

# Semiempirical LCAO calculations of electron-impact ionization cross-sections

by J. H. VAN DEN BURG and J. VAN DEN BURG

Department of Chemistry, University of Groningen, The Netherlands

(Received 15 October 1973)



pathes [17, 19]. It was suggested that the addition of the availability electron

M. O. Bonnell, *Journal of Chemical Education*, 1978, 55, 1000.

olefinic potential for describing reaction mechanisms

[8, 19]. Hence, we have examined to some extent the

calculated by the INDO potential. As expected, this method

concerning reaction mechanisms and the potential for

ing the

in

o

The results of the calculations are discussed in the following sections.

1.098 (2)

1.213 (c)

Equilibrium  $\Sigma_{g^+}$   
distance/Å

1.17

1.15

Equilibrium  $\Pi_u$

1.20

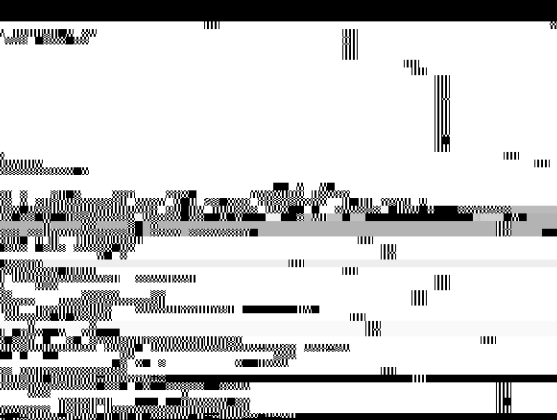
1.21

of analytical tools, as for digital filters, spectral harmonics [12], or harmonic components as defined in [13]. In order to be able to use any previous filters, are designed by the user in the program, or are they automatically generated of the ICA automatic algorithm; for fitting at any time, these are obtained by solving the equations of the model.

The first part of the paper is devoted to the description of the model, the second part to the description of the algorithm, and the third part to the results of the application of the model to the analysis of the speech signal. The first part is divided into two sections: the first section is devoted to the description of the model, and the second section to the description of the algorithm. The second part is divided into two sections: the first section is devoted to the description of the algorithm, and the second section to the results of the application of the model to the analysis of the speech signal. The third part is devoted to the results of the application of the model to the analysis of the speech signal.



The first reasonable results were obtained by calculating the total energy of the crystal using the LCAO method. The results are shown in Table 1. The wave function used was of the form

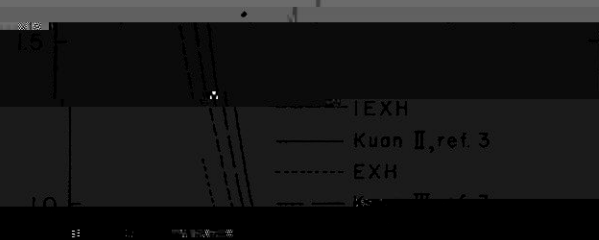
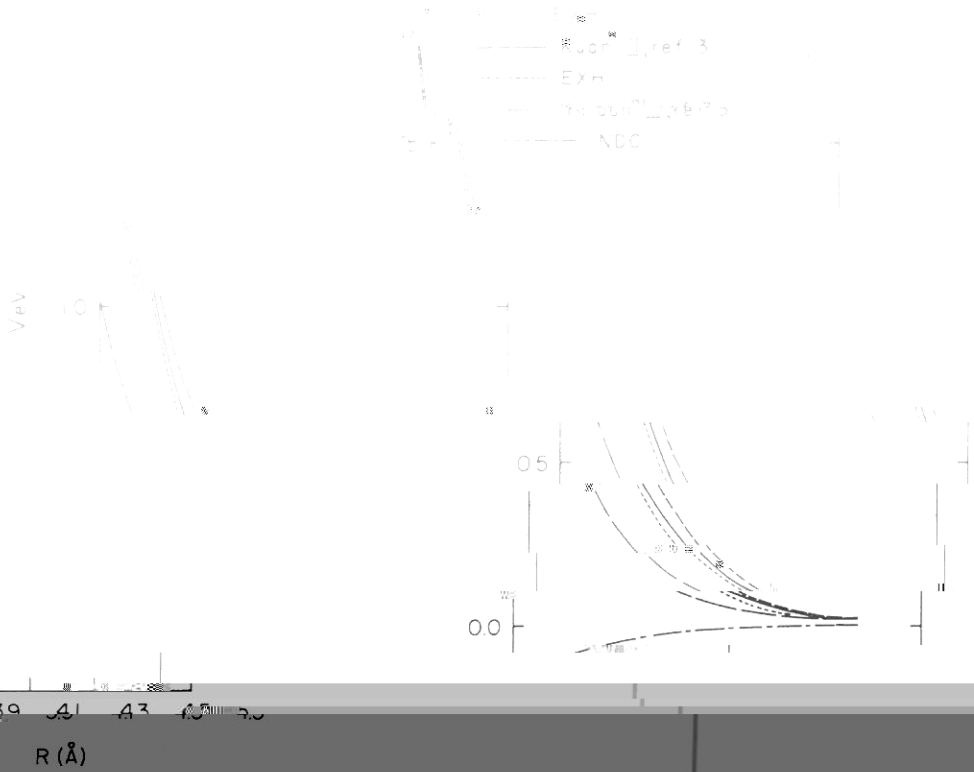


