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Frustrations in Molecular System under High Pressure

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Even at ambient pressure, liquid and solid states of room temperature ionic liquids (RTILs) are quite complicated because of a variety of charge network (scalar), molecular orientational order (vector) and coordination number (topology) based on degrees of freedom of molecular conformations. The RTILs possess a unique property such as nano-heterogeneity in spite of simple molecular system. Recently, 1-butyl-3-methylimidazolium hexafluorophosphate, [C4mim][PF6], reveals crystal polymorphs at low temperature. Furthermore, the intrinsic nature of the RTILs is enhanced under high pressure [1-3]. In [C4mim][PF6], a sequence of high pressure states is liquid-crystals-glass on compression process. A significant finding is that pressure induced "conformational glass" of [C4mim][PF6] was observed consistently by X-ray diffraction and Raman spectroscopy, where the maximum pressure was 8 GPa [3]. After decompression from the maximum pressure, the sample has completely recovered without dissociation or polymerization. A balancing between molecular packing efficiency and various cation conformers causes multistep frustrations only in one system.

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