Structures and dynamics of dense clathrate hydrates

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The ability to study the structures and dynamics of dense clathrate hydrates both at high pressures [1] and on samples recovered from high pressure [2] has enabled researchers to both more accurately characterize these materials. Studies provide insight in water potentials and the repulsive interactions between water and simple molecules or atomic species at high pressures where repulsive interactions dominate. Theses materilas are important in areas ranging from planetary science to energy or gas storage sources. In this study we will describe recent experimental and theoretical studies on dense clathrates and the closely related filled ice structures [3].

The methods employed include x-ray diffraction at both ambient and high pressure using synchrotron radiation sources, nuclear resonant inelastic x-ray scattering (NRIXS), and molecular dynamics simulations. The x-ray scattering studies at high pressure and on dense clathrates recovered from high pressure were carried out at the Advanced Photon Source, Argonne National Laboratory on samples prepared at the Nationnal Research Council of Canada.

Molecular dynamics simulations were performed using the SPC/E potential for water molecules and Lennard-Jones potentialsl for the Kr guest atoms. Analysis of the dynamics was performed using techniues described in our previous studies on calthrates [4].

The results allow characterization of the Kr guest atom dynamics in two dense forms, a hexagonal clathrate and the filled ice structure. The high quality of the NRIXS data also provides the temperature dependence of the Lamb-Mossbauer factor that provides insight into the strength of the interaction of the Kr guest atoms with the water molecules.

[1] J.S. Loveday *et al*. *Nature* (London) **410**, 661 (2001). [2] C.A. Tulk *et al*. *Phys*. *Rev*. *B* **80**, 052101 (2009). [3] J.S. Loveday *et al*. *Phys*. *Rev*. *Lett*. **87**, 215501 (2001). [4] J.S. Tse *et al*. *Nature Materials* **4**, 917 (2005)

Anorogenic magmatism, mantle plume and the assembly of Late Proterozoic Malani supercontinent

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The Trans-Aravalli Block (TAB) of the NW Indian shield is characterized by the presence of plume related anorogenic, 'within plate, high heat producing Malani magmatism' (55, 000km2; 732 Ma). TAB is characterized by high heat flow, elevated basement, and low velocity anomaly indicative of plume tectonics. The magmatism is characterized by ring structures and is indicative of extensional tectonic environment in TAB. The Siwana granites are hypersolvus with high REE abundances, with little fractionation between HREE and LREE (La/Yb: 2.3) with marked Eu anomaly (Eu/Eu*: 0.28). The Jalor granites are mainly subsolvus, with minor hypersolvus component, with lowest REE contents (La/Yb: 5) and Eu/Eu*: 0.15. The Tusham granites fall in very restricted REE range, LREE are enriched with respect to HREE, La/Yb: 17, Eu/Eu*: 0.44. The Jhunjhunu granites are subsolvus with slight enrichment of LREE La/Yb:9; Eu/ Eu*: 0.25. The mineral chemistry of biotites from Jalor, Tusham and Jhunjhunu granites show iron eurichment trend (annite rich). Due to anhydrous conditions of magma, the Jalor biotites show high FeO / MgO ratios of 6.72 whereas the lower ratios of 4.08 and 3.72 are reported from Tusham and Jhunjhunu samples respectively. The biotites fall in the anorogenic field thereby confirming the anorogenic nature of the magma. The amphiboles in the alkali granites from Siwana evolve from richterite to arfvedsonite (magmatic subsolidus trend) and the pyroxenes in alkali granites evolve from helenbergite to aegirine through aegirine angite (acmite trend). In the Jalor granites the amphiboles belong to the composition of ferro-hornblende, ferroedenitic tschermakites. The zircons in Tusham granite belong to hydrothermal and late magmetic type whereas the Jalor zircons are magmatic. The high $U0_2$ content of Tusham granites is due to high abundance of uranium in the host rock (HHP granites).