THE MO-SCF QUANTUM APPROACH OF THE 4-BUTYL-OXY-BENZAL-4 ETHYL-ANILINE (BBEA) MOLECULE. (I) QUANTUM ENERGETIC MOLECULAR CHARACTERISTICS

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Molecula de cristal licchid (LC) de tip smectic (SLC) 4-butil-oxi-benzal-4-etil-anilină (BBEA) este tratată teoretic cu mijloacele mecanicii cuantice moleculare nerelativiste, pentru prima dată în literatura cristalelor lichide (LC). Molecula BBEA/ $C_{19}H_{23}ON$ [44 nuclee, 152 electroni (110 de valență)], prin complexitatea sa structurală, ca sistem cuantic molecular, impune o tratare cuantică MO-SCF-LCAO/CNDO, în baza sa teoretică implicând ecuațiile Hartree-Fock-Roothaan, cu dezvoltare LCAO a orbitalilor moleculari (MO) şi cu parametrii PPP. Folosind un program de tip MO-SCF, calculele cuantice au fost performate în aproximația CNDO-2. Pentru BBEA, au fost obținute următoarele caracteristici cuantice MO-SCF energetice: energiile orbitale, energia electronică totală, energia moleculară totală, energia de legătură, potențialul de ionizare, potențialul de reducere şi lărgimea zonei interorbitale interzise. De asemenea, în articolul de față, rezultatele cuantice obținute pentru molecula BBEA sunt interpretate şi discutate.

The liquid crystal (LC) molecule of the smectic type (SLC) 4-butyl-oxy-benzal-4-ethyl-aniline (BBEA) is approached by means of the nonrelativistic molecular quantum mechanics for the first time in literature of the liquid crystals (LC). The BBEA molecule/$C_{19}H_{23}ON$ [44 nuclei, 152 electrons (110 of valence)] from its structural complexity as quantum molecular system imposes a MO-SCF-LCAO/CNDO quantum approach, in its theoretical basis the Hartree-Fock-Roothaan eqs. with LCAO expansion of the molecular orbitals (MO) and with PPP parameters. Using a computing program of MO-SCF type the quantum computations have been performed in the CNDO-2 approximation. The following quantum energetic MO-SCF characteristics have been obtained for BBEA: the orbital energies, the total electronic energy, the total molecular energy, the bonding energy, the ionization potential, the reduction potential and the width of the forbidden interorbital zone. In present paper the quantum results are interpreted and discussed for BBEA molecule.

Keywords: liquid crystal, smectic liquid crystal molecule, HFR eqs., BBEA molecule, quantum SCF energetic characteristics

1. Introduction

In the literature of the liquid crystals {LC} there is no published quantum study on any quantum molecular system (QMS) of LC class of the smectic type(SLC) [1,2]

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and there are no SLC molecular characteristics computed on the basis of the non-relativistic quantum molecular mechanics for any SLC molecule as far as we know in present . About two SLC molecules [4-butyl-oxy-benzal-4-ethyl-aniline (BBEA) [3] and p-n-octyl-oxy-benzoic acid (OBA) [4] we are very interested [5]. The OBA molecule is a SLC of structural species C while the BBEA molecule a SLC of species H [SLC (H)]. In present paper, we deal only with the BBEA molecule [1,2,3,5] because the CL molecule offers important discussions and interpretations about the relations between the nematic and smectic CL structures [5]. In the nematic liquid crystals(NLC) class we have published a quantum study about the p-azoxianisole (PPA) molecule [11].

The QMS as BBEA has the chemical formula $C_{19}H_{23}ON$, in its molecular structure having two benzene ring coupled a rigid group – C = N– (see Fig. 1), the whole molecule containing 44 atomic nuclei and 152 electrons (with 110 valence electrons). Our quantum approach [5] of the BBEA molecule gives MO-SCF-LCAO/CNDO-2 quantum energetic molecular characteristics and some electrical characteristics (the electronic charge density on the atom and net, the electric dipole moment and its Cartesian distribution in the whole molecule), but in the present paper we shall relate, interpret and discuss only the quantum energetic molecular characteristics:

the orbital energies ($\{e_i\}$) as eigenvalues from HFR eqs. (1), the total electronic energy (E_{el}), the total molecular energy (E_t), the bonding energy (E_b), the ionization potential (IP), the reduction potential (or the affinity of electrons) (RP) and the width of the forbidden interorbital zone (Δe), all these having the MO-SCF-LCAO quality with CNDO-2 approximation. For the computation of [($\{e_i\}$), E_{el}, E_t, E_b, IP, RP, Δe] through a SCF procedure, the used MO-SCF-LCAO/CNDO-2 computing program [5] in the beginning gives the SCF results for very important elements from program: the overlap integrals, the Coulomb integrals, the core Hamiltonian, DIFENG $(\Delta E_{el})_{ij}$ for maximum number of SCF iterations N_{ITmax}=30, and Hartree-Fock energy matrix.

