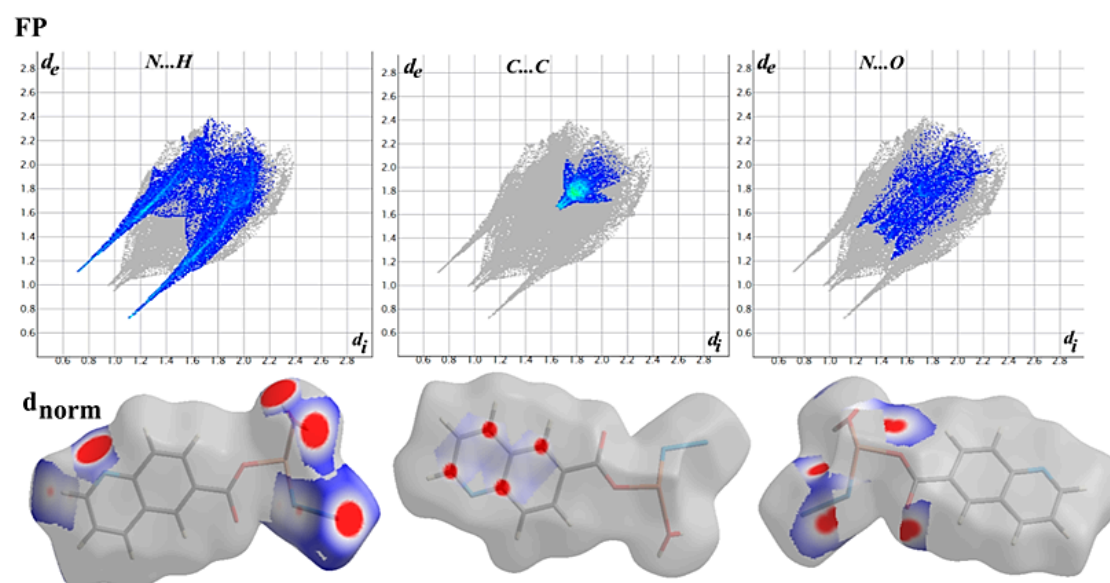


Figure S3. The FP plots and d_{norm} maps of the significant contacts in 2.

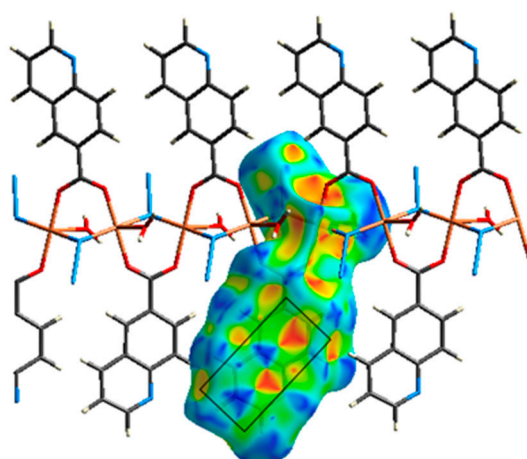


Figure S4. Red/blue triangles in SI map reveal the presence of π - π stacking interactions in complex 2.

Table S1. The %contacts in compounds **1** and **2**.

Contact	1	2
Cd-N	4.3	-
Cu-N	-	3.5
Cu-O	-	5.3
Cu-H	-	0.6
N...H	43.1	27.4
H...H	34.5	27.1
N...N	3.8	0.4
N...C	2.3	1.9
H...C	6.4	8.6
C...C	5.6	9.3
N...O	-	8.1
O...O	-	1.3
O...H	-	4.1
C...O	-	2.4

Table S2. AIM parameters (a.u.) at BCPs for complexes **1** and **2**.

