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Electronic structures and spectra of conducting anthracene derivatives

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Abstract: Theoretical studies on anthracene and a series of its derivatives were performed using the AM1 method and DFT. Based on B3LYP/6-31G(d) optimized geometries, the electronic, IR and NMR spectra of anthracene oligomers were calculated using the Indo/Cis, AM1 and B3LYP/6-31G(d) methods, respectively. The energy gaps of the oligomers decreased and the main absorptions in the electronic spectra of the oligomers were red-shifted, whereas the IR frequencies for some of the C=C and C–H bonds were blue-shifted with increasing chain length and in the presence of substituents. The ^{13}C-NMR chemical shifts of the bridged carbon atoms were upfield shifted in the presence of an electron-donating group, while the chemical shifts of the carbon atoms on the two side rings of the anthracene moiety shifted downfield in the presence of an electron-withdrawing group.

Keywords: anthracene; conducting polymer; energy gap; chemical shift; B3LYP/6-31G(d).

INTRODUCTION

Many polymers possess conductive properties, which has stimulated intensive interest of scientists. These conducting polymers are often classified into polythiophene,[1–3] polypyrrole,[4] polyheterocycles,[5,6] polyaniline[7] and polyaryl rings.[8–12] Henze *et al*. reported that the stabilities of polythiophene assemblies are enhanced with increasing chain length.[1] Methoxyl substitution in conducting polymers containing conjugated bithiazole moieties led to an improvement of the solubility.[5] For conducting copolymers of pyridine with thiophene, *n*-doped states are more stable than *p*-doped states.[6] Conducting and insulating phases are possibly located in the same polymer.[7] Polymers containing dimethyldihydropyene can be designed for optoelectronic redox switching by the introduction of a photochromic unit.[8] New phenanthroline dicarboxamide-based helical foldamers can promote the polymerization of aromatics and oligoamides for potential applica-

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tions in biology and material science.[11] Weibin *et al.* achieved the synthesis and characterization of soluble oligo(9,10-bisalkynylanthrylene)s.[12]

There are some reports on important properties of anthracene polymers, which are of interest for possible applications. Many anthracene moieties are photoluminescent, and polymers containing such units as a part of the extended π-electron system are also likely to be electroluminescent. A film of poly(anthracene-2,6-diyl) was found to be electroconducting after being doped with potassium naphthalenide polymers and ferric chloride, with conductivities of 4.0×10^{-2} and 0.12 S cm^{-1}, respectively. These film showed yellow-green luminescence.[13] Polyanthracene is partly soluble in organic solvents and its soluble part is a strong blue light emitter.[14] On the other hand, poly(9,10-anthracene diylidene) exhibits thermochromism and high thermal stability.[15–17]

However, there are only a few theoretical reports on the electronic structure and spectroscopy of anthracene derivatives. Herein, a series of such oligomers were designed to explore the effects of chain length and substituents on the energy gaps and spectra. These properties are useful to explain the conductivities and stabilities of conducting polymers.

METHODOLOGY

A linear polymer can be considered as a one-dimensional box. Electrons are delocalized and move over the whole system. Then, a minimum on the potential curve can be found. Based on the monomer anthrylene (compound **1**), compounds **2**–**4** and **5**–**11** were designed by increasing the chain length and changing the substituents, respectively (Fig. 1). The chain was elongated *via* 2,6-linkage and the substituents were inserted at the 9,10-positions on the anthrylene unit.

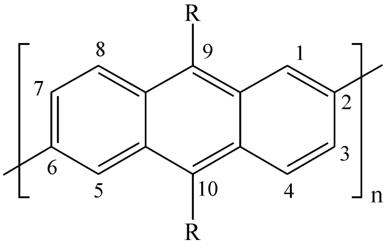

Fig. 1. The structures of compounds **1**–**11**. Compound **1**: n = 1, R = H; Compound **2**: n = 2, R = H; Compound **3**: n = 3, R = H; Compound **4**: n = 4, R = H; Compound **5**: n = 1, R = NH_2; Compound **6**: n = 1, R = NO_2; Compound **7**: n = 2, R = NH_2; Compound **8**: n = 2, R = NO_2; Compound **9**: n = 3, R = NH_2; Compound **10**: n = 3, R = NO_2; Compound **11**: n = 4, R = NH_2.

