Poster

The high pressure behaviour of $Nd(XeF_2)_3(TaF_6)_3$

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High pressure single crystal X-ray diffraction is a well-established technique in chemical crystallography, used to examine the behaviour and response of compounds to pressures in the 10s of GPa range. This enables researchers to study the phase behaviour of materials, their compression dynamics and structural phase changes, and thus infer information about the intermolecular interactions. This technique has been widely applied to a range of compounds including molecular organics,1 inorganic coordination compounds.2

The first compounds containing noble gases were discovered in 1962.[3] Since then, the chemistry of xenon, particularly in combination with fluorine, has been extensively developed.[4] The crystal structures of xenon fluorides exhibit many short intermolecular contacts as a result of the high Lewis acidity of the Xe atom. The response of these contacts to pressure can potentially lead to phase transitions, conversion of long contacts into primary bonds, or other structural changes. Research in this area has thus far been very limited, with only high pressure powder diffraction studies of XeF_2 having been reported.[5] Our current work seeks to address this and investigates the behaviour of more complex XeF_2 coordination compounds under pressure.

The compound $Nd(XeF_2)_3(TaF_6)_3$ (**1**) has provided unique insight into the phase and structural characteristics of XeF_2 coordination compounds at high pressure. Compression studies of **1** have been performed in a range of hydrostatic media, including inert gases and halocarbon oil, up to pressures of 5.5 GPa, with distinct differences in behaviour depending upon the choice of hydrostatic medium. Compression in halocarbon oil leads to a first order phase transition at 2.7 GPa characterised by collapse of channels formed along the *c* axis. Unusually, one Xe site in the high pressure phase exhibits fewer direct and long-range Xe-F interactions than at ambient pressure. Compression in noble gases has distinct behaviour from that in halocarbon oil, that will be discussed and compared.

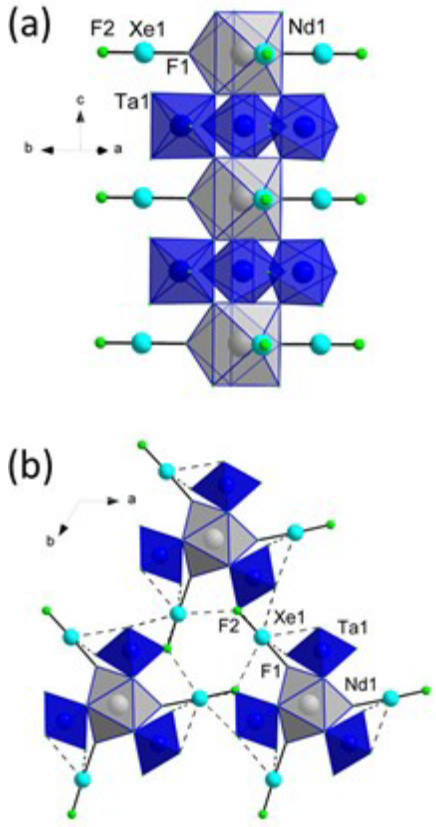

Figure 1: The crystal structure of $Nd(XeF_2)_3(TaF_6)_3$ [1] at ambient pressure and 100 K (R_1=1.45%). (a) Chains formed along the ***c*** axis. (b) Xe…F contacts connecting chains.

[1] HYPERLINK "https://pubs.acs.org/action/doSearch?field1=Contrib&text1=Alice++Dawson"A. Dawson, HYPERLINK