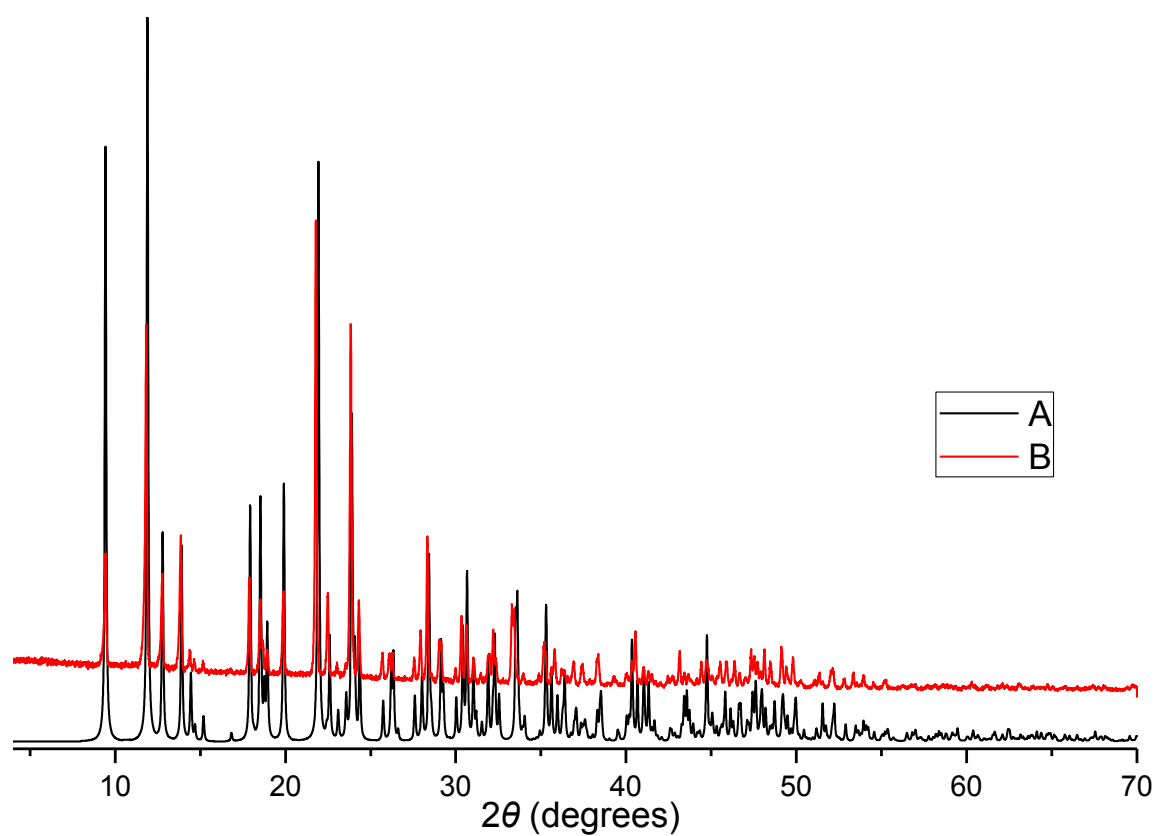


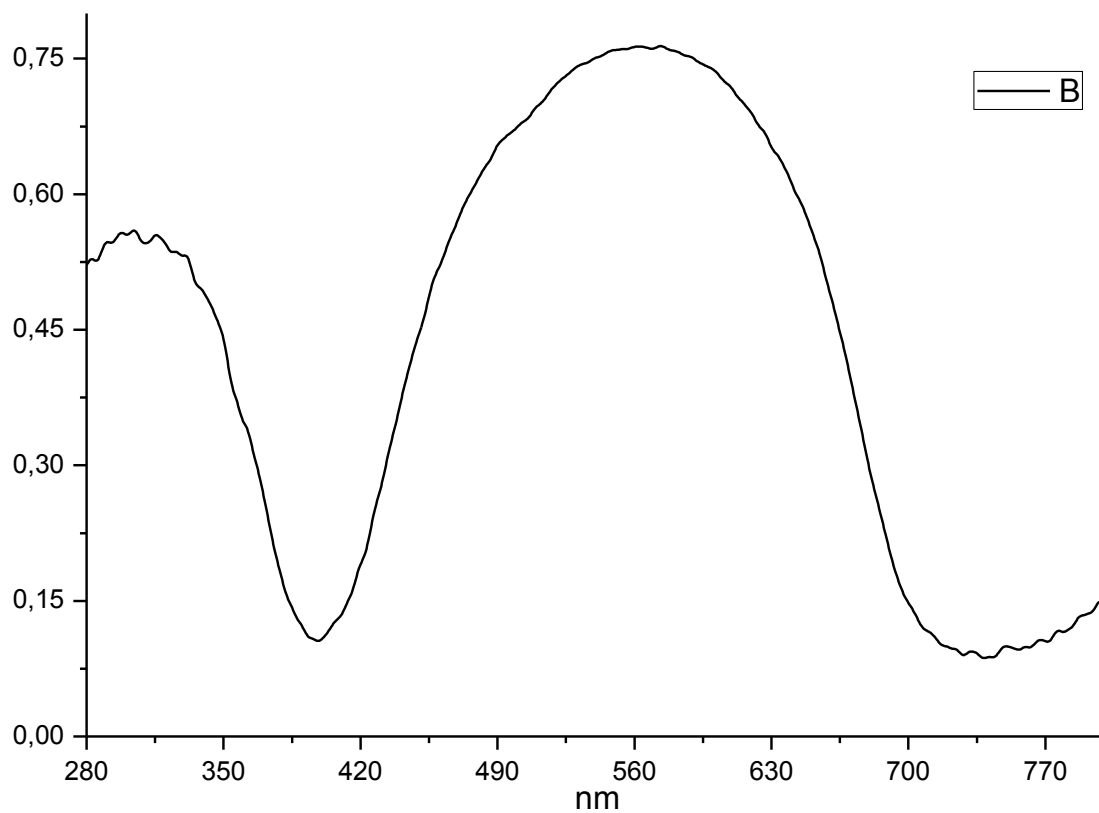
## Supporting Information

### **Peculiar Structural Findings in Coordination Chemistry of Malonamide – N,N’ diacetic acid**

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**Figure S1.** Powder pattern of 2 (a) theoretical (b) experimental



**Figure S2** The Diffuse reflectance spectra of 3

**Table S1.** Bond Distances (Å) in **1**, **2** and **3**

| <b>1</b>       | <b>2</b>         | <b>L1 in 3</b> | <b>L2 in 3</b>   |
|----------------|------------------|----------------|------------------|
| O1 C1 1.311(3) | O1 C1 1.2551(17) | O1 C1 1.297(6) | O7 C8 1.293(6)   |
| O2 C1 1.216(3) | O2 C1 1.2602(18) | O2 C1 1.239(6) | O8 C8 1.238(6)   |
| C1 C2 1.492(3) | C1 C2 1.517(2)   | C1 C2 1.513(7) | C8 C9 1.512(7)   |
