

Tert-butyl esters of 2,3-diaryl-3-arylaminopropanoic acids – stereoselective synthesis, isolation, spectroscopic and structural elucidation

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A series of seven substituted *tert*-butyl esters of 2,3-diaryl-3-arylaminopropanoic acids has been synthesized, isolated, spectroscopically and structurally elucidated. An influence of the substituents on the spectroscopic characteristics and conformations is discussed using the data of the linear-polarized IR- (IR-LD), UV-spectroscopy and ¹H-NMR. Theoretical quantum chemical calculations are carried out, with a view to explaining and supporting the experimental optical properties and the electronic structure. The stereoselective synthesis of the corresponding diastereoisomers is optimized, thus giving good yields (62–72%) and purity of the compounds

Keywords: *tert*-butyl esters of 2,3-diaryl-3-arylaminopropanoic acids, optical properties, quantum chemistry.

INTRODUCTION

The design of novel substituted β -amino acid derivatives is still interesting for organic chemistry due to their biologically important properties and the occurrence in natural products^{1–3}. The stereoselective synthesis and optimization of the synthetic pathway for the obtaining of the pure diastereoisomers in good yields is an important key for the preparation of these compounds which are useful as building blocks for β -lactams^{4–8} and peptides, containing β -amino acids^{4,6}. Herein we report the synthesis, isolation, spectroscopic and structural elucidation of seven substituted *tert*-butyl esters of 2,3-diaryl-3-arylaminopropanoic acids, depicted and numbered in Scheme 1. The optimized synthetic pathway results to formation of the pure diastereoisomers. The optical properties of the compounds (1)–(7), are fully characterized both theoretically and experimentally by means of the polarized IR- and UV-spectroscopy, as well as quantum chemical ab initio and DFT calculations. In addition ¹H-NMR measurements are applied.

EXPERIMENTAL

Materials and methods

The IR-spectra were measured on a Thermo Nicolet FTIR-spectrometer (4000–400 cm⁻¹, 2 cm⁻¹ resolution, 200 scans) equipped with a Specac wire-grid polarizer. Non-polarized solid-state IR spectra were recorded using the KBr pellets technique. The oriented samples were obtained as a suspension in a nematic liquid crystal (MLC 6815, Merck) with the presence of an isolated nitrile stretching IR-band at about 2245 cm⁻¹ additionally serving as an orientation indicator^{9–17}.

Ultraviolet (UV-) spectra were recorded on Tecan Safire Absorbance/Fluorescence XFluor 4 V 4.40 spectrophotometer operating between 190 and 900 nm, using solvent ethanol (Uvasol, Merck product) at a concentration of 2.5·10⁻⁵ M in 0.921 cm quartz cells.

The elemental analysis was carried out according to the standard procedures for C and H (as CO₂ and H₂O) and N (by the Dumas method).

The melting points were measured on Kofler apparatus and were uncorrected. The TLC was performed on the

plates of Silica Gel 60 (Merck) with hexane: acetone (6:1) as a mobile phase.

¹H NMR-Spectra were recorded on Avance DRX 250 spectrometer (250 MHz). Chemical shifts are reported relative to TMS as an internal standard.

Quantum chemical calculations are performed with the GAUSSIAN 98 and Dalton 2.0 program packages^{18,19}. The geometries of (1)–(7) are optimized at density functional theory (DFT) using the 6-311++G** basis set. The DFT method employed is B3LYP, which combines Becke's three-parameter non-local exchange function with the correlation function of Lee, Yang and Parr^{20–22}. Molecular geometries of the studied species are fully optimized by the force gradient method using Berny algorithm. For every structure, the stationary points found on the molecule potential energy hypersurfaces are characterized using standard analytical harmonic vibrational analysis. The absence of the imaginary frequencies, as well as of the negative eigenvalues of the second-derivative matrix, confirmed that the stationary points correspond to the minima of the potential energy hypersurfaces. The calculated vibrational frequencies and infrared intensities are checked to establish which kind of performed calculations are in the best agreement with the experimental data. The DFT method provides accurate vibrational data, as far as the calculated standard deviations of less than 8 cm⁻¹ are concerned, which correspond to groups, not participating in significant intra- or intermolecular interactions. A modification of the results using the empirical scaling factor 0.9614 is done to achieve better correspondence between the experimental and theoretical values^{23,24}. TD DFT and CIS calculations are performed for elucidation of the theoretical optical properties of the seven compounds in solution. The theoretical approach is described in^{9–17}.

