CALCULATION OF ONE-ELECTRON WAVE FUNCTIONS AND ENERGY LEVELS OF N-BUTANE MOLECULE ON THE BASIS OF SLATER ATOMIC ORBITALS

Faig Pashaev^{1,#}, Arzuman Gasanov², Musaver Musaev³, and Ibrahim Abbasov³

¹ Baku State University, 23 Zahid Khalilov Str., Baku, 1148, AZERBAIJAN

² War College of the Armed Forces, 136 Sh. Mehtiev Street, Baku, 1065, AZERBAIJAN

³ Azerbaijan State Oil and Industry University, 20 Azadliq Str., Baku, 1010, AZERBAIJAN

Corresponding author, faig.pasha55@gmail.com

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It is known that the application of the group theory greatly simplifies the problems of polyatomic systems possessing to any space symmetry. The symmetry properties of such systems are their most important characteristics. In such systems, the Hamilton operator is invariant under unitary symmetry transformations and rearrangements of identical particles in the coordinate system. This allows to obtain information about the character of one-electron wave functions — molecular orbitals — the considered system, i.e. to symmetrise the original wave functions without solving the Schrödinger equation.

Keywords: group theory, matrix elements, molecular orbitals, orbital energies, exponential type function.

INTRODUCTION

As a result of the dramatically increased capabilities of modern computer technology, and also significant improvement in computational quantum chemical methods, modern quantum chemistry has predictive power, capable of predicting the possibility of the existence of new chemical structures, their structure and properties, and predicting new effects. One of the methods used to quantify the physico-chemical properties of multi-electron systems (multi-electron atoms, molecules, crystals) is the molecular orbital method. However, there are certain difficulties in the theoretical study of the properties of multi-electron systems by the molecular orbital method.

Some of these difficulties are related to the number of unknown quantities involved in the equations of the molecular orbital method. The large number of equations constructed for these unknown quantities makes it difficult to solve the problem. In the case of systems with certain symmetry elements, the solution of this system of equations is simplified (Wang, 2003; Falzon and Wang, 2005; Chatterjee and Wang, 2015; Wang and Chatterjee, 2017). Regarding the

molecular orbital method, the state of an electron in a multi-electronic system is described by a one-electron wave function, called the molecular orbital. Since most of the properties of a multi-electron system are related to valence electrons motion, molecular orbitals are commonly searched in the form of linear combinations of valence atomic orbitals of atoms in the system (Downton and Wang, 2006; Shi *et al.*, 2014; Tang *et al.*, 2016; Huang *et al.*, 2018). Exponential type Gauss or Slater functions are used as atomic orbitals. It has been defined that the number of Gauss functions used to obtain the same accuracy of a physical quantity significantly exceeds the number of Slater functions (Kuang and Lin, 1997; Rico *et al.*, 2004; Guseinov, 2012; Guseinov and Mamedov, 2012; Santos *et al.*, 2014). We obtain better results using Slater functions in studying of properties of diatomic molecules in the frame of the Hartree-Fock-Roothaan method (Ahmadov *et al.*, 2019; Pashayev *et al.*, 2019). The state of an electron in the valence region is described better with the Slater functions than Gauss functions. Hence, it is advisable to use Slater-type atomic orbitals in the study of the properties of multi-electron systems in valence electron approximation (Pashayev *et al.*, 2014; Ramazanov *et al.*, 2014). The n-butane molecule has

space symmetry and belongs to the point group. In the calculations the group theory method was used, the matrix elements of the generating matrix were calculated and the symmetrised molecular orbitals of this molecule were constructed. Using the $C^{-1}HC$ similarity transformation and with considering the selection rules for the matrix elements, the Hamilton operator was reduced to a quasi-diagonal form. Energy levels corresponding to molecular orbitals have been expressed in terms of the matrix elements of the Hamilton operator H_{pq} . The Wolfsberg–Helmholz (WH) approximation was used to determine H_{pq} . The orbital energies were calculated and some characteristics of the n-butane molecule were examined. Calculations were carried out on the basis of Slater-type atomic orbitals.

THEORETICAL PART

It has been known that the symmetrisation of the original wave functions of the molecule in question consists in the possibility of decomposing reducible representations into irreducible ones, each of which, as is known, corresponds to a certain energy level (Bolotin and Stepanov, 1973; Landau and Lifshits, 2004).

