Jumping the hurdles: challenges in calculating thermal expansion coefficients from the data in the Cambridge Structural Database

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The thermal expansion coefficient of a crystalline structure is a straightforward parameter to calculate, provided that the cell parameters have been measured at least two different temperatures. Crystallographic databases, such as the Cambridge Structural Database and the Inorganic Crystal Structure Database, contain extensive data on structures analyzed at multiple temperatures, making it seemingly simple to derive thermal expansion coefficients from the available information. Understanding these coefficients is essential across various fields, including materials science, engineering, and electronics. For instance, identifying compounds with near-zero thermal expansion is crucial for applications requiring high dimensional stability, such as precision optics, aerospace components, and electronic circuits, where unwanted thermal expansion can compromise performance. Additionally, knowledge of thermal expansion behavior aids in designing resilient materials for extreme environments, such as spacecraft or high-temperature industrial processes.

However, working with large datasets containing data obtained from diverse sources presents significant challenges. Data collected in different laboratories at various times and registered in international crystallographic databases, despite meticulous curation efforts by database-maintaining organizations, often contain inconsistencies or variations that complicate analysis. This talk aims to highlight the hurdles that must be overcome to derive a meaningful and reliable set of thermal expansion coefficients from cell parameters, specifically focusing on organic compounds within the Cambridge Structural Database. The final set of thermal expansion coefficients shows, that contrary to general belief, negative thermal expansion along one or two orthogonal axes is far from rare.