This Week's Citation Classic

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Schomaker V & Trueblood K N. On the rigid-body motion of molecules in crystals. *Acta Crystallogr.* **B24**:63-76, 1968.
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The simplest proper description of the quadratic mean motion of a rigid molecule not at a center of symmetry requires a 3x3 tensor (S) with eight independent compo-nents for libration-translation correla-tion–in effect, screw motions –besides the libration (L) and translation (T) tensors previously used. [The *SCI*® indicates that this paper has been cited over 735 times since 1968.]

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"Cruickshank[1] showed in 1956 how anisotropic atomic displacement ten-sors from crystal diffraction data can be used to determine, by least-squares, two symmetric 3x3 tensors that de-scribe the effectively independent librations and translations of a rigid centrosymmetric molecule. His meth-od was widely adopted, often even for unsymmetrically sited molecules, the center of mass then usually being as-sumed to be still the effective center of libration.

"However, when Schomaker encoun-tered such a case, some handwaving convinced him that for it the motions were surely correlated rather than in-dependent, and the center of mass ir-relevant. It was not hard to formulate the problem in terms of **L**, **S**, and **T** for every possible symmetry, but testing against the voluminous available crys-tal data required a computer program that Schomaker was not prepared to write. Fortunately, Trueblood agreed to join in, having written with Peter Gant-zel a widely used program for Cruick-shank's method.

"We debugged Trueblood's first ver-sion of the *LST* program under wide beautiful skies at the Bozeman meet-ing of the American Crystallographic Association, July 1964, learning several items that had been missed in the anal-ysis. About to go on sabbatical to Nigeria and the USSR, Trueblood fin-ished the program before returning to UCLA, tested it in Fall 1965, and presented the results at the 1966 Con-gress of the International Union of Crystallography in Moscow, with suc-cessful applications to a number of compounds to illustrate the differences from Cruickshank's approach.

"Writing the paper was no easy task, for the analysis, though simple in prin-ciple, gets complicated, and the neces-sary notation was unfamiliar. We labored many months (by correspon-dence and visits up or down the Coast) and sent preliminary versions to knowl-edgeable friends. Carroll Johnson and Henri Levy referred us to Brenner's completely independent but in many details remarkably similar analysis[2] of a quite different problem.

"Why is our paper so often cited? Be-cause there are many hundreds of pre-cise anisotropic refinements of crystal structures each year, for many of which the possible rigid-body motion or segmented rigid-body motion (see, for example, Trueblood[3]) is explored. Of course, no molecule or molecular seg-ment is truly rigid, and already for his examples Cruickshank allowed for in-ternal vibrations. The need remains to *do* this routinely."

1. **Cnikkshank D W J.** The analysis of the anisotropic thermal motion of molecules in crystals. *Acta Crystallogr.* **9**:754-6, 1956.
2. **Brenner H.** Coupling between the translational and rotational Brownian motions of rigid particles of arbitrary shape. *J. Colloid Interface Sci.* **23**:407-36, 1967.
3- **Trueblood K N.** Analysis of molecular motion with allowance for intramolecular torsion. *Acta Crystallogr.* **A34**:950-4, 1978.