Keywords: high pressure, molecular solids, diffraction

MS19.P13


High pressure compounds in xenon-hydrogen mixtures
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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 hexafluoropluminate, 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 11.5 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: rare-earth hydride, neutron diffraction, rietveld

MS19.P15


High pressure structure and magnetism of one I-D magnetic material
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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.

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The external perturbations can be temperature, light irradiation, pressure, and pulsed magnetic fields all may change the magnetic coupling interaction in transition metal systems. Here, we use pressure as external force to study magneto-structural correlation.

We report here the structure and magnetic behavior of one 1-D helical chain iron complex \( \text{FeII}(\mu_{-}\text{bpt})\text{FeII}(\mu_{-}\text{COOC,H}_{2}N)\text{FeII}(\mu_{-}\text{COOC,H}_{2}N) \), in ambient conditions and under hydrostatic pressure. The complex was crystalized in a tetragonal space group \( I_{4} / a \) at ambient pressure, each iron atoms linked by one bpt and one isonicotinic acid legend, which form an infinite helical chain along the screw axis \( 4 \alpha \), at c-axis direction. The iron atoms are iron (2+) high spin state with distorted N4O2 coordinated shell.

High-pressure powder X-ray diffraction experiments from 0.03GPa to 2.79GPa pressure were carried out to understand precisely the correlation between the structure and magnetic behavior. The careful analysis of a series high pressure structures showing a pressure-induced shrinking more than 10% along the chain direction, which can describe as spring compressed 10%. This make the iron-iron distance from 4.445(2) Å at ambient pressure change significantly to 4.083(6) Å at around 2GPa. Magneto-structural correlation will be discussed. The coordinated shells of Iron (N4O2) also decrease 0.11 Å about averagely. The spin state of iron and magnetic property of title compound also will be shown in this report.

MS20.P02


**Euclidean groups in spaces of arbitrary dimensions**

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Different categories of Euclidean groups are established according to an analysis of the Fundamental theorem on Euclidean groups which is formulated and proved. The first division is into the space, subperiodic and site point groups. According to the character of the translation subgroup, the groups with the discrete, continuous and semicontinuous lattice are distinguished. The groups are classified as the crystallographic, noncrystallographic and partially crystallographic groups. In this connection, the concepts of crystallographic and space groups are amended.

Geometric classes and their splitting into arithmetic classes are defined as usual. Arithmetic classes are the natural classification units and the groups of such a class are distinguished by systems of nonprimitive translations in Seitz symbols for Euclidean operators. If the geometric class is reducible (irreducible) then the arithmetic class is either reducible or decomposable (irreducible). The factorization of the groups of decomposable or reducible classes by partial translation subgroup leads to groups of lower dimensions of the translation subgroup.

The class of the systems of nonprimitive translations which differ only by shift functions define an extension class within which the groups differ only by their location. Groups of the extension class have an extended Hermann-Mauguin symbol in the same space group, differentNew Zealand, United States of America.