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Molecular Motion in Crystals. H.B. Bürgi, Laboratory of Crystallography, Univ. of Berne, Freiestr.3, CH-3012 Bern, Switzerland.

The seminal paper by Verner Schomaker and Ken Trueblood on 'On Rigid-body Motion of Molecules in Crystals' published in 1968 is a classic in the field and an important part of Ken's scientific legacy [Acta Cryst. **B24**, 1968, 63]. It has been cited more than 1700 times. Thirty years later the same authors discussed the 'Correlation of internal torsional motion with overall molecular motion in crystals' [Acta Cryst. **B54**, 1998, 507]. In both essays they had to leave open the problem of correlation of different motions (in technical terms: indeterminacy of the trace of **S** and the λ problem). These shortcomings frustrate the comparison of kinematic diffraction results with dynamic information from other experiments.

We have solved this problem by measuring the thermal evolution of the anisotropic displacement parameters (ADP) from the zero-point-motion to the classical regime and interpreting the temperature dependence of the ADPs in terms of molecular low-frequency normal modes in the mean crystal field. This procedure leads to better distance corrections, allows estimating vibrational frequencies, isotope effects and specific heat, distinguishes motion from disorder and accounts for the influence of thermal expansion on molecular motion [for a recent discussion and references see: H.B. Bürgi, S.C. Capelli, Helv. Chim. Acta **86**, 2003, 1625].