It is evident from the figure that the LCAO and LMO methods agree reasonably well. The results are also compared with the INDO method of Pritchard and



and Pritchard (1971). The energy per molecule was found to vary from  $-15.4 \times 10^{-2}$  eV for a unit cell dimension of  $3.5 \text{ \AA}$  to  $-14.5 \times 10^{-2}$  eV for a unit cell dimension of  $4.5 \text{ \AA}$ . The slight attraction of the end-to-end interactions between  $N_2$  molecules is in accordance with the structure of  $N_2$ .

The magnitude of the interaction energy per molecule is compared with the experimental value of  $-14.5 \times 10^{-2}$  eV. The results are in good agreement with the experimental value. The results are also compared with the results of other workers (Pritchard and Pritchard, 1971; Pritchard and Pritchard, 1972; Pritchard and Pritchard, 1973; Pritchard and Pritchard, 1974; Pritchard and Pritchard, 1975; Pritchard and Pritchard, 1976; Pritchard and Pritchard, 1977; Pritchard and Pritchard, 1978; Pritchard and Pritchard, 1979; Pritchard and Pritchard, 1980; Pritchard and Pritchard, 1981; Pritchard and Pritchard, 1982; Pritchard and Pritchard, 1983; Pritchard and Pritchard, 1984; Pritchard and Pritchard, 1985; Pritchard and Pritchard, 1986; Pritchard and Pritchard, 1987; Pritchard and Pritchard, 1988; Pritchard and Pritchard, 1989; Pritchard and Pritchard, 1990; Pritchard and Pritchard, 1991; Pritchard and Pritchard, 1992; Pritchard and Pritchard, 1993; Pritchard and Pritchard, 1994; Pritchard and Pritchard, 1995; Pritchard and Pritchard, 1996; Pritchard and Pritchard, 1997; Pritchard and Pritchard, 1998; Pritchard and Pritchard, 1999; Pritchard and Pritchard, 2000; Pritchard and Pritchard, 2001; Pritchard and Pritchard, 2002; Pritchard and Pritchard, 2003; Pritchard and Pritchard, 2004; Pritchard and Pritchard, 2005; Pritchard and Pritchard, 2006; Pritchard and Pritchard, 2007; Pritchard and Pritchard, 2008; Pritchard and Pritchard, 2009; Pritchard and Pritchard, 2010; Pritchard and Pritchard, 2011; Pritchard and Pritchard, 2012; Pritchard and Pritchard, 2013; Pritchard and Pritchard, 2014; Pritchard and Pritchard, 2015; Pritchard and Pritchard, 2016; Pritchard and Pritchard, 2017; Pritchard and Pritchard, 2018; Pritchard and Pritchard, 2019; Pritchard and Pritchard, 2020; Pritchard and Pritchard, 2021; Pritchard and Pritchard, 2022; Pritchard and Pritchard, 2023; Pritchard and Pritchard, 2024; Pritchard and Pritchard, 2025).