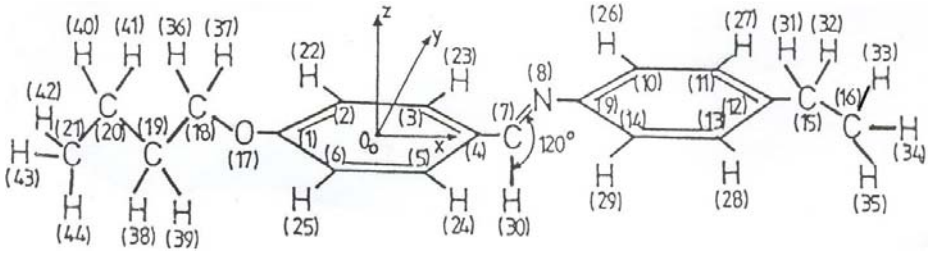

Fig. 1: The coplanar structure of the4-butyl-oxy-benzal-4-ethyl-aniline (BBEA) molecule of liquid crystal (LC) class and of the smectic type (SLC) from smectic species H [SLC(H)]and the local system of Cartesian coordinates used for the MO-SCF-LCAO/CNDO-2 quantum computations (the numbering of atoms in molecule is necessary for the input data in the computing program used).

2. Theoretical part

2.1. The MO-SCF-LCAO Roothaan equations (HFR eqs.) for the quantum study of the QMS of the LC class

Any QMS of the LC class has a great number of atoms (for ex., 44 in BBEA). This fact imposes the usage of the Hartree-Fock-Roothaan equations (HFR eqs.) from MO-SCF (molecular orbital self consistent field) theory and method [6-8], as the most good theoretical approximation for the impossible analytically accurate solving of the nonrelativistic Schrödinger quantum equation of the QMS of the LC class. The HFR eqs. as decupled equations are [5,8]:

$$\hat{F}\left|\varphi_i\right\rangle = e_i\left|\varphi_i\right\rangle \tag{1}$$

with $\hat{F}$ - the Hartree-Fock operator, $\{\left|\varphi_i\right\rangle\}$ – the molecular orbitals ({MO}), $\{e_i\}$ – the orbital energies (or eigenvalues for $\hat{F}$).

For the effective quatum computations with a computing program on the computer [5,8], (1) must be reduced to the LCAO form [6,8]:

$$\sum_{q=1}^{n_{AO}}\left(F_{pq}-e_iS_{pq}\right)c_{qi}=0 \quad \left(p=\overline{1,n_{AO}}\right) \tag{2}$$

as the LCAO Roothaan closed-shell eqs. [6], or to the matrix form:

$$\breve{F}\breve{C}=\breve{S}\breve{C}\breve{e} \tag{3}$$

with $\breve{F}$ - the Hartree-Fock matrix ($\{F_{pq}\}$ elements), $\breve{C}$ - the eigenvectors matrix ($\{c_i\}$) – the elements of matrix), $\breve{S}$ - the overlap matrix ($\{S_{pq}\}$ elements) and $\breve{e}$ - the eigenvalues matrix ($\{e_i\}$– elements). The molecular orbitals ({MO})/$\{\left|\varphi_i\right\rangle\}$ have been LCAO (linear combination of atomic orbitals {AO}) expanded:

$$\left|\varphi_i\right\rangle=\sum_{q=1}^{n_{AO}}c_{qi}\left|x_q\right\rangle \ \left(i=\overline{1,n_{MO}}\right) \tag{4}$$

using the basis of atomic orbitals $\{\left|x_q\right\rangle\}$ $\left(q=\overline{1,n_{AO}}\right)$ in number of n_{AO}. The HFR eqs. (2)/(3) are valid if it is accomplished secular equation:

$$\det\left|F_{pq}-e_iS_{pq}\right|=0 \tag{2'}$$

through its solution resulting n_{AO} orbital energies ($\{e_i\}$ $\left(i=\overline{1,n_{AO}}\right)$) and a rest ($\{e_i\}$, $i>n_{AO}\}$ representing energies for the virtual (empty) or unoccupied orbitals.