| N1 C2 1.451(3) | N1 C2 1.4546(18) | N1 C2 1.455(6) | N3 C9 1.466(6)   |
| N1 C3 1.333(3) | N1 C3 1.326(2)   | N1 C3 1.319(7) | N3 C10 1.324(7)  |
| O3 C3 1.245(3) | C3 O3 1.241(2)   | O3 C3 1.272(6) | O9 C10 1.268(6)  |
| C3 C4 1.510(3) | C3 C4 1.517(2)   | C3 C4 1.517(7) | C10 C11 1.515(7) |
| C3 C4 1.510(3) | C4 C5 1.520(2)   | C4 C5 1.518(7) | C11 C12 1.509(7) |
| O3 C3 1.245(3) | C5 O4 1.231(2)   | O4 C5 1.256(6) | O10 C12 1.275(6) |
| N1 C3 1.333(3) | C5 N2 1.319(2)   | N2 C5 1.306(6) | N4 C12 1.310(7)  |
| N1 C2 1.451(3) | N2 C6 1.448(2)   | N2 C6 1.470(6) | N4 C13 1.459(7)  |
| C1 C2 1.492(3) | C6 C7 1.520(2)   | C6 C7 1.494(7) | C13 C14 1.523(8) |
| O1 C1 1.311(3) | C7 O6 1.2487(19) | O5 C7 1.293(6) | O11 C14 1.286(6) |
| O2 C1 1.216(3) | C7 O5 1.2558(18) | O6 C7 1.249(6) | O12 C14 1.238(6) |

