$$A(\mathbf{H}) = \sum_j (f_{j,c} + f_j')[\cos(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_c - \sin(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_a] - (f_{j,a} + f_j'')[\cos(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_a + \sin(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_c] \quad (1.2.13.3a)$$

and

$$B(\mathbf{H}) = \sum_j (f_{j,c} + f_j')[\cos(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_a + \sin(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_c] + (f_{j,a} + f_j'')[\cos(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_c - \sin(2\pi\mathbf{H}\cdot\mathbf{r}_j)T_a] \quad (1.2.13.3b)$$

(McIntyre *et al.,* 1980; Dawson, 1967).

Expressions (1.2.13.3) illustrate the relation between valence-density anisotropy and anisotropy of thermal motion.

## 1.2.14. Conclusion

This chapter summarizes mathematical developments of the structure-factor formalism. The introduction of atomic asphericity into the formalism and the treatment of thermal motion are interlinked. It is important that the complexities of the thermal probability distribution function can often be reduced by very low temperature experimentation. Results obtained with the multipole formalism for atomic asphericity can be used to derive physical properties and *d*-orbital populations of transition-metal atoms (*IT* C, 1999). In such applications, the deconvolution of the charge density and the thermal vibrations is essential. This deconvolution is dependent on the adequacy of the models summarized here.

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references