Bond	$\rho(r)$	$G(r)$	$V(r)$	$H(r)$	$\nabla^2\rho(r)$
Complex 1					
Cd1-N1 ¹	0.0394	0.0571	-0.0596	-0.0025	0.2184
Cd1-N1 ³	0.0394	0.0571	-0.0596	-0.0025	0.2184
Cd1-N1	0.0544	0.0626	-0.0696	-0.0070	0.2222
Cd1-N1 ²	0.0544	0.0626	-0.0696	-0.0070	0.2222
Cd1-N4 ²	0.0498	0.0745	-0.0801	-0.0056	0.2754
Cd1-N4	0.0498	0.0745	-0.0801	-0.0056	0.2754
Complex 2					
Cu1-O2	0.0680	0.1639	-0.1792	-0.0153	0.5943
Cu1-O3	0.0684	0.1636	-0.1792	-0.0157	0.5916
Cu1-N1 ¹	0.0742	0.1589	-0.1819	-0.0230	0.5437
Cu1-N1	0.0828	0.1187	-0.1468	-0.0281	0.3624
Cu1-O1 ²	0.0108	0.0126	-0.0128	-0.0002	0.0498
Cu1-O1	0.0251	0.0369	-0.0369	0.0000	0.1477

Complex 1: ¹2-X,3-Y,-Z; ²2-X,2-Y,-Z; ³+X,-1+Y,+Z; Complex 2: ¹2-X,1/2+Y,1/2-Z; ²2-X,-1/2+Y,1/2-Z.

CheckCIF report for Complex 1

Bond precision:	C-C = 0.0030 Å	Wavelength=0.71073
Cell:	a=8.9157(3)	b=3.6913(1)
	alpha=90	beta=90.098(1)
Temperature: 100 K		gamma=90
	Calculated	Reported
Volume	762.81(4)	762.81(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H16 Cd N10	?
Sum formula	C12 H16 Cd N10	C12 H16 Cd N10
Mr	412.76	412.75
Dx,g cm-3	1.797	1.797
Z	2	2

Mu (mm-1)	1.448	1.448
F000	412.0	412.0
F000'	410.46	
h,k,lmax	10,4,27	10,4,27
Nref	1355	1338
Tmin,Tmax	0.703,0.782	0.429,1.000
Tmin'	0.689	

Correction method= # Reported T Limits: Tmin=0.429 Tmax=1.000 AbsCorr =
MULTI-SCAN

Data completeness= 0.987

Theta(max)= 24.999

R(reflections)= 0.0153(1221)

wR2(reflections)= 0.0370(1338)

S = 1.069

Npar= 115

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

[PLAT230_ALERT_2_C](#) Hirshfeld Test Diff for N1 --N2 . 5.9 s.u.

[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.595 16 Report

Alert level G

[PLAT004_ALERT_5_G](#) Polymeric Structure Found with Maximum Dimension 1 Info

[PLAT230_ALERT_2_G](#) Hirshfeld Test Diff for N2 --N3 . 5.6 s.u.

[PLAT794_ALERT_5_G](#) Tentative Bond Valency for Cd1 (II) . 2.01 Info

[PLAT804_ALERT_5_G](#) Number of ARU-Code Packing Problem(s) in PLATON 2 Info

[PLAT883_ALERT_1_G](#) No Info/Value for _atom_sites_solution_primary . Please Do !

[PLAT909_ALERT_3_G](#) Percentage of I>2sig(I) Data at Theta(Max) Still 87% Note

[PLAT910_ALERT_3_G](#) Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

[PLAT933_ALERT_2_G](#) Number of HKL-OMIT Records in Embedded .res File 9 Note

[PLAT941_ALERT_3_G](#) Average HKL Measurement Multiplicity 4.8 Low

[PLAT955_ALERT_1_G](#) Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units

[PLAT967_ALERT_5_G](#) Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree

[PLAT978_ALERT_2_G](#) Number C-C Bonds with Positive Residual Density. 5 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

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

4 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

0 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

start Validation Reply Form

_vrf_PLAT230_DENA_131_0m

;

```

PROBLEM: Hirshfeld Test Diff for   N1      --N2      .      5.9 s.u.
RESPONSE: ...
;
_vrf_PLAT911_DENA_131_0m
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=   0.595      16 Report
RESPONSE: ...
;
# end Validation Reply Form

