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Salt-bridge (SB) interaction at work in building extended supramolecular networks: Experimental and theoretical study

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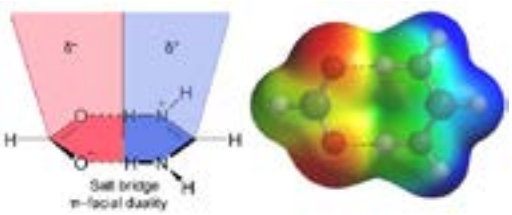
A series of pyridinium-carboxylate salts were designed prepared and structurally characterized to explore the importance of salt-bridge (SB) interactions in building self-assembled structures. We present a comprehensive analysis of the SB interaction in crystal structures of 4, 4'-Oxybis (benzoic acid) with substituted aminopyridines where the SBs displays extremely well defined geometric preferences. In the solid-state, compound exhibit lone-pair (l.p) ••• (SB)/(SB)•••π^+ assemblies while compound shows C−H•••(SB)/(SB)•••π network. Interestingly, compound exhibit two distinct networks π^+•••(SB)/(SB)•••(SB)/(SB)•••π^+ and C−H•••(SB)/(SB)•••H−C. These unexplored extended supramolecular networks are evident and explored for the first time in crystal structures. Our study also describes the duality of the salt bridge in establishing π-facial interactions with electron rich and/or electron poor moieties depending on the positive or negative nature of the SB counterpart that interacts with the SB surface. We describe the energetic and geometric features of salt-bridge interaction and explore its impact on the resultant supramolecular organization using high-level theoretical DFT-D3 calculations. The theoretical study combines the energetic features of the noncovalent forces that participate in the extended network and the characterization of the diverse interactions by means of Bader's theory of "atoms in molecules".



Recent Publications

1. Seth S K, Bauza A and Frontera A (2018) Screening polymorphism in a Ni(ii) metal–organic framework: experimental observations, Hirshfeld surface analyses and DFT studies. CrystEngComm 20(6):746-754.
2. Seth S K, Bauzá A and Frontera A (2018) Bipolar behaviour of salt-bridges: a combined theoretical and crystallographic study. New Journal of Chemistry 42:12134-12142.
3. Hossain A, Seth S K, Bauzá A, Mukhopadhyay S and Frontera A (2018) Coordination polymers based on phthalic acid and aminopyrazine ligands: on the importance of N–H•••π interactions. Polymers 10(2):182.
4. Seth S K (2018) The importance of CH•••X (X = O, π) Interaction of a New Mixed Ligand Cu(II) Coordination Polymer: Structure, Hirshfeld Surface and Theoretical Studies. Crystals 8:455.
5. Seth S K (2018) Structural characterization and Hirshfeld surface analysis of a CoII complex with imidazo[1,2-a] pyridine. Acta Cryst. E74:600-606.

Biography

Saikat Kumar Seth is an Assistant Professor of Physics at Jadavpur University, Kolkata, India. He was awarded PhD at Indian Association for the Cultivation of Science (IACS), Kolkata in 2012 and Postdoctoral at Universitat de Illes Balears, Palma, SPAIN. His area of research is X-ray Crystallography and Crystal Engineering. The focus of his research is to explore weak noncovalent interactions in the context of Crystal Engineering along with high-performance computational studies. He had published 72-research articles in various peer-reviewed journals, edited one book (National level) and contributed a book chapter in Royal Society of Chemistry (RSC). He got various awards like Young Scientist, Best Poster, Best Presentation, and Research Excellence, Outstanding Reviewer award from 4 Elsevier Journals and Publons Peer Review Award in global peer review. .

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