The effective salvation of the LCAO HFR (2) (or (3)) in the QMS of the LC class case demands for the computing of the molecular integrals an additional parametrisation. In ref. [5] we have used the Pariser-Parr-Pople (PPP) parameters [7,8] together with a CNDO (completed neglected of differential overlap) in the CNDO-2 variant [8]. A Slater determinant constructed from all the {MO} of the SLC molecule is the MO-SCF-LCAO total wave function for the considered QMS as the BBEA molecule [3].

2.2. The quantum energetic characteristics of the BBEA molecule. Quantum theoretical considerations

The atomic orbitals $(\{AO\})\{|x_q\rangle\}$ for the LCAO expansion of {MO} (4) are of the Slater type [9]. With a MO-SCF-LCAO/CNDO-2 computing program [5,8], for the BBEA molecule of the LC class (and smectic species H) [SLC(H)} we have obtained the following quantum energetic characteristics [5]: (c_1) $\{e_i\}$ –the orbital energies [as the solutions of the LCAO HFR eqs. (2) or (3)]; (c_2) E_{el} – the SCF total electronic energy; (c_3) E_t –the SCF total molecular energy; (c_4) E_b – the SCF bonding energy; (c_5) IP – the first ionization potential as the absolute value of e_i for the last occupied MO; (c_6) RP – the reduction potential (or the affinity of electrons) from e_j for the first empty (virtual) MO; and (c_7) Δe – the width of the forbidden interorbital zone as the zone between the last occupied MO and the first empty MO. The SCF total electronic energy (E_{el}) has been computed using the formula [5,6,8]:

$$E_{el} = \frac{1}{2}\sum_{p<q} P_{pq}\left(H_{pq} + F_{pq}\right) \tag{5}$$

which has the matrix elements: P_{pq} - the density matrix, H_{pq} - the core matrix and F_{pq} – the Hartree-Fock matrix. For the SCF total molecular energy (E_t) is used the relation (5) in:

$$E_t = E_{el} + E_{suppl} \tag{6}$$

where E_{suppl} is the interelectronic repulsion energy.
The SCF bonding (E_b) has been computed with

$$E_b = E_t - \sum_{I}^{Nn} E_I \tag{7}$$

having E_I as the energy of the component atom I (with N_n the number of nuclei).
For the MO-SCF-LCAO/CNDO-2 computations about the BBEA molecule, the equilibrium geometry is given in the Fig. 1 synthesising data from the LC literature (ref [1-4] on the bond and on the angles between the bonds [5] which are the input data [as experimental values obtained through ESR (electronic spin resonance) and NMR (nuclear magnetic resonance)]. The numbering of the 44 atoms from the BBEA molecule and the local system of Cartesian coordinates used in MO-SCF computation are given in the Fig. 1 also.

3. Results and Discussions

3.1. The SCF convergence from the MO-SCF-LCAO/CNDO-2 in the case of the BBEA molecule

The convergence criterion for the SCF procedure used in the MO-SCF-LCAO/CNDO-2 energetic computations for the BBEA molecule is the imposed value:

$$\varepsilon_{E\,\mathrm{el}} \leq 0.02 \text{ Hartrees} \cong 0.0137943 \text{ eV} \cong 2.20708 \cdot 10^{-21} \text{ J} \quad (8)$$

