Chemical Papers 64 (5) 645–651 (2010)
DOI: 10.2478/s11696-010-0037-3

ORIGINAL PAPER

Single crystal X-ray structure and optical properties of anthraquinone-based dyes

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Received 15 October 2009; Revised 11 February 2010; Accepted 12 February 2010

This study focuses on the preparation, single crystal X-ray diffraction, characterization, and optical properties of some anthraquinone-based dyes. The anthraquinone-based antimicrobial dye *N*-{2-[(9,10-dioxo-9,10-dihydroanthracen-1-yl)amino]-2-oxoethyl}-*N*,*N*-dimethylbutan-1-aminium chloride monohydrate (*III*) was obtained from 1-aminoanthraquinone (*I*) via 2-chloro-*N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)acetamide (*II*) using known preparation and characterization methods. Single crystal X-ray diffraction analysis of *III* revealed a monoclinic system, space group $P2_1/n$, $Z = 4$. Photoluminescence properties of anthraquinone dyes *I*–*III* were also investigated. These dyes gave an intense emission ($\lambda_{\max} = 341$ nm) upon the irradiation by UV light and showed photoluminescence quantum yields of 73 %, 66 %, and 61 % with long excited-state lifetimes of 6.87 ns, 6.14 ns, and 5.69 ns, respectively. These anthraquinone dyes are of interest as an organic light emitting material for electroluminescent devices.

Keywords: anthraquinone, antimicrobial dye, X-ray crystal structure, hydrogen bonding, photoluminescence

Introduction

Colorants having heterocyclic rings containing oxygen, nitrogen or sulfur have been widely used as dyes owing to their versatility in various high technology application areas including textiles, paper, leather, plastics, biological staining, lasers, liquid crystalline displays and ink-jet printers. Additionally, they have been used for specialized applications such as food, drug, cosmetic and photochemical production (Peters & Freeman, 1991; Kocaokutgen et al., 2005; Gregory, 1991). Anthraquinone dyes represent one of the most important dye classes used for various applications.

Azo dyes are widely used in the textile industry and they are the largest and most versatile group of synthetic organic dyes with a tremendous number of industrial applications (Øllgaard et al., 1999). Anthraquinone dyes find application in the coloration of cotton and hydrophobic synthetic fibers as well as in medicine and food chemistry (Kirk & Othmer, 1993). In contrast to the azo dyes, which have no natural counterparts, the anthraquinone chromogen provides important natural red dye sources. These dyes are moreover renowned for their outstanding fastness properties, especially to light (Gordon & Gregory, 1983). Anthraquinones have also been used as useful compounds in treating different types of cancer, especially breast cancer (Sadeghi-Aliabadi et al., 2004). Natural and synthetic derivatives of 9,10-anthracenedione, in particular, display numerous beneficial effects both in mammals and humans, e.g. antibacterial and antitrypanosomal activities.

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Cationic dyes are used in the dyeing of acrylic fibers and other cationic dyeable fibers. Some cationic dyes possess antimicrobial activity and as such have been widely applied in topical cleaning and as preservatives for food and fishery industries (Balabanova et al., 2003; Liu & Sun, 2008; Ma et al., 2003). These dyes also show photophysical properties.

Clear in-depth structural analyses of dyes allow their properties and reactivities to be easily assessed. Single crystal X-ray structure determination of dyes is important not only because it reveals molecular conformation and intra- and intermolecular interactions in solid state but also because the structural information gained from this analysis assist the understanding of the technical performance of the dyes (Singh et al., 2007; Leadbetter & Leaver, 1989). Temel et al. (1996) used heterocyclic disperse dyes for polyester coloration and in various other technical applications though without sufficient structural data (Temel et al., 1996). Additionally, there are relatively few examples of crystallographic structural data in literature (Yang et al., 2007; Malone et al., 1996). However, the study by Singh et al. (2007) showed how structural information could be linked with technical performance of the colorants. For example, brightness of some monoazo disperse dyes correlates with intramolecular hydrogen bonding interactions of the acetyl amino function and β-azo nitrogen (Singh et al., 2007). A study paralleling with this is that of Gordon and Gregory (1983), where azo dyes also having hydrogen-bonds were linked to planarity enforcement.

The search for materials for light emitting devices is an ongoing topic of interest (Chen et al., 2001; Zhao et al., 1999; Kulkarni et al., 2005). Luminescent compounds are a potential field for the application in many areas such as light emitting devices and the design of optical materials and sensors (Shinar, 2004). Thus, numerous aromatic compounds have been developed as hole transport layers in organic electroluminescent research (Pu et al., 2004). Simple quinones are completely nonfluorescent though their amino and hydroxy derivatives are often fluorescent in nature. In this respect, amino and hydroxy substituted anthraquinones show reasonably good fluorescence quantum yields. Among different excited state properties, the effect of intra- and intermolecular hydrogen bonding on the deexcitation pathways of excited amino- and hydroxyanthraquinones has been investigated. These moieties have important roles in the photoluminescence properties of these molecules (Rembold & Kramer, 1980; Dahiya et al., 2008).

