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# Electronic Supporting Information

## Two mixed-ligand cadmium(II) compounds bearing 5-nitrosopyrimidine and *N*-donor aromatic blocks: Self-assembly generation, structural and topological features, DFT studies, and Hirshfeld surface analysis

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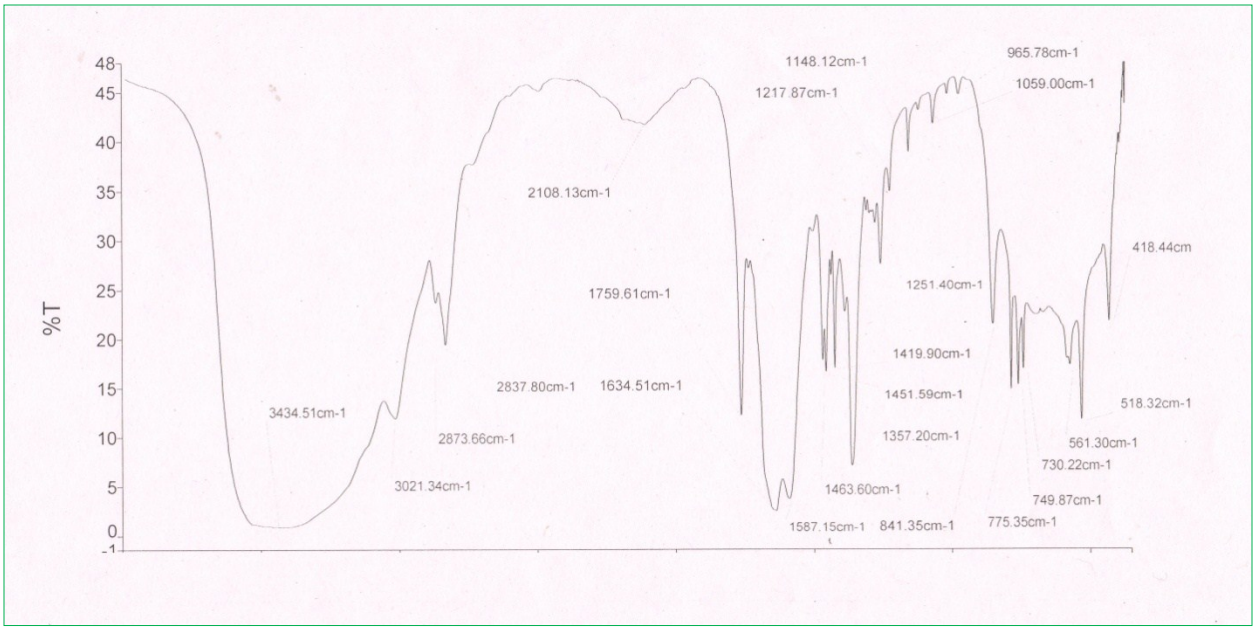


