**Supplementary Material**

Heavy metal complexes of 4-chlorodipicolinic acid - Structural, spectral and thermal correlations

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Figure S1. Comparing IR spectra of H2PDA and H2PDA-Cl ligands.

Table S1. Selected bond lengths [Å] and angles [°] for compound H2DPA-Cl·H2O.

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| --- | --- | --- | --- |
| **Bond distances** |  |  |  |
| Cl1—C1 | 1.726(2) | C2—C1  | 1.374(4) |
| O3—C7 | 1.301(4) | C2—C3  | 1.396(4) |
| O4—C7  | 1.217(4) | C7—C6  | 1.503(4) |
| O1—C4  | 1.316(3) | C6—C8  | 1.388(4) |
| O2—C4  | 1.203(4) | C3—C4  | 1.507(4) |
| N1—C6 | 1.334(4) | C1—C8  | 1.384(4) |
| N1—C3  | 1.344(4) |  |  |
| **Bond angles** |  |  |  |
| C6—N1—C3  | 116.6(2) | N1—C3—C4  | 116.6(2) |
| C1—C2—C3  | 118.0(3) | C2—C3—C4  | 119.6(3) |
| O4—C7—O3  | 125.4(3) | O2—C4—O1  | 126.0(3) |
| O4—C7—C6  | 119.2(3) | O2—C4—C3  | 123.2(3) |
| O3—C7—C6  | 115.4(2) | O1—C4—C3  | 110.8(3) |
| N1—C6—C8  | 123.9(3) | C2—C1—C8  | 119.5(2) |
| N1—C6—C7  | 119.1(3) | C2—C1—Cl1  | 120.2(2) |
| C8—C6—C7  | 117.0(3) | C8—C1—Cl1  | 120.3(2) |
| N1—C3—C2  | 123.8(3) | C1—C8—C6  | 118.2(2) |

Table S2. Possible hydrogen bonds (Å, °) for H2DPA-Cl·H2O.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **D—H···A** | **D—H** | **H···A** | **D···A** | **D—H···A** | **D—H···A** | **D—H** |
| O3—H3···O5i | 0.84 | 1.66 | 2.501(3) | 177 | O3—H3···O5i | 0.84 |
| O1—H1···O4ii | 0.84 | 1.81 | 2.578(3) | 151 | O1—H1···O4ii | 0.84 |
| O5—H5A···O3iii | 0.86(4) | 2.52(5) | 2.954(3) | 112(4) | O5—H5A···O3iii | 0.86(4) |
| O5—H5A···N1iii | 0.86(4) | 2.12(4) | 2.973(3) | 176(5) | O5—H5A···N1iii | 0.86(4) |

Symmetry codes: (i) −x+1, y+1/2, −z+1; (ii) x, y−1, z; (iii) x+1, y, z−1.

Table S3. Selected bond lengths [Å] and angles [°] for compound **1**.

|  |  |  |  |
| --- | --- | --- | --- |
| **Bond distances** |  |  |  |
| Ag1—N1  | 2.324(3) | C1—O2  | 1.227(4) |
| Ag1—O1  | 2.558(3) | C4—O3  | 1.205(4) |
| O1—C1  | 1.275(4) | C4—O4  | 1.307(4) |
| O1—H1  | 1.226(4) |  |  |
| **Bond angles** |  |  |  |
| N1i—Ag1—N1 | 153.50(15) | Ag1—O1—H1  | 121.8(17) |
| N1i—Ag1—O1i | 67.36(9) | O2—C1—O1  | 125.6(3) |
| N1—Ag1—O1i  | 121.77(9) | C4—O4—H4  | 110(4) |
| O1i—Ag1—O1 | 144.05(14) | C3—N1—Ag1  | 121.0(2) |
| C1—O1—Ag1  | 116.4(2) | C2—N1—Ag1  | 120.5(2) |
| C1—O1—H1  | 115.6(6) |  |  |

