Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information (SI) for

Bismuth 2,6-pyridinedicarboxylates: Assembly of molecular units into coordination polymers, CO_2 sorption and photoluminescence properties

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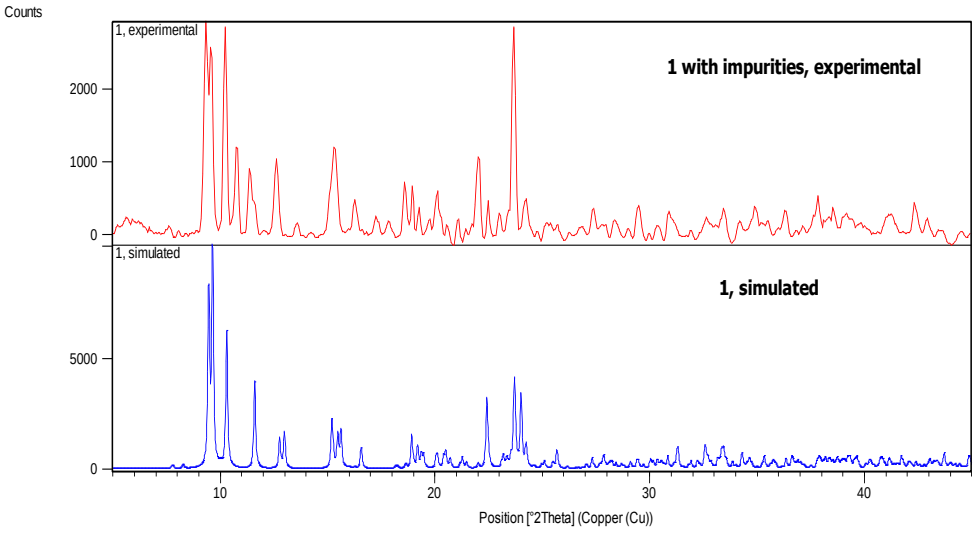


Fig. S1a, PXRD pattern for **1** (top-experimental and bottom-simulated).

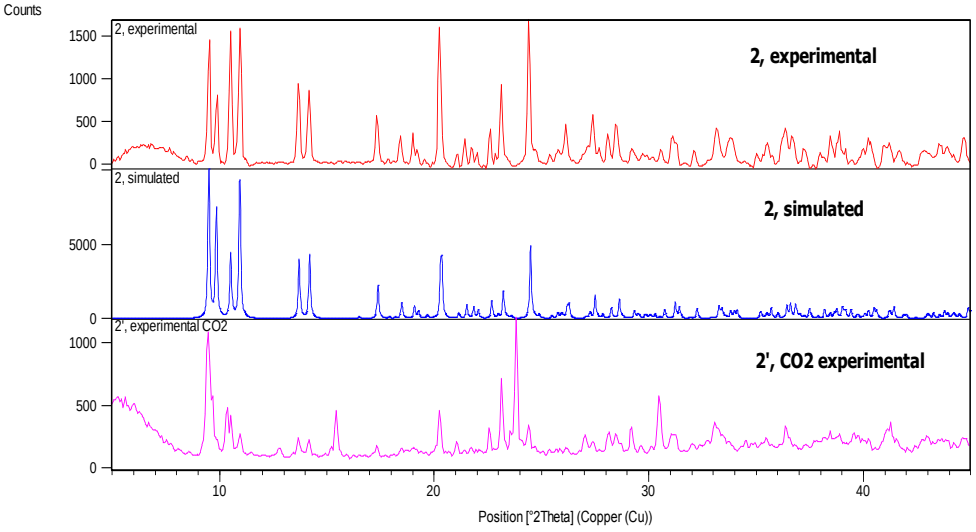


Fig. S1b, PXRD pattern for **2** (top-experimental, middle-simulated and bottom-experimental data on sample after CO2 sorption).

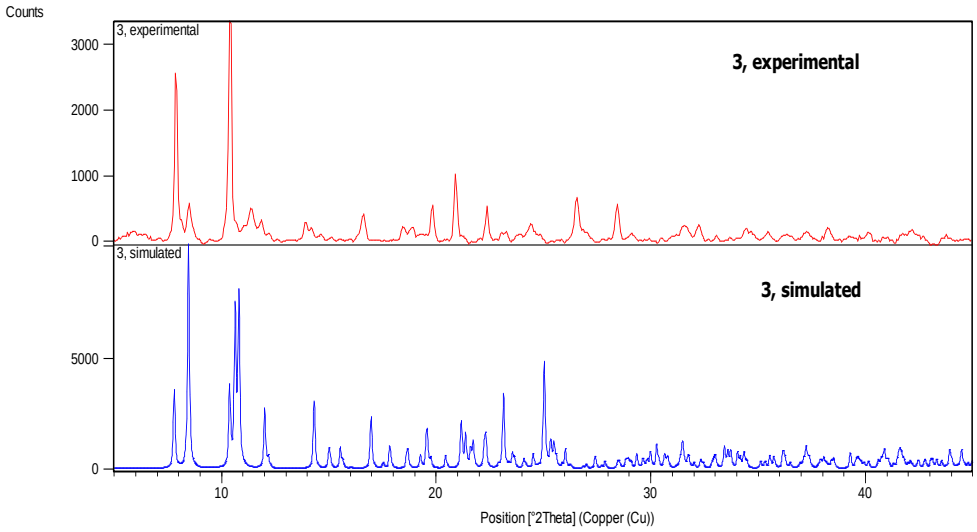


Fig. S1c, PXRD pattern for **3**(top-experimental and bottom-simulated).

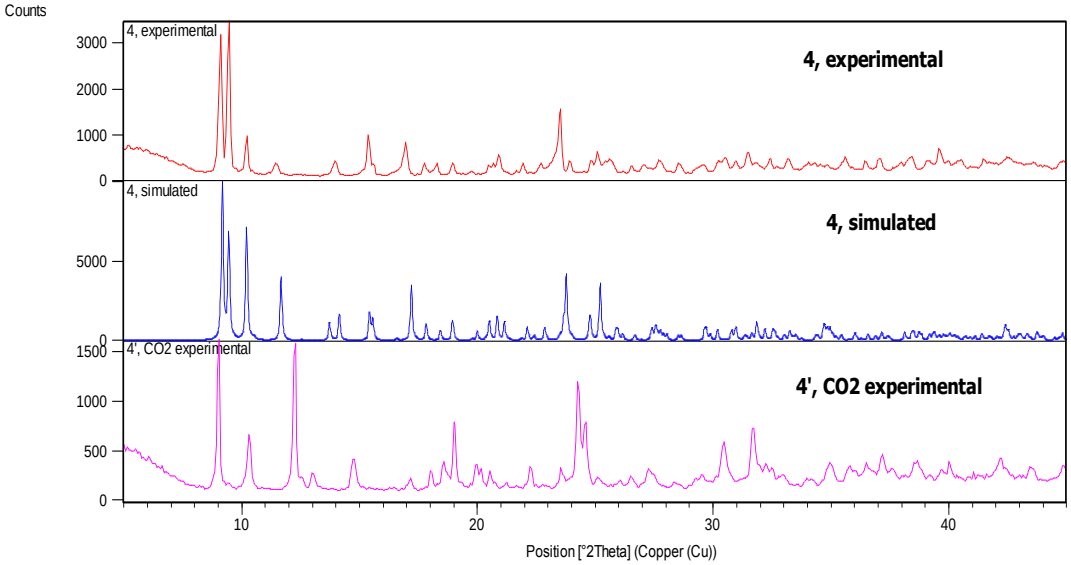


Fig. S1d, PXRD pattern for **4** (top-experimental, middle-simulated and bottom-experimental data on sample after CO2 sorption).

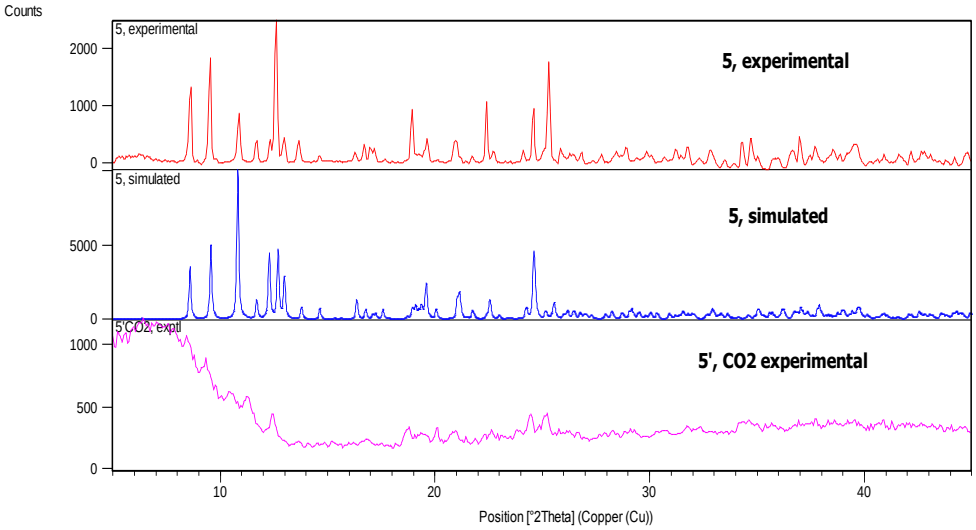


Fig. S1e, PXRD pattern for **5** (top-experimental, middle-simulated and bottom-experimental data on sample after CO2 sorption).

