

## Analysis and Illustration of Thermal Motion Covariance

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

In least-squares refinement, covariance matrix  $L$  with derivative products of structure parameters is formed and inverted to  $L^{-1}$  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  $L'$ .<sup>[2]</sup> The submatrices of  $L^{-1}$ , or  $L'^{-1}$ , 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.

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