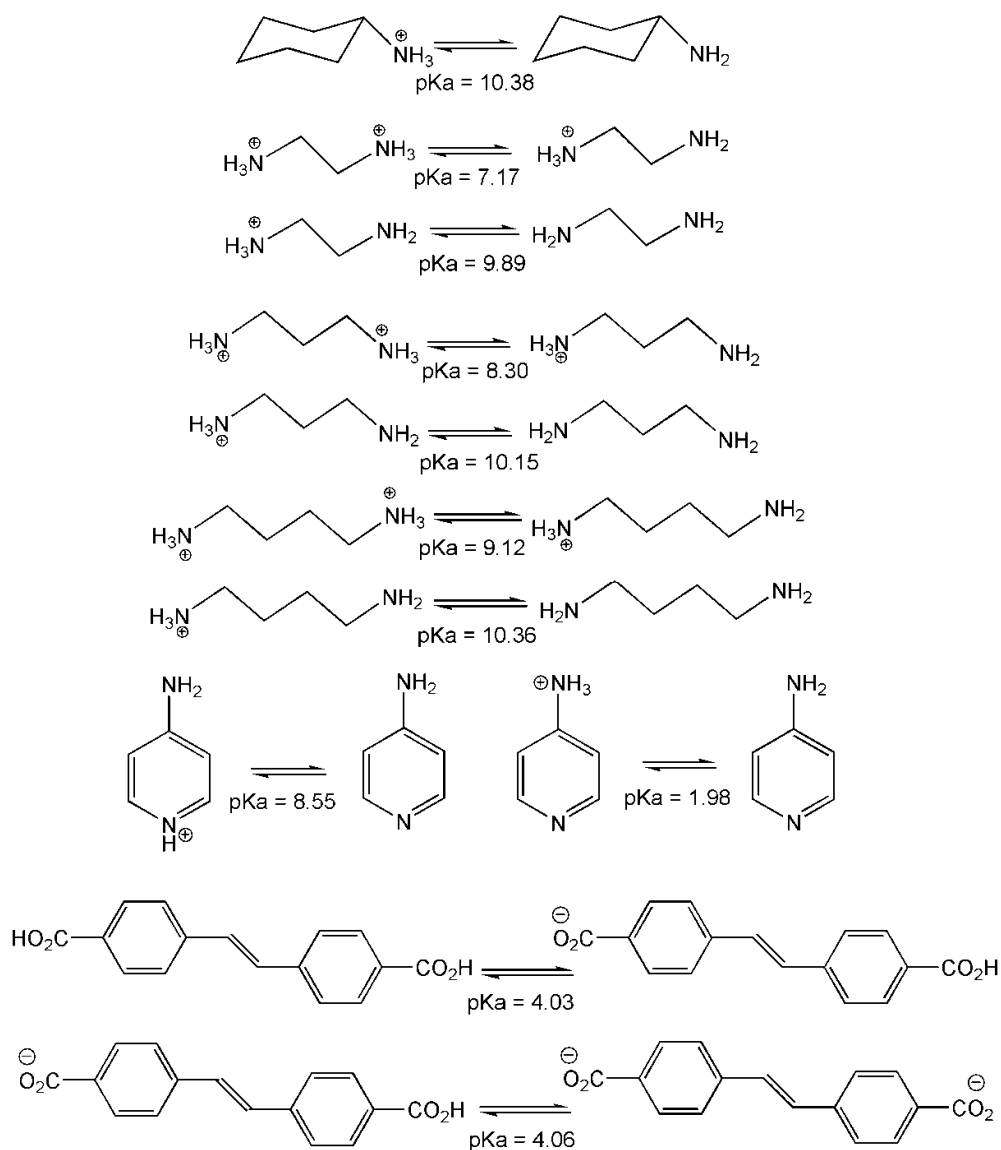


# Crystal engineering studies on the salts of trans-4,4'-stilbenedicarboxylic acid in the context of solid state [2+2] cycloaddition reaction

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## Supporting Information



Scheme S1: The pKa values of all the reactants, calculated using SPARC program (<http://ibmlc2.chem.uga.edu/sparc/>), are listed

