**Poster Sessions**

**MS19.P13**  
*Acta Cryst. (2011) A67, C331*

**High pressure compounds in xenon-hydrogen mixtures**  
Monica Amboage, Annette K. Kleppe, Andrew P. Jephcoat  
Diamond Light Source, Ltd., Harwell Science and Innovation Campus, Didcot, OX11 0DE, (UK). E-mail: monica.amboage@diamond.ac.uk

The study of binary mixtures of atomic (He, Ar, Xe, etc.) and diatomic (N₂, O₂, H₂, etc.) molecular solids is relevant for a better understanding of the interior of the giant planets. It has lead to the discovery of a new type of compound – the van der Waals (vdW) compound – and provides essential information on the interactions among simple molecules. It was long believed that group 18 elements were inert and unreactive and could not form compounds. A new chemistry field started in 1962, when the first noble gas compound, xenon hexafluoroplatinate, was synthesised [1]. Since then, many compounds have been created combining noble gases with other chemical elements [2].

Here we present a study of vDW compound formation in the xenon-hydrogen system under high pressure. We have studied several compositions (between 7% and 15% vol Xe) to map the binary phase diagram. Complex phase behaviour as a function of composition and pressure was observed with the formation of different stoichiometric phases. These novel Xe-H₂ compounds have been characterized by single-crystal and powder x-ray diffraction at beamline I15 of Diamond Light Source. We find three separate phases with orthorhombic, hexagonal and rhombohedral structures as function of pressure and composition. These novel structures will be presented in relation to other rare gas-hydrogen compounds, in particular Ar(H₂) [3], Kr(H₂) [4], and the previously reported Xe(H₂) [5].

A rare gas hydrogen system not only offers the possibility of the discovery of unusual stoichiometric compounds, but also allows the study of the hydrogen molecule in a modified environment compared to pure H₂ solid. The study of the detailed intra-molecular response of H₂ to compression can give insight into new pathways to hydrogen metallization. This has been suggested for the Ar(H₂) compound [3]. In the Ar-H system the H₂ vibron is seen to increase continuously under pressure. In contrast our Raman spectroscopic measurements on rhombohedral Xe(H₂) show shifted vibron frequencies relative to the pure (bulk) H₂ stretching mode which soften with pressure and appear to cross the pressure-frequency trajectory of the pure H₂ vibron around 50 GPa.


**Keywords:** high pressure, molecular solids, diffraction

**MS19.P15**  

**High pressure structure and magnetism of one 1-D molecular magnetic material**  
Jey-Jau Lee,² Szu-Miao Chen,³ Yu Wang³  
²National synchrotron radiation research center, Hsinchu, Taiwan, R.O.C. ³Department of Chemistry, National Taiwan University, Taipei, Taiwan, R.O.C. E-mail: jjlee@nsrcc.org.tw

Molecular magnetic materials(MMM) have been attracted much attention for increasing demands on smaller size magnetic memory devices and interest in the interpretation of the mechanism for complicated magnetic interactions. Many studies focus on investigating the magnetic coupling mechanism and the magneto -structural correlation. Many methods can be used to control magnetic property.