

*Multicomponent dithiadiazolyl crystals as a route to novel magnetic materials*

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In addition to the continued interest in dithiadiazolyl radicals (DTDAs) as components in molecular magnets, interest has been shown in the structure-property relationships of these compounds [1]. DTDAs dimerise readily in the solid state, resulting in spin pairing, and rendering them diamagnetic. It has been shown that variation in the R-group has no significant influence on the electronics of the DTDA ring [2]. It has also been shown that co-crystals of DTDAs can be made, which contain two different radicals (co-formers) in a heterodimer [3]. An experimental study is underway, whereby chosen DTDAs have been co-crystallised with one another in order to generate novel co-crystals, and in this regard a novel DTDA co-crystal will be discussed. A computational study was also done on these compounds, with Density Functional Theory calculations performed on the molecules making up the two previously known DTDA co-crystals and their co-former homodimers, as well as the novel third co-crystal, at the UB3LYP-GD3/6-311G++(d,p) level of theory to determine the energies of the heterodimers as well as homodimers. This was done to probe the stability of the co-crystal in comparison to its co-formers. Spin-unrestricted periodic calculations were also done on the known co-crystals and co-formers to further investigate thermodynamic properties such as lattice energies, in order to gain an understanding of the driving force behind co-crystal stability. The results of the experimental study will be compared to computational results.

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[3] Allen, C., Haynes, D. A., Pask, C. M. and Rawson, J. M. (2009). *CrystEngComm.*, 11(10), 2-5.



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