For the surveillance of the SCF convergence process and for a good SCF quality of the computed quantum energetic characteristics. The criterion (8) has been used for the difference of SCF total electronic energy (E_{el}) values between two successive iterations:

$$\text{DIFENG} \equiv \left|\left(\Delta E_{el}\right)\right| = \left|\left(E_{el}\right)_j - \left(E_{el}\right)_i\right| \equiv \left|\left(\Delta E_{el}\right)_{ij}\right| \quad (9)$$

at a SCF cycle of 30 iterations maximum. The reach of SCF convergence pre-established in (8) is given graphically in the Fig. 2 through the dependence:

$$\left|\left(\Delta E_{el}\right)\right| = f\left(N_{it}\right) \quad (10)$$

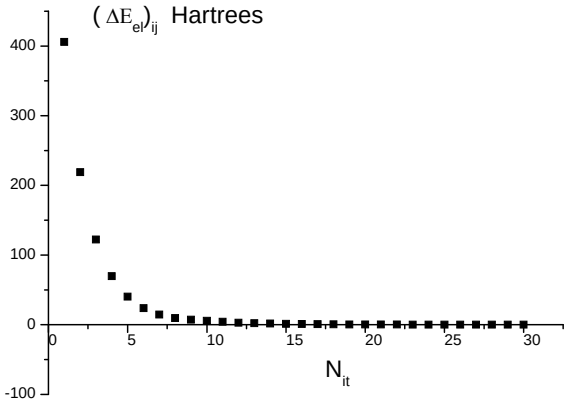

Fig. 2: The SCF convergence from the MO-SCF procedure of the quantum energetic computations in the case of the BBEA molecule through the dependence $\left|\left(\Delta E_{el}\right)_{ij}\right| = f\left(N_{it}\right)$ (10) with the accomplishment of the convergence criterion (8).

with N_{it} – the number of iterations. The plotting of the graph from fig. 2 has been made with the SCF values $\{(\Delta E_{el})_{ij}\}$ enlisted in the table 1.

Table 1

$\{(\Delta E_{el})_{ij}\}$ in the case of BBEA molecule and the SCF convergence obtained for N_{it} of 30 iterations maximum (in 1 a.u.H = 1 Hartree)*

N_{it}	$(\Delta E_{el})_{ij}$ (Hartrees)	N_{it}	$(\Delta E_{el})_{ij}$ (Hartrees)	N_{it}	$(\Delta E_{el})_{ij}$ (Hartrees)
1	-405.75485	11	-4.14020	21	-0.22015
2	-218.98312	12	-3.04266	22	-0.16486
3	-122.29504	13	-2.25116	23	-0.12451
4	-69.76593	14	-1.67554	24	-0.09198
5	-40.04327	15	-1.25067	25	-0.06860
6	-23.69781	16	-0.93292	26	-0.05084
7	-14.55664	17	-0.69916	27	-0.03906
8	-9.63306	18	-0.52301	28	-0.02948
9	-7.26563	19	-0.39197	29	-0.02130
10	-5.64471	20	-0.29327	30	-0.01703

*Obs. $\left|\left(\Delta E\right)_{29\to 30}\right| = 0.01703$ Hartrees = 0.01175 eV = $1.87932 \cdot 10^{-21}$ J < $\varepsilon_{E_{el}}$ (8)

The plotted graph from the fig.2 shows that at N_{it} = 30 the convergence criterion (8) is accomplished because in the last iteration the value $|(\Delta E)|$ is given through 0.01703 Hartrees < 0.02 Hartrees as the pre-established and imposed value for the 30 SCF iterations.

3.2. The orbital energies {e_j} of the BBEA molecule. The MO-SCF-LCAO/CNDO-2 energetic spectrum

The present paper gives the MO-SCF-LCAO/CNDO-2 quantum energetic results obtained with the computing program of the SCF quality described in ref. [5] as a computing program adapted through the PPP parameters [8] adapting the CNDO-2 version of CNDO. The SCF results as the orbital energies {e_j} are the eigenvalue from (1) obtained through (2) for the 110 valence electrons (from the total of 152, the rest being core electrons) of the BBEA molecule as QMS of the closed-shell type (having 152 electrons). The table 2 includes the values of the orbital energies indicating the 55 molecular orbitals completely (double) occupied with the 110 valence electrons, because the all orbital energies {e_j} $\left(i=\overline{1,55}\right)$ have negative values. These energies are eigenvalues of the Hartree-Fock operator $\hat{F}$ from the HFR eqs. (1) which has been written for the LCAO form (2) with the input data for the 44 atoms of the BBEA molecule through the geometrical structure from fig.1 (giving the values for the bonds and angles). Also, the table 2 shows {e_j} $\left(i=\overline{56,107}\right)$ having positive values, these representing the energies of the empty (virtual) orbital electronic levels, when the BBEA molecule will be excited some virtual levels becoming occupied.

Table 2.

