

Microwave methods for the synthesis of paddlewheel diruthenium compounds with N,N-donor ligands

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Supplementary material: Single crystal X-ray characterisation of compounds 1-4

[Ru₂(DPhT)₄] (1), CCDC 814431 and [Ru₂(DPhT)₄]·THF (1·THF), CCDC 814432

Two crystals were solved in the case of compound 1: one of them was isolated from a reaction with EtOH as a solvent, and the other one from a reaction with THF. The two structures display identical space group and very similar cell parameters, as a consequence of the molecular packing of the paddlewheel unit. The difference between the two structures lies in the solvent present in the voids of the crystal. In the case of the data set obtained from the crystal isolated from the reaction carried out with the optimised conditions (CCDC 814432), the residual electron density found in the voids could not be assigned to a particular molecule. The PLATON routine SQUEEZE was applied to the data set, giving a number of electrons located in the void that could correspond to a triethylamine molecule (used as a reagent). In the case of the crystal obtained from the reaction with THF (CCDC 814431), a disordered molecule of this solvent could be placed at the voids.

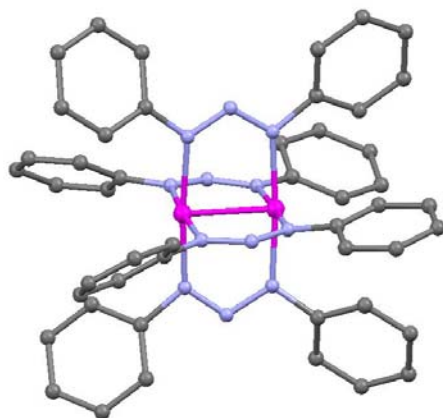


Figure S1. Molecular plot of [Ru₂(DPhT)₄] (1). Hydrogen atoms have been omitted for clarity.

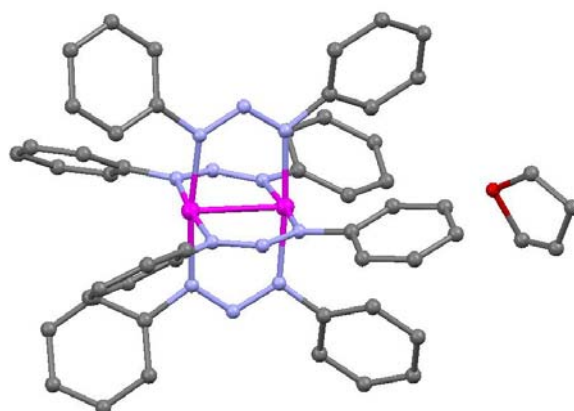


Figure S2. Molecular plot of [Ru₂(DPhT)₄]·THF (1·THF). Hydrogen atoms have been omitted for clarity.

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[Ru₂(DFPhT)₄] (2), CCDC 766373

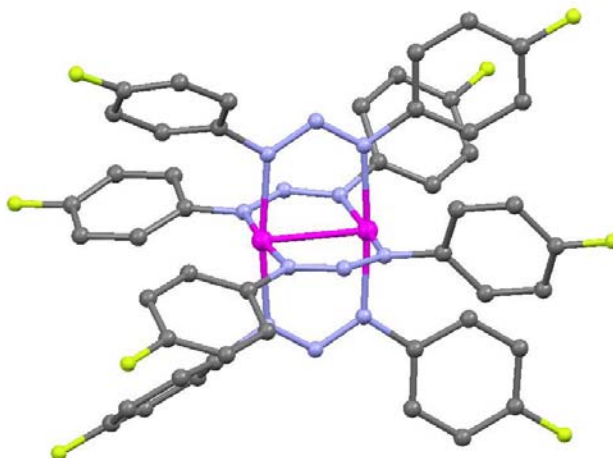


Figure S3. Molecular plot of [Ru₂(DFPhT)₄] (2). Hydrogen atoms have been omitted for clarity.

[Ru₂Cl(DPhF)₄] (3), CCDC 814433

A similar structure is found in the literature[†] as a pentane solvate of this diruthenium molecular species that crystallises in the same space group and displays slightly shorter cell parameters. The structure solved by us displays an identical molecular packing and has also disordered solvent in the voids located among the paddlewheel species, but in our case the electron density has been attributed to disordered water molecules.

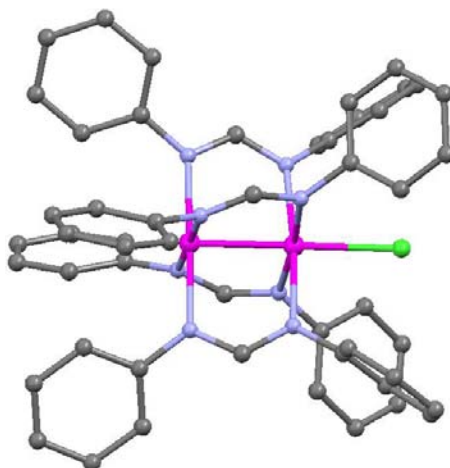


Figure S4. Molecular plot of [Ru₂Cl(DPhF)₄] (3). Hydrogen atoms have been omitted for clarity.

[†] J. L. Bear, B. Han, S. Huang, K. M. Kadish, *Inorg. Chem.*, 1996, **35**, 3012.

[Ru₂Cl(DAniF)₄] (4), CCDC 814434

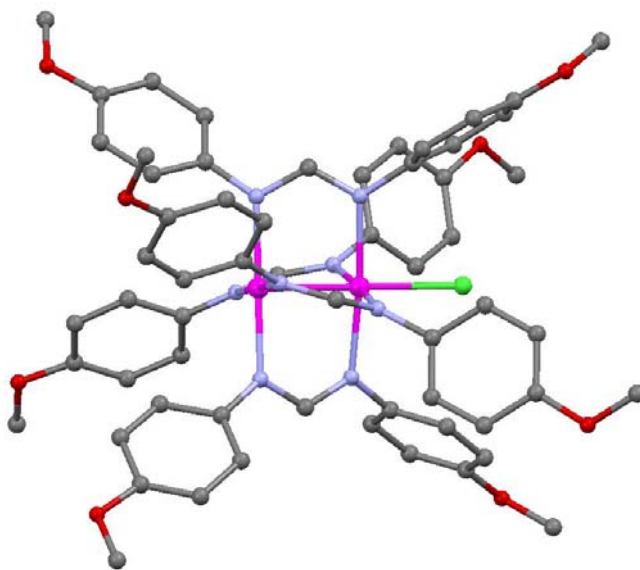


Figure S5. Molecular plot of [Ru₂Cl(DAniF)₄] (4). Hydrogen atoms have been omitted for clarity.