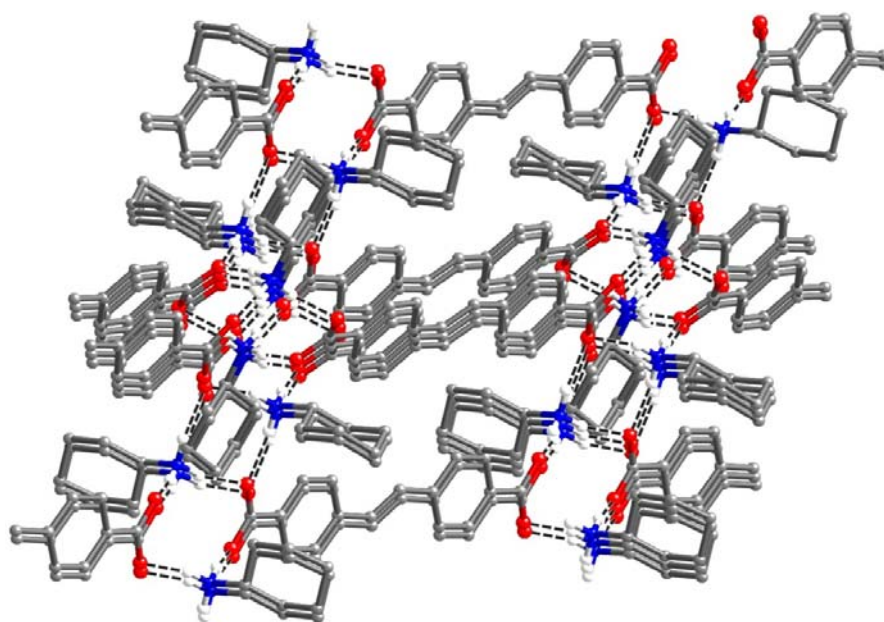


Fig S1. A perspective view of the packing structure of **1** approximately along *a* direction.

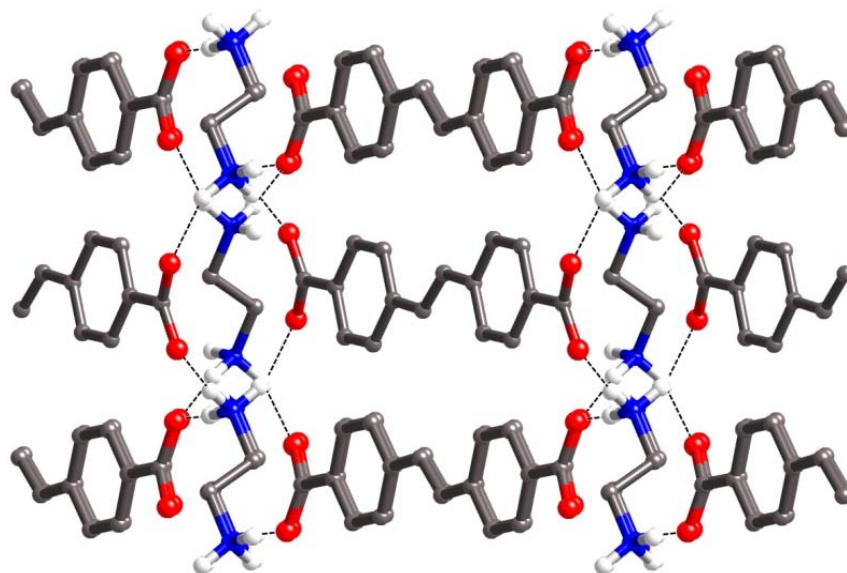


Fig S2. Packing structure of **2**, viewed approximately along *c* direction.

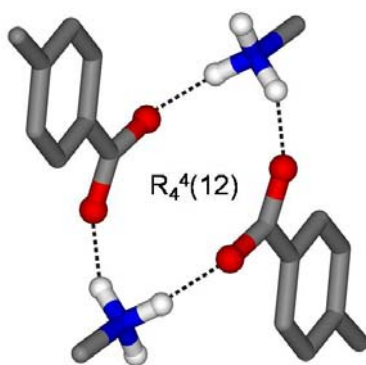


Fig S3. The graph set notation of hydrogen bonded ring present in **2**.

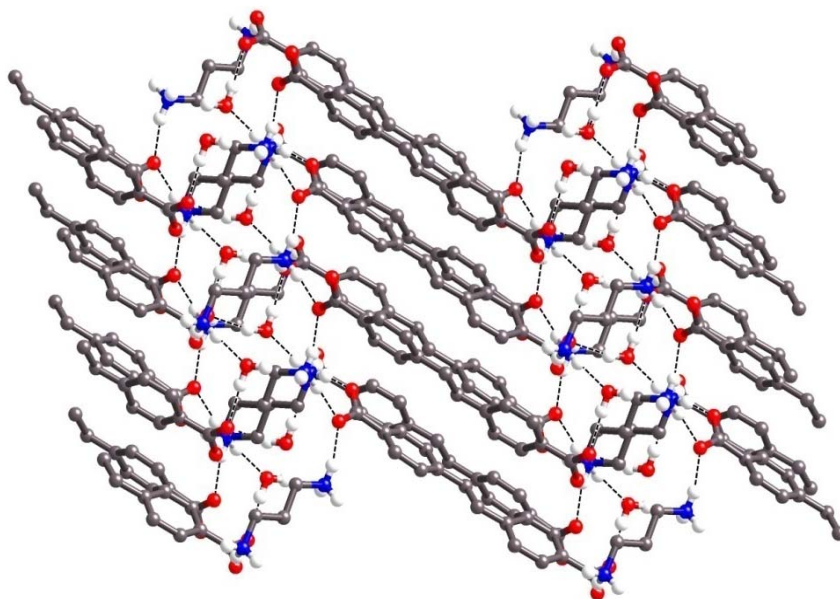


Fig S4. A view of packing along *b*-axis shows that the components are packed in zigzag manner in **3**.