The SCF orbital energies {e_j} $\left(i=\overline{1,107}\right)$ from the MO-SCF-LCAO/CNDO-2 quantum approach of BBEA for its 110 valence electrons (**) [in 1 a.u.H = 1 Hartree = 0.6897164 eV]

No. (*)	e_i $\left(i=\overline{1,36}\right)$	No. (*)	e_i $\left(i=\overline{37,72}\right)$	No. (*)	e_i $\left(i=\overline{73,107}\right)$					
1	-1.9146	19	-1.0218	37	-0.6907	55	-0.4121	73	0.2950	91	0.3927
2	-1.8980	20	-1.0061	38	-0.6602	56	0.1324	74	0.3007	92	0.4035
3	-1.7796	21	-0.9981	39	-0.6508	57	0.1343	75	0.3011	93	0.4049
4	-1.7022	22	-0.9357	40	-0.6248	58	0.1430	76	0.3048	94	0.4137
5	-1.6381	23	-0.9139	41	-0.6060	59	0.1512	77	0.3130	95	0.4381
6	-1.5780	24	-0.9038	42	-0.6003	60	0.1569	78	0.3167	96	0.4519
7	-1.4256	25	-0.8807	43	-0.5856	61	0.2507	79	0.3204	97	0.4527
8	-1.4105	26	-0.8562	44	-0.5769	62	0.2609	80	0.3214	98	0.4587
9	-1.3962	27	-0.8438	45	-0.5658	63	0.2653	81	0.3264	99	0.4597
10	-1.3401	28	-0.7903	46	-0.5468	64	0.2710	82	0.3307	100	0.4665
11	-1.2401	29	-0.7701	47	-0.5302	65	0.2751	83	0.3379	101	0.4750
12	-1.1843	30	-0.7591	48	-0.5197	66	0.2783	84	0.3386	102	0.4826
13	-1.1571	31	-0.7540	49	-0.5144	67	0.2806	85	0.3511	103	0.4931
14	-1.1282	32	-0.7243	50	-0.5084	68	0.2852	86	0.3589	104	0.5207
15	-1.0953	33	-0.7142	51	-0.4919	69	0.2863	87	0.3682	105	0.5298
16	-1.0900	34	-0.7048	52	-0.4719	70	0.2869	88	0.3742	106	0.5449
17	-1.0805	35	-0.7046	53	-0.4449	71	0.2871	89	0.3784	107	0.5585
18	-1.0642	36	-0.6908	54	-0.4358	72	0.2914	90	0.3861		

(*) the numbering of the eigenvectors {c_i} the eqs (2) and (3)
(**) the BBEA molecule has 152 electrons, the rest of 42 electrons are core electrons and quantum energetic information is included in the core Hamiltonian results.

The excitation of the BBEA molecule can be made placing the SLC(H) molecules of this class in an external electrical field, case in which the Hartree-Fock operator $\hat{F}$ from the HFR eqs. (1)-(3) will contain the term of external electrical interaction as molecular hamiltonian term. A future paper will can treat the effects of the this placing of the BBEA molecule in external electrical fields about the MO-SCF-LCAO/CNDO-2 quantum results.

The MO-SCF-LCAO/CNDO-2 energetic spectrum of the orbital energies levels in the BBEA molecule for its 110 valence electrons has been treated through graphical means in the figure 3 which shows other important energetic levels as the last occupied level of -0.4121 Hartrees = -0.37555 eV ≡ e_{55} and, respectively the first unoccupied (empty or virtual) level of +0.1324 Hartrees ≡ e_{56}. Also, the fig. 3 shows the SCF forbidden interorbital zone Δe.

