Gas Phase Electron Diffraction

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1. . Introduction

Electrons have both wave and particle properties, so they are diffracted by atoms and molecules, but can also be observed as distinct particles. Both properties are used in the electron diffraction experiment, which gives information about distances between atoms in gas-phase molecules.[1-3]

2. Theory

The theory of gas phase electron diffraction is hardly a new topic. It is well established for decades and has been thoroughly described in the literature. Consequently, it will not be dealt with in such depth here. The purpose of this part is to serve as a primer such that the subsequent descriptions of the ultrafast gas-phase electron diffraction experimental and theoretical methodology may be understood in the context of the much more familiar field of conventional gas-phase electron diffraction.

3. Experiments and Applications

Electron diffraction is the most widely applicable technique for determining structures of gaseous molecules. However, locating light atoms in molecules which contain heavy atoms can be difficult, and it is also limited in resolving interatomic distances which are similar to one another. In both these respects it is complementary to liquid crystal NMR spectroscopy. We have therefore developed ways of performing combined analyses of the data from both these experiments, and from rotational spectroscopy. We can thus derive structures which are much more accurate and complete than can be obtained using one technique by itself.

4. Conclusion

Combining all these experimental data with flexible restraints derived from ab initio or DFT calculations is a further technique developed here, known as the SARACEN

method. This allows us to determine accurate structures of much larger and more complex molecules.

[1] L. O. Brockway, Reviews of modern physics, volume 8, number 3, 231-266 (1936)

[2] Stereochemical Applications of Gas-Phase Electron Diffraction. Part A: The Electron Diffraction Technique, edited by I. Hargittai and M. Hargittai (VCH, New York, 1988).

[3]. http://www.ged.chem.ed.ac.uk/structure/ged.html