Table S4. Possible hydrogen bonds (Å, °) for compound **1**.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **D—H···A** | **D—H** | **H···A** | **D···A** | **D—H···A** | **D—H···A** | **D—H** |
| O1—H1···O1i | 1.23(1) | 1.23(1) | 2.451(5) | 177(9) | O1—H1···O1i | 1.23(1) |
| O1—H1···O2i | 1.23(1) | 2.58(1) | 3.371(4) | 120(1) | O1—H1···O2i | 1.23(1) |
| O4—H4···O5ii | 0.84(3) | 1.70(3) | 2.532(4) | 171(5) | O4—H4···O5ii | 0.84(3) |
| O5—H5A···O2iii | 0.84(6) | 1.87(6) | 2.686(4) | 162(5) | O5—H5A···O2iii | 0.84(6) |
| O5—H5B···O3iv | 0.76(6) | 2.17(6) | 2.933(4) | 176(5) | O5—H5B···O3iv | 0.76(6) |

Symmetry codes: (i) −x+1, y, −z+1/2; (ii) x+1, y, z; (iii) x+1/2, y+1/2, z; (iv) −x+2, y, −z+1/2.

Table S5. Selected bond lengths [Å] and angles [°] for compound **2**.

|  |  |  |  |
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| **Bond distances** |  |  |  |
| Cd1—O6  | 2.2944(19) | Cd1—O5ii  | 2.440(2) |
| Cd1—N1  | 2.299(2) | O1—C1  | 1.273(3) |
| Cd1—O5  | 2.3145(19) | O1—Cd1i  | 2.3469(18) |
| Cd1—O1i  | 2.3469(18) | C1—O2  | 1.241(3) |
| Cd1—O3  | 2.3887(19) | C4—O4  | 1.239(3) |
| Cd1—O1  | 2.4286(18) | C4—O3  | 1.266(3) |
| **Bond angles** |  |  |  |
| O6—Cd1—N1  | 93.44(7) | O1i—Cd1—O1  | 73.63(7) |
| O6—Cd1—O5  | 113.33(7) | O3—Cd1—O1  | 137.86(6) |
| N1—Cd1—O5  | 139.11(7) | O6—Cd1—O5ii  | 155.59(7) |
| O6—Cd1—O1i  | 82.79(7) | N1—Cd1—O5ii  | 91.05(7) |
| N1—Cd1—O1i  | 141.93(7) | O5—Cd1—O5ii  | 77.20(7) |
| O5—Cd1—O1i  | 74.61(6) | O1i—Cd1—O5ii  | 78.96(7) |
| O6—Cd1—O3  | 98.12(7) | O3—Cd1—O5ii  | 105.92(7) |
| N1—Cd1—O3  | 69.56(7) | O1—Cd1—O5ii  | 75.47(6) |
| O5—Cd1—O3  | 76.25(7) | C1—O1—Cd1i  | 134.67(17) |
| O1i—Cd1—O3  | 148.51(6) | C1—O1—Cd1  | 118.96(16) |
| O6—Cd1—O1  | 83.95(6) | Cd1i—O1—Cd1  | 106.37(7) |
| N1—Cd1—O1  | 68.31(7) | O2—C1—O1  | 126.6(2) |
| O5—Cd1—O1  | 141.27(6) | O4—C4—O3  | 126.8(3) |

Symmetry codes: (i) −x+1, −y+1, −z; (ii) −x, −y+1, −z.

Table S6. Possible hydrogen bonds (Å, °) for compound **2**.

|  |  |  |  |  |  |  |
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| **D—H···A** | **D—H** | **H···A** | **D···A** | **D—H···A** | **D—H···A** | **D—H** |
| O5—H5A···O6i | 0.84(2) | 2.04(3) | 2.819(3) | 155(3) | O5—H5A···O6i | 0.84(2) |
| O5—H5B···O2ii | 0.81(2) | 1.80(3) | 2.578(3) | 159(3) | O5—H5B···O2ii | 0.81(2) |
| O6—H6A···O3iii | 0.97 | 1.81 | 2.673(3) | 147 | O6—H6A···O3iii | 0.97 |
| O6—H6B···O4iv | 0.88 | 1.74 | 2.608(3) | 170 | O6—H6B···O4iv | 0.88 |

Symmetry codes: (i) x−1, y, z; (ii) −x+1, −y+1, −z; (iii) x+1, y, z; (iv) −x, −y, −z.