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Supramolecular architectures and luminescent properties of salts containing flexible bis(pyridyl) cations with aliphatic diamine spacer: Effects of inorganic anions, alkalinity and conformation of the bis(pyridyl) cations

Tong-Peng Liu, Li-Hua Huo, Zhao-Peng Deng, Hui Zhao and Shan Gao

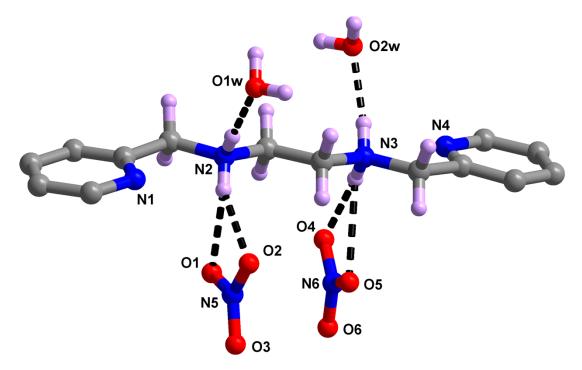


Fig. S1 Molecular structure of salt 5 with the hydrogen bonds denoted as black dashed lines.

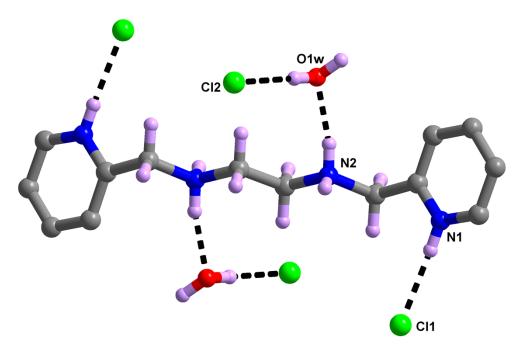


Fig. S2 Molecular structure of salt 11 with the hydrogen bonds denoted as black dashed lines.

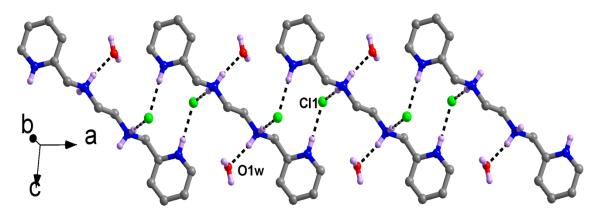


Fig. S3 Chain structure of salt 11 formed by the interconnection of Cl1 anions and H_4M3^{2+} cations.

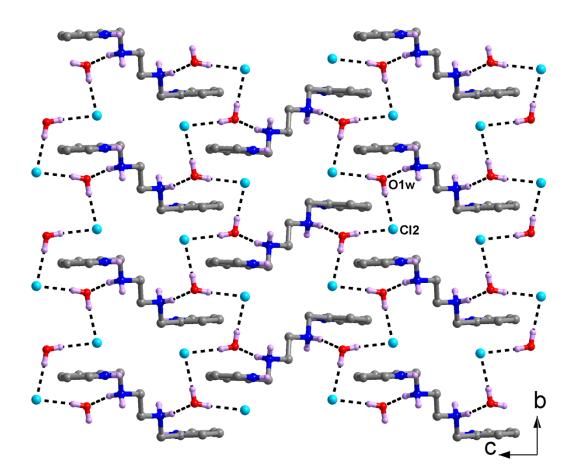


Fig. S4 Layer structure of salt 11 formed by the interconnection of Cl2 anions, O1w and H_4M3^{2+} cations.

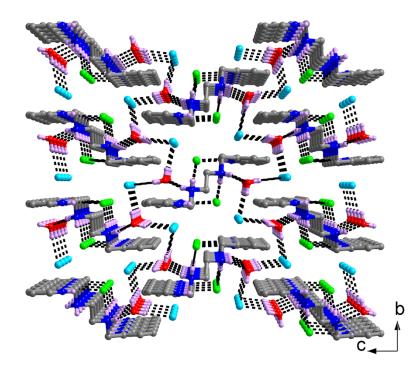


Fig. S5 Supramolecular network of salt 11.

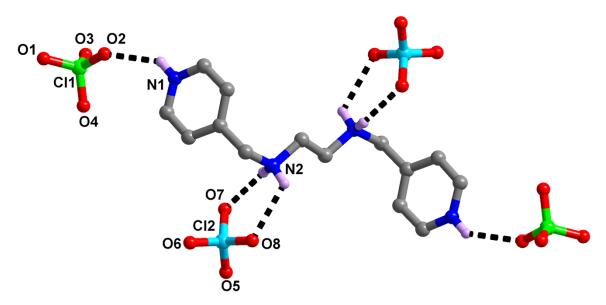


Fig. S6 Molecular structure of salt 15 with the hydrogen bonds denoted as black dashed lines.

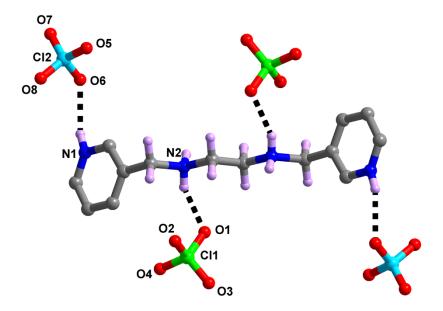


Fig. S7 Molecular structure of salt 16 with the hydrogen bonds denoted as black dashed lines.