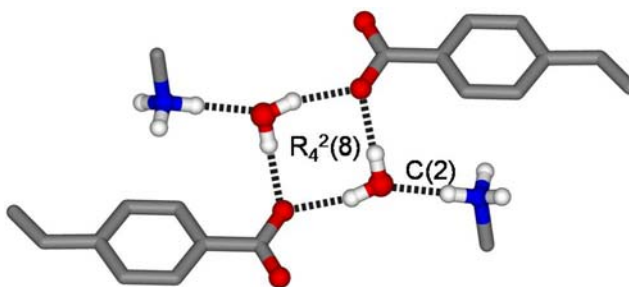


Fig S5. The graph set notation of the hydrogen bonded motifs in **3**.

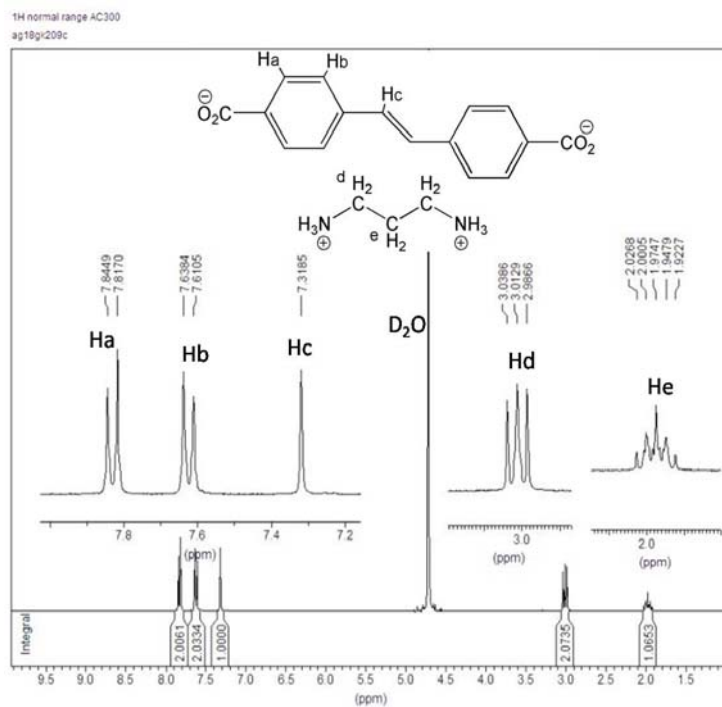


Fig S6. <sup>1</sup>H NMR spectrum (300 MHz, D<sub>2</sub>O) of **3** before UV irradiation.

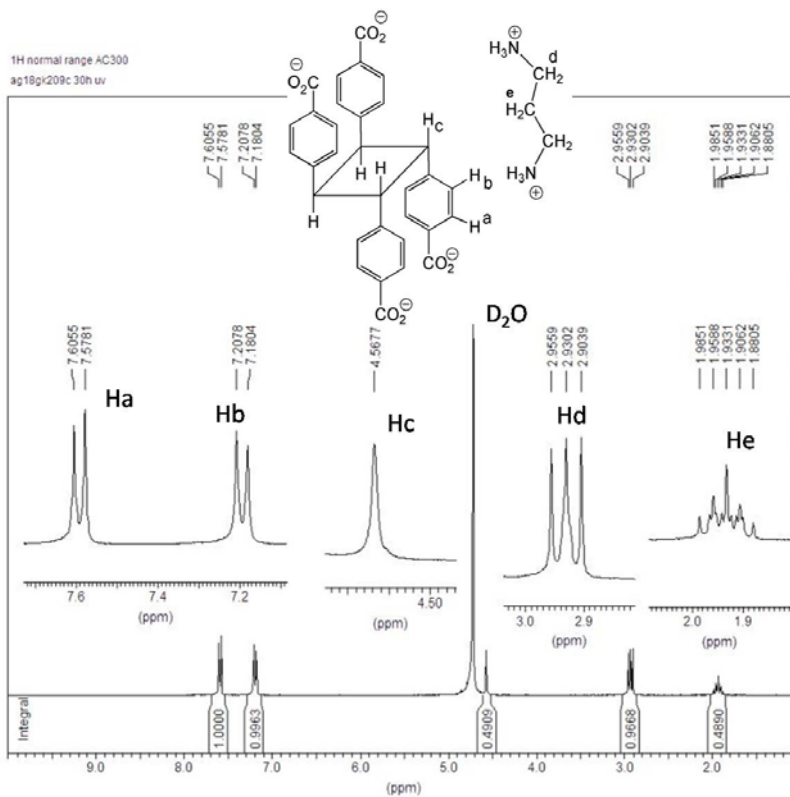


Fig S7. <sup>1</sup>H NMR spectrum (300 MHz, D<sub>2</sub>O) of **3** after 30 h of irradiation showing quantitative dimerization.

