Supplementary Material (ESI) for New Journal of Chemistry

Self-Assembly of Fe^{III} Complexes *via* Hydrogen Bonded Water Molecules into Supramolecular Coordination Networks

Ian McKeogh, Jonathan P. Hill, Emily S. Collins, Thomas McCabe, Annie K. Powell Wolfgang Schmitt*

Electronic Supplemental Information

Enlarged figures of the crystal structure of **1**

Enlarged figures of the crystal structure of **2**

Comparison of IR and UV-VIS spectra of **1** and **3**

Enlarged and additional TEM images of **3**

Hydrogen bonds in **2** [Å and °]

Correspondence to schmittw@tcd.ie

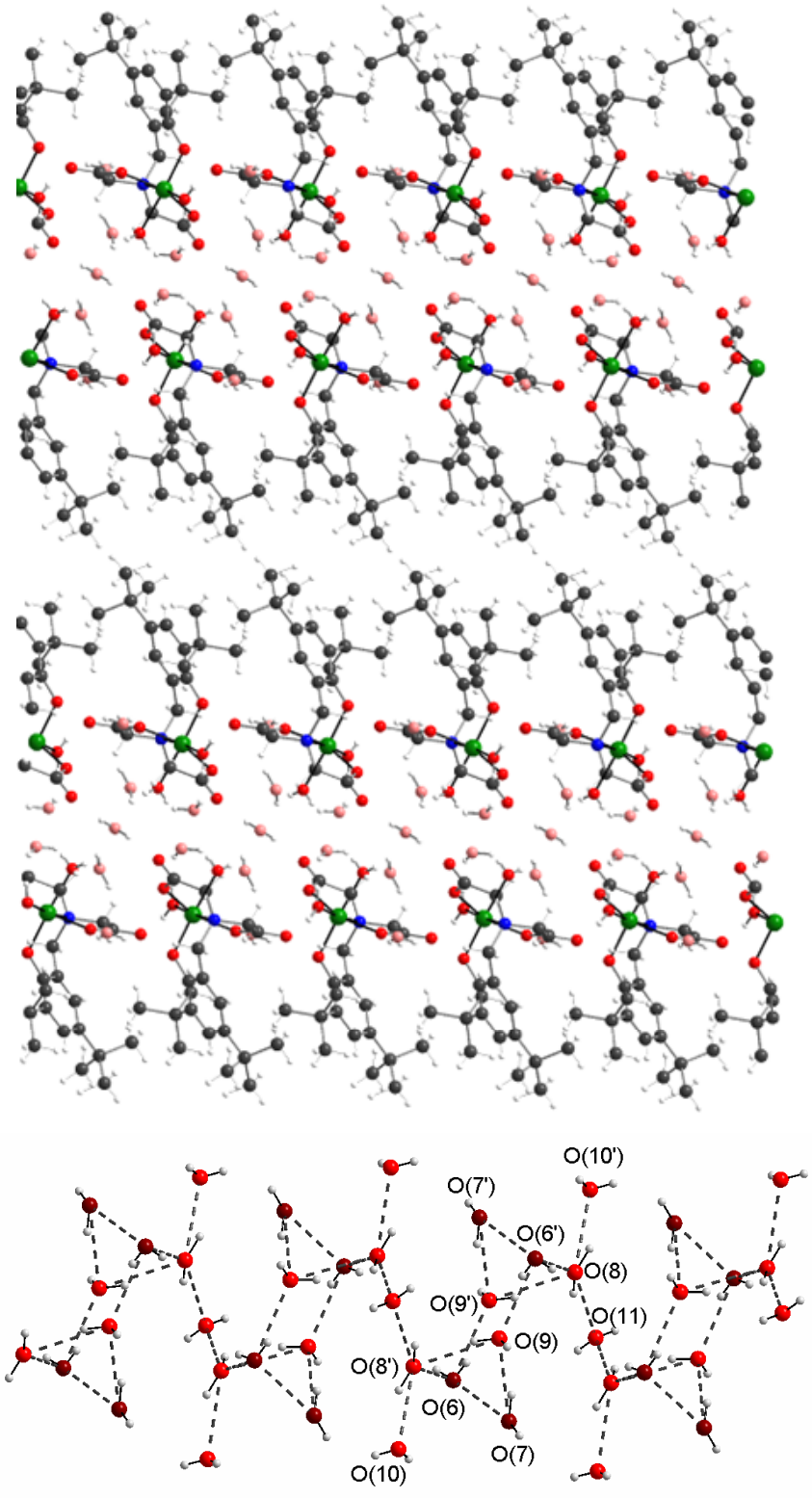

Fig. S1. Layered lamellar structure of **1**, view in the direction of the crystallographic *b* axis (top) and hydrogen bonded network of constitution and coordination (darker red) water molecules in the hydrophilic region of **1** (bottom, ‘ corresponds to *1-x, 1-y, 1-z* positions).

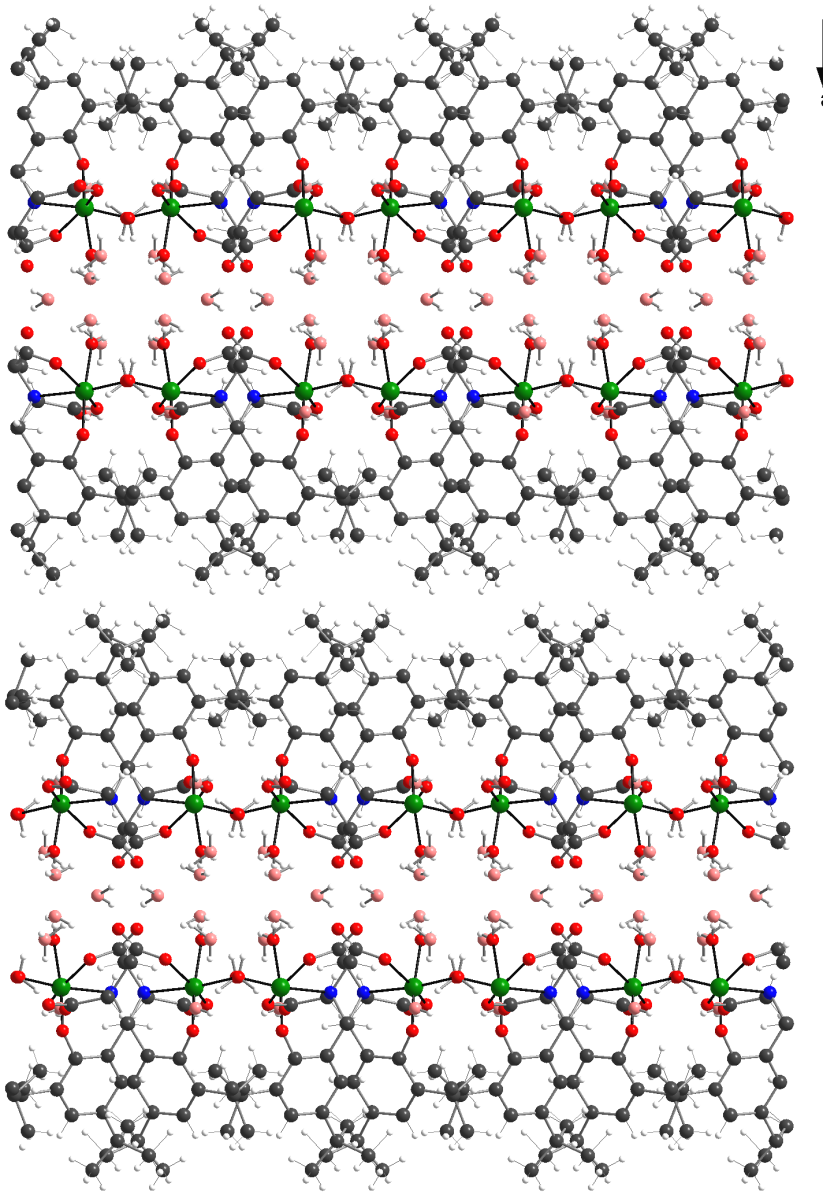

Fig. S2. Layered lamellar structure of **1**, viewed in the direction of the crystallographic *c* axis.

