On the Incompleteness of Atomic Models

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When working with incomplete models at a conventional resolution of about 2-3 Å, one may suppose for simplicity that unknown atoms may be found with the given probability at any point of the unit cell. Then the contribution of these atoms to structure factors can be taken into account statistically. This allows a proper modification of target values and a choice of the weighting scheme to be done [1].

When working at a resolution of 1 Å or higher, the model incompleteness changes its aspect. The conventional model of spherical atoms cannot describe the density deformation caused by interatomic interactions, and this discrepancy is significant for high-resolution structure factors. While all atoms are well defined at such a resolution, refinement without special precaution gives too large values for ADPs in order to 'cover' the deformation density missed in the model. At the same time, an introduction of multipolar models [2] may lead to overfitting the data. An intermediate model of dummy bond electrons was shown [3] to be capable to reduce the distortion of the ADPs even when the model is refined at the resolution of order of 0.9 Å that is not yet adequate for refinement of multipolar models.

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