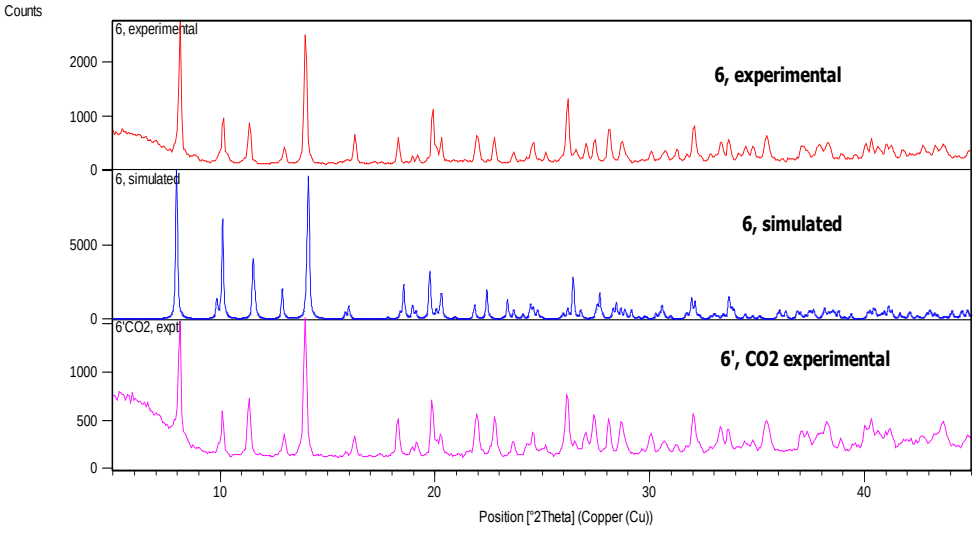


Fig. S1f, PXRD pattern for **6** (top-experimental, middle-simulated and bottom-experimental data on sample after CO2 sorption).

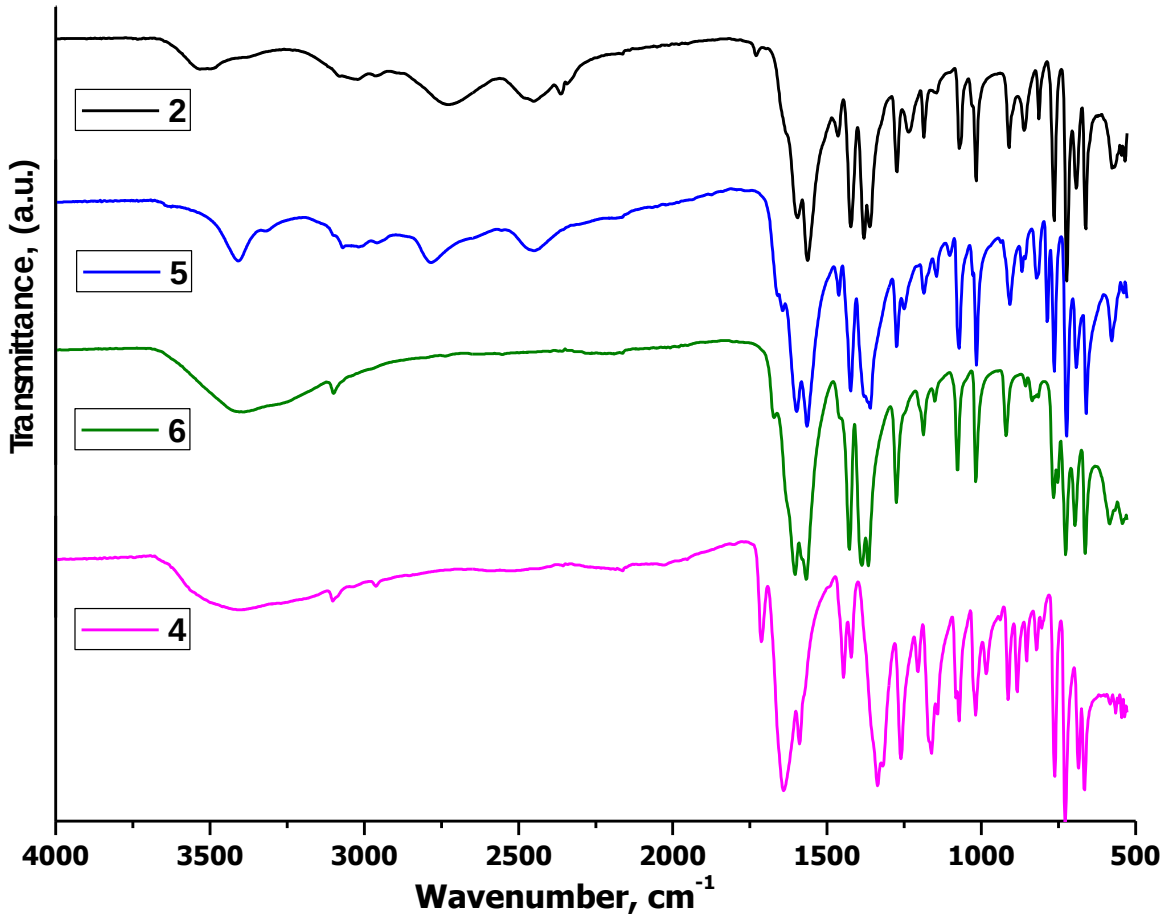


Fig. S2a, IR spectra of compound **2**-**6**.

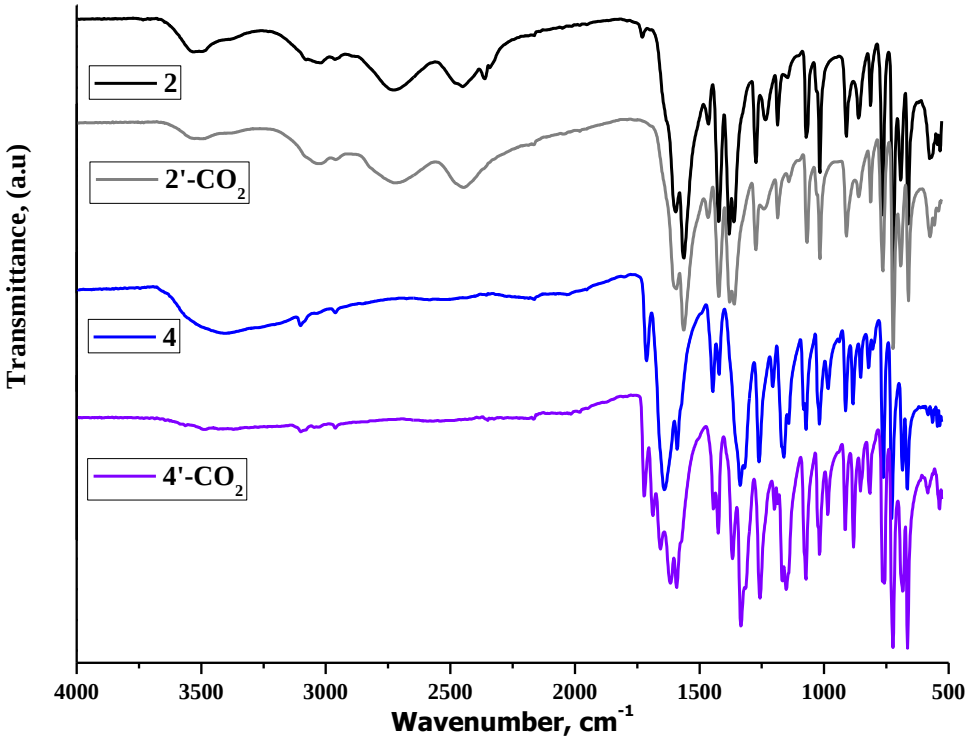


Fig. S2b, IR spectra of compound **2**,**4** and their respective CO_2 sorption samples .

