Pramāṇa, Vol. 8, No. 2, 1977, pp. 99-107. © Printed in India.

Electron momentum distributions and Compton profiles of some molecules with FSGO model

S R GADRE, R RAMASWAMY* and P T NARASIMHAN†
Department of Chemistry, Indian Institute of Technology, Kanpur 208016
* Present address: Department of Chemistry, Princeton University, Princeton, New Jersey 08540, U.S.A.

MS received 7 July 1976; in revised form 2 November 1976

Abstract. The electron momentum distributions and the Compton profiles (within the impulse approximation) of H_2, LiH, methane, water, acetylene, ethylene, ethane cyclopropane and cyclobutane have been calculated using the floating spherical Gaussian orbital (FSGO) wavefunctions. The agreement of the single-FSGO Compton profiles with the corresponding experimental or the Hartree-Fock (HF-SCF) theoretical ones is fairly good in most of the cases examined. The advantages and drawbacks of using the FSGO model for the calculation of Compton profiles are discussed.

Keywords. Electron momentum distributions; Compton profiles; FSGO model of molecular structure.

1. Introduction

Recently there has been a revival of interest in the electron momentum distributions (EMD) and Compton profiles (CP) of molecules. (For review, see Epstein and Tanner 1976). In the present paper, we shall confine our attention to the theoretical calculation of CP's of some small molecules. The first calculation of the shape of the Compton line for H_2 was done by Hicks (1937) using valence-bond wavefunction of Weinbaum (1933). Duncanson and Coulson (1941) calculated CP's of methane, ethane, ethylene and acetylene. Epstein and Lipscomb (1970) presented a general algorithm for obtaining EMD's using HF-SCF wavefunctions of polyatomic molecules. This algorithm was applied to evaluate CP's of hydrocarbons using a localized molecular orbital (LMO) approach (Epstein 1970). Some more studies using LMO approach have been recently reported (Smith and Whangbo 1974) for a number of molecules including hydrocarbons. The CP of water has been calculated using a variety of wavefunctions and compared with recent experimental results (Tanner and Epstein 1974). The effect of hydrogen bonding on the CP of water has also been examined in detail (Whangbo *et al* 1974). Thus, with growing interest on the theoretical side and the use of

† To whom all correspondence should be addressed.