



A Neutral Zwitterionic Molecular Solid

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Résumé en anglais We report on the acid ethylenedithiotetrathiafulvaleneamidoglycine (EDT-TTF-CO-NH-CH₂-CO₂H; 1; EDT-TTF=ethylenedithiotetrathiafulvalene) and the 1:1 adduct [(EDT-TTF).+CO-NH-CH₂-(CO₂)−][(EDT-TTF)-CO-NH-CH₂-(CO₂H)]·CH₃OH (2), a new type of hydrogen-bonded, 1:1 acid/zwitterion hybrid embrace of redox peptidics into a two-dimensional architecture, an example of a system deliberately fashioned so that oxidation of π-conjugated cores toward the radical-cation form would interfere with the activity of the appended ionizable residues in the presence of a templating base during crystal growth. First-principles calculations demonstrate that, notwithstanding preconceived ideas, a metallic state is more stable than the hole-localized alternatives for a neat 1:1 neutral acid/zwitterion hybrid. The inhomogeneous Coulomb field associated with proton-shared, interstacks O-H⋯O hydrogen bonds between the ionizable residues distributed on both sides of the two-dimensional π-conjugated framework leads, however, to a weak hole localization responsible for the activated but high conductivity of 1 S cm^{−1}. This situation is reminiscent of the role of the environment on electron transfer in tetraheme cytochrome c, in which the protonation state of a heme propionate becomes paramount, or ion-gated transport phenomena in biology. These observations open rather intriguing opportunities for the construction of electronic systems at the interface of chemistry and biology.

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DOI 10.1002/chem.201001875 [18]

Liens

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