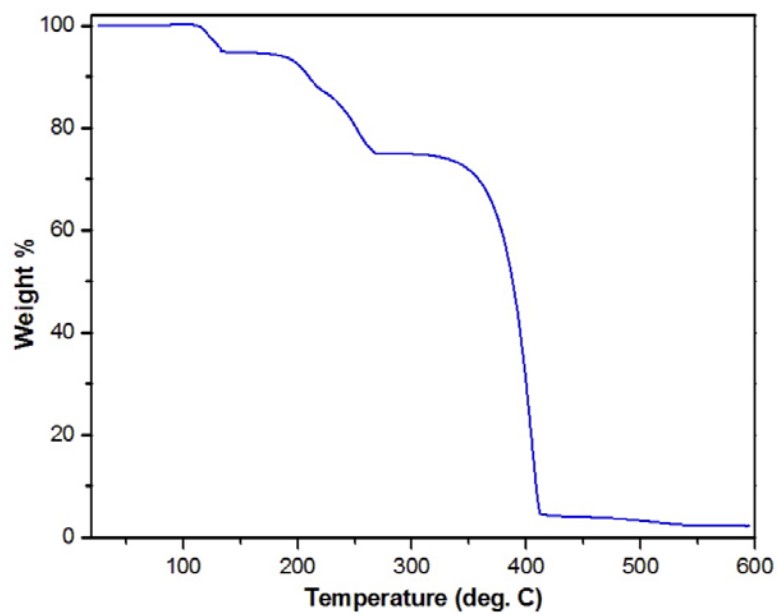


Fig S8. Thermogravimetric analysis for the salt **3**. 5.2% wt. loss above 100 °C shows strong hydrogen bonding interactions present in the lattice.

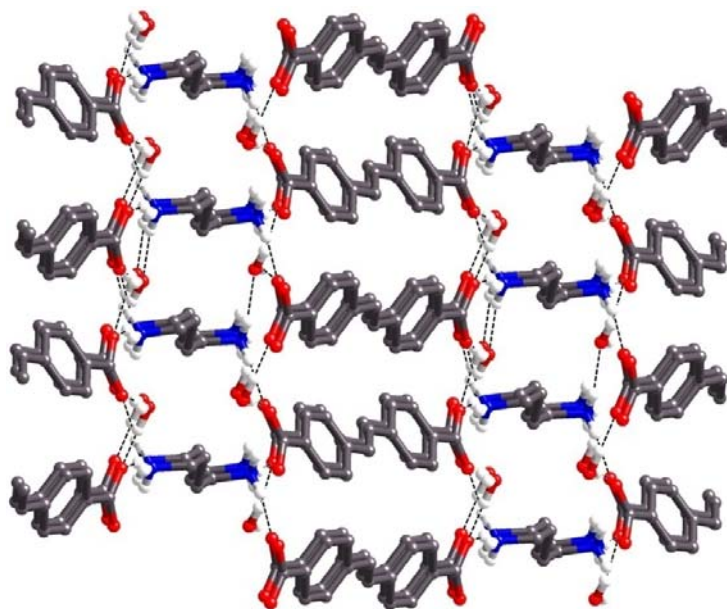


Fig S9. A perspective view of the packing structure of **4**.

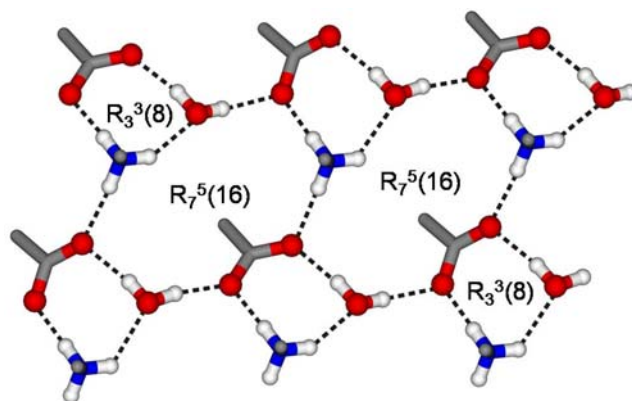


Fig S10. The graph set notation of the hydrogen bonded motifs present in **4**.