**Table S2.** Analysis of all centroid distances found in **3**.

| Cg(I) | Res(I) | Cg(J)   | [ARU(J)]  | CgCg     | Transformed J Plane P, Q, R, S | Alpha  | Beta | Gamma | CgI_Perp | CgJ_Perp | Slippage |
|-------|--------|---------|-----------|----------|--------------------------------|--------|------|-------|----------|----------|----------|
| Cg(1) | [1]    | > Cg(3) | [2555.01] | 4.335(3) | 0.9792 0.1393 0.1476           | 4.3920 | 5.18 | 42.11 | 6.89     | 2.963    | 3.216    |
| Cg(1) | [1]    | > Cg(3) | [2655.01] | 4.432(3) | 0.9792 0.1393 0.1476           | 2.1676 | 5.18 | 39.47 | 35.75    | 3.596    | 3.421    |
| Cg(1) | [1]    | > Cg(4) | [2555.01] | 3.250(3) | 0.9870 0.1563 0.0378           | 5.0402 | 2.39 | 13.13 | 15.40    | 3.134    | 3.165    |
| Cg(1) | [1]    | > Cg(4) | [2655.01] | 3.516(3) | 0.9870 0.1563 0.0378           | 1.5714 | 2.39 | 9.00  | 8.38     | 3.478    | 3.473    |
| Cg(1) | [1]    | > Cg(6) | [2555.01] | 4.222(3) | 0.9898 0.1252 0.0676           | 4.5207 | 0.51 | 41.06 | 41.55    | 3.160    | 3.184    |
| Cg(1) | [1]    | > Cg(6) | [2655.01] | 3.978(3) | 0.9898 0.1252 0.0676           | 2.1101 | 0.51 | 29.75 | 29.24    | 3.471    | 3.454    |
| Cg(2) | [1]    | > Cg(3) | [2555.01] | 5.517(3) | 0.9792 0.1393 0.1476           | 4.3920 | 7.38 | 53.65 | 56.09    | 3.078    | 3.270    |
| Cg(2) | [1]    | > Cg(4) | [2555.01] | 4.096(3) | 0.9870 0.1563 0.0378           | 5.0402 | 2.77 | 40.35 | 37.58    | 3.246    | 3.121    |
| Cg(2) | [1]    | > Cg(4) | [2655.01] | 4.910(3) | 0.9870 0.1563 0.0378           | 1.5714 | 2.77 | 43.96 | 46.72    | 3.366    | 3.534    |
| Cg(2) | [1]    | > Cg(6) | [2555.01] | 3.847(3) | 0.9898 0.1252 0.0676           | 4.5207 | 2.70 | 32.78 | 34.10    | 3.186    | 3.235    |
| Cg(2) | [1]    | > Cg(6) | [2655.01] | 4.282(3) | 0.9898 0.1252 0.0676           | 2.1101 | 2.70 | 36.97 | 36.43    | 3.445    | 3.421    |
| Cg(3) | [1]    | > Cg(5) | [2545.01] | 3.864(3) | 0.9960 0.0887 0.0044           | 1.0699 | 8.76 | 32.96 | 32.57    | 3.256    | 3.242    |
| Cg(3) | [1]    | > Cg(5) | [2645.01] | 4.325(3) | 0.9960 0.0887 0.0044           | 5.6025 | 8.76 | 39.90 | 37.81    | 3.417    | 3.318    |
| Cg(4) | [1]    | > Cg(5) | [2545.01] | 3.986(3) | 0.9960 0.0887 0.0044           | 1.0699 | 4.35 | 36.55 | 39.35    | 3.082    | 3.202    |
| Cg(4) | [1]    | > Cg(5) | [2645.01] | 4.539(3) | 0.9960 0.0887 0.0044           | 5.6025 | 4.35 | 41.30 | 37.71    | 3.590    | 3.410    |
| Cg(5) | [1]    | > Cg(6) | [2555.01] | 3.288(3) | 0.9898 0.1252 0.0676           | 4.5207 | 4.20 | 7.40  | 8.77     | 3.250    | 3.260    |
| Cg(5) | [1]    | > Cg(6) | [2655.01] | 3.425(3) | 0.9898 0.1252 0.0676           | 2.1101 | 4.20 | 5.07  | 9.20     | 3.381    | 3.412    |

