

# Alexandra M Z Slawin

## Professor of Chemical Crystallography

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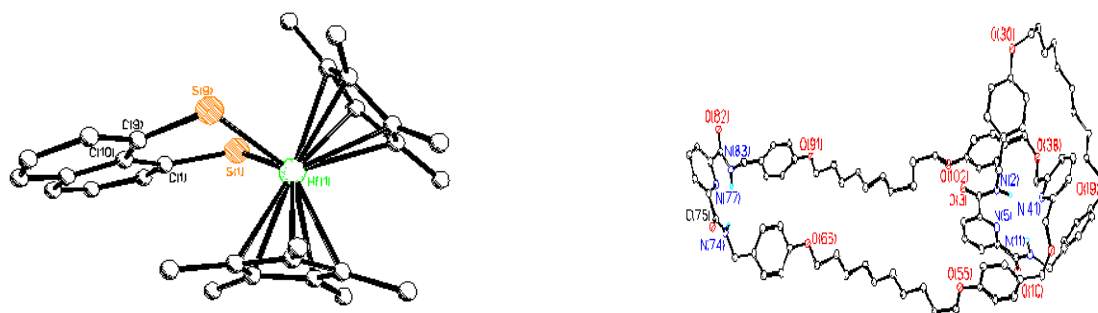
Research Interests: Chemical Crystallography, Structure solution and structure activity relationships. Automation of crystallography.



<http://chemistry.st-and.ac.uk/staffmember.php?id=amzs>

We are interested in single crystal X-ray studies on a wide range of inorganic and organic molecules. New structures are related to biological and/or macroscopic properties (e.g. conductivity) using a variety of graphics-based (molecular modelling) techniques. Particular topics include: new enforced distortions in disubstituted naphthalens and rotaxanes.

We have an enviable range of high quality equipment <http://chemistry.st-and.ac.uk/staff/amzs/group/>, with three high brilliance rotating anode based systems, a benchtop diffractometer and a robotically controlled system. All of our equipment is fitted with Low temperature facilities.



*Figures*. Left: A typical small organometallic structure. The X-ray structure of  $\text{Cp}^*\text{Hf}(\text{S}_2\text{C}_{10}\text{H}_6)$ , red prism; 0.1, 0.1, 0.1 mm; orthorhombic,  $a = 18.074(2)$ ,  $b = 8.4295(11)$ ,  $c = 16.721(2)$  Å,  $V = 2547.5(6)$  Å<sup>3</sup>,  $Z = 4$ ,  $\text{Pna}2_1$ , 14755 reflections, 4039 independent ( $R_{\text{int}} = 0.0252$ ), 3773 observed reflections to give conventional  $R = 0.0195$ . Dataset collected in 45 minutes at 93 K using MM-007/VariMax-Mo/Mercury CCD and X-stream LT apparatus. Right: A medium-sized organic structure. This structure solved completely at the first attempt. Colorless prism; 0.1, 0.1, 0.1 mm; monoclinic,  $V = 8401$  Å<sup>3</sup>. Dataset collected in ca 10 hours at 173 K using Cu MM-007/Blue/Saturn 92 and X-stream LT apparatus. Sample courtesy of D. Leigh and B. Walker (University of Edinburgh)

### SELECTED RECENT PUBLICATIONS

[http://chemistry.st-and.ac.uk/staff/amzs/group/full\\_pubs.html](http://chemistry.st-and.ac.uk/staff/amzs/group/full_pubs.html)

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