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Accurate determination of bound coherent neutron scattering lengths using Bragg diffraction

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Bound coherent scattering lengths $b(\text{coh})$ are one of the basic properties of any isotope, and many experimental neutron techniques in condensed matter as well as in nuclear physics rely on these values, determined by many different scientists over decades and collected in various tables. But many of the values listed in these respectable references have large experimental uncertainties, including possible systematic errors, due largely to having been measured decades ago with neutron instrumentation that has since greatly improved.

Therefore, we use the advantages of modern neutron powder diffraction (NPD), like very good counting statistics even on sub-gram samples, for a redetermination of $b(\text{coh})$ of important isotopes.

The measurement of integrated Bragg peak intensities $I(\text{hkl})$ using NPD has the huge advantage that only the *relative* peak intensities are affected by a change in one of the sample's $b(\text{coh})$, such that there is no need to normalize the data to an absolute intensity scale, being therefore much less prone to systematic errors than are other techniques used for $b(\text{coh})$ determination. Rietveld refinement then provides the structure factor $F(\text{hkl})$, and in the case of fixed atomic positions, $F(\text{hkl})$ depends only on $b(\text{coh})$ which thus can be determined directly. The strategy for an accurate determination of $b(\text{coh})$ is therefore to use binary or ternary compounds with well-known crystal structures and ideally with a small number of free positional parameters.

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