K11 **Novel Structures in "Simple" Metals.** Malcolm I McMahon, *School of Physics and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh EH9 3JZ, U.K. E-mail: mim@ph.ed.ac.uk*

Keywords: Incommensurate; High pressure; Metals

At ambient pressure, the metallic elements typically adopt simple high-symmetry crystal structures. However, at high pressures, the relative movement of different atomic energy levels can result in the formation of structures characterised by a degree of directional bonding. The structures of these high-pressure phases can be extremely complex, and it is only with recent advances in high-pressure single-crystal and powder-diffraction techniques that the structures of many of them have been determined. In the group 1, 2, and 15 elements, we have found a number of incommensurate composite structures comprising interpenetrating host and guest structures [1]; transitions between these composite structures [2]; modulations of the host and guest structures; and a transition to a composite structure with a "liquid" guest component [3]. In the group 16 elements, we have found an incommensurate modulated structure [4] that is stable over a wide range of pressure and temperature. In this talk I will review the recent results on these "simple" metals.

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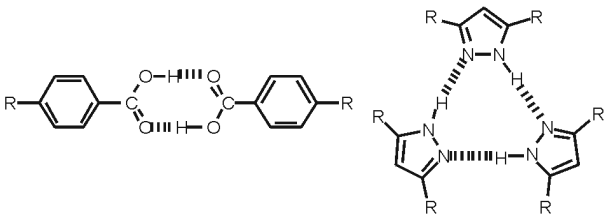
K12 **An analysis of the 'Resonance Assisted Hydrogen Bond' (RAHB) Concept and its Application to Pyrazole Clusters.** José Elguero, *Instituto de Química Médica, CSIC, Juan de la Cierva 3, E-28006 Madrid, Spain.*
E-mail: iqmbe17@iqm.csic.es

Keywords: RAHB; Pyrazole; Dynamic Solid-State NMR

The lecture will be divided in three parts. In the first one the curious fact that pyrazoles are one of the two classes of compounds (the other being benzoic acids) that frequently show proton transfer in the solid state (SSPT) will be summarized [1-6]. Special emphasis will be put on the necessary conditions for this phenomenon to be observed which will be discussed in relation with the number of protons transferred in the process.



In the second part, the various reasons why pyrazoles crystallize in six different patterns (catemers, dimers, trimers, tetramers, and hexamers) will be examined in order to find some regularities [7-9]. The connectivity between the centroids of the five-membered rings is a useful way to represent the catemers. Since the RAHB concept (developed for β-diketones [10]) was applied unsuccessfully to pyrazoles [11], in the last part of the lecture this concept will be analyzed theoretically for the paradigmatic case of acetylacetone using NMR (mainly coupling constants but also chemical shifts) as a tool [12].

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