Zeitschrift für Physikalische Chemie Neue Folge, Bd. 99, S. 97—106 (1976)

Electronic Structures of Cyclopropenone and Aminocyclopropenones

By

TSUNETOSHI KOBAYASHI

The Institute for Solid State Physics, The University of Tokyo, Roppongi, Minato, Tokyo (Japan)

With 1 figure

(Received June 5, 1975)

The electronic structures of cyclopropenone, aminocyclopropenone, *N*,*N*-dimethylaminocyclopropenone, diaminocyclopropenone and bisdimethylaminocyclopropenone were studied theoretically with a semiempirical INDO ASMO LCAO SCF CI method. The Mulliken populations, the dipole moments, the orbital energies, especially in relation to the photoelectron spectra, and the electronic excitation energies of these compounds were discussed.

Die elektronischen Strukturen von Cyclopropenon, Aminocyclopropenon, *N*,*N*-Dimethylaminocyclopropenon, Diaminocyclopropenon und Bisdimethylaminocyclopropenon wurden mit einer semiempirischen INDO ASMO LCAO SCF CI Methode theoretisch untersucht. Die Mulliken-Populationen, die Dipolmomente, die Orbitalenergien, besonders in bezug auf die Photoelektronenspektren, und die elektronischen Anregungsenergien dieser Verbindungen wurden diskutiert.

Introduction

Cyclopropenone is interesting from both theoretical and experimental points of view. In cyclopropenone a highly strained unsaturated three-membered ring and an electron-withdrawing carbonyl group are incorporated with each other in the simplest and most symmetrical way.

In this paper the electronic structures of cyclopropenone(I), and its amino derivatives, that is, aminocyclopropenone(II), *N*,*N*-di-