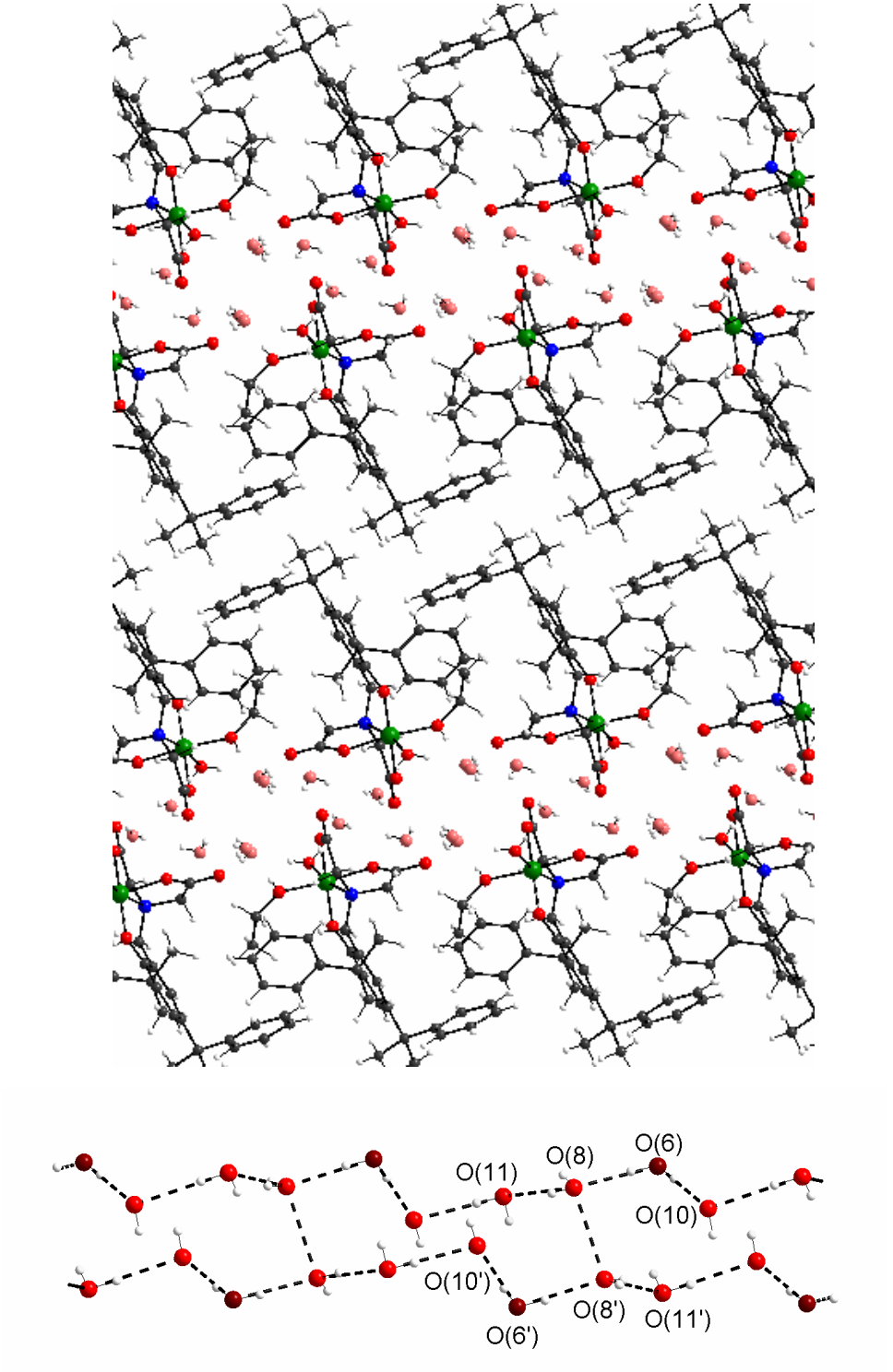

Fig. S3. Layered lamellar structure of **2**, view in the direction of the crystallographic *b* axis (top) and hydrogen bonded network of constitution and coordination (darker red) water molecules