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Looking for Hydrogen Atoms in X-ray Data. Bruce Noll, Thomas Fehlner, Sundargopal Ghosh, Hong Yan., Dept. of Chemistry & Biochemistry, Univ. of Notre Dame, 260b Stepan Hall of Chemistry and Biochemistry, Notre Dame, IN 46556-5670 USA.

Crystallographers are sometimes asked to locate hydrogen atoms that play an important role in the structure, but cannot easily be fit to a geometric model. Of course, X-ray data is not the first choice for such a task, but it is satisfying to locate these hydrogens to generate agreement between the crystal structure and the spectroscopic data. While many of the hydrogens can be located by difference map, many remain hidden, especially those near heavy atoms like transition elements. Difference maps with a large number of residual peaks are often sufficient to reveal these hydrogens. Similarly, difference maps using only data below $(\sin\theta)/\lambda=0.35$ may reduce the extraneous peaks caused by the metal atoms and highlight the missing hydrogens. Each method has borne fruit, but often one or two hydrogens remain hidden. Even after finding some of these hydrogens, it remains to choose an appropriate method to model them. Their proximity to the heavy atoms makes full refinement difficult. Often some can be refined, while others must be constrained. A few examples will be presented and the audience will be encouraged to offer their tips and tricks for divining missing hydrogens.