Full geometry optimization of these compounds without any symmetry restriction was performed step by step using the AM1 method and DFT at the B3LYP/STO-3G, B3LYP/3-21G and B3LYP/6-31G(d) levels (the optimized geometry of compound **11** at B3LYP/6-31G(d) level is shown in Fig. S1 in the Supplement, available only in electronic form at http://www.shd.org.rs/jscs).

The AM1 method and DFT in the Gaussian 03 program[18] were successfully employed to study the electronic structures and spectroscopic characteristics of supramolecular complexes,[19–22] intramolecular hydrogen bonding species,[23] conducting polymers[24,25] and carbon clusters.[26–29] Based on the B3LYP/6-31G(d) optimized geometries of the compounds, the configuration interaction was investigated using the Indo/Cis method.[30] By exciting electrons from the 14 highest occupied molecular orbits into the 14 lowest unoccupied orbits, this led to the generation of 196 configurations. Subsequently, the IR frequencies were computed using the AM1 method. Finally, ^{13}C-NMR chemical shifts were calculated using the Giao method at the B3LYP/6-31G(d) level.

RESULTS AND DISCUSSION

LUMO–HOMO energy gaps

The LUMO–HOMO energy gaps of the unsubstituted compounds **1**–**4** gradually decreased with increasing value of n (Table I); those of compounds **5**, **7**, **9** and **11** with R = NH_2 and of compounds **6**, **8** and **10** with R = NO_2 showed the same regularity. With decreasing energy gap, electrons can be easily excited from the ground state and, hence, the conductivities of the oligomers increased over those of the monomers. It was experimentally shown that the energy gap of oligo(9,10-bialkynylanthrylene)s decreased from 2.60 (n = 1) to 2.31 eV (n = 5),[12] supporting the above calculation results. The energy gaps of polyanthrylene, and its derivatives substituted by amino and nitrate groups were predicted *via* the extrapolation method to be 2.95, 2.38 and 2.73 eV.[25] On the other hand, the energy gaps of compounds **5** and **6** are less than that of compound **1**, owing to the presence of the substituents. The electron-donating group affects the energy gap more than the electron-withdrawing group. Comparing the energy gaps of compounds **7**–**10** with that of compound **1**, the same conclusion as above can be drawn. The HOMO energy of the oligomer increased, and the energy gap decreased in the presence of the electron-donating group,[31] which supports the present calculations. Therefore, the presence of substituents decreases the energy gaps, improves the conductivities and also enhances the solubilities of the oligomers.

TABLE I. Several variables of compounds **1**–**11** optimized at the B3LYP/6-31G(d) level

Variable	Compounds										
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
Energy gap / eV	3.599	3.230	3.045	2.995	2.902	3.182	2.615	2.913	2.463	2.760	2.393
η / eV	1.800	1.615	1.523	1.478	1.451	1.591	1.308	1.457	1.232	1.380	1.197
χ / eV	3.429	3.480	3.506	3.520	2.803	4.652	2.871	4.780	2.910	4.849	2.926
IP / eV	5.228	5.095	5.028	4.997	4.254	6.243	4.178	6.236	4.141	6.229	4.122
EA / eV	1.629	1.865	1.983	2.042	1.352	3.061	1.563	3.323	1.678	3.469	1.729

In addition to C2–C6 coupling of the anthracene units in Fig. 1, coupling at the 9,10-positions was also considered. The energy gaps of the analogous oligomers (n = 1, 2, 3) formed *via* 9,10-linkages were calculated to be 3.599, 2.144 and 1.158 eV at the B3LYP/6-31G(d) level, respectively. The energy gaps decreased with increasing chain length. Compared with those obtained for 2,6-linkages in Table 1, the energy gaps of the oligomers with 9,10-linkage become small. Since C9 and C10 are located at the middle positions of the anthracene unit, the 9,10-lingkage is favorable for the overlapping of the electron cloud between neighboring anthracene units. Hence, polyanthracenes formed *via* 9,10-linkages will exhibit better conductivities than those formed *via* 2,6-lingkages.

