EXPERIMENTAL DETERMINATION OF PARTIAL CHARGES WITH ELECTRON DIFFRACTION

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Atomic partial charges, integral for understanding molecular interactions and behavior, lack a precise quantum mechanical definition, posing complexity. Their determination is vital in theoretical chemistry, material sciences, and molecular dynamics simulations. Existing methods prioritize practicality over accuracy, necessitating innovation. This study introduces a novel experimental approach for determining partial charges, utilizing electron diffraction, crystal structure refinement, and ionic scattering factors. Integrated into electron crystallography workflows, this method requires no specialized software. Validated with amino acid crystals, it simplifies charge determination, enhances chemical modeling, and reduces noise in Fourier maps. The technique highlights fine structural details, including hydrogen atoms, usually requiring dynamic structure refinement. This promises a more precise understanding of molecular structures, applicable across chemical and material science disciplines.