5.11: R factor

The term ***R* factor** in crystallography is commonly taken to refer to the 'conventional' *R* factor

\(R =

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\),

a measure of agreement between the amplitudes of the structure factors calculated from a crystallographic model and those from the original X-ray diffraction data. The *R* factor is calculated during each cycle of least-squares structure refinement to assess progress. The final *R* factor is one measure of model quality.

More generally, a variety of *R* factors may be determined to measure analogous residuals during least-squares optimization procedures. Where the refinement attempts to minimize the deviates of the squares of the structure factors (refinement against F^2), the *R* factor based on F^2 is used to monitor the progress of refinement:

\(R(F^2) =

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\).

Likewise, refinement against *I* can be tracked using the Bragg *R* factor

\(R_B =

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\).

Even for refinement against F^2 or *I*, the 'conventional' *R* factor may be calculated and quoted as a measure of model quality, in order to compare the resulting quality of models calculated at different times and with different refinement strategies.

The *R* factor is sometimes described as the **discrepancy index**.