

## Supporting information

**Table S1** Selected geometric parameters (Å, °) for (I)

|                             |             |                              |             |
|-----------------------------|-------------|------------------------------|-------------|
| Al1—O11W                    | 1.8896 (15) | Al2—O21W                     | 1.8760 (13) |
| Al1—O12W                    | 1.8799 (13) | Al2—O22W                     | 1.8810 (16) |
| Al1—O13W                    | 1.8740 (14) | Al2—O23W                     | 1.8930 (14) |
| O12W—Al1—O11W               | 89.45 (6)   | O21W <sup>ii</sup> —Al2—O22W | 89.68 (6)   |
| O12W—Al1—O11W <sup>i</sup>  | 90.55 (6)   | O21W—Al2—O22W                | 90.32 (6)   |
| O13W—Al1—O11W               | 90.93 (6)   | O21W—Al2—O23W                | 90.26 (6)   |
| O13W <sup>i</sup> —Al1—O11W | 89.07 (6)   | O21W <sup>ii</sup> —Al2—O23W | 89.74 (6)   |
| O13W—Al1—O12W               | 89.22 (6)   | O22W—Al2—O23W <sup>ii</sup>  | 89.63 (6)   |
| O13W <sup>i</sup> —Al1—O12W | 90.78 (6)   | O22W—Al2—O23W                | 90.37 (6)   |

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

**Table S2** Selected geometric parameters (Å, °) for (II)

|               |             |                             |             |
|---------------|-------------|-----------------------------|-------------|
| Co1—O11W      | 2.1042 (17) | Co1—O16W                    | 2.0368 (19) |
| Co1—O12W      | 2.1074 (17) | Co2—O21W                    | 2.0513 (18) |
| Co1—O13W      | 2.1852 (17) | Co2—O22W                    | 2.1073 (19) |
| Co1—O14W      | 2.0640 (17) | Co2—O23W                    | 2.0715 (17) |
| Co1—O15W      | 2.0343 (18) |                             |             |
| O11W—Co1—O12W | 174.53 (6)  | O16W—Co1—O11W               | 92.29 (7)   |
| O11W—Co1—O13W | 84.79 (6)   | O16W—Co1—O12W               | 87.18 (7)   |
| O12W—Co1—O13W | 100.63 (6)  | O16W—Co1—O13W               | 87.52 (7)   |
| O14W—Co1—O11W | 93.44 (7)   | O16W—Co1—O14W               | 92.06 (7)   |
| O14W—Co1—O12W | 81.14 (7)   | O21W—Co2—O22W               | 89.77 (9)   |
| O14W—Co1—O13W | 178.16 (6)  | O21W <sup>i</sup> —Co2—O22W | 90.23 (9)   |
| O15W—Co1—O11W | 94.50 (7)   | O21W—Co2—O23W               | 90.11 (7)   |
| O15W—Co1—O12W | 86.37 (7)   | O21W—Co2—O23W <sup>i</sup>  | 89.89 (7)   |
| O15W—Co1—O13W | 89.76 (7)   | O23W—Co2—O22W <sup>i</sup>  | 90.39 (8)   |
| O15W—Co1—O14W | 90.88 (7)   | O23W—Co2—O22W               | 89.61 (8)   |
| O15W—Co1—O16W | 172.42 (7)  |                             |             |

Symmetry code: (i)  $-x+2, -y+1, -z$ .

**Table S3** Selected geometric parameters (Å, °) for (III)

|               |             |                             |             |
|---------------|-------------|-----------------------------|-------------|
| Mg1—O11W      | 2.069 (2)   | Mg1—O16W                    | 2.023 (2)   |
| Mg1—O12W      | 2.0695 (19) | Mg2—O21W                    | 2.0471 (17) |
| Mg1—O13W      | 2.1321 (18) | Mg2—O22W                    | 2.0961 (19) |
| Mg1—O14W      | 2.0178 (19) | Mg2—O23W                    | 2.0391 (17) |
| Mg1—O15W      | 2.036 (2)   |                             |             |
| O11W—Mg1—O12W | 174.72 (7)  | O16W—Mg1—O11W               | 90.37 (9)   |
| O11W—Mg1—O13W | 86.78 (7)   | O16W—Mg1—O12W               | 88.10 (8)   |
| O12W—Mg1—O13W | 98.30 (7)   | O16W—Mg1—O13W               | 91.06 (8)   |
| O14W—Mg1—O11W | 89.41 (8)   | O16W—Mg1—O15W               | 172.81 (9)  |
| O14W—Mg1—O12W | 85.60 (8)   | O21W <sup>i</sup> —Mg2—O22W | 90.26 (8)   |
| O14W—Mg1—O13W | 174.89 (8)  | O21W—Mg2—O22W               | 89.73 (8)   |
| O14W—Mg1—O15W | 89.96 (8)   | O23W <sup>i</sup> —Mg2—O21W | 90.06 (7)   |
| O14W—Mg1—O16W | 92.37 (9)   | O23W—Mg2—O21W               | 89.94 (7)   |
| O15W—Mg1—O11W | 96.46 (9)   | O23W—Mg2—O22W               | 89.59 (8)   |
| O15W—Mg1—O12W | 85.29 (8)   | O23W—Mg2—O22W <sup>i</sup>  | 90.41 (8)   |
| O15W—Mg1—O13W | 87.08 (7)   |                             |             |