Synthesis

Preliminary experiments²⁵ for the optimization of the reaction of *tert*-butyl phenylacetate and benzylideneaniline revealed that good yields and stereoselectivity for the product (1) was obtained by performing the reaction in PTC (phase-transfer catalysis) conditions. The compounds (1)–(7) were prepared according to the following procedure: Aqueous sodium hydroxide (50%, 5 mL) is added to the magnetically stirred solution of *tert*-butyl phenylacetate (10

mmol) and the corresponding arylmethylideneaniline (Schiff base) (10 mmol) in 5 mL CH_3CN , using benzyltriethylammonium chloride (TEBA) (0.5 mmol) as a PTC. Thus prepared acetonitrile solutions are stirred at room temperature for 1h (for compounds **1**, **3**–**7**) or 24 h (for compound **2**). Water (50 mL) was added and the solid was collected and washed with water to the neutral. The following diastereomeric ratios were observed ($^1\text{H-NMR}$) for the crude products (*erythro*/*threo* ratio is 85:15 for compounds **1**, **3** and **5**; 95:5 for **4**, **6**, **7** and 15:85 for compound **2**). After recrystallization the main diastereoisomers of the products (**1**)–(**7**) were isolated with 62–72% yields. The configuration of the isolated diastereoisomers is determined, using their $^1\text{H-NMR}$ spectra and literature data²⁶ for the similar compounds.

erythro-(**1**): m.p. 186–188°C (benzene/hexane); Yield 70%; found C, 80.39%, H, 7.50%, N, 3.75%; calcd. [$\text{C}_{25}\text{H}_{27}\text{NO}_2$], C, 80.40%, H, 7.29%, N, 3.75%. $^1\text{H-NMR}$ (CDCl_3): 1.18 (s, 9H), 3.77 (d, 1H, $J = 10.1$ Hz), 4.88 (d, 1H, $J = 10.1$ Hz), 6.39 (d, 2H); 6.59 (t, 1H), 6.98 (t, 2H), 7.16–7.51 (m, 10H); *threo*-(**2**): m.p. 144–146°C (ethanol); Yield 44%; found C, 80.51%, H, 7.42%, N, 3.87%; calcd. [$\text{C}_{26}\text{H}_{29}\text{NO}_2$], C, 80.59%, H, 7.54%, N, 3.61%. $^1\text{H-NMR}$ (CDCl_3): 1.34 (s, 9H), 2.24 (s, 3H), 3.93 (d, 1H, $J = 6.9$ Hz), 4.88 (d, 1H, $J = 6.9$ Hz), 5.09 (br s, 1H), 6.32 (d, 2H), 6.53 (d, 1H), 6.88 (d, 1H), 7.00 (d, 1H), 7.13–7.6 (m, 10H); *erythro*-(**3**): m.p. 149–151°C (ethanol/ethyl acetate); Yield 66%; found C, 80.85%, H, 7.28%, N, 3.71%; calcd. [$\text{C}_{26}\text{H}_{29}\text{NO}_2$], C, 80.59%, H, 7.54%, N, 3.61%. $^1\text{H-NMR}$ (CDCl_3): 1.18 (s, 9H), 2.12 (s, 3H), 3.76 (d, 1H, $J = 10.1$ Hz), 3.83 (br s, 1H, 4.87), (d, 1H, $J = 10.1$ Hz), 6.19 (d, 2H), 6.41 (d, 1H), 6.87 (t, 1H), 7.23–7.55 (m, 10H); *erythro*-(**4**): m.p. 160–162°C (hexane); Yield 63%; Found C, 80.83%, H, 7.36%, N, 3.61%; calcd. [$\text{C}_{26}\text{H}_{29}\text{NO}_2$], C, 80.59%, H, 7.54%, N, 3.61%. $^1\text{H-NMR}$: 1.18 (s, 9H), 2.12 (s, 3H), 3.76 (d, 1H, $J = 10.1$ Hz), 4.84 (d, 1H, $J = 10.1$ Hz), 6.30 (d, 2H), 6.79 (d, 2H), 7.4–7.50 (m, 10H); *erythro*-(**5**): m.p. 150–152°C (ethanol/ethyl acetate); Yield 62%; Found C, 73.82%, H, 6.11%, N, 3.70%; calcd. [$\text{C}_{25}\text{H}_{26}\text{ClNO}_2$], C, 73.61%, H, 6.42%, N, 3.43%. $^1\text{H-NMR}$ (CDCl_3): 1.22 (s, 9H), 3.85 (d, 1H, $J = 9.7$ Hz), 4.65 (d,