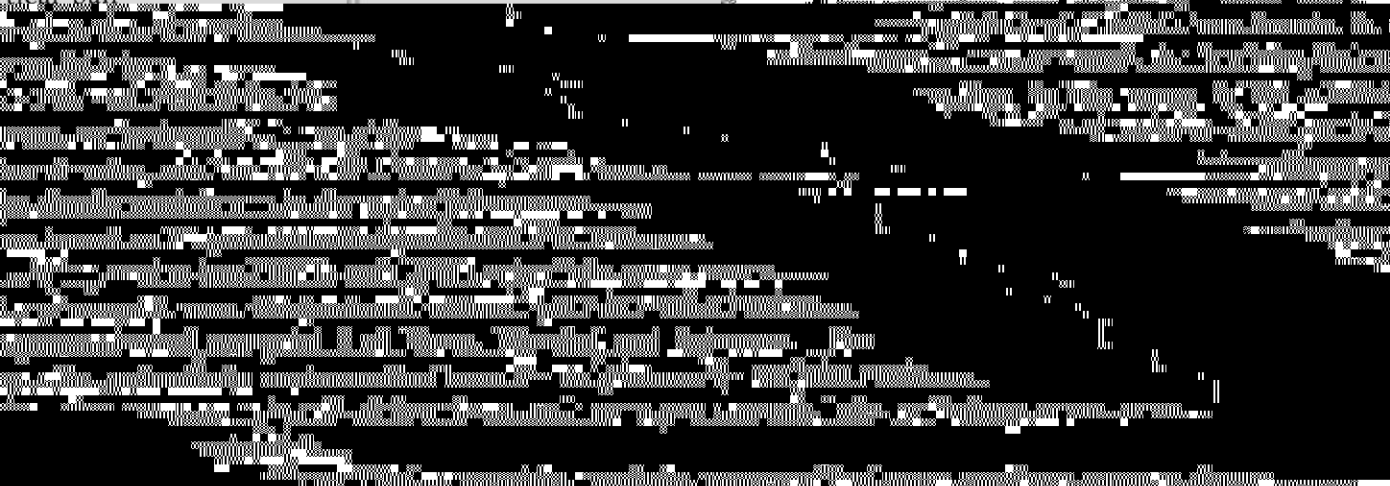


...omized according to the experimental procedure...  
 ...EXH, EXH and NDC theories. (a) Linear...  
 ...plane configuration...

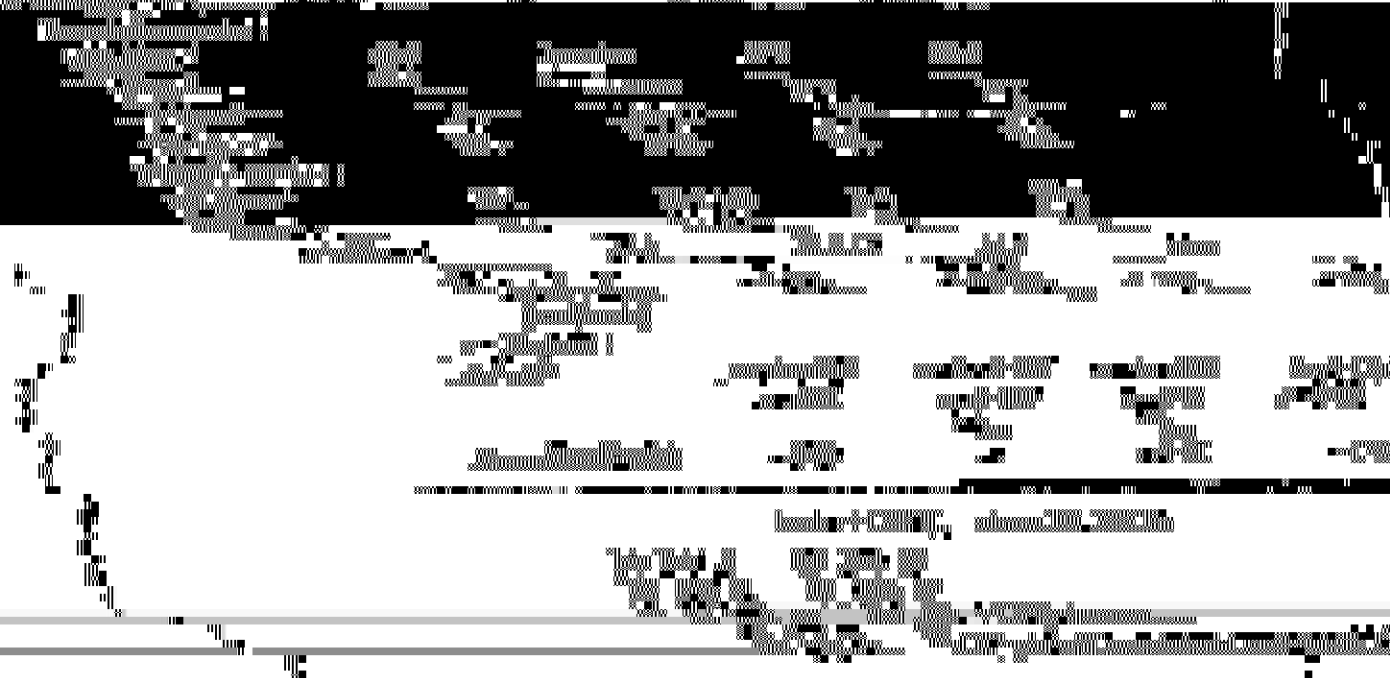
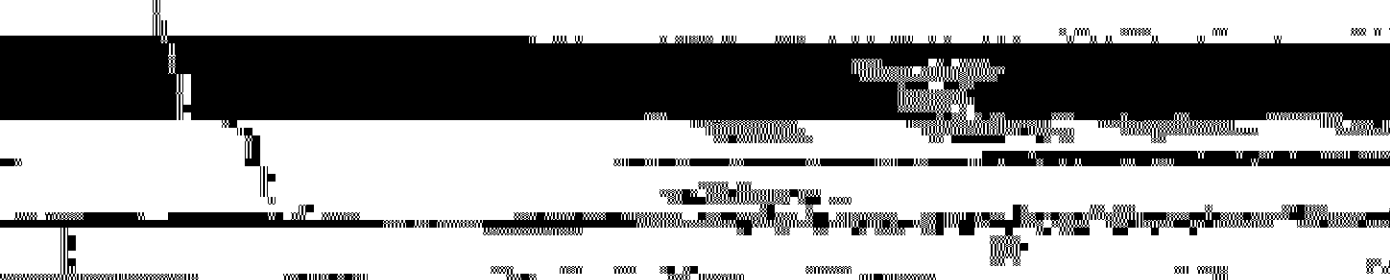
...  
 ...  
 ...