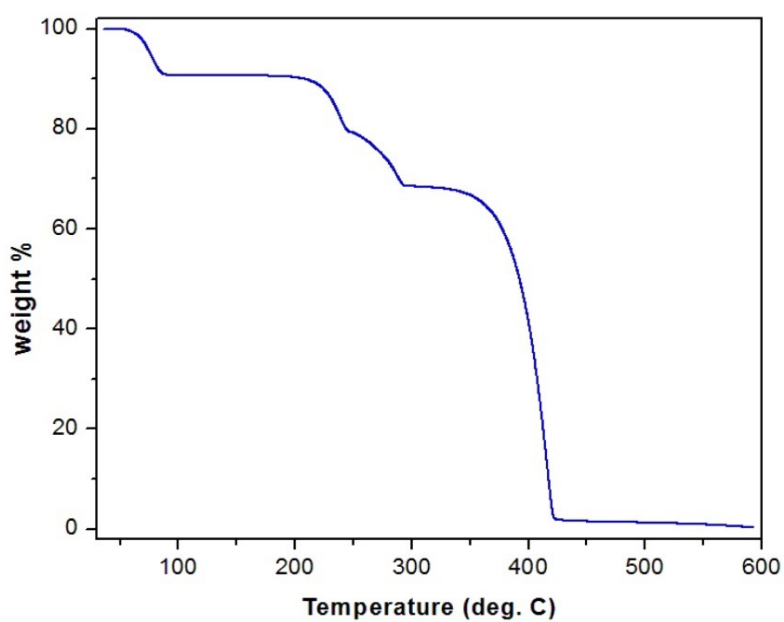


Fig S11. Thermogravimetric analysis for the salt **4**. Calculated 9.2% and observed water loss is 9.3%.

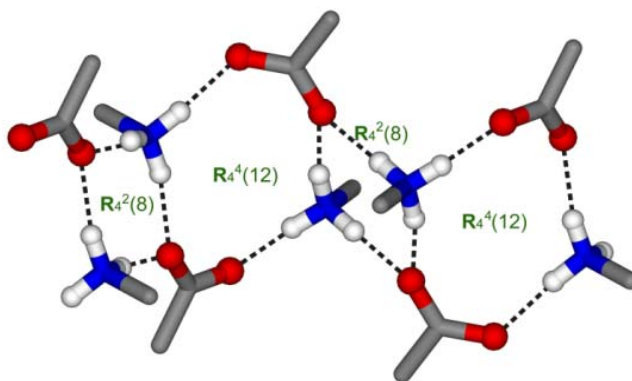


Fig S12. The graph set notation of the hydrogen bonded motifs present in **5**.



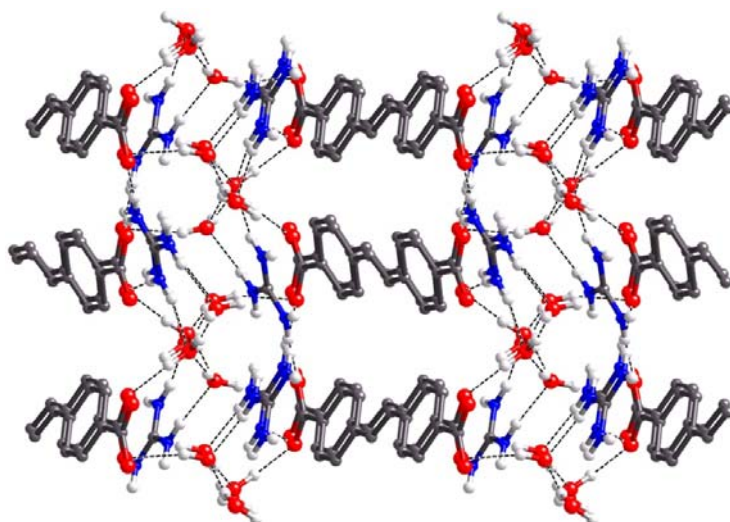


Fig S13. The packing structure of the salt **6** that shows various kinds of hydrogen bonding interactions played by the cations, anions and water molecules.

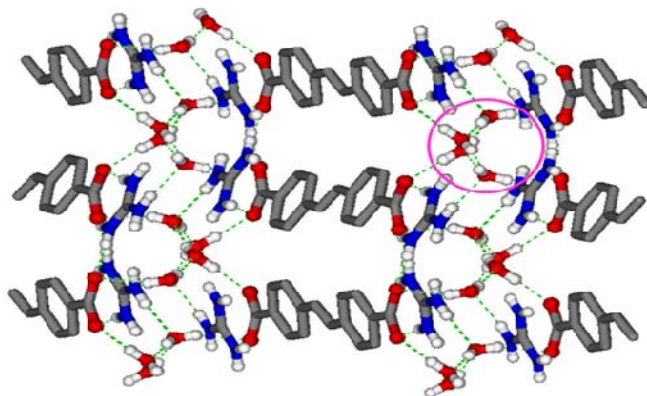


Fig S14. A perspective view of packing diagram along 'c' direction in **6**. Water cluster is shown in pink circle.

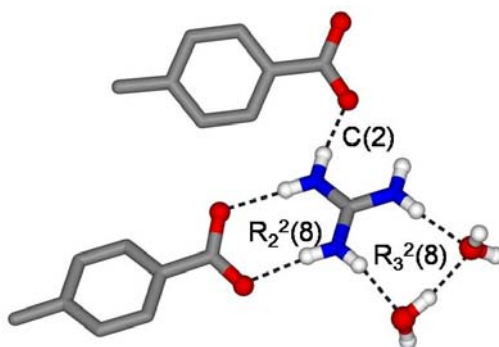


Fig S15. The graph set notation of the motifs in **6**.