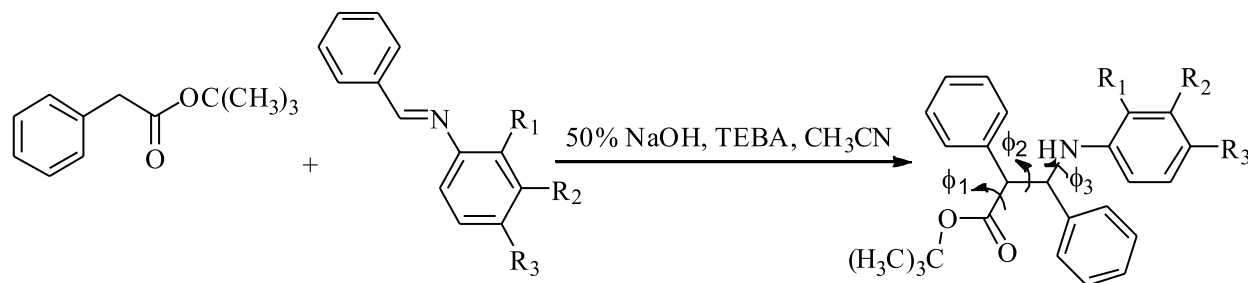
$J = 4.2$ Hz), 4.90 (dd, 1H, $J_1 = 9.7$ Hz, $J_2 = 4.3$ Hz), 6.41 (dd, 1H), 6.49 (dt, 1H), 6.88 (dt, 1H), 7.09 (dd, 1H), 7.24–7.48 (m, 10H); *erythro*-(**6**): m.p. 157–159°C (ethanol/ethyl acetate); Yield 71%; found C, 73.86%, H, 6.61%, N, 3.50%; calcd. [$\text{C}_{25}\text{H}_{26}\text{ClNO}_2$], C, 73.61%, H, 6.42%, N, 3.43%. $^1\text{H-NMR}$ (CDCl_3): 1.19 (s, 9H), 3.76 (d, 1H, $J = 10.0$ Hz), 3.96 (br s, 1H), 4.87 (dd, $J_1 = 10.0$ Hz, $J_2 = 4.1$ Hz), 6.25 (dd, 1H), 6.37 (t, 1H), 6.55 (dd, 1H), 6.88 (t, 1H), 7.22–7.47 (m, 10H); *erythro*-(**7**): m.p. 154–156°C (hexane); Yield 71%; found C, 73.87%, H, 6.13%, N, 3.43%; calcd. [$\text{C}_{25}\text{H}_{26}\text{ClNO}_2$], C, 73.61%, H, 6.42%, N, 3.43%. $^1\text{H-NMR}$ (CDCl_3): 1.19 (s, 9H), 3.76 (d, 1H, $J = 10.0$ Hz), 3.91 (br s, 1H), 4.84 (d, $J = 10.0$ Hz), 6.31 (d, 2H), 6.93 (d, 2H), 7.25–7.47 (m, 10H).

RESULT AND DISCUSSION

The performed conformational analysis is carried out by the variation of the dihedral angles ϕ_1 – ϕ_3 (Scheme 1). The potential energy surphases show series of conformational minima are obtained with the energy values E less than 0.5 kJ/mol.

The theoretical geometry parameters and the most stable form are compared with the available crystallographic data of the derivatives of 3-hydroxy-2,3-diphenylpropanoic acid^{27,28}. The main difference is obtained comparing the dihedral -N-C-C-C(O)- angle values show a difference of 2.1° , thus indicating an excellent correlation between the theoretical and experimental geometry parameters. The obtained $z = 2$ proposed a Davydov splitting effect of corresponding IR-spectra in crystalline state of pairs of maxima with different polarization according to the theoretical background in^{9–17}. The group theory proposed a close to the co-linear orientation of the $\bar{\nu}_{\text{NH}}$ and $\bar{\nu}_{\text{C=O}}$ in the frame of the isolated molecule of (**2**) as well as in the frame of the unit cell. The corresponding dihedral angle of both transition moments is $11.2(4)^\circ$. In contrast the out-of-plane vibrations of the aromatic fragments would be eliminated at a different dichroic ratios.