[ 2555] = -x,1/2+y,1/2-z, [ 2655] = 1-x,1/2+y,1/2-z, [ 2545] = -x,-1/2+y,1/2-z, [ 2645] = 1-x,-1/2+y,1/2-z

**Table S3.** Analysis of C-O...Cg interactions found in **3** (O..Cg < 4.0 Å, Gamma < 30.0 Deg)

| Y--X(I)     | Res(I) | Cg(J) | [ARU(J)]  | X..Cg    | Transformed J-Plane P, Q, R, S | X-Perp              | Gamma   | Y-X..Cg  | Y..Cg Y-X,Pi |
|-------------|--------|-------|-----------|----------|--------------------------------|---------------------|---------|----------|--------------|
| C(3)-O(3)   | [1]    | Cg(3) | [2555.01] | 3.346(5) | -0.9792 0.1393-0.1476          | 4.3920 3.265 12.66  | 76.4(3) | 3.288(6) | 1.61         |
| C(3)-O(3)   | [1]    | Cg(3) | [2655.01] | 3.490(5) | -0.9792 0.1393-0.1476          | -2.1676 3.294 19.25 | 85.6(3) | 3.620(6) | 1.61         |
| C(12)-O(10) | [1]    | Cg(2) | [2545.01] | 3.459(5) | -0.9936-0.1109-0.0228          | 0.8104 3.349 14.48  | 72.8(3) | 3.313(6) | 4.13         |
| C(12)-O(10) | [1]    | Cg(2) | [2645.01] | 3.317(5) | -0.9936-0.1109-0.0228          | -5.8454 3.307 4.54  | 90.3(3) | 3.561(6) | 4.13         |

**Table S4.** Analysis of Ring-Metal Interactions with distance Cg-Cu <4.0 Å found in **3**

| Cg(I) | Res(I) | Me(J)   | [ARU(J)]   | Cg(I)-Me(J) | MeJ_Perp | Beta  |
|-------|--------|---------|------------|-------------|----------|-------|
| Cg(1) | [ 1]   | > Cu(2) | [ 2555.01] | 3.413       | 3.120    | 23.89 |
| Cg(1) | [ 1]   | > Cu(2) | [ 2655.01] | 3.713       | 3.517    | 18.69 |
| Cg(4) | [ 1]   | > Cu(1) | [ 2545.01] | 3.308       | 3.176    | 16.26 |
| Cg(4) | [ 1]   | > Cu(1) | [ 2645.01] | 3.961       | 3.436    | 29.82 |
| Cg(5) | [ 1]   | > Cu(2) | [ 2555.01] | 3.479       | 3.102    | 26.93 |
| Cg(6) | [ 1]   | > Cu(1) | [ 2545.01] | 3.652       | 3.161    | 30.05 |
| Cg(6) | [ 1]   | > Cu(1) | [ 2645.01] | 3.779       | 3.469    | 23.36 |

[ 2555] = -X, 1/2+Y, 1/2-Z, [ 2655] = 1-X,1/2+Y,1/2-Z, [ 2545] = -X,-1/2+Y,1/2-Z, [ 2645] = 1-X,-1/2+Y,1/2-Z