In the present paper the n-butane (C_4H_{10}) molecule is regarded in the coordinate system in such a way that its center of mass is located at the origin of coordinates. Figure 1 depicts the schematic diagram of the C_4H_{10} molecule. According to this diagram, Cartesian coordinates of carbon and hydrogen atoms were determined (Table 1). The point group C_{2h} contains symmetry elements: I , C_2 , σ_h and i . C_2 is the rotation axis of the second order, the σ_h plane coincides with the XOY plane and the C_2 axis with the Z axis.

The valence orbitals of the carbon atoms $2s$ -, $2p_x$ -, $2p_y$ -, $2p_z$ and $1s$ — AO of hydrogen atoms were chosen as the basis functions of the n-butane molecule. Molecular orbitals were constructed from a linear combination of atomic orbitals (Minkin *et al.*, 2010):

$$U_i = \sum_{q=1}^m c_{qi} \chi_q \quad (1)$$

Here C_{qi} is the unknown coefficient, χ_q is the atomic orbitals, and the selected number of atomic orbitals for calculations is $m = 26$. We considered the transformation of basis functions in the symmetry operations in group C_{2h} and constructed matrices of order 26 for each element of the group. The combination of these matrices is a reducible representation of the C_{2h} point group for the C_4H_{10} molecule. Using the formula

$$m_i = \frac{1}{N} \sum \chi^+ (\Gamma_i / g) \chi (\Gamma / g) \quad (2)$$

the number of irreducible representations was calculated. Here, N is the order of group, $\chi(\Gamma_i / g)$ is the character of irreducible representation of Γ_i , and $\chi(\Gamma / g)$ is the character of reducible representation of Γ . The direct sum of the point group of the molecule under consideration was obtained as follows:

Fig. 1. Structural diagram of the molecule n-butane (Feng Wang, 2003)

Table 1. Cartesian coordinates of atoms in the n-butane molecule

Atom	Coordinate	X	Y	Z
C ₁		-2.53433	3.52434	0
H ₁		-4.47698	4.21117	0
H ₂		-1.56302	4.21117	1.68238
H ₃		-1.56302	4.21117	-1.68238
C ₂		-2.53433	0.61319	0
H ₄		-3.50566	-0.07365	-1.68238
H ₅		-3.50566	-0.07363	1.68238
C ₃		0.21034	-0.35719	0
H ₆		1.18166	0.32964	-1.68238
H ₇		1.18166	0.32964	1.68238
C ₄		0.21034	-3.26834	0
H ₈		0.76010	-3.95516	-1.68238
H ₉		2.15299	-3.95516	0
H ₁₀		-0.76010	-3.95516	1.68238

$$\Gamma = 9A_g + 4A_u + 4B_g + 9B_u \quad (3).$$

Subscripts g and u refer, respectively, to symmetric and antisymmetric symmetry transformations.

Using the matrices of the reducible representation of the point group C_{2h} of the n-butane molecule, as well as the tables of the characters of the irreducible representations (Bolotin and Stepanov, 1973; Landau and Lifshits, 2004) of this point group, the elements of the generating matrix C were calculated. The elements of the columns of the generating matrix coincide with the coefficients C_{qi} of the basis functions χ_q in (1) (Bolotin and Stepanov, 1973). In accordance with formula (1), symmetrised molecular orbitals of the n-butane molecule were constructed:

$$U_1 = \frac{1}{\sqrt{2}} (\chi_8 + \chi_{14}) = \frac{1}{\sqrt{2}} (\chi_{200}^C + \chi_{200}^C)$$

$$U_2 = \frac{1}{2} (\chi_{12} + \chi_{13} + \chi_{18} + \chi_{19}) = \frac{1}{2} (\chi_{100}^{H_4} + \chi_{100}^{H_5} + \chi_{100}^{H_6} + \chi_{100}^{H_7})$$

$$U_3 = \frac{1}{2} (\chi_5 + \chi_6 + \chi_{24} + \chi_{25}) = \frac{1}{2} (\chi_{100}^{H_1} + \chi_{100}^{H_2} + \chi_{100}^{H_8} + \chi_{100}^{H_9})$$

$$U_4 = \frac{1}{2} (\chi_5 + \chi_6 - \chi_{24} - \chi_{25}) = \frac{1}{2} (\chi_{100}^{H_1} + \chi_{100}^{H_2} - \chi_{100}^{H_8} - \chi_{100}^{H_9})$$

$$U_5 = \frac{1}{\sqrt{2}} (\chi_1 + \chi_{20}) = \frac{1}{\sqrt{2}} (\chi_{200}^{C_1} + \chi_{200}^{C_4})$$