The IR-spectroscopic elucidation of the pure diastereoisomers in the solid-state (Fig. 1) is obtained by means of the Linear-dichroic infrared (IR-LD) spectroscopic



- $R_1 = R_2 = R_3 = \text{H}$ (**1**);
- $R_1 = \text{CH}_3$, $R_2 = R_3 = \text{H}$ (**2**);
- $R_2 = \text{CH}_3$, $R_1 = R_3 = \text{H}$ (**3**);
- $R_3 = \text{CH}_3$, $R_1 = R_2 = \text{H}$ (**4**);
- $R_1 = \text{Cl}$, $R_2 = R_3 = \text{H}$ (**5**);
- $R_2 = \text{Cl}$, $R_1 = R_3 = \text{H}$ (**6**);
- $R_3 = \text{Cl}$, $R_1 = R_2 = \text{H}$ (**7**)

Scheme 1. Chemical diagram of *tert*-butyl esters of 2,3-diaryl-3-arylamino propanoic acids (**1**)–(**7**)

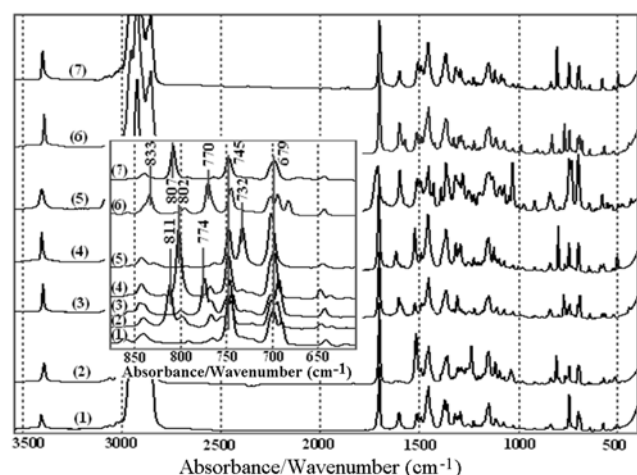


Figure 1. IR-spectra of (1)-(7) in solid-state in KBr pellets; The corresponding IR-spectroscopic region within 900–600 cm^{-1} shown in the small figure

measurements. The application of the reducing-difference procedure result to the experimental IR-assignment of the spectroscopic characteristics. The presence of the CH_3 - or Cl-substituents weakly affects on the peak positions on the characteristics IR-maxima of the compounds (1)-(7) (Fig. 1). The $\bar{\nu}_{\text{NH}}$ and $\bar{\nu}_{\text{C=O}}$ stretching vibrations are affected about 11 cm^{-1} depending of the type of the substituents. In plane vibrations of the aromatic fragments within 1650–1450 cm^{-1} differ about 4 cm^{-1} . These substituents significantly affect only the out-of-plane vibrations of the phenyl-fragments, observing within 800–600 cm^{-1} (Fig. 1). The application of the reducing-difference procedure of the $\bar{\nu}_{\text{NH}}$ IR-band leads to strong reduction of corresponding $\bar{\nu}_{\text{C=O}}$ maximum, which is in accordance with the theoretical conformations (Scheme 2). The same is valid for the elimination of the out-of-plane vibrations of the aromatic fragments (Fig.2), at different dichroic ratio, which is also in accordance with the predicted and experimentally observed geometries of (1)-(7).

