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Contribution of X-ray crystallography to the full description of Molecular Switches behavior under Pressure at Variable Temperature

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Since the development of Diamond Anvil Cell¹, the investigations of materials under high pressure (HP) did not stop to increase. Nevertheless, obtaining **HP structural data** is still a challenge especially when combining several thermodynamic variables such as **pressure and temperature**, or when data are recorded on **molecular materials**.

Addressing the additional difficulties due to molecular compounds necessary includes methodology developments in order to access to a reliable characterization, taking account their specificities. Surprisingly, though the scientific community still develops new technics to get accurate data at very high pressure, working with **soft material at pressure bellow 1 GPa is still challenging**. For example, structural data under pressure represent less than 1% of the CSD data base.

Spin CrossOver (SCO) materials are molecular complexes that can switch from a Low Spin (LS) to a High Spin (HS) state upon physical stimuli like pressure, opening potential piezo-switch based applications². The structure-properties relationships of such compounds at ambient conditions are now well established,³ but their crystallographic investigation under pressure remains very scarcely reported even though new, unexplained or very rare behaviors are observed in numerous examples⁴. Typically, despite the crucial role of polymorphism on such materials, full (P, T) **phase-diagrams of SCO molecular switches are almost unexplored**. In this communication, we show how powerful is crystallography to investigate pressure induced phenomena using **HP single crystal diffraction** as well as **in situ HP Powder X-Ray Diffraction (PXRD)**. Thanks to these techniques, we present the full description of SCO compounds along their transitions and explore pressure induced phenomena taking place on **low pressure range with extremely small pressure steps**. Beyond the rare determination of the bulk moduli of HS and LS states at different temperatures, such investigations reveal unusual behaviours like negative linear compressibility or unexpected pressure induced phase transitions (fig. 1).

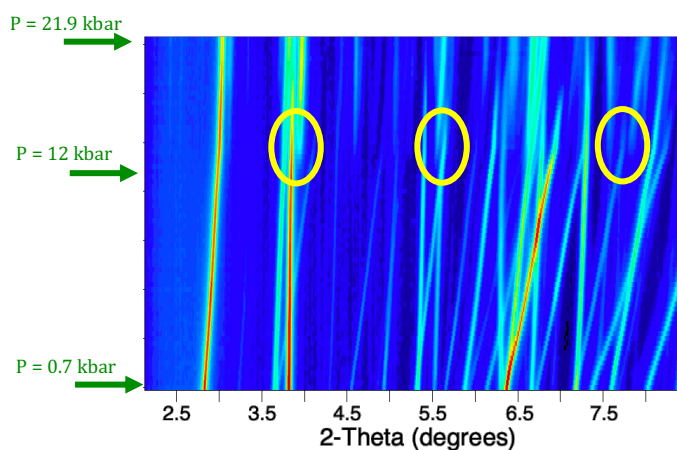


Figure 1: Pressure dependence of PXRD diagram of a SCO compound showing a structural transition around 12 kbar.

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