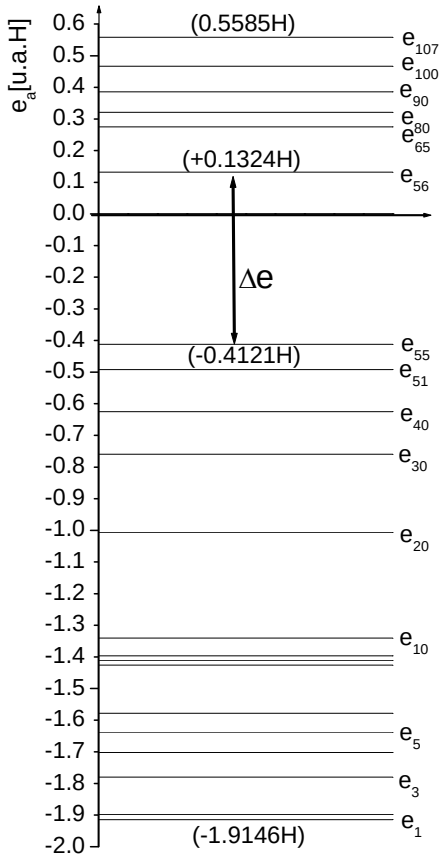

Fig. 3: The MO-SCF-LCAO/CNDO-2 energetic spectrum of the orbital energies levels in the case of BBEA molecule, through its the 110 valence electrons (from total 152 electrons, the rest of 42 as core electrons). Also, is illustrated the SCF forbidden interorbital zone of width $\Delta e = e_{56} - e_{55}$ = 0.5445 Hartrees = 0.37555 eV (between the last occupied level and the first unoccupied level). Each $e_i < 0$ $\left(i = \overline{1,55}\right)$ shows that the energy level is double occupied with valence electrons.

3.3. The quantum energetic characteristics obtained from the SCF results for the orbital energies. {IP, RP and Δe}

(a) IP as the (first) ionization potential (see ref. [8] is given through the SCF energy of the last orbital molecular occupied with two valence electrons and its value has +0.4121 Hartrees = +0.2842321 eV ≅ +0.45477 $\cdot 10^{-19}$ J, when is respected the physical mathematical definition for IP. Such, IP ≅ $|e_{55}|$ (see the table 2) can be extracted from $\{e_i\}$ $\left(i=\overline{1,107}\right)$ and used as SCF energetic value for the information about the excitation of the BBEA molecule in the ionisation process and we have:

$$(IP)_{BBEA} \equiv |e_{55}| \cong 0.28423 \text{ eV} = 0.45477 \cdot 10^{-19} \text{ J} \qquad (11)$$

The energetic level e_{55} is illustrated in the fig. 3.

(b) RP as the reduction potential (or the affinity of electrons) is obtained through the SCF energy of the first molecular orbital unoccupied (empty or virtual) but the negative sign (see ref. [8]):

$$(RP)_{BBEA} = -e_{56} = \text{-0.1324 Hartrees} \cong \text{-0.09132 eV} \qquad (12)$$

if we use the table 2 with the values of the orbital energies for the BBEA molecule.

When we compare (11) with (12), we obtain:

$$(IP)_{BBEA} \cong 3.11254|RP| \qquad (13)$$

The relation (13) shows that in the BBEA molecule the electron acceptor character determinates over the electron donor character. This fact is confirmed through the width of the SCF forbidden interorbital zone Δe (see rel. (14)).

(c) The SCF forbidden interorbital zone Δe is defined as:

$$(\Delta e)_{BBEA} = e_{56} - e_{55} \equiv IP + |RP| \qquad (14)$$

being determined as energetic width of the value $|e_{55}| > e_{56}$. This value has +0.5445 Hartrees = 0.37555 eV ≅ 6.0088 $\cdot 10^{-20}$ J and shows that the BBEA molecule has the electron acceptor character dominating its electron donor character. This SCF energetic fact it can see from the fig. 3 showing the width Δe and for the BBEA molecule as QMS of SLC(H) class can be have possible implications of electrical nature for the dipolmoment, respectively quadrupole moment, also about the interaction the BBEA molecule at micro and macromolecular levels. With the SCF results (12), (13) and (14), in future paper we shall can discuss the same SCF energetic results obtained for the PPA (p-azoxy-anisole) molecule as nematic liquid crystal class compared with the same results for the BBEA molecule as smectic liquid crystal class.