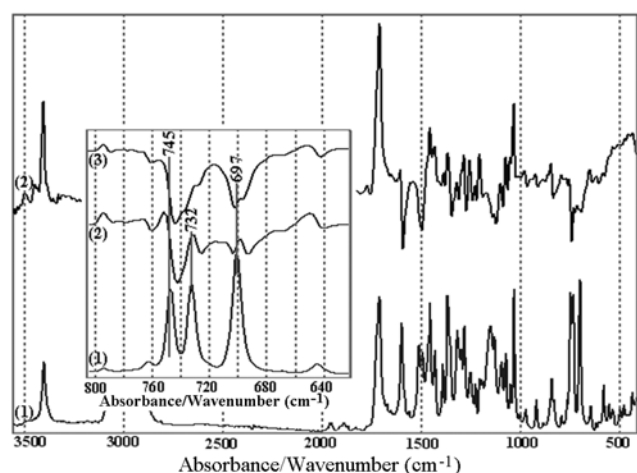
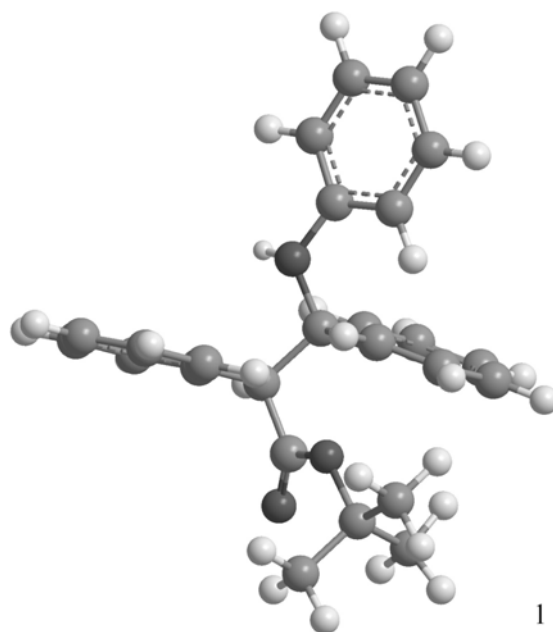
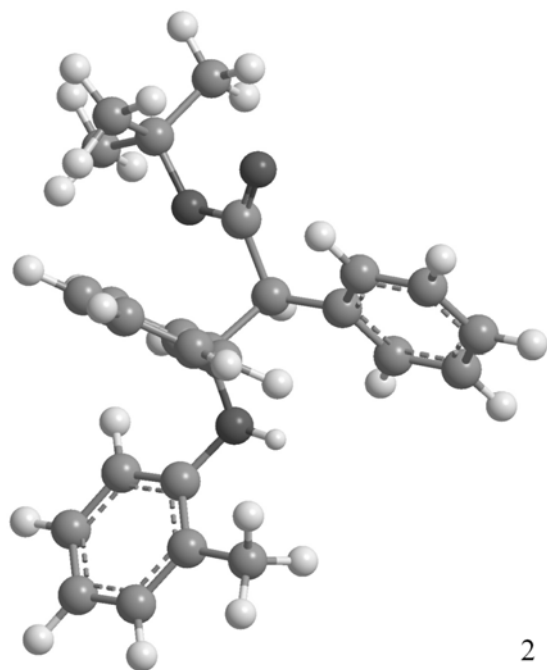


Figure 2. Non-polarized IR- (1) and difference IR-LD (2) spectra of (5); Small figure: Non-polarized IR-(1), difference (2) and reduced IR-LD (3) spectra after elimination the band at 732 cm^{-1} within 800–600 cm^{-1} IR-region

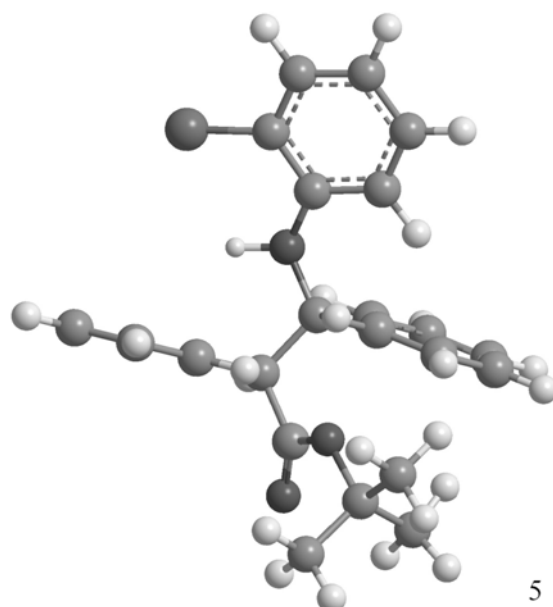
The experimental electronic spectra of (1)-(7), depicted in Fig. 3, show the typical for the phenyl-systems UV-bands at about 210 nm (ϵ_v about 11 000 $\text{L}\cdot\text{mol}^{-1}\cdot\text{cm}^{-1}$) and at about 248 nm (ϵ_v about 2000 $\text{L}\cdot\text{mol}^{-1}\cdot\text{cm}^{-1}$) of the K- and