```

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

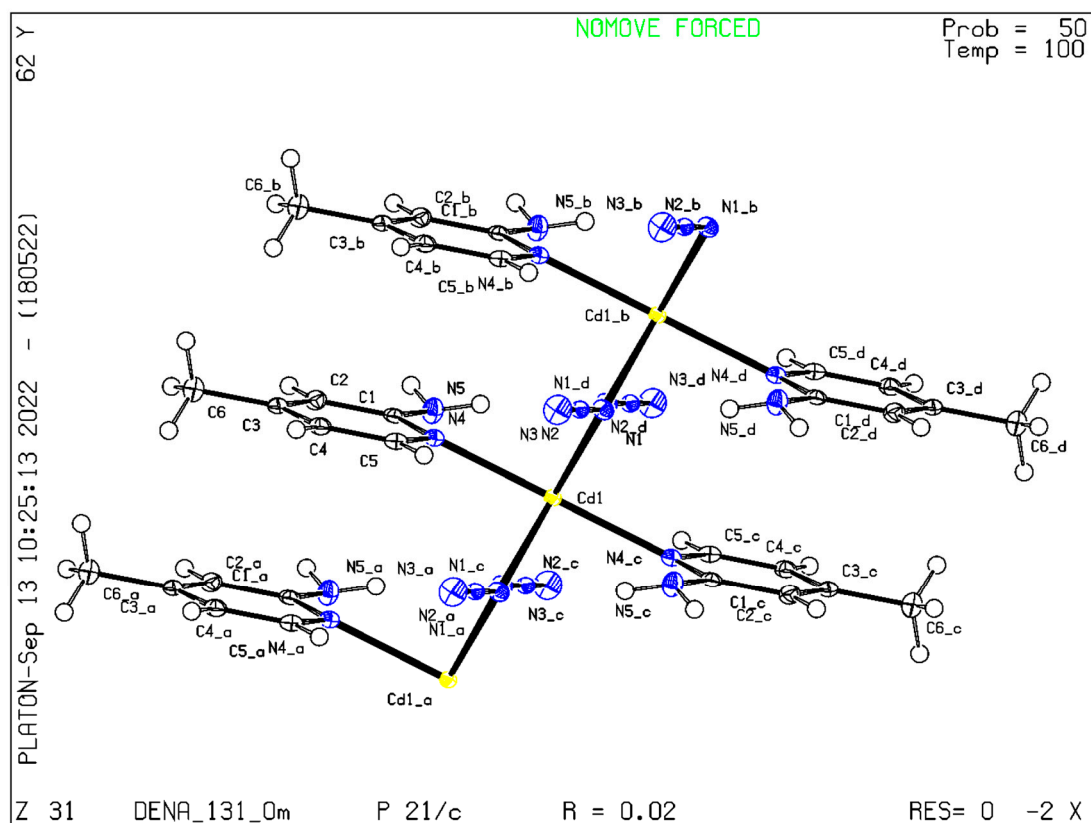
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 18/05/2022; check.def file version of 17/05/2022

Datablock DENA_131_0m - ellipsoid plot



CheckCIF report for Complex 2

Bond precision:	C-C = 0.0065 Å	Wavelength=0.71073
Cell:	a=8.0773(5) b=6.4187(3) c=20.9267(12)	
	alpha=90 beta=96.499(2) gamma=90	
Temperature:	100 K	
Volume	Calculated 1077.99(10)	Reported 1077.99(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C10 H8 Cu N4 O3	?
Sum formula	C10 H8 Cu N4 O3	C10 H8 Cu N4 O3
Mr	295.75	295.74

Dx,g cm-3	1.822	1.822
Z	4	4
Mu (mm-1)	2.032	2.032
F000	596.0	596.0
F000'	597.48	
h,k,lmax	9,7,23	8,7,23
Nref	1559	1542
Tmin,Tmax	0.651,0.784	0.812,1.000
Tmin'	0.620	