3.4. The fundamental quantum MO-SCF-LCAO/CNDO-2 energetic characteristics {E_{el}, E_t, E_b} of the BBEA molecule

Using the quantum relations (5), (6) and (7) [entirely presented in ref. [8] and very developed and detailed in ref. [5], the quantum energies: (a) E_{el} - as the SCF total electronic energy, (b) E_t – as the SCF total molecular energy and (c) E_b – as the bonding energy, with their formulas (5)-(7) adopted for a MO-SCF-LCAO/CNDO-2 computing program ([5], [8]), have been obtained for the BBEA (4-butyl-oxy-benzal-4-ethyl aniline) molecule having the following values [5]:

$$\left(E_{el}\right)_{BBEA} = -933.688 \text{ Hartrees} = -643.9799 \text{ eV} = -1.03037 \cdot 10^{-16} \text{ J} \quad (15)$$

$$\left(E_{t}\right)_{BBEA} = -182.786 \text{ Hartrees} = -126.0705 \text{ eV} = -2.01713 \cdot 10^{-17} \text{J} \quad (16)$$

$$\left(E_{b}\right)_{BBEA} = -21.802 \text{ Hartrees} = -15.0372 \text{ eV} = -2.40595 \cdot 10^{-18} \text{ J} \quad (17)$$

Because in the whole LC literature for the none of the three obtained quantum energies of the BBEA molecule there are no values for confrontation and comparison, we assert that the SCF quality of these values [(15)-(17)] is ensured through the SCF convergence of the computing procedure which discharges the convergence criterion (8) [see tab. 1 and the secv. 3.1]. In ref. [5] we have compared the (E_{el}/N_e) values for the BBEA molecule and the PPA (p-azoxyanisole) molecule [for the total number of electrons N_e (152 in BBEA and 136 in PAA)] as the average electronical energy per electron. The results are: $(E_{el}/N_e)_{BBEA} \cong -6.1468$ Hartrees, respectively $(E_{el}/N_e)_{PPA} \cong -6.3188$ Hartrees, through $(E_{el})_{BBEA}$ from (15) and $(E_{el})_{PAA} \cong -871.997$ Hartrees (ref. [5]). The good agreement between the average electronical energies per electron for BBEA and PAA shows that $(E_{el}/N_e)_{BBEA} \cong 0.97278\ (E_{el}/N_e)_{PAA}$ or $(E_{el}/N_e)_{PPA} = 1.02798\ (E_{el}/N_e)_{BBEA}$. This fact has significance for the good quality of the SCF convergence in the SCF procedure of computing program used and for the good quality of the MO-SCF-LCAO/CNDO-2 quantum values of E_{el} in the BBEA and PPA cases.

If we shall estimate for the bonding energy (E_b) an average value through the Pauling values (ref. [10]) of the energies of all direct chemical bonds between the 44 atoms of the BBEA molecule, then we have the statistical "classical" value:

$$E_b = -2.456604 \cdot 10^{-18} \text{ J} = -15.353776 \text{ eV} \cong -22.261 \text{ Hartrees} \quad (18)$$

Between values (17) and (18) for the same BBEA molecule is a relative error of 2.1053%.

4. Final specifications

The all MO-SCF results from present paper are obtained [5] through the running the MO-SCF-LCAO/CNDO-2 program [8] (in FORTRAN language) adapted for the quantum molecular system considered from the liquid crystal (LC) molecules class. The computing program has been running at the Computing Centre of the Nuclear Reactor of the IFIN Bucharest-Magurele for the doctors thesis (in theoretical physics at "Babes Bolyai" University, Faculty of Physics, Cluj-

Napoca) [5] and are performed with the help of the strong (at that calendar date) SYS-V7 group of computers [5]. For the BBEA molecule the total run time has been 10763 seconds (approx. 3 hours). The all results from present paper are unpublished results.

5. Conclusions

(1) The present paper shows the unpublished results which have been obtained for a quantum molecular system from the liquid crystal (LC) class of smectic (S) type (SLC) and of species H (SLC(H)) which is 4-butyl-oxy-benzal-4-ethyl-aniline (BBEA) molecule.
(2) All the computed quantum characteristics are of energetic type and these have the MO-SCF-LCAO/CNDO-2 quality.
(3) In the LC literature there is no quantum study about the BBEA molecule and there are no LC molecular characteristics computed on the basis of the nonrelativistic quantum molecular mechanics. For this fact, we offer for publication our quantum SCF results from ref. [5].
(4) Important aspects about the quantum SCF energetic molecular characteristics (E_{el}, E_t, E_b, IP, RP, Δe) are given and commented in the manner of the MO-SCF Roothaan theory and method [6] for the BBEA molecule having in view that the BBEA is a SLC(H) molecule. For the same SLC(H) molecule a future paper will give quantum SCF electrical characteristics which are obtained simultaneously with those quantum SCF energetic.

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