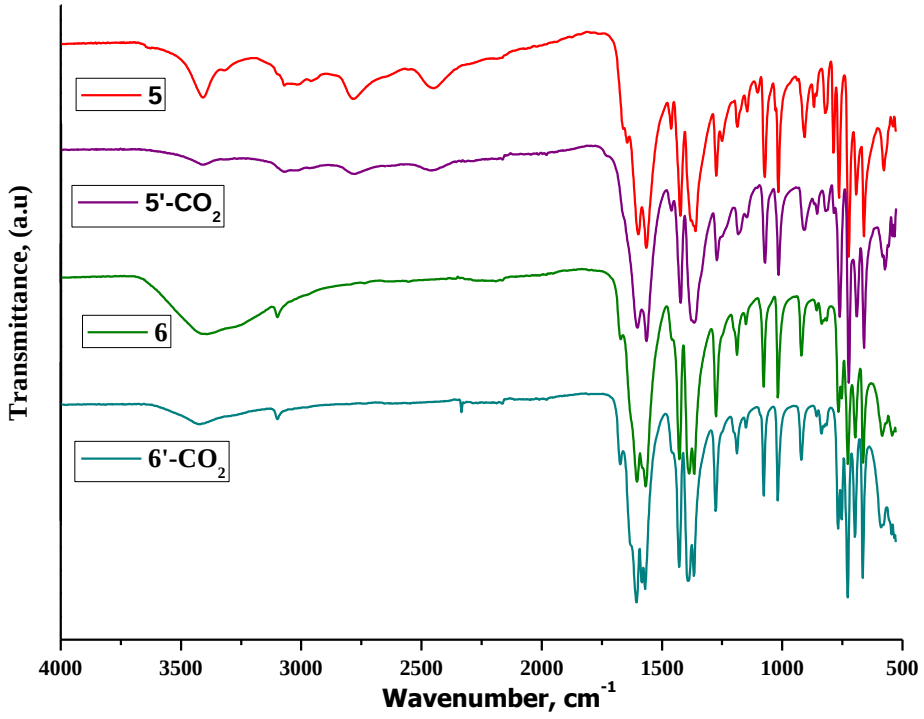


Fig. S2c, IR spectra of compound **5**,**6** and their respective CO_2 sorption samples .

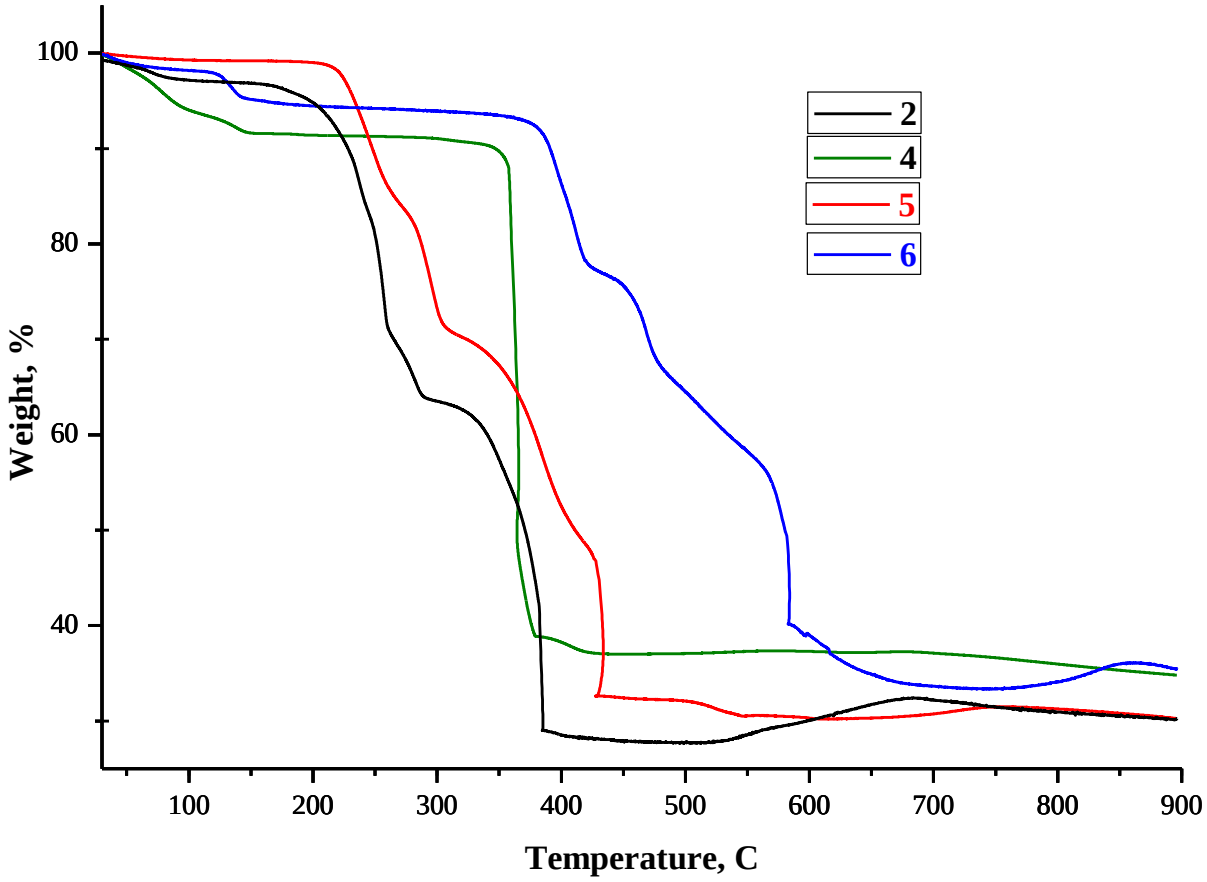


Fig. S3a, TGA plots of compounds **2**-**6**.

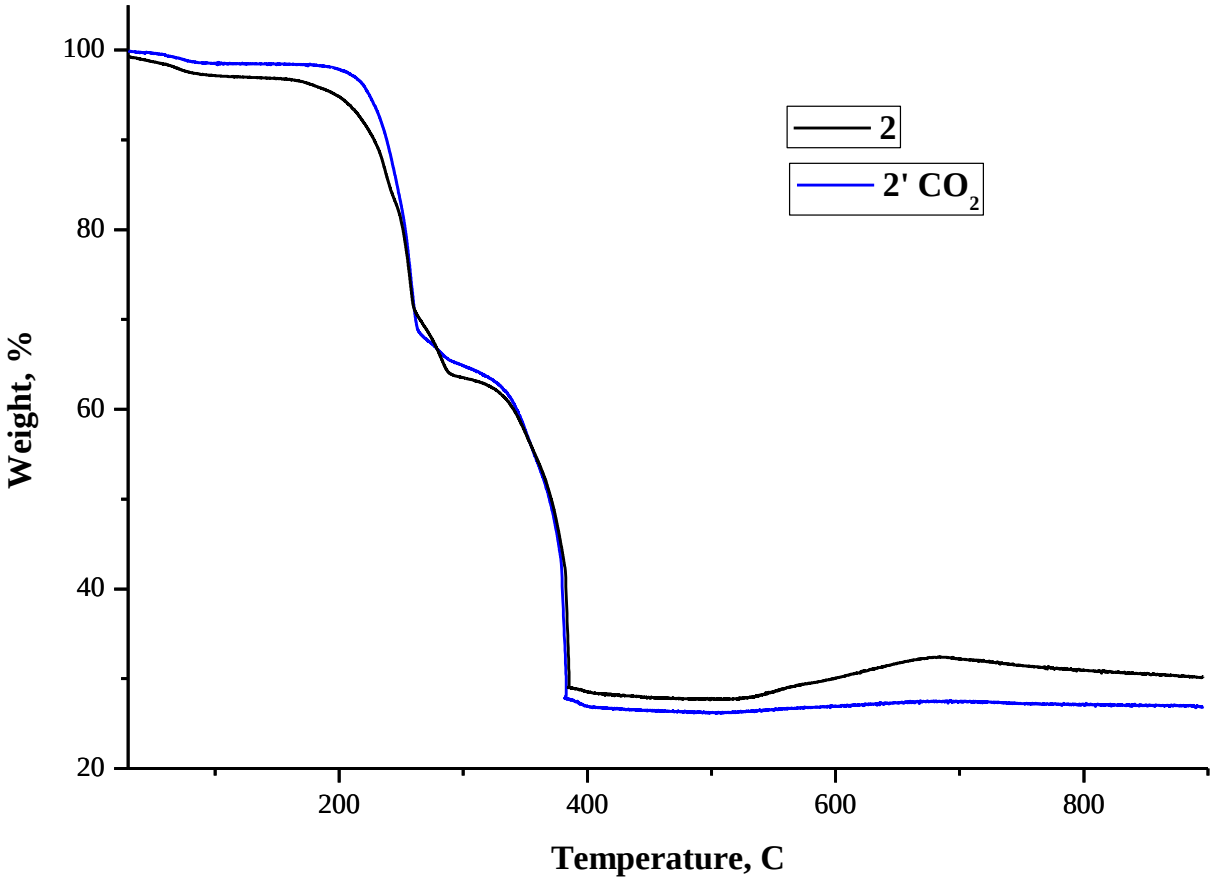


Fig. S3b, TGA plots of compound **2** and its CO_2 sorption sample .