**Fig. S1** IR Spectrum of $[Cd_2(\mu_2\text{-}H_2Vi)_4(benzim)_2]\cdot 2MeOH$ (**1**)

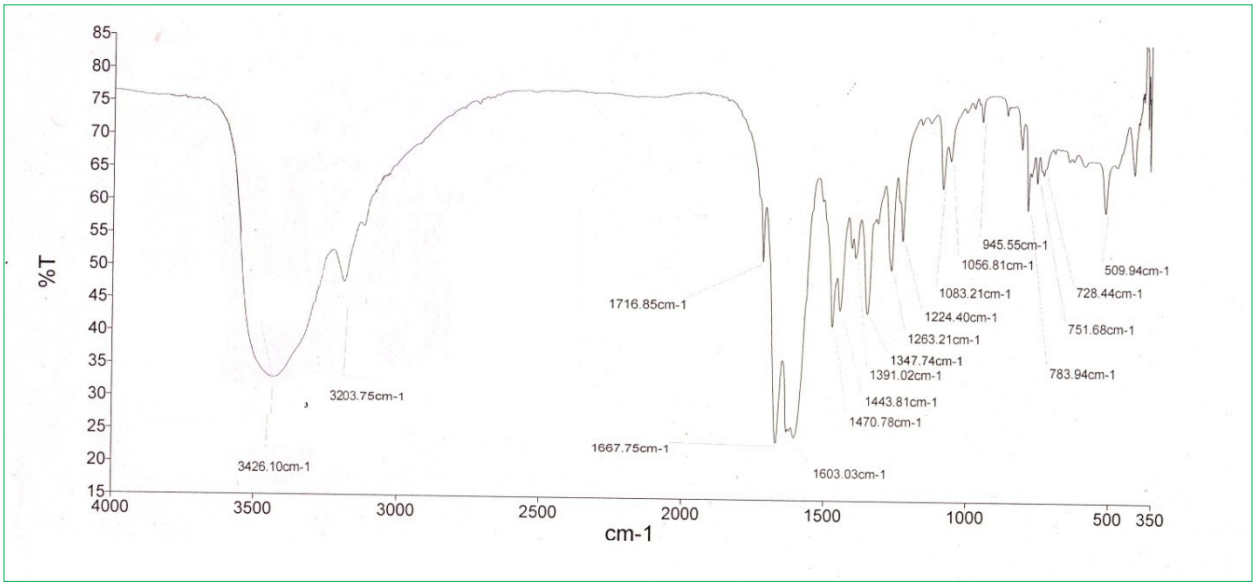


**Fig. S2** IR Spectrum of $[Cd(\mu_2\text{-}DMV)(DMV)(2\text{-}apy)]_n$ (**2**)

**Table S1** Bond Lengths for 1.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Cd | O10 | 2.3274(16) | N20 | Cd[1] | 2.5798(18) |
| Cd | O11[1] | 2.2892(16) | N20 | C20 | 1.328(3) |
| Cd | O21 | 2.4799(17) | N21 | C21 | 1.367(3) |
| Cd | O22[1] | 2.4007(17) | N21 | C22 | 1.380(3) |
| Cd | N10 | 2.3933(17) | N22 | C22 | 1.373(3) |
| Cd | N20[1] | 2.5798(18) | N22 | C23 | 1.376(3) |
| Cd | N30 | 2.2763(19) | N30 | C30 | 1.359(4) |
| O10 | C13 | 1.234(2) | N30 | C36 | 1.378(3) |
| O11 | Cd[1] | 2.2892(16) | N31 | C30 | 1.340(4) |
| O11 | N10 | 1.280(2) | N31 | C31 | 1.379(4) |
| O12 | C11 | 1.222(3) | C10 | C11 | 1.459(3) |
| O13 | C12 | 1.222(3) | C10 | C13 | 1.456(3) |
| O20 | C23 | 1.223(3) | C20 | C21 | 1.456(3) |
| O21 | N20 | 1.277(2) | C20 | C23 | 1.458(3) |
| O22 | Cd[1] | 2.4007(17) | C31 | C32 | 1.385(4) |
| O22 | C21 | 1.234(3) | C31 | C36 | 1.404(4) |
| O23 | C22 | 1.205(3) | C32 | C33 | 1.389(6) |
| N10 | C10 | 1.314(3) | C33 | C34 | 1.398(6) |
| N11 | C11 | 1.380(3) | C34 | C35 | 1.383(4) |
| N11 | C12 | 1.363(3) | C35 | C36 | 1.405(4) |
| N12 | C12 | 1.370(3) | O1S | C1SB | 1.412(12) |
| N12 | C13 | 1.356(2) | O1S | C1SA | 1.401(10) |