environment as  $\theta$ , and the field  $F$  is calculated as  $F = \frac{1}{L} \int \theta dx$ . The first derivative of the field is  $F' = \frac{1}{L} \int \theta' dx$ .

the phenomenological potential  $\Phi$  is calculated by



The function  $\Phi(x)$  is calculated as  $\Phi(x) = \frac{1}{L} \int \theta dx$ .



...of the RDO theory for describing ground state energy,  $\mu$  and interactions in atomic crystals had been previously

...significantly better than EXPT results. The  $\mu$  number was found to have abss s

...the energy of the ground state of the system. The energy of the ground state of the system is given by the minimum of the energy functional  $E[\psi]$  with respect to the wave function  $\psi$ . The energy functional is given by  $E[\psi] = \int \psi^* H \psi d\tau$ , where  $H$  is the Hamiltonian operator and  $\tau$  is the volume element. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives.

...the energy of the ground state of the system. The energy of the ground state of the system is given by the minimum of the energy functional  $E[\psi]$  with respect to the wave function  $\psi$ . The energy functional is given by  $E[\psi] = \int \psi^* H \psi d\tau$ , where  $H$  is the Hamiltonian operator and  $\tau$  is the volume element. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives.

...the energy of the ground state of the system. The energy of the ground state of the system is given by the minimum of the energy functional  $E[\psi]$  with respect to the wave function  $\psi$ . The energy functional is given by  $E[\psi] = \int \psi^* H \psi d\tau$ , where  $H$  is the Hamiltonian operator and  $\tau$  is the volume element. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives.

...the energy of the ground state of the system. The energy of the ground state of the system is given by the minimum of the energy functional  $E[\psi]$  with respect to the wave function  $\psi$ . The energy functional is given by  $E[\psi] = \int \psi^* H \psi d\tau$ , where  $H$  is the Hamiltonian operator and  $\tau$  is the volume element. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives. The energy functional is a functional of the wave function  $\psi$  and its derivatives.



inability of the paramagnons to interact with their potential lattice ions, or  
rather, the  $\gamma$ -paramagnon dispersion is dispersive, whereas a para-  
magnon dispersion dependent on band interaction could explain this transition [56].  
Unfortunately this potential has never been examined relative  
explaining the solid lattice vibrations.

and absorption coefficients  $\epsilon_{\text{max}}$  and  $\lambda_{\text{max}}$  are the maximum of the absorption coefficient  $\epsilon$  and the wavelength  $\lambda$  at which  $\epsilon$  is maximum,  $p$  is the index of the unit cell