Some important variables

Conducting polymers generally display poor thermodynamic stabilities due to their expanded conjugated structures. The improvement of their stability is a main problem. The influence of substituents on stability was investigated in this study. The ionization potential (*IP*), electron affinity (*EA*), absolute hardness (η) and absolute electron negativity (χ) (Table I) changed linearly as the chain length increased. The *IP* and η values of compounds **1**–**4** decreased with increasing n. Thus, polyanthrylene easily looses electrons and its thermal stability becomes worse. Simultaneously the *EA* and χ of compounds **1**–**4** grew more, leading to the easy reduction of polyanthrylene. Then the polymer is reactive. The experimental *IP* values of the substituted anthrylene decreased from 5.45 (n = 1) to 5.29 eV (n = 5), whereas the *EA* values increased from 2.85 (n = 1) to 2.98 eV (n = 5),[12] supporting the above calculation results. Observing the values of the four variables of compounds **5**, **7**, **9** and **11** and **6**, **8** and **10**, it can be concluded that the polyanthrylenes substituted by electron-withdrawing and donating groups also possess sensitive redox characteristics.

The *IP* and *EA* values of compound **5** are lower than those of compound **1**, thus it is easy inject holes into compound **5**. The *IP* and *EA* values of compound **6** are higher than those of compound **1**, thus compound **6** easily catch electrons. Hence, the presence of the electron-donating group leads to easy oxidation, whereas the electron-withdrawing group stimulates reduction of the substituted polyanthrylenes. The η values of compounds **5** and **6** are lower than that of compound **1**, thus the presence of the substituents does not improve the thermal stability of the polymer.

Intrinsic conducting materials with large *EA* and χ values, such as compounds **6**, **8** and **10**, are likely to undergo *n*-doping. Compounds **5**, **7**, **9** and **11** of lower *IP* have a low oxidation potential, resulting in a low resistance and good conductivity. For example, the anthrylene pentamer with the electron-donating group displays a large charge carrier mobility of 2.95×10^{-3} cm^2 V$^{-1}\cdot$s^{-1}.[12]

Electronic absorption spectra

The main absorption peaks in the electronic spectrum of compound **1** were calculated to be at 215.8, 230.6, 276.6 and 317.4 nm. The first absorption at 317.4 nm was scaled by the multiplier 1.18, although its oscillator strength, 0.0109, was small compared with the experimental result 375 nm.[14] There was a large red-shift in the absorptions at 228.1, 267.4, 296.1, 354.4 and 364.6 nm of compound **2** compared with those of compound **1** (Fig. 2; the electronic spectra of other compounds are given in Fig. S2 of the Supplement). Simultaneously, the bands of compound **2** are split and broadened due to its low symmetry because the two anthrylene planes are not coplanar in the presence of the large steric effect. The absorptions at 235.2 and 362.4 nm of compound **3** were red-shifted relative to 228.1 and 354.4 nm of compound **2**. Those at 306.5 and 366.0 nm of compound **4** were also red-shifted in comparison with 304.3 and 362.4 nm of compound **3**. Thus, the main absorption bands were red-shifted as the chain length increased, which is in agreement with the experimental conclusion that the first UV absorptions of substituted anthrylene are red-shifted as *n* increases from 1 to 5.[12]