$$U_6 = \frac{1}{\sqrt{2}} (\chi_1 - \chi_{20}) = \frac{1}{\sqrt{2}} (\chi_{200}^{C_1} - \chi_{200}^{C_4})$$

$$\begin{aligned}
U_7 &= \frac{1}{\sqrt{2}} (\chi_0 - \chi_{15}) = \frac{1}{\sqrt{2}} (\chi_{211}^{C_2} - \chi_{211}^{C_3}) \\
U_8 &= \frac{1}{2} (\chi_{12} + \chi_{13} - \chi_{18} - \chi_{19}) = \frac{1}{2} (\chi_{100}^{H_4} + \chi_{100}^{H_5} - \chi_{100}^{H_6} - \chi_{100}^{H_7}) \\
U_9 &= \frac{1}{\sqrt{2}} (\chi_{11} + \chi_{17}) = \frac{1}{\sqrt{2}} (\chi_{210}^{C_2} + \chi_{210}^{C_3}) \\
U_{10} &= \frac{1}{\sqrt{2}} (\chi_{10} + \chi_{16}) = \frac{1}{\sqrt{2}} (\chi_{21-1}^{C_2} + \chi_{21-1}^{C_3}) \\
U_{11} &= \frac{1}{\sqrt{2}} (\chi_7 + \chi_{26}) = \frac{1}{\sqrt{2}} (\chi_{100}^{H_3} + \chi_{100}^{H_{10}}) \\
U_{12} &= \frac{1}{\sqrt{2}} (\chi_7 - \chi_{26}) = \frac{1}{\sqrt{2}} (\chi_{100}^{H_3} - \chi_{100}^{H_{10}}) \\
U_{13} &= \frac{1}{\sqrt{2}} (\chi_3 - \chi_{22}) = \frac{1}{\sqrt{2}} (\chi_{21-1}^{C_1} - \chi_{21-1}^{C_4}) \\
U_{14} &= \frac{1}{\sqrt{2}} (\chi_4 + \chi_{23}) = \frac{1}{\sqrt{2}} (\chi_{210}^{C_1} + \chi_{210}^{C_4}) \\
U_{15} &= \frac{1}{\sqrt{2}} (\chi_2 - \chi_{21}) = \frac{1}{\sqrt{2}} (\chi_{211}^{C_1} - \chi_{211}^{C_4}) \\
U_{16} &= \frac{1}{\sqrt{2}} (\chi_2 + \chi_{21}) = \frac{1}{\sqrt{2}} (\chi_{211}^{C_1} + \chi_{211}^{C_4}) \\
U_{17} &= \frac{1}{\sqrt{2}} (\chi_4 - \chi_{23}) = \frac{1}{\sqrt{2}} (\chi_{210}^{C_1} - \chi_{210}^{C_4}) \\
U_{18} &= \frac{1}{\sqrt{2}} (\chi_3 + \chi_{22}) = \frac{1}{\sqrt{2}} (\chi_{21-1}^{C_1} + \chi_{21-1}^{C_4}) \\
U_{19} &= \frac{1}{\sqrt{2}} (\chi_{10} - \chi_{16}) = \frac{1}{\sqrt{2}} (\chi_{21-1}^{C_2} - \chi_{21-1}^{C_3}) \\
U_{20} &= \frac{1}{2} (\chi_{12} - \chi_{13} + \chi_{18} - \chi_{19}) = \frac{1}{2} (\chi_{100}^{H_4} - \chi_{100}^{H_5} + \chi_{100}^{H_6} - \chi_{100}^{H_7}) \\
U_{21} &= \frac{1}{\sqrt{2}} (\chi_{11} - \chi_{17}) = \frac{1}{\sqrt{2}} (\chi_{210}^{C_2} - \chi_{210}^{C_3}) \\
U_{22} &= \frac{1}{\sqrt{2}} (\chi_9 + \chi_{15}) = \frac{1}{\sqrt{2}} (\chi_{211}^{C_2} + \chi_{211}^{C_3}) \\
U_{23} &= \frac{1}{\sqrt{2}} (\chi_8 - \chi_{14}) = \frac{1}{\sqrt{2}} (\chi_{200}^{C_2} - \chi_{200}^{C_3}) \\
U_{24} &= \frac{1}{2} (\chi_{12} - \chi_{13} - \chi_{18} + \chi_{19}) = \frac{1}{2} (\chi_{100}^{H_4} - \chi_{100}^{H_5} - \chi_{100}^{H_6} + \chi_{100}^{H_7}) \\
U_{25} &= \frac{1}{2} (\chi_5 - \chi_6 + \chi_{24} - \chi_{25}) = \frac{1}{2} (\chi_{100}^{H_1} - \chi_{100}^{H_2} + \chi_{100}^{H_8} - \chi_{100}^{H_9}) \\
U_{26} &= \frac{1}{2} (\chi_5 - \chi_6 - \chi_{24} + \chi_{25}) = \frac{1}{2} (\chi_{100}^{H_1} - \chi_{100}^{H_2} - \chi_{100}^{H_8} + \chi_{100}^{H_9})
\end{aligned}$$

