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Structural study of the bulk and local compressibilities of the mixed organic/inorganic [(CH3)4N][FeCl4] compound

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Mixed organic/inorganic crystals as [(CH3)4N]FeCl4 (Ref. 1) are receiving considerable attention due to their simple structure consisting of organic (CH3)4N+ and inorganic FeCl4- tetrahedra, being precursors of magnetic ionic liquids with FeCl4- as the most common anion (Ref.2). The incorporation of magnetic anions (as FeCl4-) makes them attractive for modifying their thermodynamic properties by applying external magnetic fields or illumination (Ref.3).
In spite of its relevance, the vibrational and electronic structures of FeCl4- anions remain yet unexplored, in part due to the scarce number of mixed organic/inorganic crystals incorporating FeCl4- anions in the structure, apart from the strong absorption of these materials in the visible-ultraviolet range. This is due to low-lying, spin and parity allowed electric-dipole charge-transfer transitions, forming the material band gap. Furthermore, these materials can be easily compressed due to the small bulk modulus (K ≤ 10 GPa) in comparison to the local bulk moduli of both organic and inorganic tetrahedra, being more than an order of magnitude higher, as it was recently shown in [(CH3)4N]2MnX4 (X: Cl,Br) compound (Ref.4).
This work reports investigations on the structure of isostructural compounds [(CH3)4N]FeCl4 and [(CH3)4N]GaCl4 as a function of pressure with the aim of determining the compression mechanisms governing the crystal bulk and molecular tetrahedra. We have obtained the equation-of-state for the crystal and both tetrahedral ions, the organic (CH3)4N+ and inorganic (Fe,Ga)Cl4- by means of x-ray diffraction and Raman spectroscopy in the 0 –15 GPa range. The comparison between the local and bulk compressibilities allows us to conclude that molecular tetrahedra are harder to compress than the crystal bulk, due the strong intramolecular covalent bonds in comparison to the weak intermolecular hydrogen bonds.
A full report on the structure of these compounds and their associated properties will be presented at the conference.

References

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Caption (s) - Add figures as attached files (2 fig. max)

Bulk and local equation of states of [(CH3)4N]FeCl4 and GaCl4-, respectively.

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