in the hydrophilic region of **2** (bottom, ‘ corresponds to –x, y, 0.5-z positions).

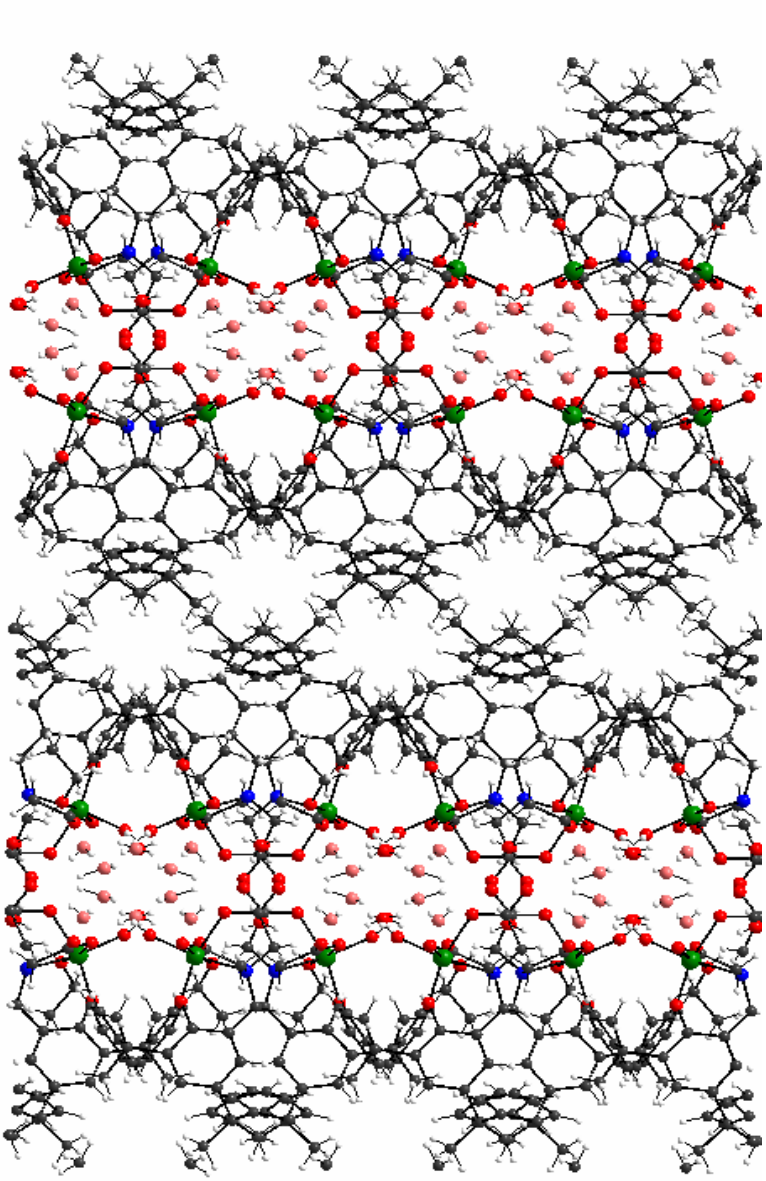

Fig. S4. Layered lamellar structure of **2**, view in the direction of the crystallographic *c* axis.