To determine the energy levels corresponding to symmetrised molecular orbitals the similarity transformation C^{-1} was used, where C was the generating matrix, was the Hamilton operator. Using the similarity transformation and tak-

ing into account the selection of the matrix elements, the Hamilton operator was reduced to a quasi-diagonal form. As a result of the calculations, the orbital energies were expressed in terms of the matrix elements H_{pq} :

$$\begin{aligned}
\varepsilon_1 &= \frac{1}{2} (H_{8,8} + H_{8,14} + H_{14,8} + H_{14,14}) \\
\varepsilon_2 &= \frac{1}{4} (H_{12,12} + H_{12,13} + H_{12,18} + H_{12,19} + H_{13,12} + H_{13,13} + H_{13,18} \\
&\quad + H_{13,19} + H_{18,12} + H_{18,13} + H_{18,18} + H_{18,19} + H_{19,12} + H_{19,13} \\
&\quad + H_{19,18} + H_{19,19}) \\
\varepsilon_3 &= \frac{1}{4} (H_{5,5} + H_{5,6} + H_{5,24} + H_{5,25} + H_{6,5} + H_{6,6} + H_{6,24} \\
&\quad + H_{6,25} + H_{24,5} + H_{24,6} + H_{24,24} + H_{24,25} + H_{25,5} + H_{25,6} \\
&\quad + H_{25,24} + H_{25,25}) \\
\varepsilon_4 &= \frac{1}{4} (H_{5,5} + H_{5,6} - H_{5,24} - H_{5,25} + H_{6,5} + H_{6,6} - H_{6,24} \\
&\quad - H_{6,25} - H_{24,5} - H_{24,6} + H_{24,24} + H_{24,25} + H_{25,5} - H_{25,6} \\
&\quad + H_{25,24} + H_{25,25}) \\
\varepsilon_5 &= \frac{1}{2} (H_{1,1} + H_{1,20} + H_{20,1} + H_{20,20}) \\
\varepsilon_6 &= \frac{1}{2} (H_{1,1} - H_{1,20} - H_{20,1} + H_{20,20}) \\
\varepsilon_7 &= \frac{1}{2} (H_{9,9} - H_{9,15} - H_{15,9} + H_{15,15}) \\
\varepsilon_8 &= \frac{1}{4} (H_{12,12} + H_{12,13} - H_{12,18} - H_{12,19} + H_{13,12} + H_{13,13} - H_{13,18} \\
&\quad - H_{13,19} - H_{18,12} - H_{18,13} + H_{18,18} + H_{18,19} - H_{19,12} - H_{19,15} \\
&\quad + H_{19,18} + H_{19,19}) \\
\varepsilon_9 &= \frac{1}{2} (H_{11,11} + H_{11,17} + H_{17,11} + H_{17,17}) \\
\varepsilon_{10} &= \frac{1}{2} (H_{10,10} + H_{10,16} + H_{16,10} + H_{16,16}) \\
\varepsilon_{11} &= \frac{1}{2} (H_{7,7} + H_{7,26} + H_{26,7} + H_{26,26}) \\
\varepsilon_{12} &= \frac{1}{2} (H_{7,7} - H_{7,26} - H_{26,7} + H_{26,26}) \\
\varepsilon_{13} &= \frac{1}{2} (H_{3,3} - H_{3,22} - H_{22,3} + H_{22,22}) \\
\varepsilon_{14} &= \frac{1}{2} (H_{4,4} + H_{4,23} + H_{23,4} + H_{23,23}) \\
\varepsilon_{15} &= \frac{1}{2} (H_{2,2} - H_{2,21} - H_{21,2} + H_{21,21}) \\
\varepsilon_{16} &= \frac{1}{2} (H_{2,2} + H_{2,21} + H_{21,2} + H_{21,21}) \\
\varepsilon_{17} &= \frac{1}{2} (H_{4,4} - H_{4,23} - H_{23,4} + H_{23,23})
\end{aligned}$$