Symmetry code: (i)  $-x+2, -y+1, -z$ .**Table S4** Selected geometric parameters (Å, °) for (IV)

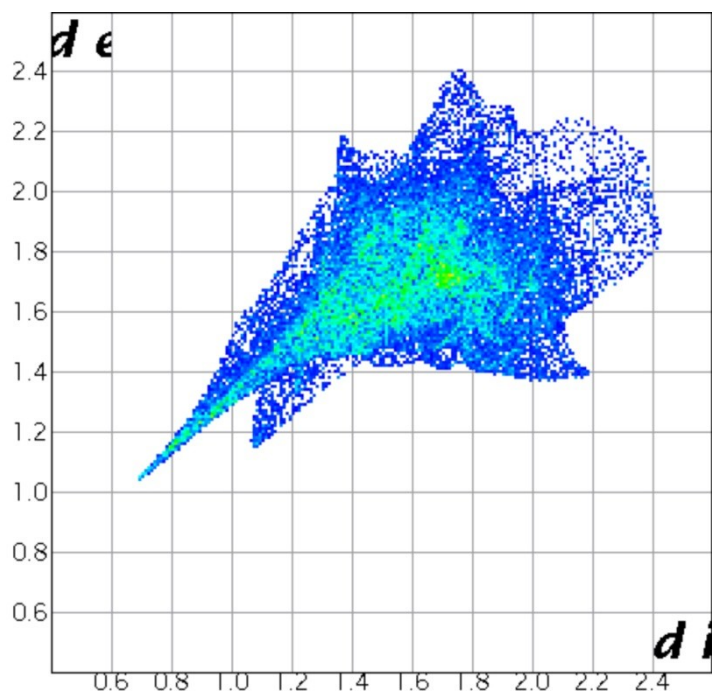
|                           |             |                          |             |
|---------------------------|-------------|--------------------------|-------------|
| Ni1—O1W                   | 2.0590 (17) | Ni1—O3W                  | 2.0588 (13) |
| Ni1—O2W                   | 2.0503 (13) |                          |             |
| O2W—Ni1—O1W               | 91.67 (6)   | O2W—Ni1—O3W              | 92.96 (5)   |
| O2W <sup>i</sup> —Ni1—O1W | 88.33 (6)   | O3W—Ni1—O1W              | 93.37 (6)   |
| O2W—Ni1—O3W <sup>i</sup>  | 87.04 (5)   | O3W—Ni1—O1W <sup>i</sup> | 86.63 (6)   |

Symmetry code: (i)  $-x+1, -y+2, -z$ .**Table S5** Selected geometric parameters (Å, °) for (V)

|         |             |         |             |
|---------|-------------|---------|-------------|
| Zn1—O1W | 2.097 (2)   | Zn1—O3W | 2.0996 (18) |
| Zn1—O2W | 2.0813 (19) |         |             |

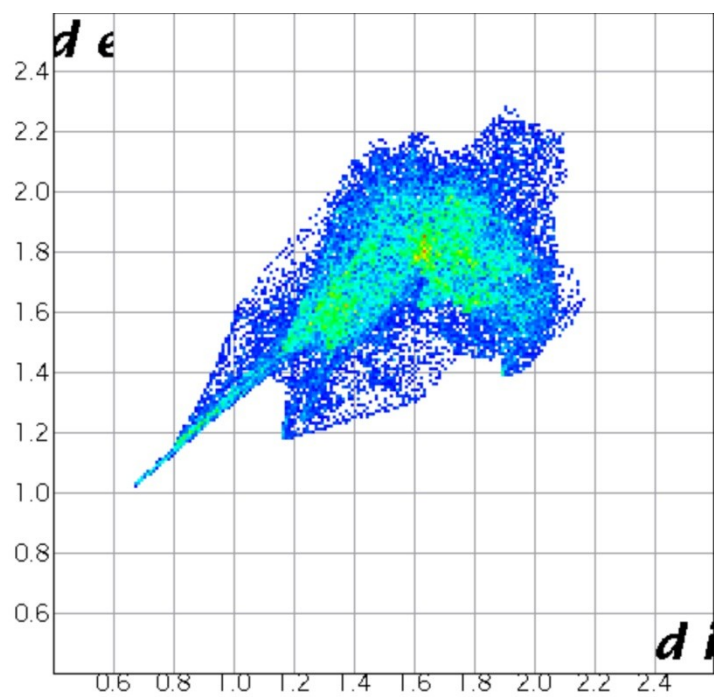
|                          |           |                          |           |
|--------------------------|-----------|--------------------------|-----------|
| O1W—Zn1—O3W <sup>i</sup> | 86.88 (8) | O2W—Zn1—O1W              | 91.46 (8) |
| O1W—Zn1—O3W              | 93.12 (8) | O2W—Zn1—O3W <sup>i</sup> | 87.20 (7) |
| O2W—Zn1—O1W <sup>i</sup> | 88.54 (8) | O2W—Zn1—O3W              | 92.80 (7) |