[1]-x,2-y,1-z

**Table S2** Bond Angles for 1.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O10 | Cd | O21 | 96.42(6) | C36 | N30 | Cd | 133.69(18) |
| O10 | Cd | O22[1] | 84.95(6) | C30 | N31 | C31 | 107.6(3) |
| O10 | Cd | N10 | 69.13(6) | N10 | C10 | C11 | 125.96(18) |
| O10 | Cd | N20[1] | 118.09(6) | N10 | C10 | C13 | 113.77(17) |
| O11[1] | Cd | O10 | 169.62(7) | C13 | C10 | C11 | 120.22(17) |
| O11[1] | Cd | O21 | 76.46(7) | O12 | C11 | N11 | 120.16(19) |
| O11[1] | Cd | O22[1] | 101.09(7) | O12 | C11 | C10 | 125.1(2) |
| O11[1] | Cd | N10 | 115.10(6) | N11 | C11 | C10 | 114.73(17) |
| O11[1] | Cd | N20[1] | 72.26(7) | O13 | C12 | N11 | 122.1(2) |
| O21 | Cd | N20[1] | 120.23(5) | O13 | C12 | N12 | 121.32(19) |
| O22[1] | Cd | O21 | 172.18(6) | N11 | C12 | N12 | 116.56(18) |
| O22[1] | Cd | N20[1] | 65.20(6) | O10 | C13 | N12 | 119.72(18) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N10 | Cd | O21 | 73.77(6) | O10 | C13 | C10 | 123.85(18) |
| N10 | Cd | O22[1] | 113.80(7) | N12 | C13 | C10 | 116.42(17) |
| N10 | Cd | N20[1] | 75.48(6) | N20 | C20 | C21 | 113.70(17) |
| N30 | Cd | O10 | 91.37(7) | N20 | C20 | C23 | 126.27(18) |
| N30 | Cd | O11[1] | 81.52(7) | C21 | C20 | C23 | 119.96(17) |
| N30 | Cd | O21 | 92.43(7) | O22 | C21 | N21 | 119.67(19) |
| N30 | Cd | O22[1] | 79.82(7) | O22 | C21 | C20 | 123.88(19) |
| N30 | Cd | N10 | 154.07(8) | N21 | C21 | C20 | 116.45(18) |
| N30 | Cd | N20[1] | 130.12(7) | O23 | C22 | N21 | 122.0(2) |
| C13 | O10 | Cd | 115.79(13) | O23 | C22 | N22 | 122.3(2) |
| N10 | O11 | Cd[1] | 119.99(13) | N22 | C22 | N21 | 115.73(19) |
| N20 | O21 | Cd | 114.93(13) | O20 | C23 | N22 | 119.37(19) |
| C21 | O22 | Cd[1] | 118.22(14) | O20 | C23 | C20 | 125.27(19) |
| O11 | N10 | Cd | 124.63(13) | N22 | C23 | C20 | 115.36(18) |
| O11 | N10 | C10 | 119.20(17) | N31 | C30 | N30 | 112.8(3) |
| C10 | N10 | Cd | 115.84(13) | N31 | C31 | C32 | 131.9(3) |
| C12 | N11 | C11 | 126.34(18) | N31 | C31 | C36 | 105.2(2) |
| C13 | N12 | C12 | 125.38(17) | C32 | C31 | C36 | 122.9(3) |
| O21 | N20 | Cd[1] | 124.28(13) | C31 | C32 | C33 | 115.9(3) |
| O21 | N20 | C20 | 119.90(17) | C32 | C33 | C34 | 121.9(3) |
| C20 | N20 | Cd[1] | 114.78(13) | C35 | C34 | C33 | 122.4(3) |
| C21 | N21 | C22 | 125.62(18) | C34 | C35 | C36 | 116.4(3) |
| C22 | N22 | C23 | 126.54(19) | N30 | C36 | C31 | 110.5(2) |
| C30 | N30 | Cd | 120.64(18) | N30 | C36 | C35 | 129.0(2) |
| C30 | N30 | C36 | 103.8(2) | C31 | C36 | C35 | 120.5(3) |

[1]-x,2-y,1-z

**Table S3** Bond Lengths for 2.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Cd1 | O1 | 2.3164(19) | N2 | C3 | 1.390(3) |
| Cd1 | O3[1] | 2.3611(19) | N2 | C5 | 1.466(3) |
| Cd1 | O4[1] | 2.4272(19) | N3 | C4 | 1.350(3) |
| Cd1 | O5 | 2.3481(18) | N4 | C7 | 1.378(3) |
| Cd1 | N3 | 2.511(2) | N4 | C8 | 1.389(3) |
| Cd1 | N6 | 2.369(2) | N4 | C12 | 1.476(4) |
| Cd1 | N7 | 2.301(2) | N5 | C8 | 1.370(4) |
| O1 | C1 | 1.237(3) | N5 | C9 | 1.402(3) |
| O2 | C2 | 1.209(3) | N5 | C11 | 1.474(4) |
| O3 | Cd1[2] | 2.3611(19) | N6 | C10 | 1.345(3) |
| O3 | C3 | 1.216(3) | N7 | C13 | 1.345(3) |

| | | | | | |
|---|---|---|---|---|---|
| O4 | Cd1[2] | 2.4273(19) | N7 | C17 | 1.355(4) |
| O4 | N3 | 1.256(3) | N8 | C13 | 1.338(4) |
| O5 | C7 | 1.231(3) | C1 | C4 | 1.438(3) |
| O6 | C8 | 1.209(3) | C3 | C4 | 1.438(3) |
| O7 | C9 | 1.210(3) | C7 | C10 | 1.446(3) |
| O8 | N6 | 1.257(3) | C9 | C10 | 1.452(4) |
| N1 | C1 | 1.372(3) | C13 | C14 | 1.416(4) |
| N1 | C2 | 1.380(3) | C14 | C15 | 1.346(6) |
| N1 | C6 | 1.476(3) | C15 | C16 | 1.388(5) |
| N2 | C2 | 1.382(3) | C16 | C17 | 1.364(4) |