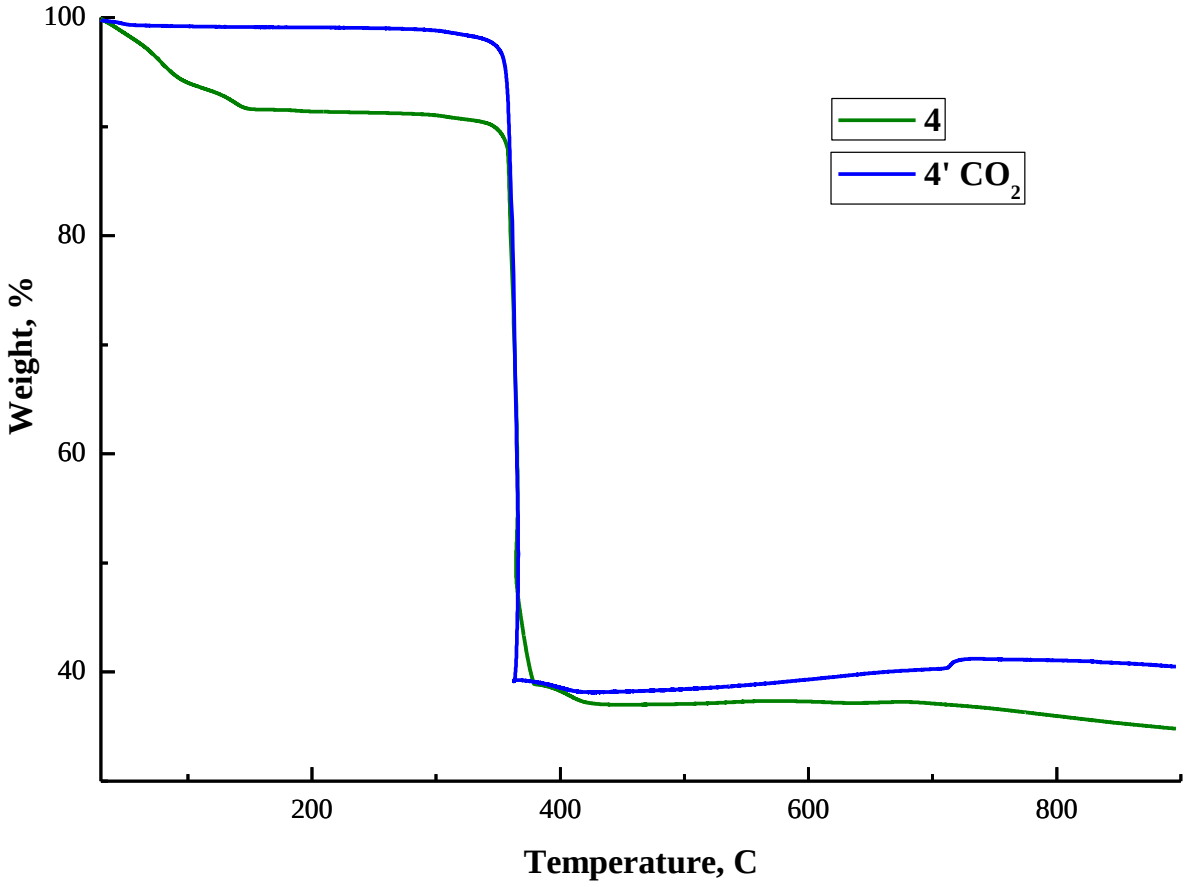


Fig. S3c, TGA plots of compound **4** and its CO_2 sorption sample .

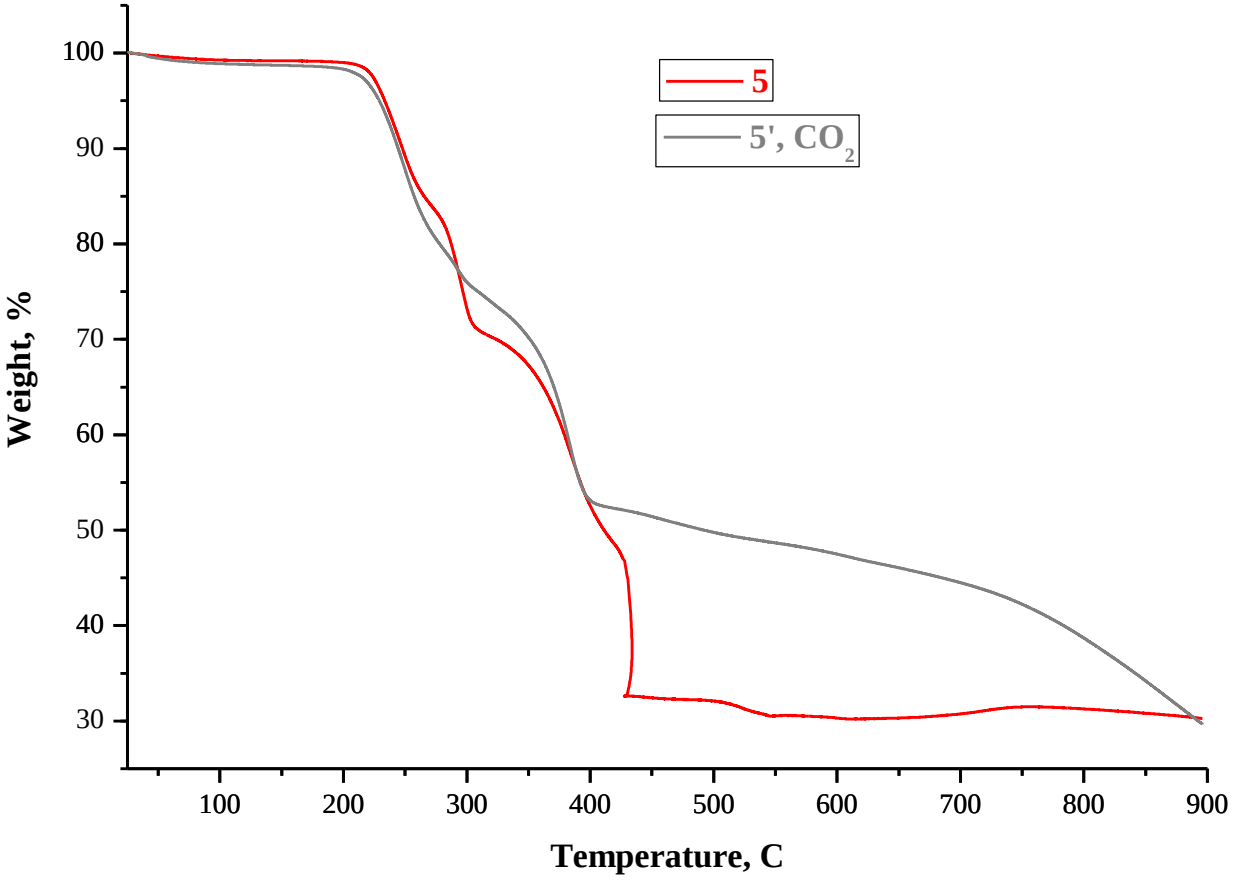


Fig. S3d, TGA plots of compound **5** and its CO_2 sorption sample .

