

## MS13 Structural Characterization of Functional Materials

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TTF-based hydrogen-bonded organic frameworks: porous conducting crystalline materials

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### Abstract

Hydrogen-bonded organic frameworks, or HOFs, are porous molecular-based crystalline materials that are self-assembled through hydrogen bonding interactions.<sup>1</sup> Similar to other porous materials such as MOFs and COFs, HOFs have been used in multiple applications, including gas storage, separation, encapsulation, or proton conductivity, among others.<sup>2</sup> A major advantage of HOFs is the lack of formation of strong coordination bonds (as in MOFs) or covalent bonds (as in COFs), thus being easily synthesised in mild conditions, which facilitates their processing, one of the major drawbacks of MOFs and COFs.

Herein we will present the preparation of porous conducting HOFs through the use of tetrathiafulvalene-tetrabenzoic acid, H4TTFB, a molecule that has been previously used in the construction of conductive MOFs and COFs.<sup>3</sup> By tuning the synthetic conditions, three different polymorphs have been obtained, all of them presenting open structures and suitable TTF stacking for efficient orbital overlap.<sup>3</sup> Interestingly, two of these polymorphs present a zwitterionic character with a positively charged TTF core and a negatively charged carboxylate group, resulting in an efficient charge transport with no need of post-synthetic treatment (e.g., electrochemical oxidation or doping). In fact, experimental conductivities of 10–6 S·cm<sup>-1</sup> are observed. On the contrary, a non-zwitterionic HOF based on the same ligand behaves as an insulator despite the suitable stacking of the TTF units.

### References

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