Triethylphosphine: a 'molecular gear' enabling single-crystal-to-single-crystal phase transitions

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Stimulus-responsive molecular materials are highly desirable because of the wide range of their potential applications. In particular, switching of physical properties opens application pathways for molecular materials as sensors or actuators. Controllable roperty switching can be achieved by inducing single-crystal-to-single-crystal (SCSC) phase transitions. Identifying (supra)molecular motifs that increase probability of SCSC is thus important to understand property switching and forward materials design.

Here I will present a few instances where SCSC phase transtions could be induced by temperature[2] or pressure variation[3,4] in the crystal structures of **organogold(I) triethylphosphines, leading to noticeable changes in mechanical or optical properties of the analyzed solids.** Despite its relatively small size and large flexibility, the $–PEt_3$ moiety fullfills all criteria[1] for being a "molecular gear", which in favourable crystalline environment can ensure occurrence of ordered, predictable and reversible structural changes. The mechanism of these transitions may be envisaged as initiated by a rotation of a single $–PEt_3$ group in a double layer (a single gear movement), followed by adjacent phosphines adjusting their conformations as a result of steric strain.

Structural changes underlying phase transitions could be partly captured in the course of rapid high-pressure **single-crystal X-ray diffraction** experiments conducted at the ESRF synchrotron facility, showing that with carefully planned experiments[5] detailed structural analysis under high pressure conditions is nowadays attainable with a high level of accuracy even for larger, labile molecular systems.

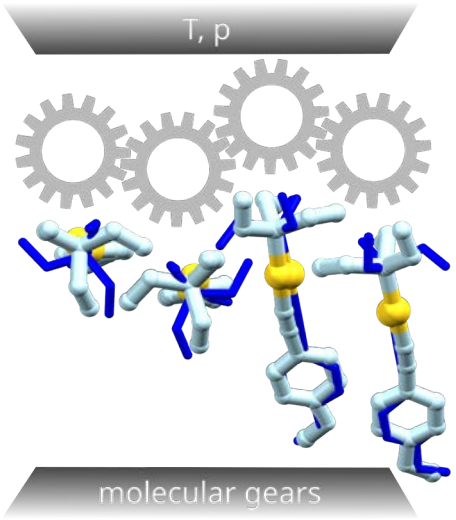

Figure 1.

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