Supporting Information

Hydrogen Bonds in Bis(1*H*-benzimidazole-κN^3)cadmium(II) Dibenzoate: Hirshfeld Surface Analysis and AIM Perspective

Jia-Jun Wang,[1,2] Li-Nan Dun,[1,2] Bao-Sheng Zhang,[1,2]

Zhong-Hui Wang,[3] He Wang,[1,2] Chuan-Bi Li,[1,2,*] Wei Liang[1,2,*]

[1] *Key Laboratory of Preparation and Application of Environmental Friendly Materials, Ministry of Education, Jilin Normal University, Changchun 130103, China*

[2] *Chemistry Department of Jilin Normal University, Siping 136000, China*

[3] *Sulfuric Acid Plant, Jilin Petrochemical Company Acrylonitrile Factory, Jilin 132021, China*

Corresponding author: E-mail: li_c_b@163.com (Chuan-Bi Li);

E-mail: 16433576@qq.com (Wei Liang)

Table SI

Table SI Short Ring/[C–H···*Cg*(π-ring)] Interactions. [*Cg–Cg*/(H···*Cg*) Distances in Å and Angles *α, β,* γ in º]

Cg(I)		Cg(1)	Cg(2)	Cg(2)	C(I)-H(I)	C_{20}-H_{20}	C_{20}-H_{20}
Cg(J)		Cg(2)[a]	Cg(3)[b]	Cg(4)[b]	Cg(J)	Cg(5)[c]	Cg(6)[c]
Cg-Cg		3.677(2)	3.968(2)	3.700(2)	C···Cg	3.487(4)	3.634(4)
	P	-0.3331	-0.3801	-0.3815	P	0.1487	0.1585
Transformed	Q	0.1920	-0.1808	-0.1845	Q	0.9649	0.9575
J-Plane	R	-0.9231	-0.9071	-0.9258	R	0.2164	0.2409
	S	2.0825	-2.6796	-2.6637	S	12.3496	12.4764
α		3.0(2)	2.9(2)	2.97(17)			
β		17.7	25.3	16.8	H-Prep	-2.57	-2.56
γ		18.6	28.2	19.2	γ	1.17	23.75
CgI_Perp		-3.4856(16)	-3.4958(18)	-3.4943(18)	C-H···Cg	169	150
CgJ_Perp		-3.5029(18)	-33.5427(13)	-3.5427(13)	H···Cg	2.57	2.80
Slippage		1.117	1.0698	1.067	C-H···π	78	77

Symmetry codes: a = -x, ½ + y, ½ - z; b = -x, -½ + y, ½ - z; c = ½ - x, ½ + y, z.

The Representations and Definitions

The Representations and Definitions:

Cg(I) = Plane number I (= ring number in () above)

Cg(J) = Center of gravity of ring J (Plane number above)

α = Dihedral Angle between Planes I and J (º)

β = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (º)

γ = Angle Cg(I)-->Cg(J) vector and normal to plane J (º)
or Angle between Cg-H vector and ring J normal

Cg-Cg = Distance between ring Centroids (Å)

CgI_Perp = Perpendicular distance of Cg(I) on ring J (Å)

CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Å)

Slippage = Distance between Cg(I) and Perpendicular Projection of Cg

H-Perp = Perpendicular distance of H to ring plane J

C-H···Cg = C-H-Cg angle (º)

C···Cg = Distance of C to Cg (Å)

C-H, π = Angle of the C-H bond with the π-plane (i.e.' Perpendicular = 90º, Parallel = 0º)

5-Membered Ring (1) N1 --> C15 --> N2 --> C16 --> C21 -->

6-Membered Ring (2) C2 --> C3 --> C4 --> C5 --> C6 --> C7 -->

6-Membered Ring (3) C16 --> C17 --> C18 --> C19 --> C20 --> C21 -->

9-Membered Ring (4) N1 --> C15 --> N2 --> C16 --> C17 --> C18 --> C19 --> C20 --> C21

5-Membered Ring (5) N3 --> C22 --> N4 --> C23 --> C28 -->

9-Membered Ring (6) N3 --> C22 --> N4 --> C23 --> C24 --> C25 --> C26 --> C27 --> C28 -->

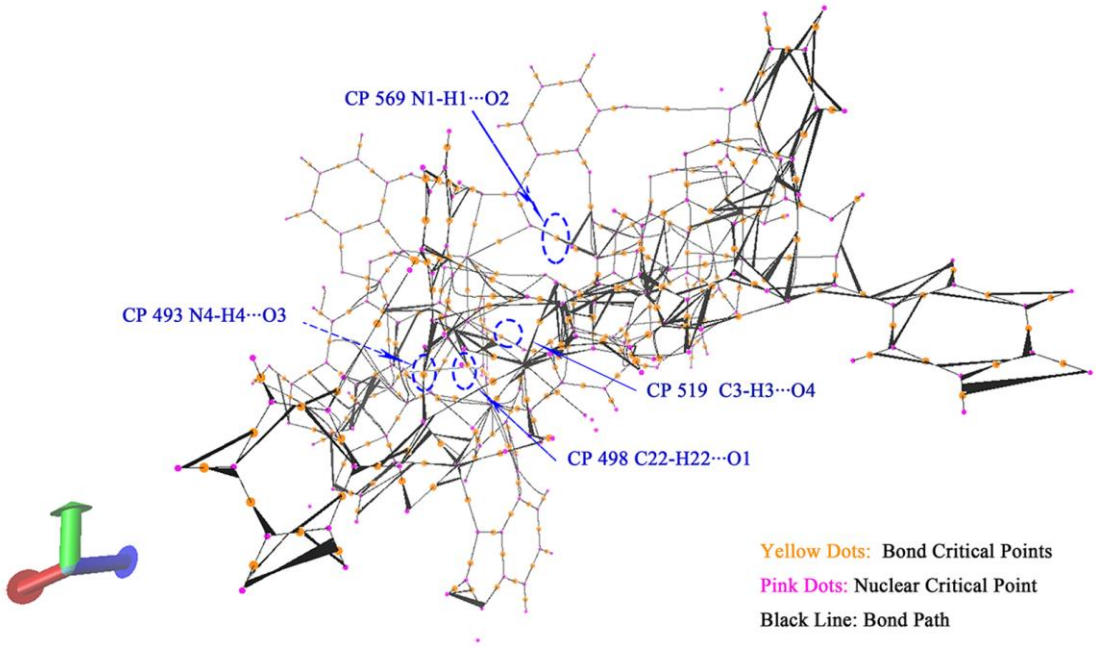

Fig. S1 The hydrogen bonds with full BCPs (yellow dots) and Nuclear Critical Points (NCPs, pink ball) and the bond paths of the three coordination units model of the compound.

Note:

1. The Fig. S1 Produced from The VMD Software.[a]
2. The NCP and BCP from the CPs.pdb and the bond paths are come from the Path.pdb file (open them with VMD), the CPs.pdb file and Paths.pdb file are produced from the Multiwfn software.
3. The Number of CPs can be found from the GaussView software (open the CPs.pdb with GaussView, the C atom represented the NCP, the N atom represented the BCP). The Order and the information of the CPs can be found in the CPprop.txt

[a] W. Humphrey, A. Dalke, and K. Schulten. VMD - Visual Molecular Dynamics. *J. Mol. Graphics*, **1996**, *14*, 33-38. **DOI:** 10.1016/0263-7855(96)00018-5