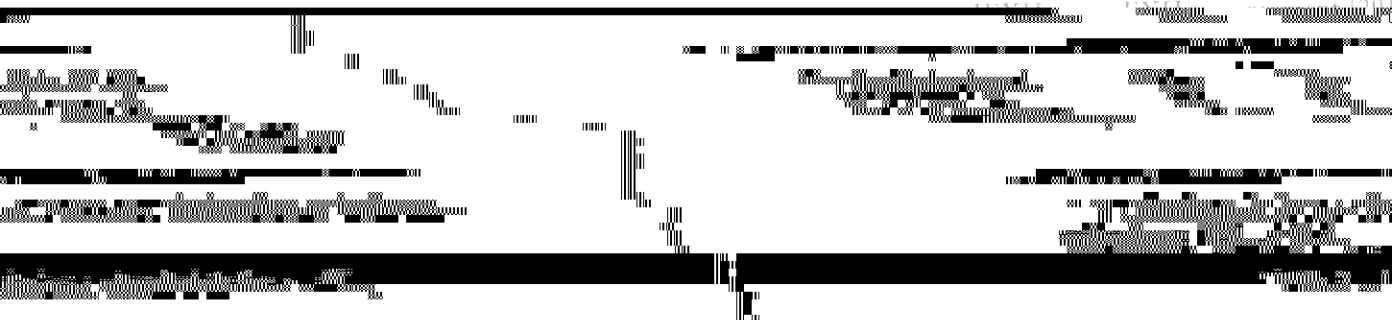


the effect of the amount of disorder on the distribution of the  $N_0$  values.

It is expected that the model calculated by the EYH

should give a good approximation to the spin density distribution. The addition of corrections to the spin density distribution...  
singularity at surface effects may give a small increase in the...  
is unlike the situation in the case of a diamond of  $111\bar{1}$  boron...  
graphite (110) by a factor of more than 10. This is due to the...  
strongly perturbs the cluster states.

Adjusted quadrangle...



...different...  
...calculation...  
...distance dependence...  
...obtained

here for the positive solution is, therefore, shorter than that for the negative solution. The rapid convergence of the potential to the ionization potential of the valence orbitals is also observed.

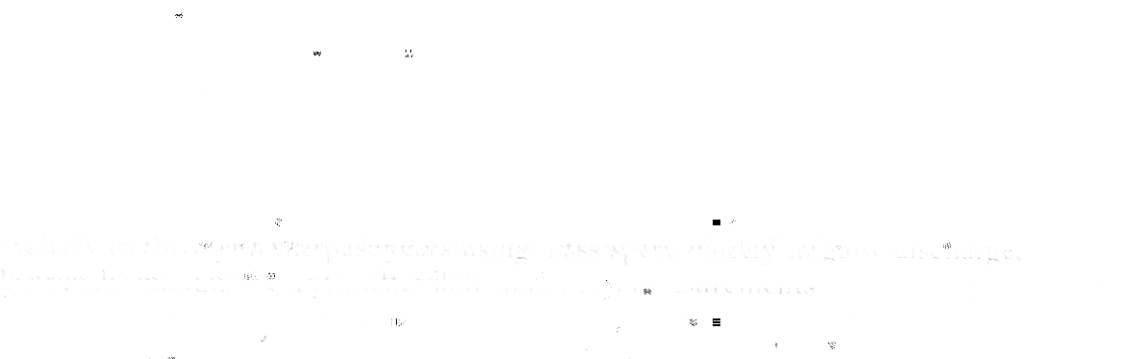


Figure 1. Ionization potential and ionization energy of the valence orbitals of the polymer chain. The potential energy is calculated from the Hartree-Fock method. The ionization energy of the valence orbitals is calculated from the Hartree-Fock method. The potential energy curve is smooth and shows a clear dip at approximately 50 Å.

The potential energy curve is smooth and shows a clear dip at approximately 50 Å.

stability was associated with a  $15\%$  reduction in the calculations of

(10) The decrease in the calculations of the calculations of

to  $0.1\text{ eV}$  by the calculations of the calculations of

experimental value of  $0.5 \pm 0.1\text{ eV}$  [31]. The EXH

9. SUMMARY AND CONCLUSIONS

FBX, FFA, and FND resin-impregnated C-AP methods were evaluated as test as-  
sessment methods to assess quality of hydraulic fracturing. A significant  
agreement has been found between the methods.