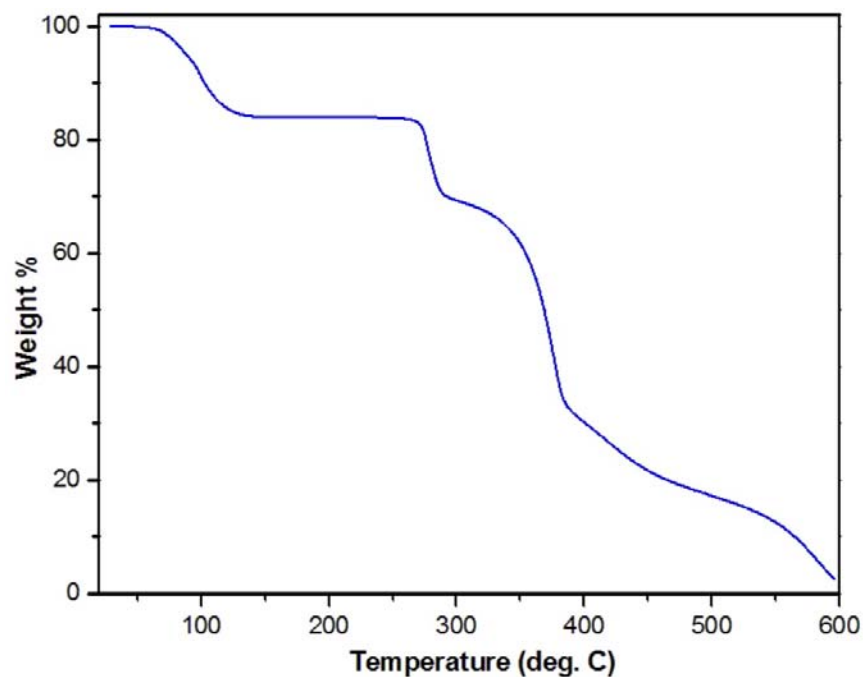


Fig S16. TGA of the salt **6**: both the observed and calculated water losses are 15.7%.

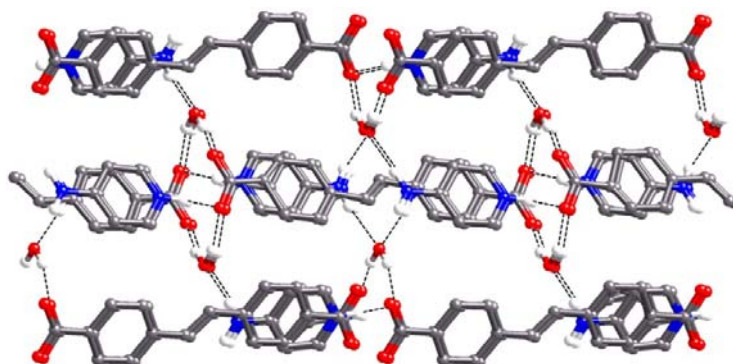


Fig S17. The packed crystal diagram of the salt **7** that shows various kinds of hydrogen bonding interactions played by the cations, anions and water molecules.

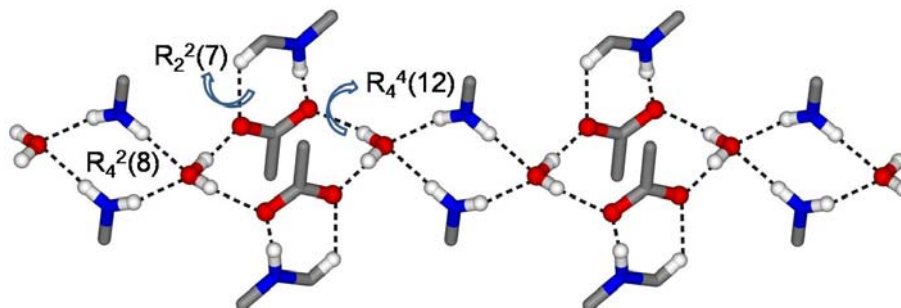


Fig S18. The graph set H-bonded motifs present in the crystal structure of **7**.