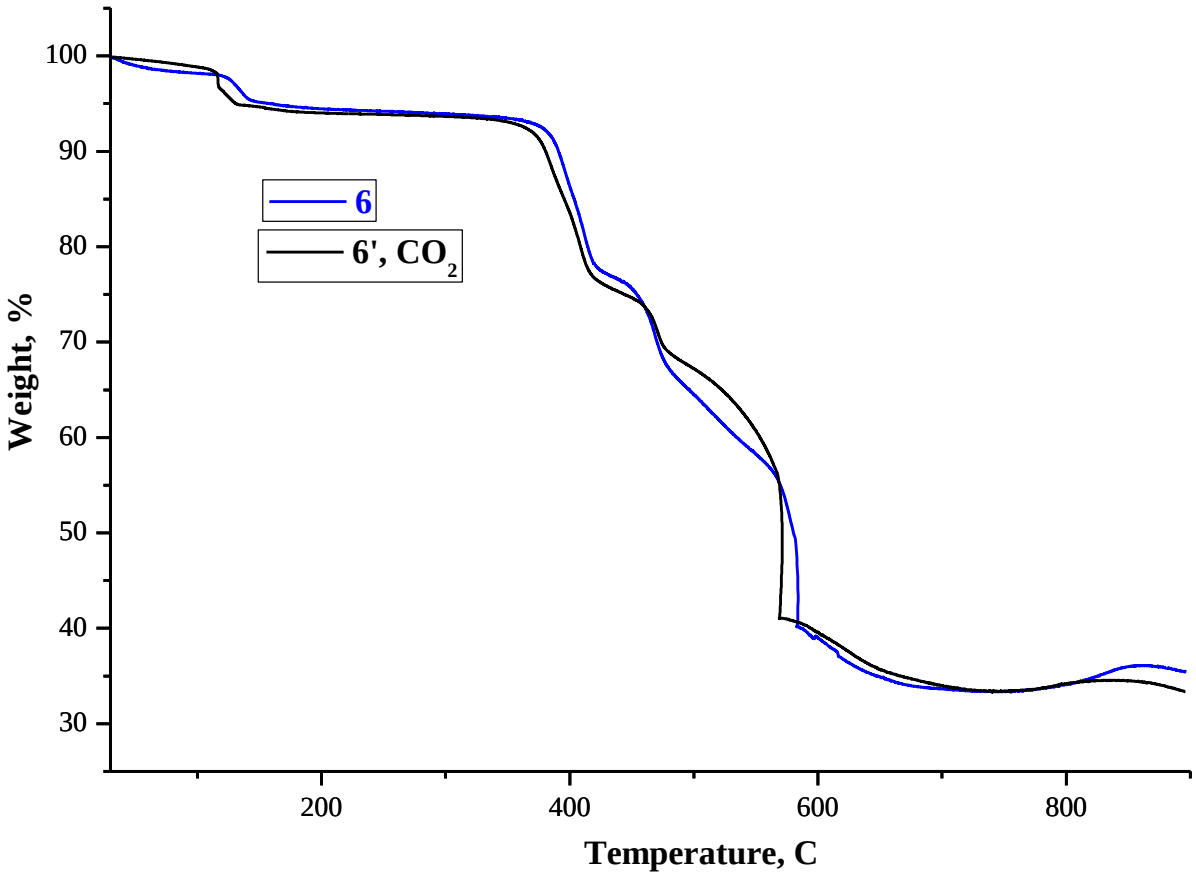


Fig. S3e, TGA plots of compound **6** and its CO_2 sorption sample .

Special details of the refinement of the single crystal diffraction data.

In compound 2, two of the N-H and N-C bond distances are restrained to obtain a stable refinement by using the Dfix command.
DFIX N3 H3a 0.95 0.01
DFIX N3 H3b 0.95 0.01
DFIX N4 C32 1.485 0.01
DFIX N4 C31 1.485 0.01

In compound 3, two of the N-H bond distances are restrained to obtain a stable refinement by using the Dfix command.
DFIX N4 H4A 0.95 0.01
DFIX N4 H4B 0.95 0.01

In compound 6, two of the O-H bond distances are restrained to obtain a stable refinement by using the Dfix command.
DFIX O9 H1 0.85 0.01
DFIX O9 H9 0.85 0.01

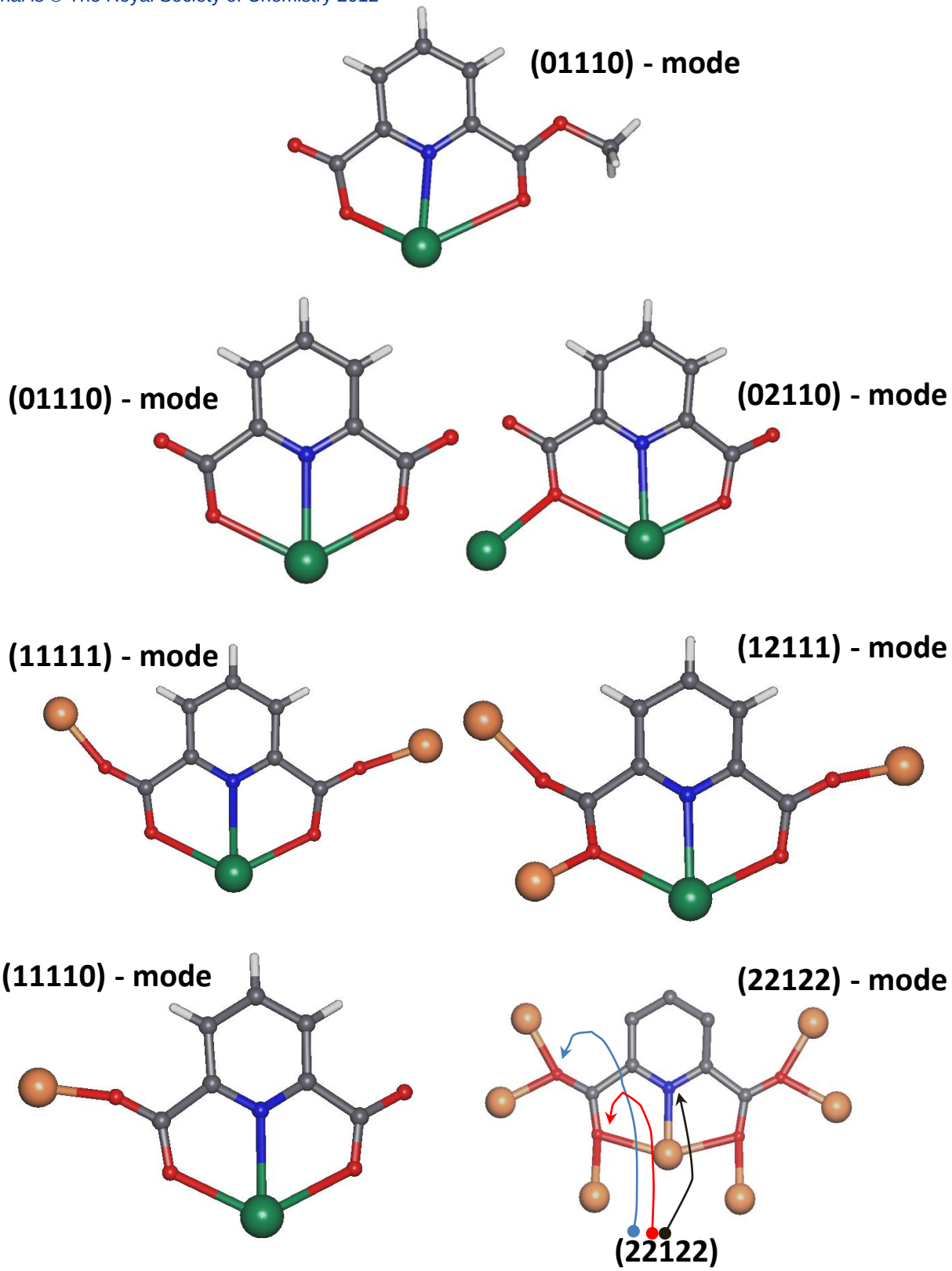
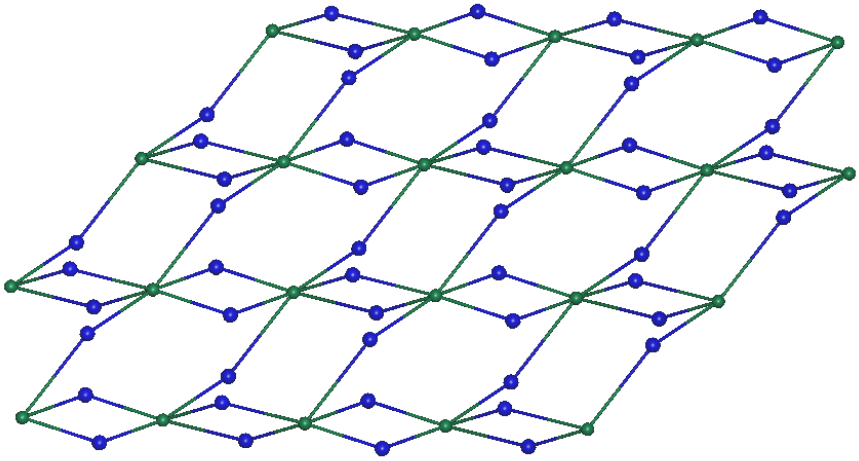
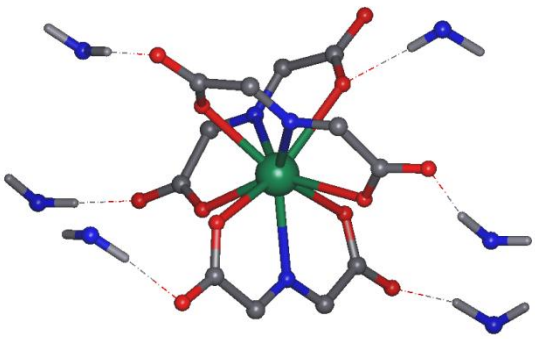


Fig. S4, Various coordination modes exhibited by pdcme and pdc anions in compounds **1**-**6**.