[1]-x,1/2+y,1/2-z; [2]-x,-1/2+y,1/2-z

**Table S4** Bond Angles for 2.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O1 | Cd1 | O3[1] | 143.75(6) | C9 | N5 | C11 | 118.2(3) |
| O1 | Cd1 | O4[1] | 72.26(6) | O8 | N6 | Cd1 | 121.84(15) |
| O1 | Cd1 | O5 | 84.66(7) | O8 | N6 | C10 | 120.9(2) |
| O1 | Cd1 | N3 | 66.48(6) | C10 | N6 | Cd1 | 116.85(15) |
| O1 | Cd1 | N6 | 141.28(7) | C13 | N7 | Cd1 | 127.80(18) |
| O3[1] | Cd1 | O4[1] | 71.49(7) | C13 | N7 | C17 | 118.2(2) |
| O3[1] | Cd1 | N3 | 149.78(7) | C17 | N7 | Cd1 | 114.02(18) |
| O3[1] | Cd1 | N6 | 69.99(7) | O1 | C1 | N1 | 118.7(2) |
| O4[1] | Cd1 | N3 | 138.72(7) | O1 | C1 | C4 | 124.5(2) |
| O5 | Cd1 | O3[1] | 96.62(8) | N1 | C1 | C4 | 116.9(2) |
| O5 | Cd1 | O4[1] | 91.22(7) | O2 | C2 | N1 | 121.5(2) |
| O5 | Cd1 | N3 | 84.18(6) | O2 | C2 | N2 | 121.5(2) |
| O5 | Cd1 | N6 | 69.37(6) | N1 | C2 | N2 | 117.0(2) |
| N6 | Cd1 | O4[1] | 133.94(7) | O3 | C3 | N2 | 118.3(2) |
| N6 | Cd1 | N3 | 82.28(7) | O3 | C3 | C4 | 125.1(2) |
| N7 | Cd1 | O1 | 90.26(8) | N2 | C3 | C4 | 116.6(2) |
| N7 | Cd1 | O3[1] | 89.21(8) | N3 | C4 | C1 | 111.9(2) |
| N7 | Cd1 | O4[1] | 90.03(7) | N3 | C4 | C3 | 127.5(2) |
| N7 | Cd1 | O5 | 174.13(7) | C3 | C4 | C1 | 120.6(2) |
| N7 | Cd1 | N3 | 91.11(7) | O5 | C7 | N4 | 118.9(2) |
| N7 | Cd1 | N6 | 113.53(7) | O5 | C7 | C10 | 124.4(2) |
| C1 | O1 | Cd1 | 120.85(16) | N4 | C7 | C10 | 116.7(2) |
| C3 | O3 | Cd1[2] | 136.64(19) | O6 | C8 | N4 | 120.8(3) |
| N3 | O4 | Cd1[2] | 137.90(17) | O6 | C8 | N5 | 121.4(3) |
| C7 | O5 | Cd1 | 115.88(15) | N5 | C8 | N4 | 117.8(2) |
| C1 | N1 | C2 | 124.7(2) | O7 | C9 | N5 | 119.9(3) |
| C1 | N1 | C6 | 118.9(2) | O7 | C9 | C10 | 125.4(3) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C2 | N1 | C6 | 115.9(2) | N5 | C9 | C10 | 114.7(2) |
| C2 | N2 | C3 | 124.0(2) | N6 | C10 | C7 | 113.3(2) |
| C2 | N2 | C5 | 116.5(2) | N6 | C10 | C9 | 125.1(2) |
| C3 | N2 | C5 | 119.1(2) | C7 | C10 | C9 | 121.6(2) |
| O4 | N3 | Cd1 | 122.50(16) | N7 | C13 | C14 | 120.4(3) |
| O4 | N3 | C4 | 121.2(2) | N8 | C13 | N7 | 119.3(2) |
| C4 | N3 | Cd1 | 116.33(15) | N8 | C13 | C14 | 120.3(3) |
| C7 | N4 | C8 | 123.8(2) | C15 | C14 | C13 | 119.8(3) |
| C7 | N4 | C12 | 118.9(2) | C14 | C15 | C16 | 120.1(3) |
| C8 | N4 | C12 | 117.3(2) | C17 | C16 | C15 | 117.9(3) |
| C8 | N5 | C9 | 125.2(2) | N7 | C17 | C16 | 123.6(3) |
| C8 | N5 | C11 | 116.6(2) | | | | |

[1]-x,1/2+y,1/2-z; [2]-x,-1/2+y,1/2-z

**Table S5** Hydrogen Bonds for 1.

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N11 | H11 | O12[1] | 0.86 | 1.96 | 2.818(2) | 172.2 |
| N12 | H12 | O20[2] | 0.86 | 2.21 | 2.824(2) | 128.3 |
| N12 | H12 | O21[2] | 0.86 | 2.02 | 2.807(2) | 151.1 |
| N21 | H21 | O1S[3] | 0.86 | 1.95 | 2.807(3) | 178.5 |
| C30 | H30 | O11[3] | 0.93 | 2.25 | 2.852(3) | 121.6 |

[1]1-x,2-y,2-z; [2]1-x,2-y,1-z; [3]-x,2-y,1-z

**Table S6** Hydrogen Bonds for 2.

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| N8 | H8A | O8 | 0.86 | 2.16 | 3.000(3) | 165.2 |
| N8 | H8B | O8[1] | 0.86 | 2.29 | 2.998(3) | 140.0 |

[1]-x,1-y,-z