Symmetry code: (i)  $-x+1, -y+2, -z$ .



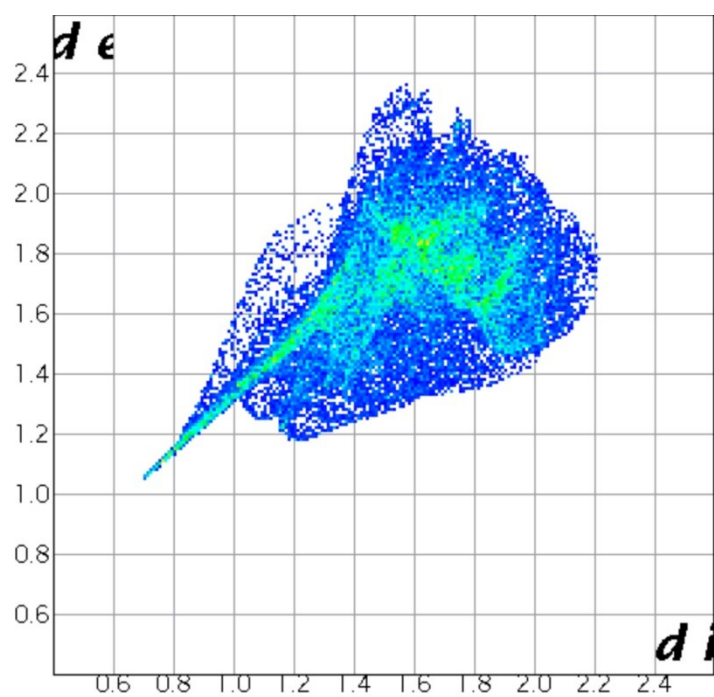
**Figure S1**

Two-dimensional fingerprint plots of **2ap** cation in compound **I**.



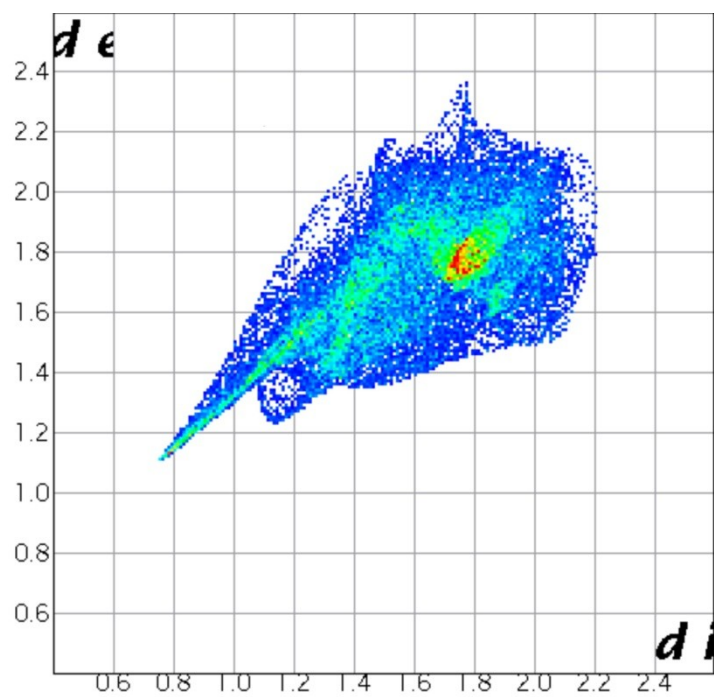
**Figure S2**

Two-dimensional fingerprint plots of **2ap** cation in compound **II**.



**Figure S3**

Two-dimensional fingerprint plots of **2ap** cation in compound **IV**.



**Figure S4**

Two-dimensional fingerprint plots of **2ap** cation in compound **VI**.