For description this coordination mode notation see: ***Chem. Mater.*, 1997, 9, 6.**





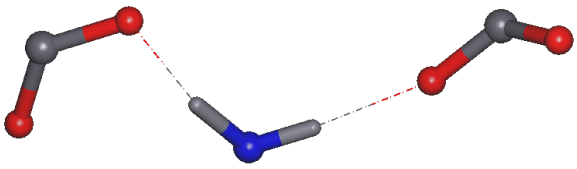


Fig. S5, The view of (4,4)-connected square lattice (sql) / Shubnikov tetragonal plane net topology in **1**.
The view of the 6-connecting H-bonded Bi-coordination unit and the 2-connecting dma cation in the above net (not all the atoms are shown for clarity).

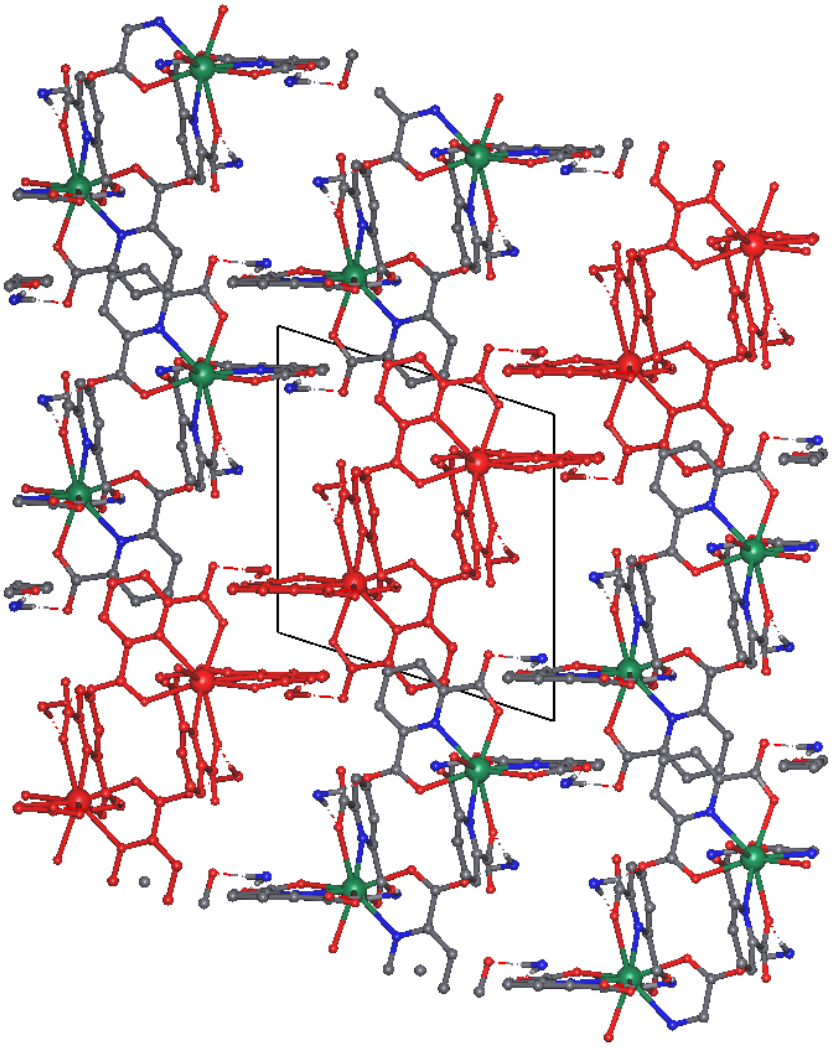


Fig. S6, The view of H-bonded layers staked along the *b* axis in **1**, involving a week pi-pi interaction from the pyridyl rings of the adjacent layers.

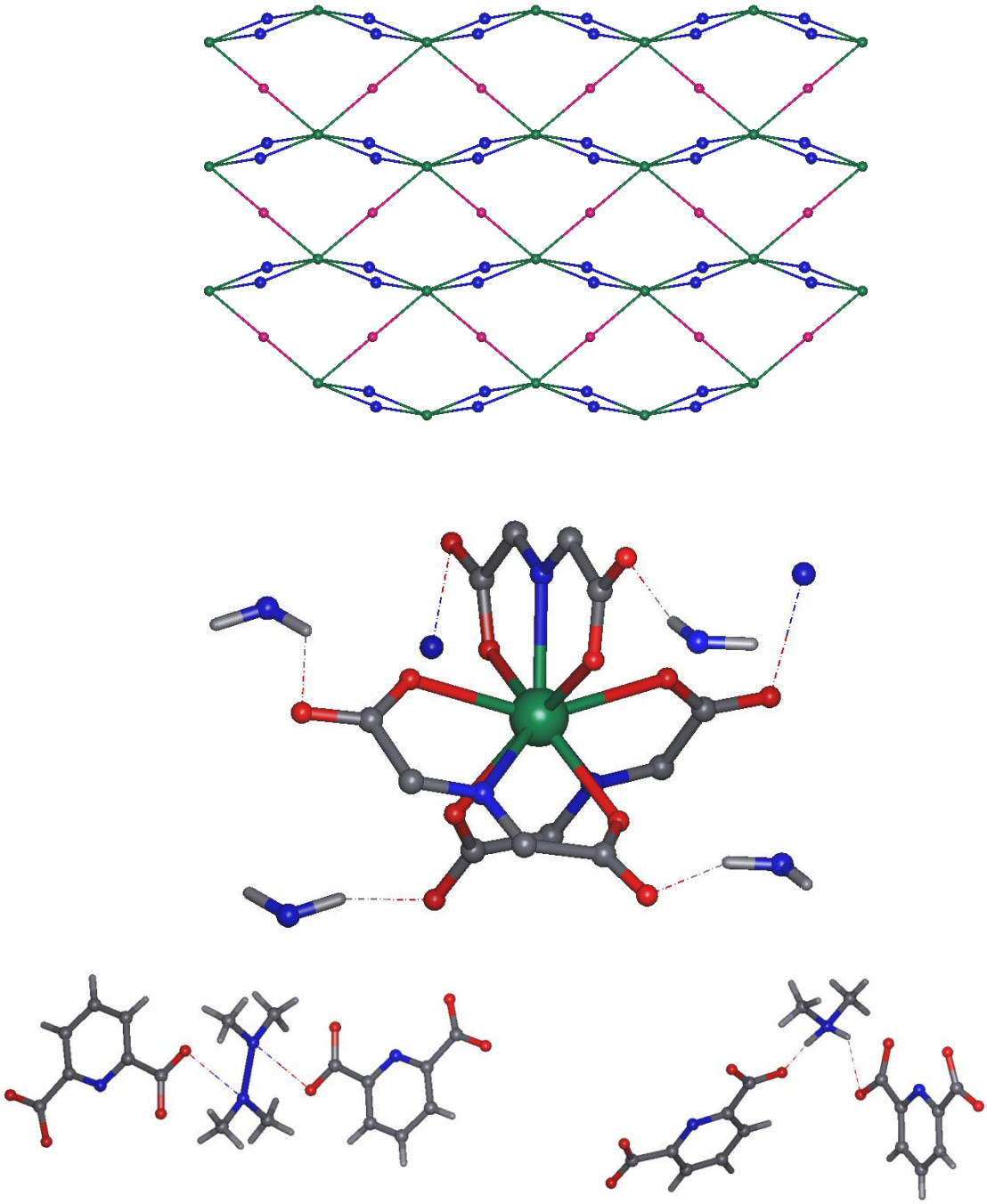


Fig. S7, The view of (4,4)-connected square lattice (sql) / Shubnikov tetragonal plane net topology in **2**.
The view of the 6-connecting H-bonded Bi-coordination unit and two types of 2-connecting dma cations in the above net.
(Purple-dimeric dma cations and blue-single dma cation in the net)
(not all the atoms are shown for clarity).