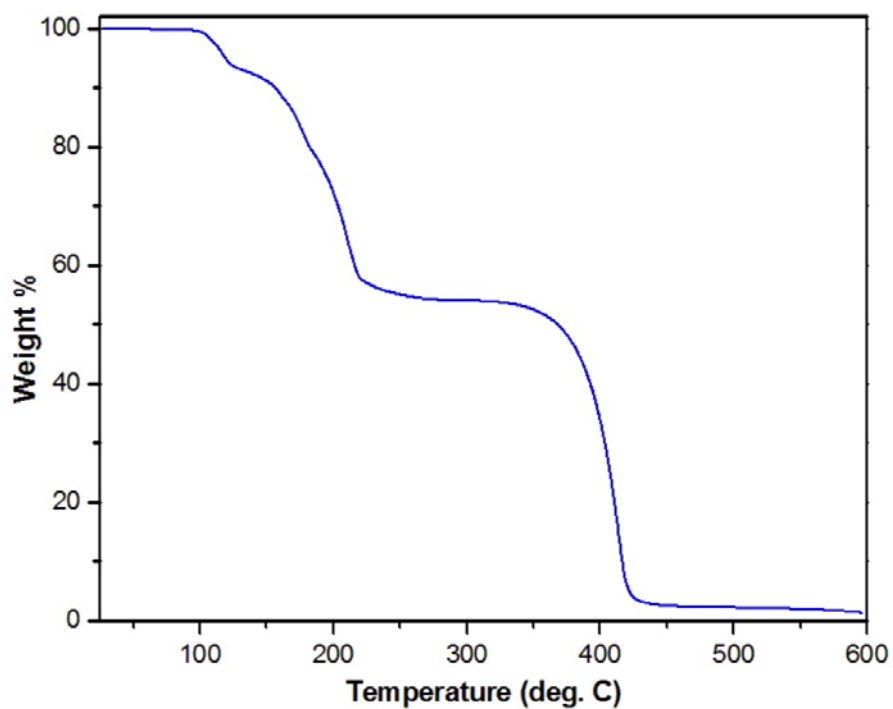


Fig S19. TGA for the salt **7**: the observed water loss is 7.15%, where the calculated water loss is 7.31%.

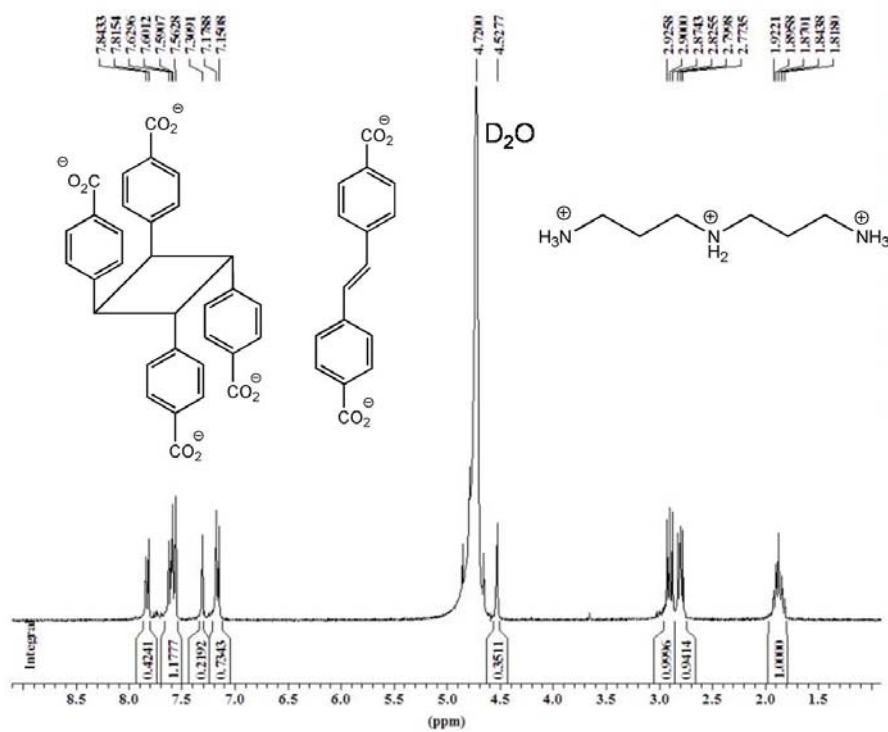


Fig S20. <sup>1</sup>H NMR spectrum of the salt **9** after UV irradiation for 40 h that shows 62% photodimerization.

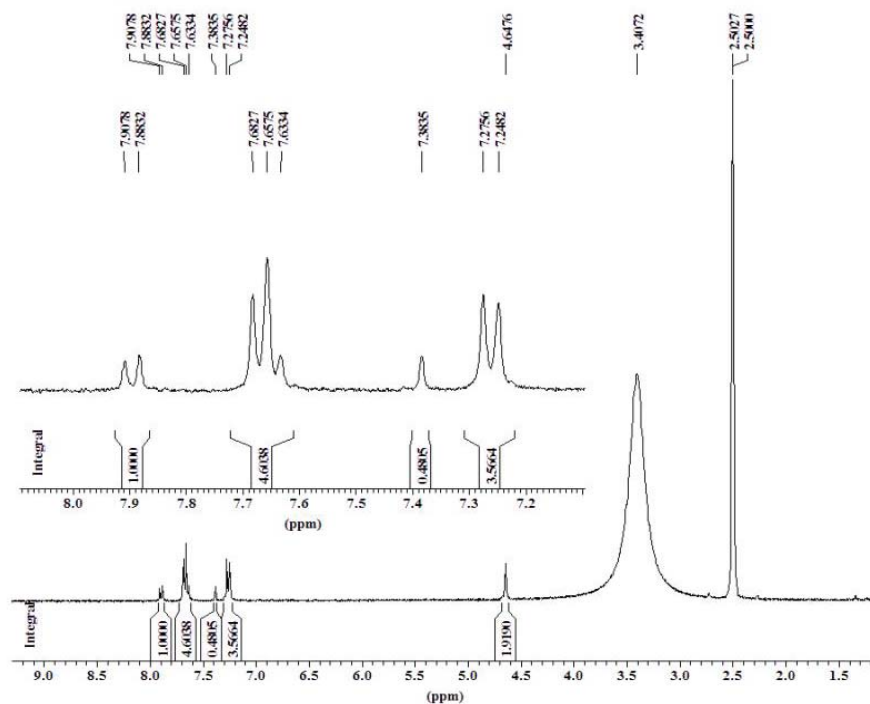


Fig S21. <sup>1</sup>H NMR spectrum of the diammonium salt of SDC, **10** after UV irradiation for 50 h that shows 80% photodimerization.

