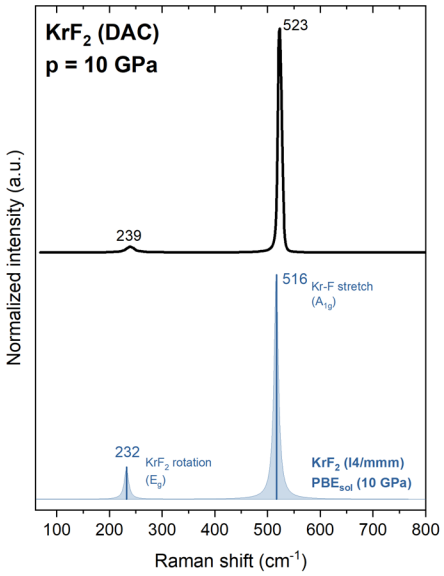
High-pressure experiments on $XePtF_6$ – the first noble gas compound

Klemen MOTALN (Jožef Stefan Institute, Slovenia)
Sylwia OLSZEWSKA (Cardinal Stefan Wyszynski University in Warsaw, Poland)
Miha VIRANT (Jožef Stefan Institute, Slovenia)
Erik URAN (Jožef Stefan Institute, Slovenia)
Olha SANKO (Jožef Stefan Institute, Slovenia)
Ana SILJANOVSKA VIRANT (Jožef Stefan Institute, Slovenia)
Kristian RADAN (Jožef Stefan Institute, Slovenia)
Mirela DRAGOMIR (Jožef Stefan Institute, Slovenia)
Nico GIORDANO (Deutsches Elektronen-Synchrotron DESY, Germany)
Bjorn WEHINGER (European Synchrotron Radiation Facility, France)
Dominik KURZYDŁOWSKI (Cardinal Stefan Wyszynski University in Warsaw, Poland)
Matic LOZINŠEK (Jožef Stefan Institute, Slovenia)

Abstract

Although the demonstration of noble-gas reactivity represents one of the most significant breakthroughs of 20th-century inorganic chemistry, the first noble-gas compound, $XePtF_6$ ($XeF_2 \cdot PtF_4$) [1], lacks comprehensive structural characterization, and its geometry and atom connectivity remain to be elucidated [2]. Ternary Xe-Pt-F compounds, however, could serve as important systems for benchmarking theoretical methods and deepening our understanding of Lewis acid-base interactions and chemical bonding in noble-gas compounds [3].

In a recent study, we proposed several structural models of $XePtF_6$ through density functional theory calculations, which were derived from experimentally determined crystal structures of XeF_2–MF_4 (M = Cr, Mn) analogues [4]. Here, we present diamond anvil cell experiments in which laser-heated recrystallization, single-crystal diffraction, and confocal Raman microscopy were combined with solid-state modelling, resulting in the first successful structural determination of $XePtF_6$. Furthermore, we experimentaly explored the high-pressure reactivity within the Xe–Pt–F system, as well as the thermodynamic stability of compressed krypton difluoride.



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