$$\begin{aligned}
\varepsilon_{18} &= \frac{1}{2} (H_{3,3} + H_{3,22} + H_{22,3} + H_{22,22}) \\
\varepsilon_{19} &= \frac{1}{2} (H_{10,10} - H_{10,16} - H_{16,10} + H_{16,16}) \\
\varepsilon_{20} &= \frac{1}{4} (H_{12,12} - H_{12,13} + H_{12,18} - H_{12,19} - H_{13,12} + H_{13,13} - H_{13,18} \\
&\quad + H_{13,19} + H_{18,12} - H_{18,13} + H_{18,18} - H_{18,19} - H_{19,12} + H_{19,13} \\
&\quad - H_{19,18} + H_{19,19}) \\
\varepsilon_{21} &= \frac{1}{2} (H_{11,11} - H_{11,17} - H_{17,11} + H_{17,17}) \\
\varepsilon_{22} &= \frac{1}{2} (H_{9,9} + H_{9,15} + H_{15,9} + H_{15,15}) \\
\varepsilon_{23} &= \frac{1}{2} (H_{8,8} - H_{8,14} - H_{14,8} + H_{14,14}) \\
\varepsilon_{24} &= \frac{1}{4} (H_{12,12} - H_{12,13} - H_{12,18} + H_{12,19} - H_{13,12} + H_{13,13} + H_{13,18} \\
&\quad - H_{13,19} - H_{18,12} + H_{18,13} + H_{18,18} - H_{18,19} + H_{19,12} - H_{19,13} \\
&\quad - H_{19,18} + H_{19,19}) \\
\varepsilon_{25} &= \frac{1}{4} (H_{5,5} - H_{5,6} + H_{5,24} - H_{5,25} - H_{6,5} + H_{6,6} - H_{6,24} \\
&\quad + H_{6,25} - H_{24,5} + H_{24,6} + H_{24,24} - H_{24,25} - H_{25,5} + H_{25,6} \\
&\quad - H_{25,24} + H_{25,25}) \\
\varepsilon_{26} &= \frac{1}{4} (H_{5,5} - H_{5,6} - H_{5,24} + H_{5,25} - H_{6,5} + H_{6,6} - H_{6,24} \\
&\quad - H_{6,25} - H_{24,5} + H_{24,6} + H_{24,24} - H_{24,25} + H_{25,5} - H_{25,6} \\
&\quad - H_{25,24} + H_{25,25})
\end{aligned}$$

COMPUTER CALCULATIONS

Since analytically it is impossible to calculate the H_{pq} values, various semi-empirical methods are used. In the present paper we used one of the variants of the molecular orbitals method — the WH method (Fedorov *et al.*, 2006). According to this method, the diagonal elements of the H_{pq} matrix taken with the opposite sign are equated to the ionisation energy of the corresponding valence states of the atoms that make up the molecule. The values of ionisation potentials used for the valence states of carbon and hydrogen atoms are as follows:

$$(2s|c|2s) = -0.772096 \text{ a.u.}$$

$$(2p|c|2p) = -0.419161 \text{ a.u.}$$

$$(1s|H|1s) = -0.499786 \text{ a.u.}$$

According to the WH method, the off-diagonal matrix elements are calculated by the formula (Fedorov *et al.*, 2006).

$$H_{pq} = \frac{1}{2} k S_{pq} (H_{pp} + H_{qq}) \quad (4)$$

The parameter k is assumed to be 1.75 (Fedorov *et al.*, 2006).

$$S_{pq} = \int \chi_p^* \chi_q dv \quad (5)$$

the overlap integral.

The Slater function used in our calculations is given by:

$$\chi_q \equiv \chi_{nlm}(\xi, \vec{r}) = \frac{(2\xi)^{n+1/2}}{\sqrt{(2n)!}} r^{n-1} e^{-\xi r} S_{lm}(\theta, \varphi) \quad (6)$$

$S_{lm}(\theta, \varphi)$ is the real spherical function; ξ is the exponential parameter (Bessis and Bessis, 1981), its value was calculated using the available data.