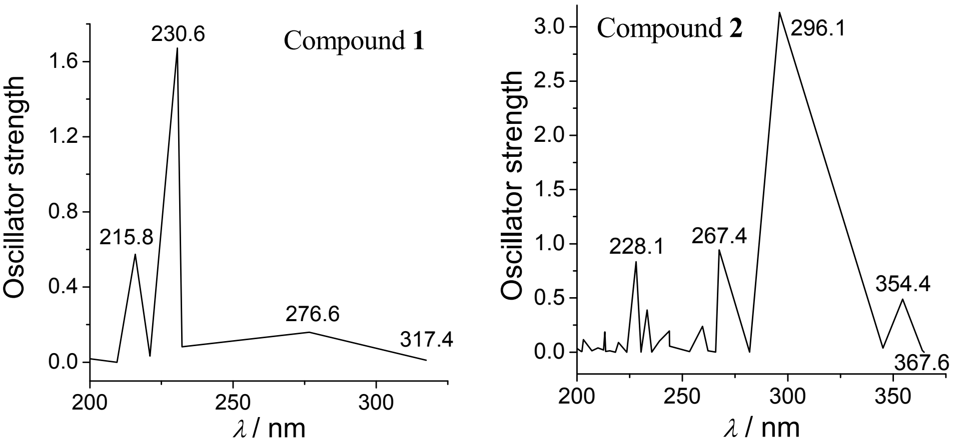

Fig. 2. The electronic spectra of compounds **1** and **2** calculated by the Indo/Cis method.

The first peak of compound **5** appeared at 395.2 nm, arising from the π-π* transition of the HOMO (39) to the LUMO (40), in view of the valence electrons of the Indo method. This absorption was red-shifted compared with that of compound **1**, which was caused by substitution with NH_2 groups. The contribution coefficients of the P_z atomic orbitals of the two nitrogen atoms to the HOMO (39) are 0.2256 and –0.2256, and those to the LUMO (40) are both –0.1104. Obviously, the atomic orbitals of the nitrogen atoms participate in the formation of the molecular orbitals and play an important role in the frontier orbitals. This effect results in a decrease of the energy gap and red-shifts of the main electronic transitions. Similarly, the main peaks of compounds **5**, **7**, and **9** are sequentially red-shifted.

The main peaks of compound **6**, appearing at 257.0 and 296.4 nm, were red-shifted compared with 230.6 and 276.6 nm of compound **1**. This is caused by the substitution of the NO_2 group. These two absorptions of compound **6** are blue-shifted in contrast to 262.5 and 395.2 nm of compound **5**. The presence of the electron-donating group in compound **5** leads to a smaller energy gap. The strongest peaks at 257.0, 287.2 and 292.0 nm of compounds **6**, **8** and **10** were gradually red-shifted, which is ascribed to the lower energy gap and decrease in symmetry with elongation of the chain length.

IR spectra

The stabilities of polymers are related to the delocalization of electrons and strength of the main chain bonds, which can be reflected in the IR spectra. The main absorption peaks in the IR spectrum of compound **1** were calculated to be at 723.4, 880.7 and 3289.0 cm^{-1}. The first two bands are assigned to the C–H out-of-plane deformation vibrations, which are consistent with the experimental results of 725 and 883 cm^{-1}.[14] The last one is attributed to the C–H stretching vibration. There were large blue-shifts in the absorptions at 736.0, 903.2 and 3289.9 cm^{-1} of compound **2** relative to those of compound **1** (Fig. 3; the IR spectra of the other compounds are given in Fig. S3 of the Supplement). Simultaneously, the number of the absorptions increased with increasing chain length. These absorptions of compound **2** were further blue-shifted to 737.5, 908.0 and 3290.0 cm^{-1} in compound **3**. This indicates that the C–H bonds were strengthened with enlargement of the conjugation system and delocalization of the electrons.

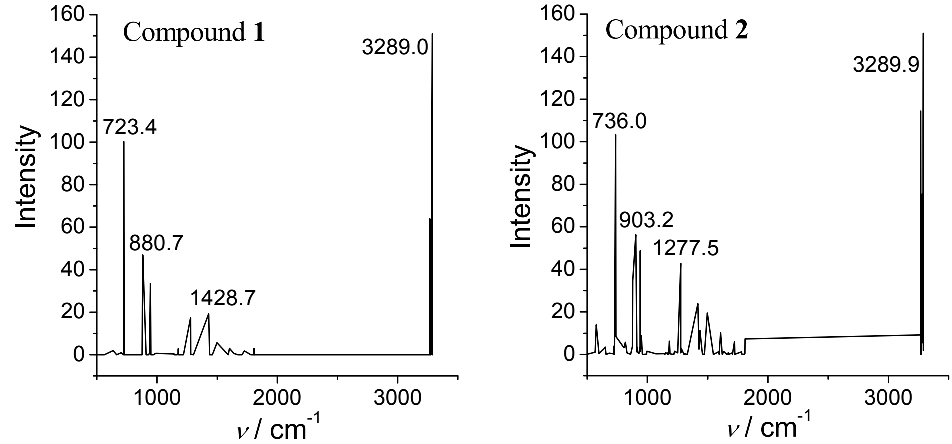

Fig. 3. The IR spectra of compounds **1** and **2** calculated by the AM1 method.