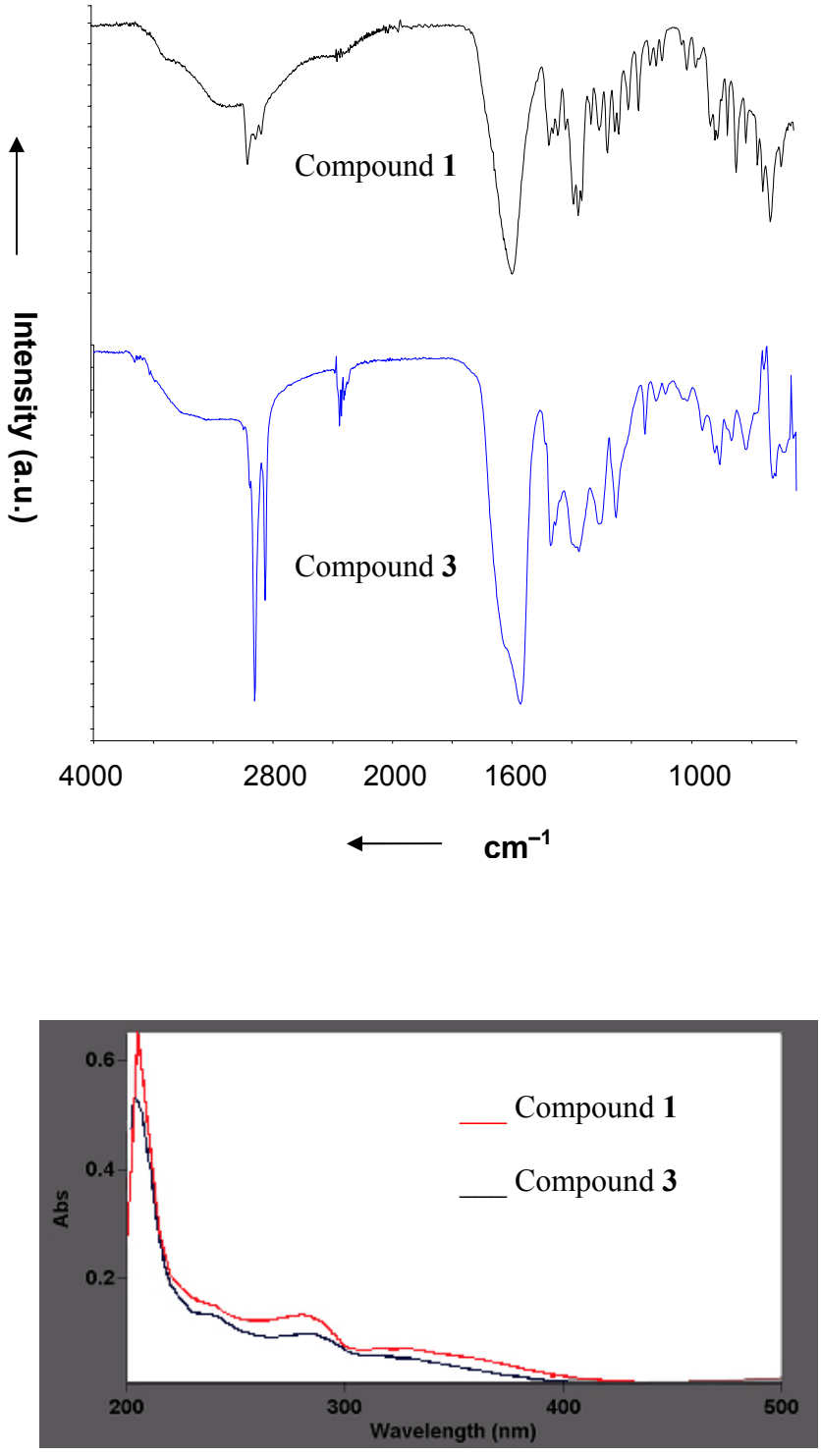

Fig. S5. Comparison of IR (top) and UV-VIS (bottom) spectra of **1** and **3**.