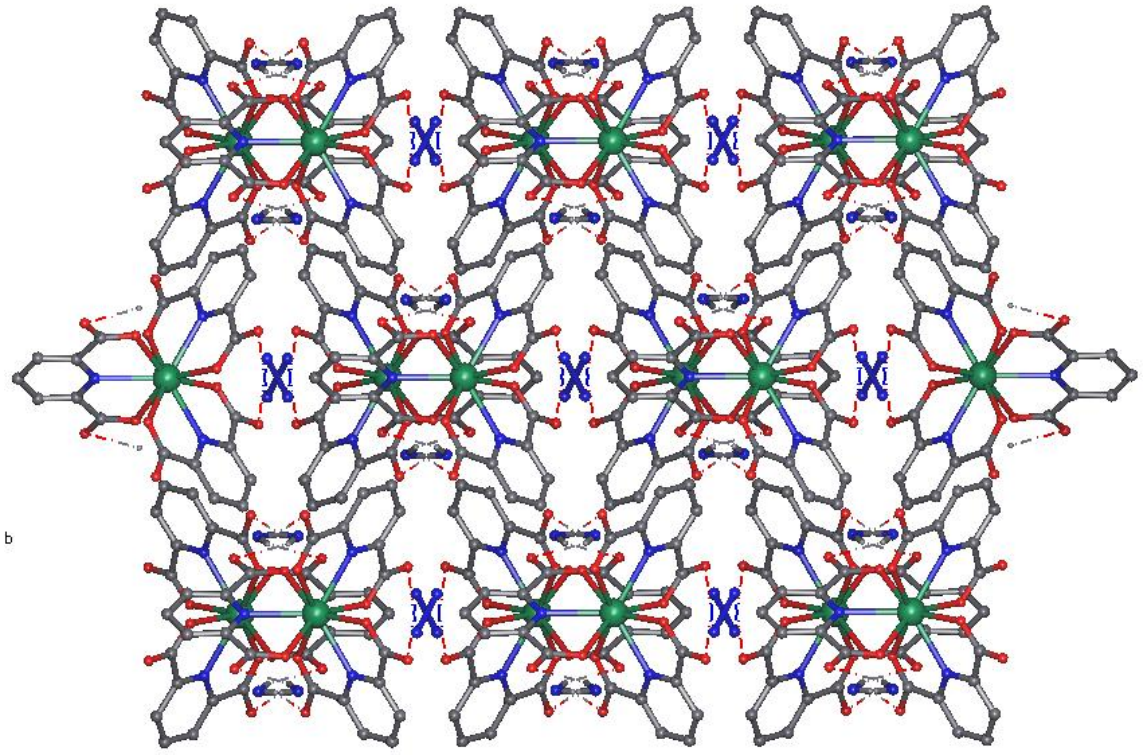


Fig. S8, The view of H-bonded layers staked along the *c* axis in **2**, involving a week pi-pi interaction from the pyridyl rings of the adjacent layers.

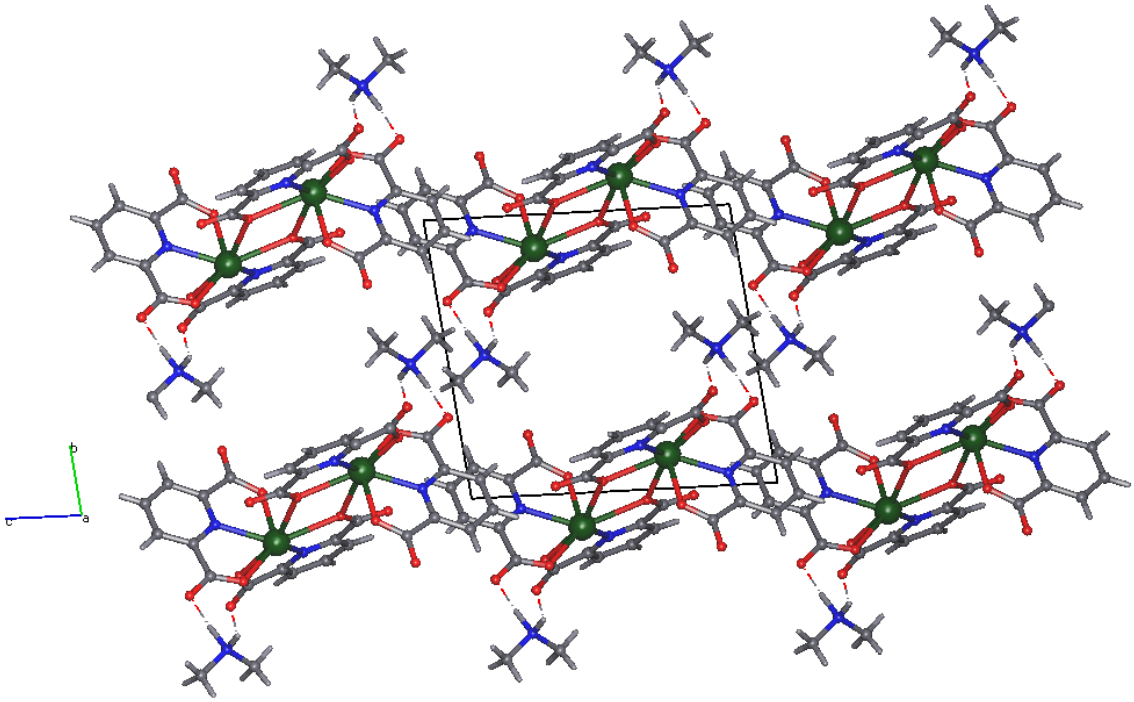


Fig. S9, The view of H-bonded chains packed along the *a* axis in **3**, involving a week pi-pi interaction from the pyridyl rings of the adjacent chains.

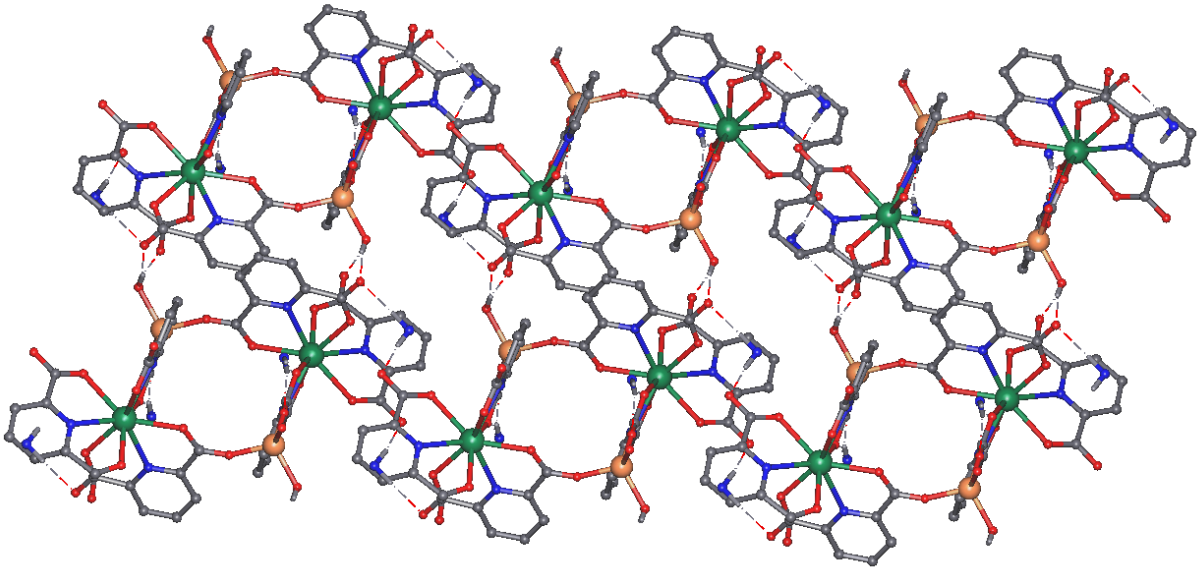


Fig. S10, The view of H-bonded layers packed along the *a* axis in **5**, involving a H-bonding interactions, through the terminal water molecule coordinated to the lithium cation from one layer to the pdc anions of the adjacent layer of the adjacent chains.