The main IR absorptions of compound **5** were at 846.4, 1660.8 and 3292.7 cm^{-1}, *i.e.*, blue-shifted relative to the corresponding bands of compound **1** at 880.7, 1428.7 and 3289.0 cm^{-1}. The absorption at 1660.8 cm^{-1} of compound **5** is generated by the stretching vibration of the C=C bonds, which is basically consistent with the experimental frequency at 1597 cm^{-1} of the C=C bonds in polynaphthylene.[10] The IR band at 1660.8 cm^{-1} of compound **5** could be due to deformation vibration of the N–H bond of the primary aromatic amine. The presence of the electron-donating groups in compound **5** elevates the electron density on the anthrylene ring and strengthens the C=C and C–H bonds. The main absorptions at 850.0, 3292.9 and 3363.8 cm^{-1} arising from the C–H and N–H bonds in compound **7** were blue-shifted compared with those of compound **5**. The N–H stretching vibration at 3363.8 cm^{-1} in compound **7** is less strong than the O–H stretching vibration at 3383 cm^{-1} in polynaphthylene.[10] The absorption at 1658.8 cm^{-1} resulting from the C=C bonds in compound **7** was red-shifted relative to that of compound **5**. The main absorptions at 853.4, 3293.3 and 3364.7 cm^{-1} in compound **9** were blue-shifted, whereas the absorption at 1658.1 cm^{-1} was red-shifted in comparison with the corresponding bands in compound **7**. The electron density on the anthrylene ring decreased as the chain length increased, leading to a weakening of the C=C bonds and a strengthening of the C–H and N–H bonds.

The main IR absorptions caused by the C–H bonds of compounds **6**, **8** and **10** compared with those of compounds **5**, **7** and **9** were blue-shifted, whereas those arising from the C=C bonds were red-shifted. The absorptions near 1867 cm^{-1} of compounds **6**, **8** and **10** resulted from N=O bonds, which were stronger than the C=O bonds with an experimental stretching frequency at 1743 cm^{-1}.[32] The π-electron density on the anthrylene ring was delocalized in the presence of the $-NO_2$, which reduced the strength of the C=C bonds.

NMR spectra

The change in electron density of the carbon atoms and symmetry of the oligomers can be observed in the NMR spectra, which are helpful in understanding the stabilities of polymers. The chemical shifts δ of the hydrogen atoms in the ^{1}H-NMR spectra of compounds **1**–**3** were calculated to be in the ranges 5.4–9.2, 5.3–11.9 and 5.3–12.1 ppm, respectively. Thus, the range of the δ values of the hydrogen atoms was enlarged and the δ data were shifted downfield with increasing n. The electrons on the hydrogen atoms were delocalized and the shielding effect was reduced with the increasing chain length. The δ data of the hydrogen atoms on the naphthylene ring were determined to be at 7.1–7.6 ppm,[10] which supports the above calculation.

The δ values of the carbon atoms in the ^{13}C-NMR spectrum of compound **1** appeared in the range 126.2–195.9 ppm. The absorption at 126.2 ppm arose from C(9) and C(10), whereas the absorption at 195.9 ppm is ascribed to C(11)–C(14). The δ data of C(2) and C(6) for the linkage of the two anthrylene rings in compound **2** were shifted downfield to 167.1 ppm (Fig. 4; the NMR spectra of the other compounds are given in Fig. S4 of the Supplement), and the C–C bond was weakened because of the formation of the dimer. In the naphthylene oligomer, the δ values of the two linkage carbon atoms were also downfield shifted from 118.7 to 120.6 ppm.[10] The ^{13}C-NMR absorptions of compound **3** were split because of the decreased symmetry. The δ data of C(9) and C(10) in compound **5** were shifted downfield to 130.1 ppm, while those of C(11)–C(14) were shifted upfield till 170.3 ppm. The situation was similar for compound **7**. The presence of the electron-donating group decreased the electron density on the neighboring carbon atoms but increases that on the bridged carbon atoms. The δ data of C(9) and C(10), and C(11)–C(14) in compound **6** were shifted upfield to 87.2 and 184.4 ppm, respectively, while those of C(1), C(4), C(5) and C(8), and C(2), C(3), C(6) and C(7) were shifted downfield to 159.6 and 169.2 ppm, respectively. A similar regularity was observed in the bands of compound **8**. The presence of the electron-withdrawing group reduces the electron density on the two side rings, but elevates that on the middle ring in the anthrylene unit.

