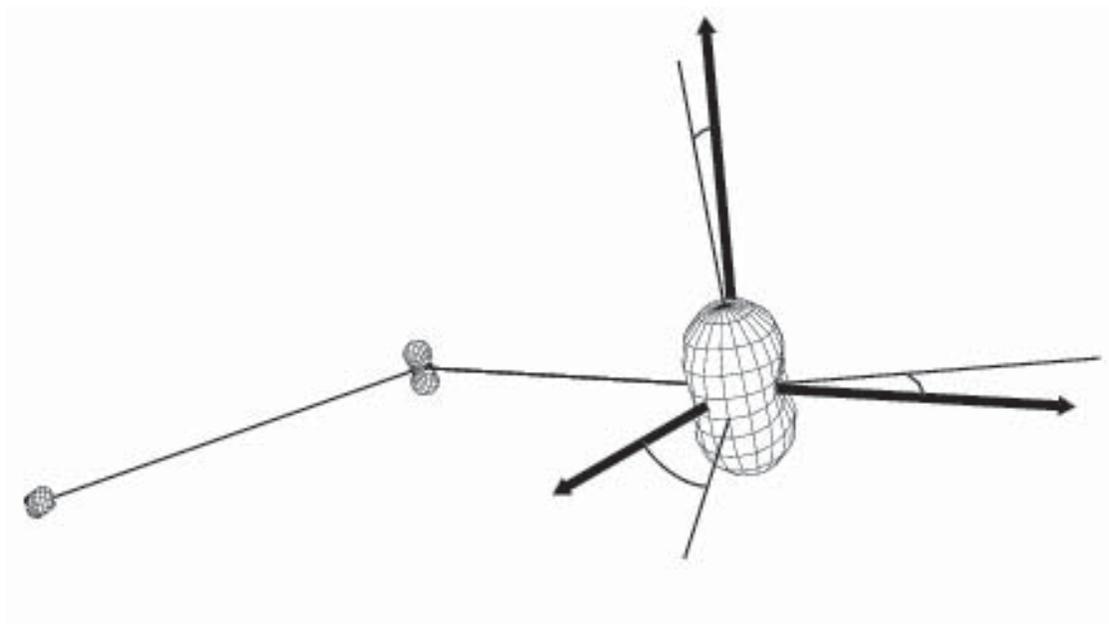


MS29-01 | MODELLING OF HYDROGEN ATOMS IN CRYSTALLOGRAPHY – AN OVERVIEW

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Hydrogen is the most abundant element in the universe, and - because of the role of water - the most abundant element in living matter. Most organic molecules have a skin of - often labile - hydrogen atoms which thereby facilitate the interactions between molecules, as well as determine properties like charge and pH.

Because of its light mass, its polarizability and the fact that only one electron is associated to the atom, it is a difficult atom to model, seen with a crystallographer's eyes. Yet there are more than a million crystal structures containing hydrogen in the structural databases.

I will present an overview of how crystallographers have modeled hydrogen atoms historically, but will especially put focus on the state of the art - and try to sketch what is appearing in the horizon.