1



2



5

Scheme 2. The most stable conformers of (1), (2) and (5)

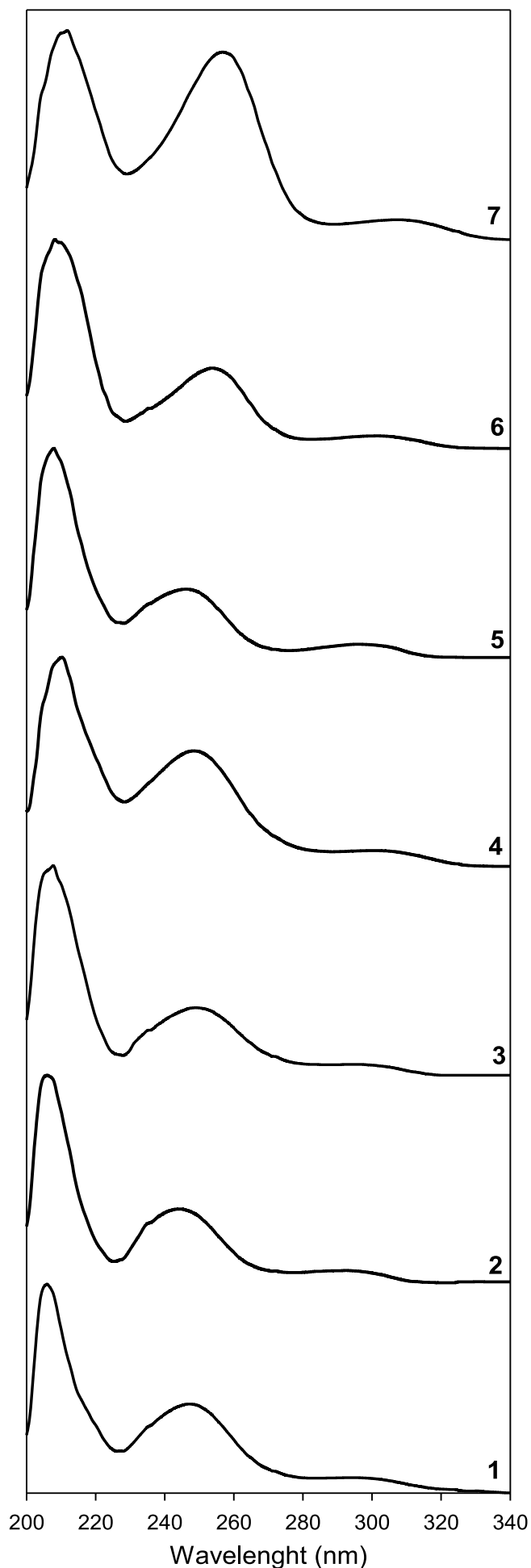
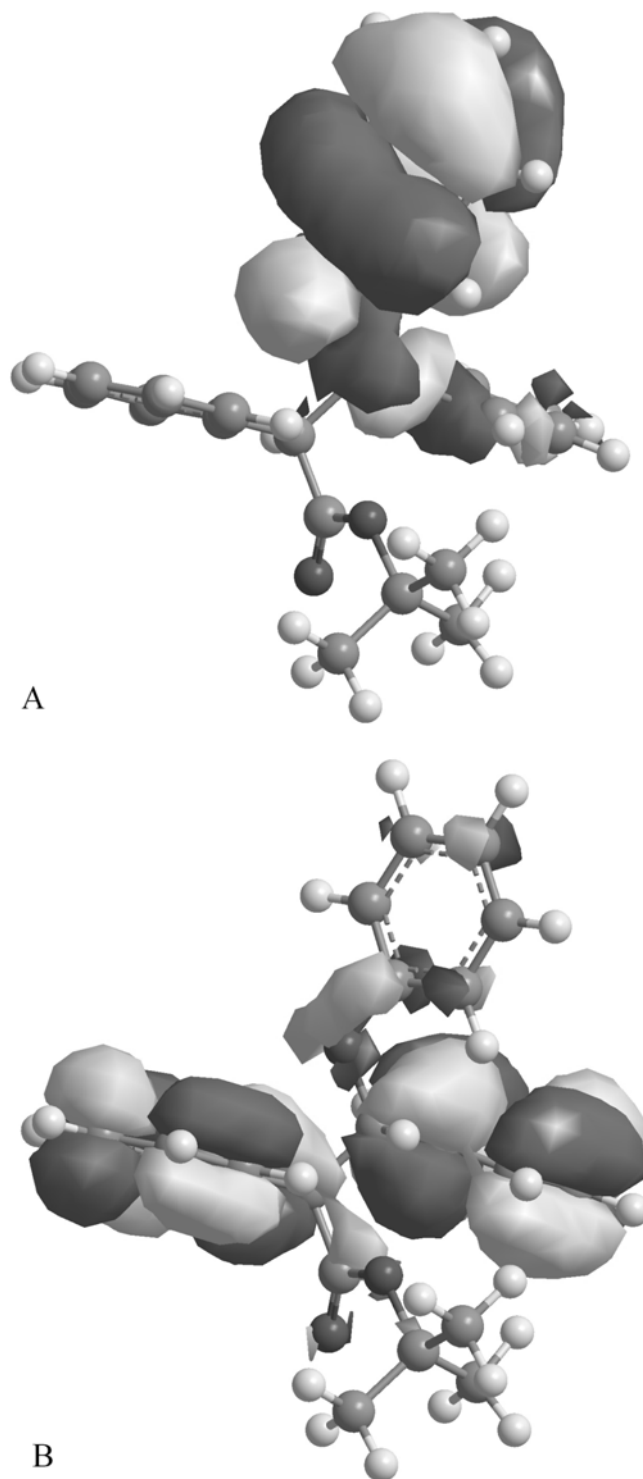