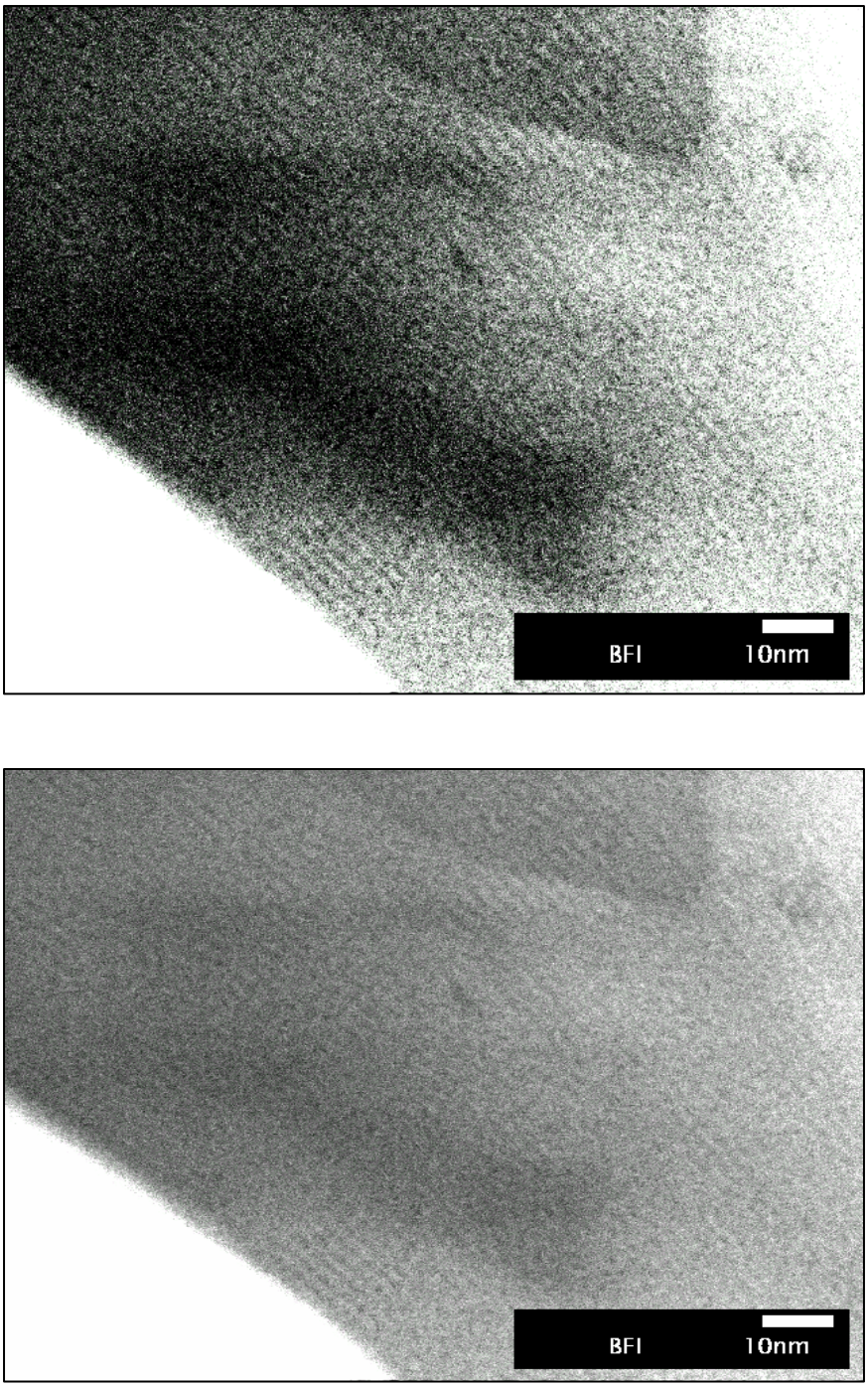

Fig. S7. Enlarged and additional TEM images of **3**.