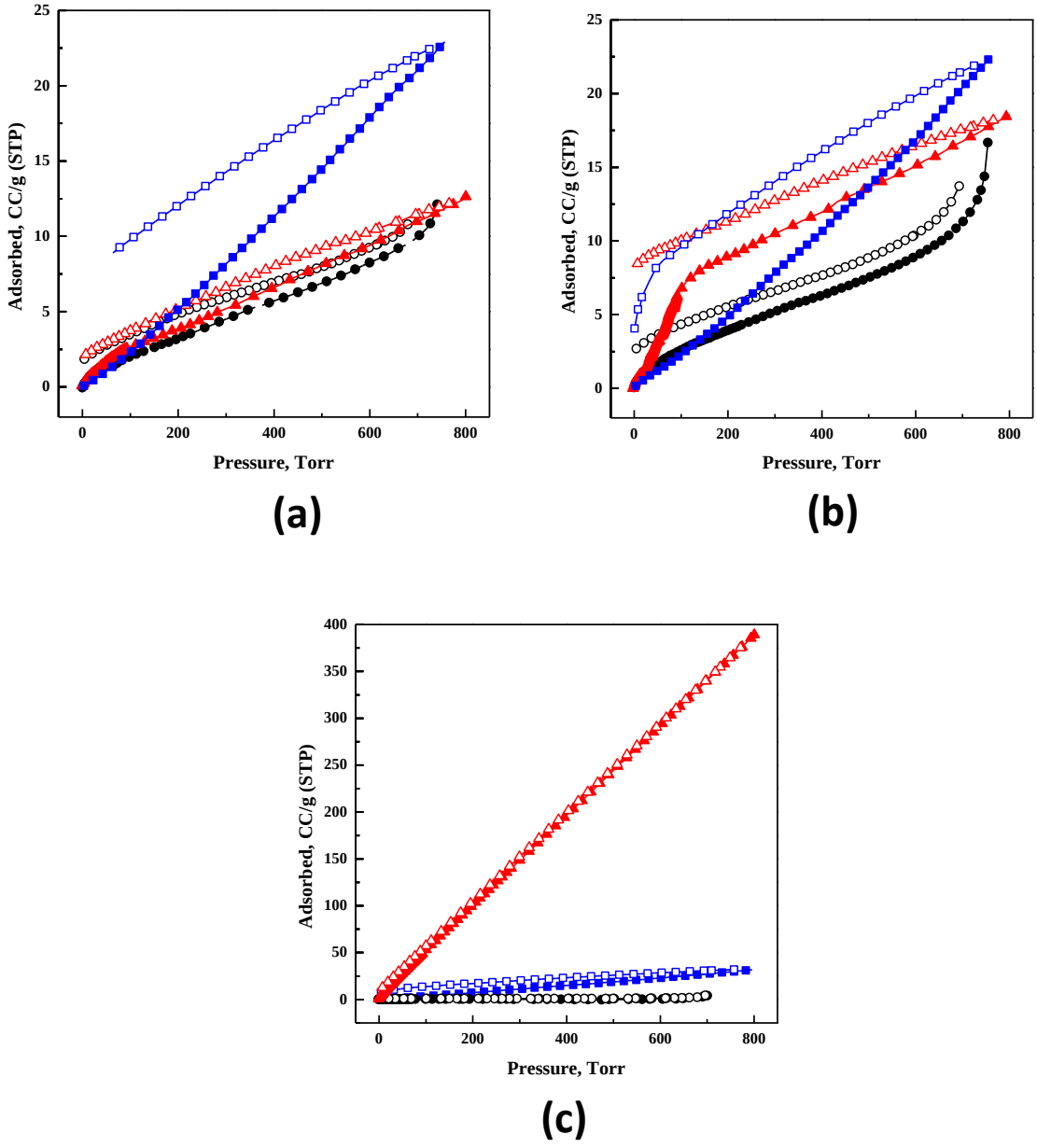


Fig. S11, Gas sorption isotherms for activated samples of **2** (a), **4** (b) and **5** (c), shows the uptake of CO2 at 275 K (blue squares), N_2 at 77 K (black circles) and H_2 at 77 K (red triangles). Solid and open symbols indicate gas sorption and desorption, respectively.

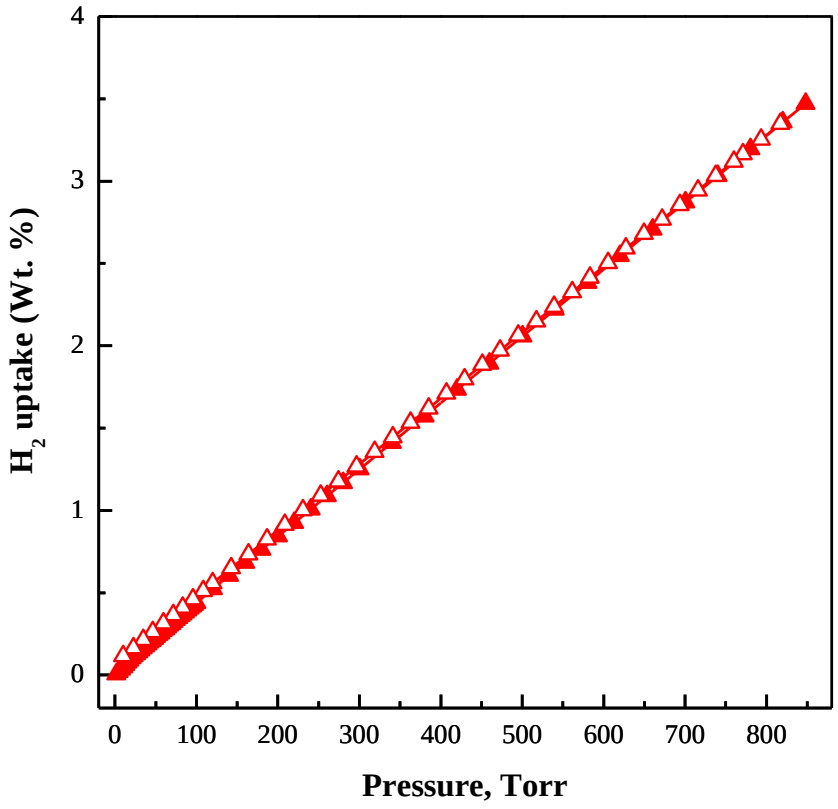


Fig. S12, H_2 sorption isotherms for activated samples **5** at 77 K. Solid and open symbols indicate gas sorption and desorption, respectively.

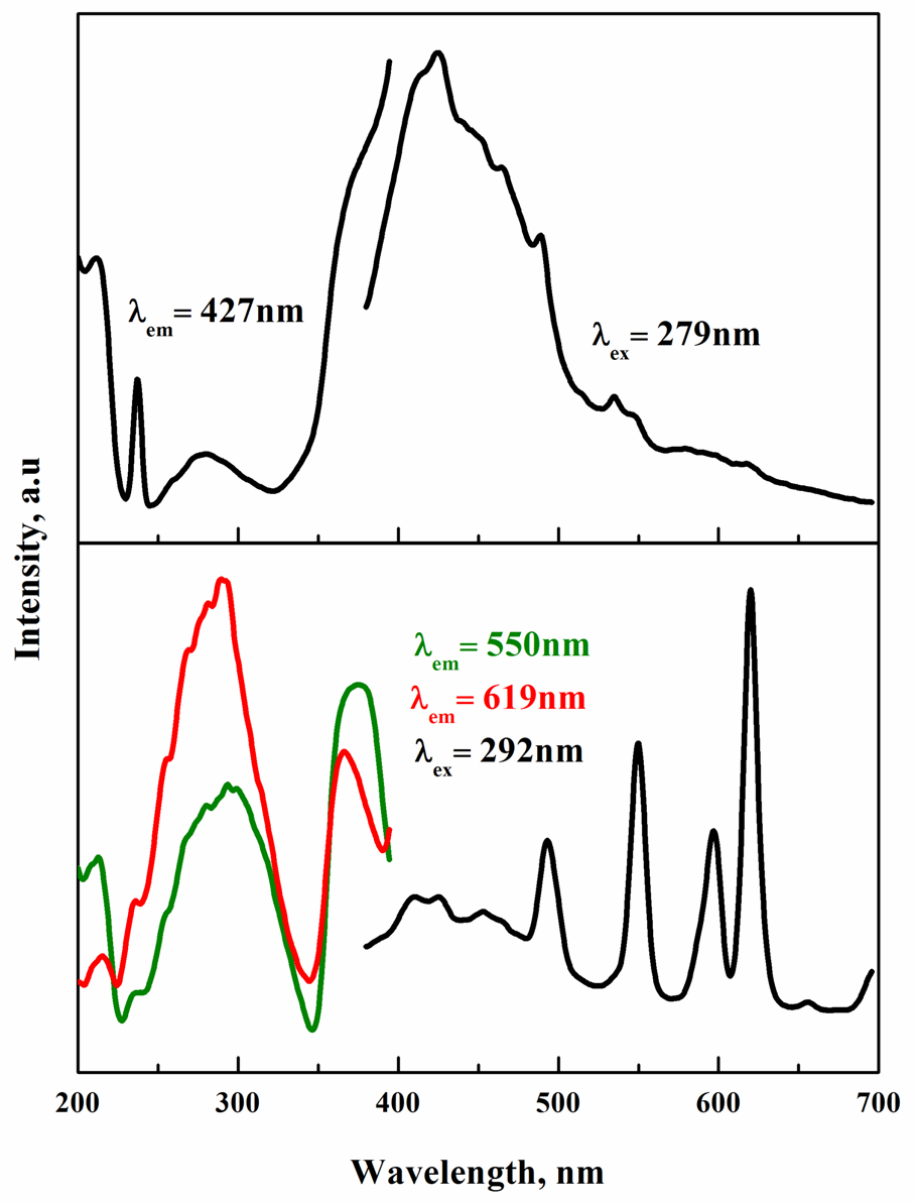


Fig. S13, Photoluminescence spectra of undoped **4**, top and **4a** (5 mol% Tb + 5 mol% Eu), bottom.