

**Dr Julie Fisher**

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**EPSRC Studentship – NMR Studies of Host-Guest Complexes.**

Dr Julie Fisher.

The EPSRC have funded a project grant to explore novel metallo-cages with particular reference to their potential use as nano-vessels. To this end a post-doctoral worker has been appointed (Nov. 2011), under the supervision of Dr. Hardie, to conduct the synthetic aspects of the project and the x-ray crystallographic characterisations. The grant also funds a PhD, under the supervision of Dr. Julie Fisher, to enable NMR investigations of the cages themselves in solution, but more importantly of the host-guest properties of these. A variety of NMR techniques will be utilised including standard 1D and 2D data analysis, nuclear Overhauser (nOe) measurements, and acquisition of diffusion ordered (DOSY) data for the direct determination of molecular weight, molecular shape and, where appropriate, binding constant determination.

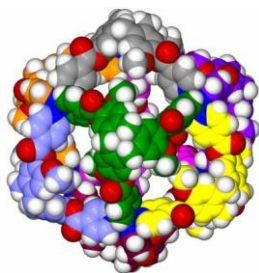


Fig. 1 Stella octangula cage

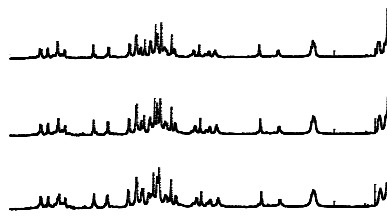


Fig. 2 VT NMR spectra

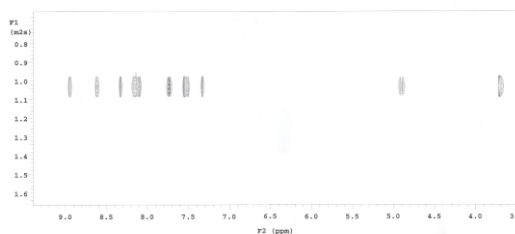


Fig. 3 DOSY spectrum

In many cases these discrete assemblies are hollow, however this 'void' will be occupied by smaller 'guest' molecules such as solvent or counter-ions. There is growing interest in utilising these spaces to investigation interactions or reactions between guest molecules which for a number of reasons may not be favourable in the bulk solvent. The cage may be functionalised to change the size of the cavity, to introduce stereochemical features in the interior, to introduce hydrogen bonding potential, and so on. All of these possibilities will be explored in this project.

The student will interact with the post-doctoral worker to discuss results and contribute to some of the molecular design decisions. The student, together with the post-doctoral worker will have the opportunity to perform some molecular modelling studies on more interesting systems, through our collaboration with Dr. Sarah Harris (Physics).

The studentship may start from January 2012 and the stipend would be at the standard research council rate (~ £13,895 pa for 2011/12). Applications for this studentship, which will be accepted until the studentship is filled, should be directed to Anna Luty, School of Chemistry, University of Leeds, Leeds LS2 9JT and can be made online via the following link: <http://www.chem.leeds.ac.uk/postgraduate-research/how-to-apply.html>

Please contact Dr Julie Fisher ([j.fisher@chem.leeds.ac.uk](mailto:j.fisher@chem.leeds.ac.uk)) for further details about this project.

**References**

1. 'Stellated polyhedral assembly of a topologically complicated Pd<sub>4</sub>L<sub>4</sub> "Solomon cube"'  
T.K. Ronson, J.Fisher, L.P. Harding, P.J. Rizkallah, J.E. Warren, M.J.Hardie. *Nature Chemistry*, **1**, 212-216 (2009)
2. 'Star-burst prisms with cyclotrimeratrylene-type ligands: a [Pd<sub>6</sub>L<sub>8</sub>]<sup>12+</sup> stella octangular.'  
T.K. Ronson, J. Fisher, L.P. Harding and M.J. Hardie. *Angew. Chem.Int. Ed* **46**, 9086-9088 (2007)