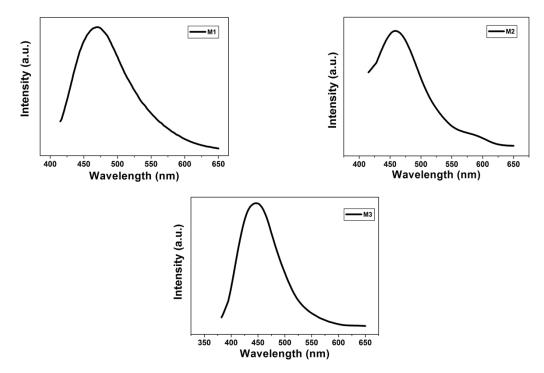


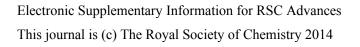
Fig. S8 Emission spectra of organic molecules M1-M3 in the solid-state at room temperature.

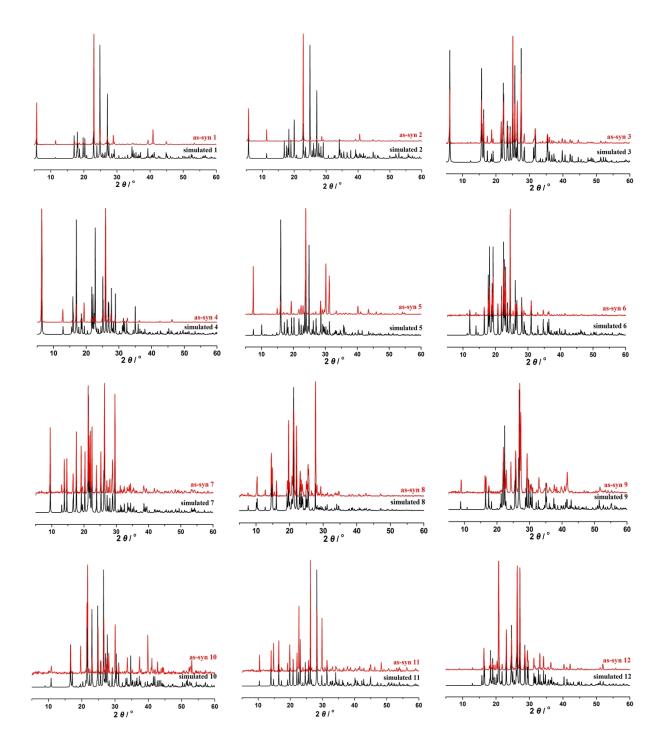
Powder X-ray diffraction (PXRD)

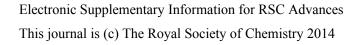
Powder X-ray diffraction (PXRD) patterns for solid samples of salts **1-17** are measured at room temperature as illustrated in Fig. S9. The patterns are highly similar to their simulated ones (based on the single-crystal X-ray diffraction data), indicating that the single-crystal structures are really representative of the bulk of the corresponding samples.

Thermogravimetric analysis (TGA)

The thermal stability of the seventeen salts were analyzed on crystalline samples by thermogravimetric analyses (TGA) from room temperature to 600 °C at a rate of 10 °C min⁻¹ under atmosphere. As shown in Fig. S10, the thermal stability of the chlorates is lower than the thermal stability of the perchlorates but higher than that of corresponding nitrates without considering the first weight loss of water molecules. The main weight loss of the seventeen salts is falling in beginning from 157 °C, 151 °C, 135 °C, 141 °C, 131 °C, 200 °C, 205 °C, 198 °C, 168 °C, 155 °C, 155 °C, 136 °C, 138 °C, 130 °C, 195 °C, 210 °C and 216 °C, respectively. Moreover, a minor weight loss corresponding to the water molecules is observed for salts **3**, **5**, **6** and **11** in the range of 57-85 °C (obsv. 8.84%; calc. 8.91%), 50-72 °C (obsv. 8.86%; calc. 8.91%), 70-89 °C (obsv. 7.45%; calc. 7.52%) and 54-85 °C (obsv. 8.56%; calc. 8.49%), respectively.







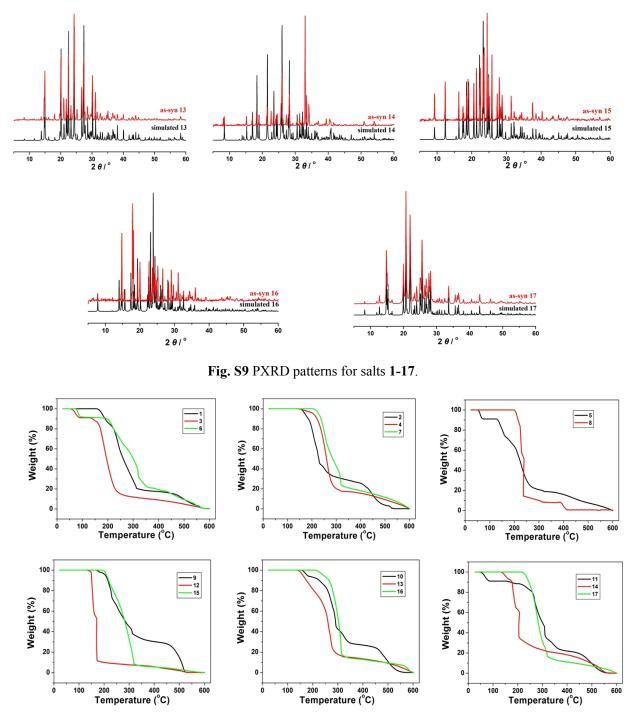


Fig. S10 TG curves of salts 1-17 under atmosphere.