E0007

Analysis and Illustration of Thermal Motion Covariance. Carroll K. Johnson and Michael N. Burnett, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA.

An extension of ORTEP is planned to portray statistical correlation[1] of thermal motion ellipsoids.

In least-squares refinement, covariance matrix **L** with derivative products of structure parameters is formed and inverted to $\mathbf{L}^{-1}$ for parameter shift and standard error calculation. Position-position, position-thermal, and thermal-thermal submatrices in **L** can be replaced by multivariate Hermite polynomial tensors of order 2, 3, and 4, respectively, forming $\mathbf{L}'$.[2] The submatrices of $\mathbf{L}^{-1}$ or $\mathbf{L}'^{-1}$ provide the basis for an ORTEP-4 *covariance skeleton* drawing shown within and interconnecting the regular thermal ellipsoids. It may also be shown as a separate drawing.

[1] M. L. Stein, **Interpolation of Spatial Data: Some Theory for Kriging**, Springer, 1999.
[2] C. K. Johnson, *New Computational Techniques, Particularly for Refinement*, in **Computational Needs and Resources in Crystallography**, National Academy of Sciences, 1973, p 48-57.