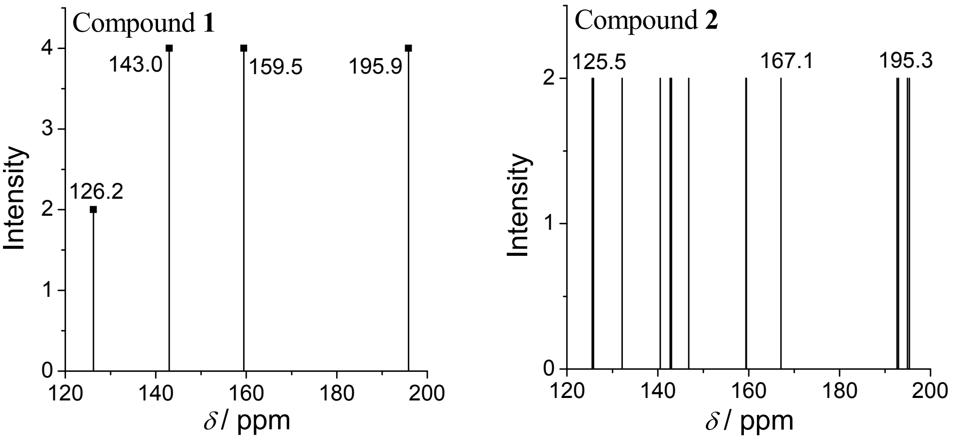

Fig. 4. ^{13}C-NMR spectra of compounds **1** and **2** calculated on the B3LYP/6-31G(d) level.

CONCLUSIONS

The electronic structures and spectroscopic characteristics of the anthrylene oligomers were affected by the chain length and substituents. The energy gaps of the oligomers decreased with increasing number of repeating units, thus polyanthrylene becomes a conducting polymer. The presence of the substituents decreases the energy gaps of the oligomers. Substitution by NO_2 or NH_2 groups and elongation of the chain length lead to red-shifts of the main absorptions in the electronic spectra of the oligomers. The electron density on the bridged carbon atoms in the anthrylene ring was elevated on substitution by amino groups; thus the C=C and C–H bonds are strengthened. The anthrylene polymer with the amino groups was predicted to be a better conducting material because of its lower oxidation potential and energy gap.

SUPPLEMENT

Available in electronic form only (http://www.shd.org.rs/JSCS/).

И З В О Д

ЕЛЕКТРОНСКА СТРУКТУРА И СПЕКТРИ ПРОВОДНИХ ДЕРИВАТА АНТРАЦЕНА

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Теоријске студије антрацена и серије његових деривата изведене су помоћу AM1 методе и DFT. На основу B3LYP/6-31G(d) оптимизованих геометрија израчунати су електронски, IR и NMR спектри антраценових олигомера помоћу Indo/Cis, AM1 and B3LYP/6-31G(d) метода, респективно. Разлике у енергетским нивоима олигомера се смањују, а главни апсорпциони максимуми им се померају ка црвеном делу спектра, док су IR фреквенције неких C=C and C–H веза померене ка плавом делу спектра са повећањем дужине ланца и у присуству супституента. ^{13}C-NMR хемијска померања чворних атома угљеника померају се ка мањим δ вредностима у присуству електрон-донорских група, док се δ вредности угљеникових атома спољашњих прстенова антраценских делова молекула повећавају у присуству електрон-акцепторских група.

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