Figure 3. UV-spectra of (1)-(7) in ethanol solution at concentration $2.5 \cdot 10^{-5}$ M and 0.921 cm quartz cell

B-bands. The intramolecular transfer leads to observation of the weak band about 300 nm with ϵ , about $1000 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$. The corresponding HOMO and LUMO MOs illustrate the origin of this UV-band in all of the compound (1)-(7). The distributions for the HOMO and LUMO of the lowest single excited state show the discussed optical absorption. These data are in accordance with the theoretically predicted UV-spectra in the same solvent (Table 1, Fig. 3). The presence of the CH_3 - or Cl-substituents affects the UV-maxima about 10 nm and a hyperchromic effect of about $300 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ of the B-bands is observed in the cases of corresponding derivatives (5)-(7), which could be explained with the presence of Cl-substituent.



Scheme 3. HOMO (A) and LUMO (B) MOs of (1)

Table 1. Theoretical and experimental UV-spectra of (1)-(7) in ethanol solution

Compound	(1)	(2)	(3)	(4)	(5)	(6)	(7)
	λ [nm]						
Exp.	200	206	206	203	205	202	202
	245	248	250	252	244	254	257
	298	302	307	303	303	300	300
Theor. (f)	187 (0.2221)	193 (0.1997)	189 (0.1999)	187 (0.2006)	200 (0.2681)	202 (0.2823)	202 (0.2889)
	240 (0.1278)	242 (0.1200)	244 (0.1213)	241 (0.1218)	240 (0.1431)	243 (0.1318)	241 (0.1226)
	303 (0.0067)	303 (0.0192)	303 (0.0141)	303 (0.0163)	301 (0.0101)	300 (0.0100)	300 (0.0103)

CONCLUSION

The synthetic pathway for the obtaining of seven *tert*-butyl esters of 2,3-diaryl-3-arylaminopropanoic acids is reported, leading to the yields of 62–72%. The compounds were isolated, spectroscopically and structurally determined by means of the polarized IR- and UV-spectroscopy and ¹H-NMR. The presence of methyl- or chlor- substituents weakly affects on the positions of the characteristic IR bands of the compounds studied. In the electronic spectra of the Cl-containing compounds a hyperchromic effect is observed. Theoretical quantum chemical calculations are also performed with a view to supporting and explaining the corresponding electronic spectra in the solution.

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