$$\xi_{2s}(C) = 1.45677; \quad \xi_{2p_x}(C) = \xi_{2p_y}(C) = \xi_{2p_z}(C) = 1.68211$$

$$\xi_{1s}(H) = 1.0.$$

r, θ, φ are the spherical coordinates of electrons. The expressions of the base Slater atomic orbitals taking into account the values of the parameters ξ and expression (5) are obtained in the following form:

$$\chi_{2s}(c) \equiv \chi_{211}^c(1.45677; \vec{r}) = \frac{1.47406}{\sqrt{\pi}} \cdot r \cdot e^{-1.45677 \cdot r} \quad (7)$$

$$\chi_{2p_x}(c) \equiv \chi_{211}^c(1.68211; \vec{r}) = \frac{3.66953}{\sqrt{\pi}} \cdot r \cdot e^{-1.68211 \cdot r} \sin \theta \cdot \cos \varphi \quad (8)$$

$$\chi_{2p_y}(c) \equiv \chi_{211}^c(1.68211; \vec{r}) = \frac{3.66953}{\sqrt{\pi}} \cdot r \cdot e^{-1.68211 \cdot r} \sin \theta \cdot \sin \varphi \quad (9)$$

$$\chi_{2p_z}(c) \equiv \chi_{210}^c(1.68211; \vec{r}) = \frac{3.66953}{\sqrt{\pi}} \cdot r \cdot e^{-1.68211 \cdot r} \cos \theta \quad (10)$$

$$\chi_{1s}(H) \equiv \chi_{100}^H(1; \vec{r}) = \frac{e^{-r}}{\sqrt{\pi}} \quad (11)$$

To calculate the overlap integrals S_{pq} we used well-known analytical expressions (Guseinov and Mamedov, 2008; Pashaev, 2009; Gasanov and Pashaev, 2016), including the values of the Cartesian coordinates of the atomic nuclei in the molecular coordinate system.

According to formula (4) the values of the H_{pq} matrices were calculated and the orbital energies of the n-butane molecule were found (in a.u.).

$$\varepsilon_1 = -1.334141, \quad \varepsilon_2 = -0.897712, \quad \varepsilon_3 = -0.863092,$$

$$\varepsilon_4 = -0.852767, \quad \varepsilon_5 = -0.787302, \quad \varepsilon_6 = -0.756890,$$

$$\varepsilon_7 = -0.615851, \quad \varepsilon_8 = -0.594016, \quad \varepsilon_9 = -0.546923,$$

$$\varepsilon_{10} = -0.506367, \quad \varepsilon_{11} = -0.504228, \quad \varepsilon_{12} = -0.495344,$$

$$\varepsilon_{13} = -0.423958, \quad \varepsilon_{14} = -0.419809, \quad \varepsilon_{15} = -0.419402,$$

$$\varepsilon_{16} = -0.418920, \quad \varepsilon_{17} = -0.418513, \quad \varepsilon_{18} = -0.424364,$$

$$\varepsilon_{19} = -0.331955, \quad \varepsilon_{20} = -0.309041, \quad \varepsilon_{21} = -0.291399,$$

$$\varepsilon_{22} = -0.222471, \quad \varepsilon_{23} = -0.210051, \quad \varepsilon_{24} = -0.198375,$$

$$\varepsilon_{25} = -0.242076, \quad \varepsilon_{26} = -0.141209$$

26 valence electrons occupy energy levels starting from the lowest to the highest one. As a result of calculations, we have obtained

$$\varepsilon_{HOMO} = \varepsilon_{13} = -11.536579 \text{ eV}$$

$$\varepsilon_{LUMO} = \varepsilon_{14} = -11.423678 \text{ eV}$$

We have also determined the ionisation energy of the n-butane molecule:

$$I = -\epsilon_{13} = -11.536579 \text{ eV}$$

CONCLUSION

The obtained results confirmed that by applying the methods of group theory we can obtain information on some properties of molecules on the basis of Slater functions. The results show that the study of the properties of multi-electron systems by quantum mechanical methods is significantly facilitated by the application of group theory. One-electron wave functions describing the state of electrons — molecular orbitals are in the form of a linear combination of atomic orbitals. The unknown coefficients in the linear combination are calculated using group theory. The orbital energies corresponding to the molecular orbitals are ultimately expressed by the overlap integrals. Analytical expressions in the scientific literature are used to calculate the overlap integrals of Slater-type atomic orbitals.

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ATSEVIŠĶU ELEKTRONU VIĻŅU FUNKCIJU UN ENERĢIJAS LĪMEŅU APRĒĶINS N-BUTĀNA MOLEKULAI, PAMATOJOTIES UZ SLEITERA ATOMA ORBITĀĻU BĀZES FUNKCIJĀM

Rakstā apskatīts aprēķina veids, lai iegūtu informāciju par molekulu īpašībām, pamatojoties uz Sleitera atoma orbitāļu bāzes funkcijām.