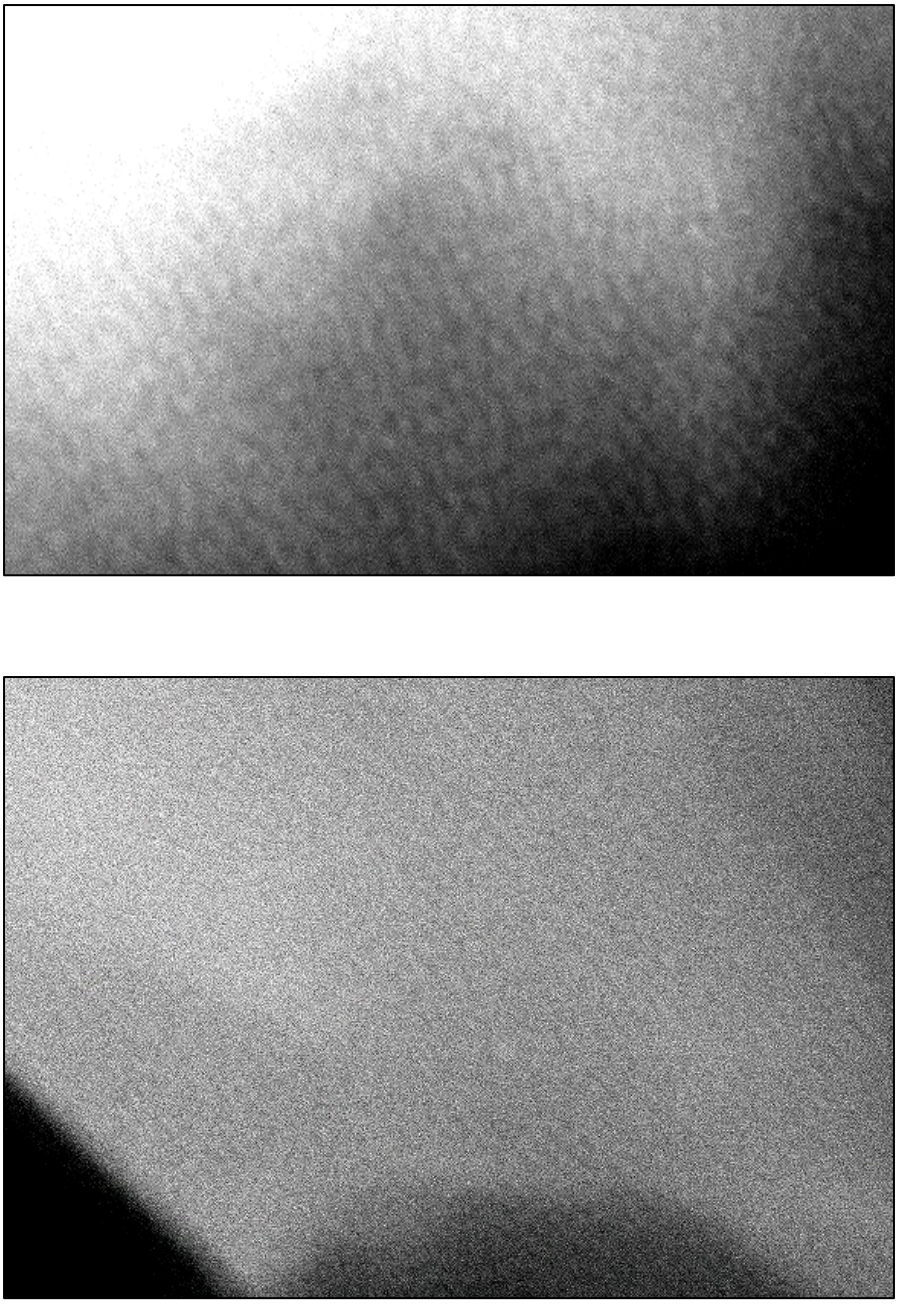

Fig. S8. Enlarged and additional TEM images of **3**.