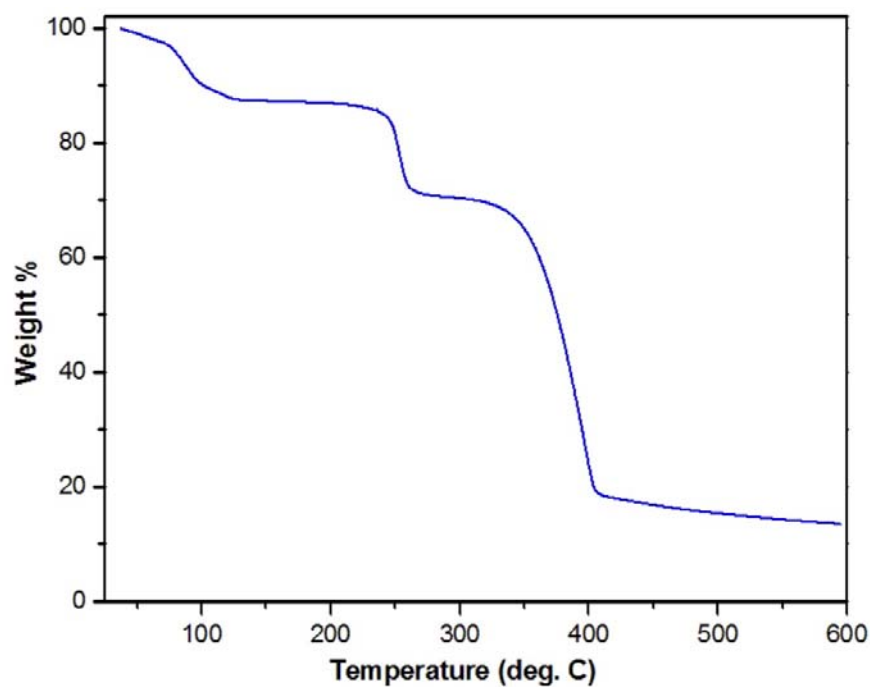


Fig S22. TGA of the salt **9**. Calculated weight loss for the composition  $C_{60}H_{70}N_6O_{12} \cdot 8H_2O$  is 11.88% and found water loss is 12.1%. Hence it supports the elemental analysis to determine the correct composition.

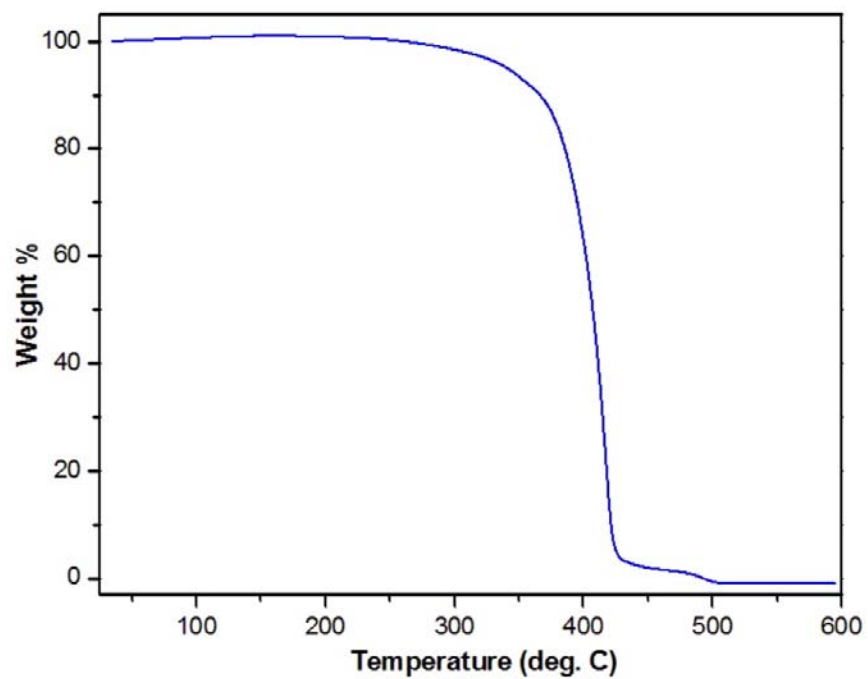


Fig S23. TGA for the salt **10**. It shows that the salt is anhydrous and supports for the correct composition.