Correction method= # Reported T Limits: Tmin=0.812 Tmax=1.000 AbsCorr =
MULTI-SCAN

Data completeness= 0.989

Theta(max)= 23.347

R(reflections)= 0.0367(1092)

wR2(reflections)= 0.0939(1542)

S = 1.064

Npar= 163

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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575

Calculated sin(theta_max)/wavelength = 0.5576

Author Response: The crystal was damaged during the measurements

Alert level C

<u>PLAT088_ALERT_3_C</u>	Poor Data / Parameter Ratio	9.46	Note
<u>PLAT213_ALERT_2_C</u>	Atom O2 has ADP max/min Ratio	3.1	prolat
<u>PLAT213_ALERT_2_C</u>	Atom C1 has ADP max/min Ratio	3.8	oblate
<u>PLAT230_ALERT_2_C</u>	Hirshfeld Test Diff for N1 --N2 .	7.0	s.u.
<u>PLAT341_ALERT_3_C</u>	Low Bond Precision on C-C Bonds	0.0065	Ang.
<u>PLAT905_ALERT_3_C</u>	Negative K value in the Analysis of Variance ...	-4.794	Report
<u>PLAT911_ALERT_3_C</u>	Missing FCF Refl Between Thmin & STh/L=	0.558	16 Report

Alert level G

<u>PLAT002_ALERT_2_G</u>	Number of Distance or Angle Restraints on AtSite	3	Note
<u>PLAT004_ALERT_5_G</u>	Polymeric Structure Found with Maximum Dimension	1	Info
<u>PLAT171_ALERT_4_G</u>	The CIF-Embedded .res File Contains EADP Records	1	Report
<u>PLAT172_ALERT_4_G</u>	The CIF-Embedded .res File Contains DFIX Records	2	Report
<u>PLAT480_ALERT_4_G</u>	Long H...A H-Bond Reported H10 ..N2 .	2.67	Ang.
<u>PLAT794_ALERT_5_G</u>	Tentative Bond Valency for Cu1 (II) .	2.17	Info
<u>PLAT860_ALERT_3_G</u>	Number of Least-Squares Restraints	2	Note
<u>PLAT883_ALERT_1_G</u>	No Info/Value for _atom_sites_solution_primary .		Please Do !
<u>PLAT909_ALERT_3_G</u>	Percentage of I>2sig(I) Data at Theta(Max) Still	40%	Note
<u>PLAT910_ALERT_3_G</u>	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
<u>PLAT933_ALERT_2_G</u>	Number of HKL-OMIT Records in Embedded .res File	1	Note
<u>PLAT965_ALERT_2_G</u>	The SHELXL WEIGHT Optimisation has not Converged		Please Check
<u>PLAT967_ALERT_5_G</u>	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
<u>PLAT978_ALERT_2_G</u>	Number C-C Bonds with Positive Residual Density.	1	Info

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Validation response form

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start Validation Reply Form

_vrf_PLAT088_Morsy_Cu16_0m

;

PROBLEM: Poor Data / Parameter Ratio 9.46 Note

RESPONSE: ...

;

_vrf_PLAT213_Morsy_Cu16_0m

;

PROBLEM: Atom O2 has ADP max/min Ratio 3.1 prolat

RESPONSE: ...

;

_vrf_PLAT230_Morsy_Cu16_0m

;

PROBLEM: Hirshfeld Test Diff for N1 --N2 . 7.0 s.u.

RESPONSE: ...

;

_vrf_PLAT341_Morsy_Cu16_0m

;

PROBLEM: Low Bond Precision on C-C Bonds 0.0065 Ang.

RESPONSE: ...

;

_vrf_PLAT905_Morsy_Cu16_0m

;

PROBLEM: Negative K value in the Analysis of Variance ... -4.794 Report

RESPONSE: ...

;

_vrf_PLAT911_Morsy_Cu16_0m

;

PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.558 16 Report

RESPONSE: ...

;

end Validation Reply Form

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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.

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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

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PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock Morsy_Cu16_0m - ellipsoid plot