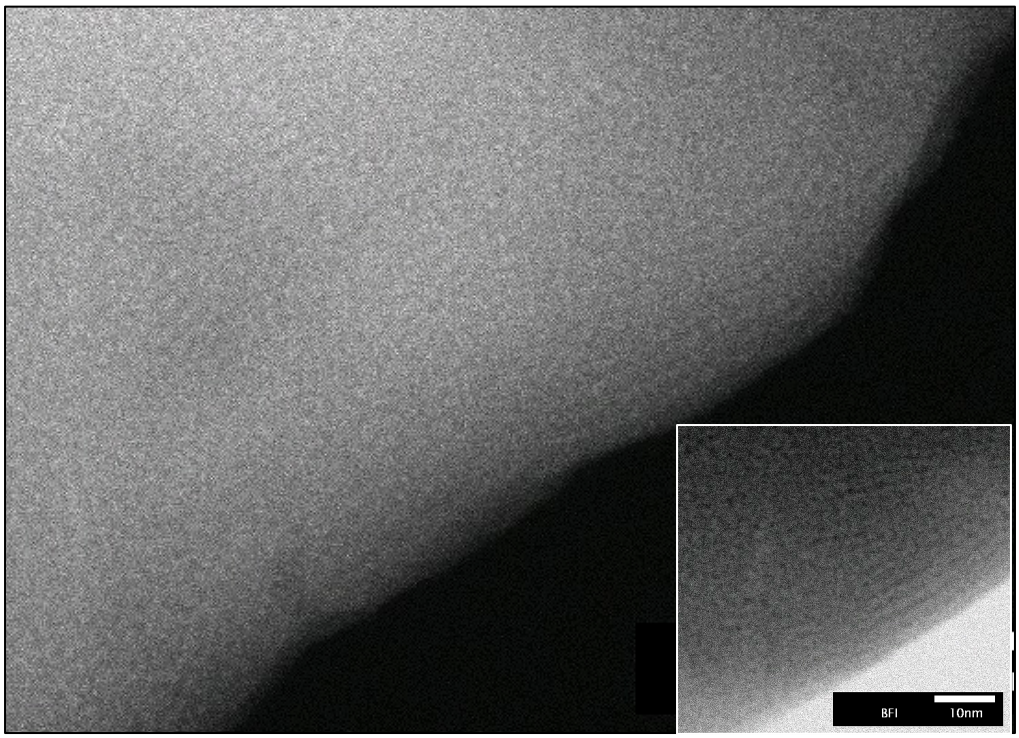

Fig. S9. Enlarged and additional TEM images of **3**.

Table S1. Hydrogen bonds in **2** [Å and °].

D-H...A	**d(D-H)**	**d(H...A)**	**<(DHA)**	**d(D...A)**
O11-H11B...O10[x, -y, z+1/2]	0.836(16)	2.048(17)	175(3)	2.882(3)
O8-H8A ...O11	0.806(16)	1.981(17)	169(3)	2.777(2)
O6-H6B ...O8	0.821(15)	1.821(15)	174(2)	2.639(2)
O6-H6A ...O10	0.839(15)	1.781(15)	176(2)	2.618(2)
O7-H7A ...O9	0.80(3)	1.81(3)	175(3)	2.607(2)
O8-H8B ...O3[x, -y, z+1/2]	0.810(16)	1.942(16)	175(3)	2.750(2)
O9-H9B ...O5[-x, y, -z+1/2]	0.844(16)	2.32(2)	141(2)	3.026(2)
O9-H9A ...O3[x, -y+1, z+1/2]	0.870(16)	1.897(17)	176(3)	2.766(2)
O11-H11A ...O4[-x, y, -z+1/2]	0.826(16)	2.08(2)	148(2)	2.810(2)

D: donor atom; A aceptor atom; d distance; < angle