Antimicrobial anthraquinone dyes are important in textile industry because they are used in the dyeing of acrylic fibers and other cationic dyeable fibers. Anthraquinone dyes linking quaternary ammonium salts are cationic surface active compounds that can provide combined effects: disinfection, surface activation and antihistatic properties (Patrauchan & Oriel, 2003; Sun & Ma, 2005). Previous work in our laboratories regarding the synthesis and characterization of various new dyes, their transition metal complexes and some of their properties were reported (Kurtoğlu et al., 2008, 1999a, 1999b; Kurtoğlu & Baydemir, 2007; Serin & Kurtoğlu, 1994; Aslantas et al., 2007; Birbiçer et al., 1999). In this study, anthraquinone-based dyes were prepared and chemical structure of the final product (*III*) was characterized. The main objective of this research was to analyze single crystal X-ray structure of the antimicrobial anthraquinone dye *N*-{2-[(9,10-dioxo-9,10-dihydroanthracen-1-yl)amino]-2-oxoethyl}-*N*,*N*-dimethylbutan-1-aminium chloride monohydrate and to investigate optical properties of the three anthraquinone dyes in the solution. These dyes were found to exhibit photoluminescence, giving intense emission upon UV irradiation.

Experimental

All solvents were of reagent grade and purified according to standard procedures. 9,10-Diphenylanthracene, 1-aminoanthraquinone, *N*,*N*-dimethylbutylamine, and chloroacetyl chloride were purchased from Sigma–Aldrich Co. (Germany) All chemicals were of reagent grade and used without further purification. 2-Chloro-*N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-acetamide (*II*) and *N*-{2-[(9,10-dioxo-9,10-dihydroanthracen-1-yl)amino]-2-oxoethyl}-*N*,*N*-dimethylbutan-1-aminium chloride monohydrate (*III*) were prepared using known methods (Ma et al., 2003; Martelli et al.,1988; Sun & Ma, 2005).

Elemental analyses were performed using a LECO CHNS 932 elemental analyzer. The FTIR spectra (KBr) were recorded on a Shimadzu 8300 FTIR spectrometer (in the range of 4000–400 cm^{-1}). ^{1}H NMR spectra (300 MHz) were recorded on a Bruker FT-NMR spectrometer. Crystal data were collected on a Rigaku R-AXIS RAPID-S diffractometer. Melting points were obtained using an Electrothermal LDT 9200 apparatus in open capillaries. Photoluminescent properties of compounds *I*–*III* were studied using a Perkin–Elmer LS55 spectrometer. All samples were prepared in spectrophotometric grade methanol and analyzed in a 1 cm optical path quartz cuvette. Solution concentration of *I*–*III* in methanol was 10^{-5} mol L^{-1} and the samples were excited at 283 nm wavelength. Photoluminescence quantum efficiencies of *I*–*III* were calculated using 9,10-diphenylantracene as the standard (Guilbault, 1990; Gilbert & Baggott, 1991; Osaheni & Jenekhe, 1994).

A pale yellow needle crystal of *III* (obtained by recrystallization from ethyl acetate) with dimensions of 0.2 mm × 0.2 mm × 0.30 mm was used for the X-ray analysis. The diffraction experiment was carried out in a four-circle Rigaku R-AXIS RAPID-S diffractometer equipped with a two-dimensional area

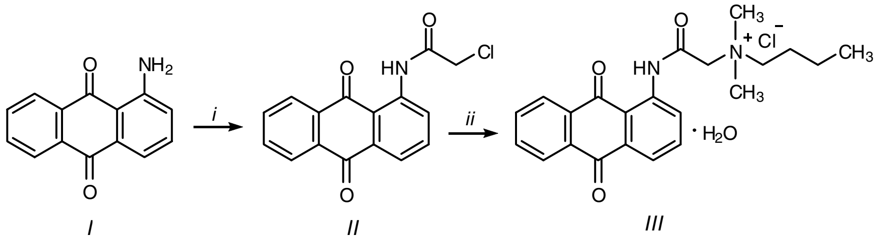

Fig. 1. Reaction scheme for the preparation of dye *III*. Reaction conditions: *i*) chloroacetyl chloride, dimethylacetamide, chloroform, r.t.; *ii*) *N*,*N*-dimethylbutylamine, dimethylformamide, 95 °C.

Table 1. Crystal data and structure refinement for *III*^{a}

Empirical formula	$C_{22}H_{25}ClN_2O_3 \cdot H_2O$
Formula mass	418.91
Temperature, T (K)	293(2)
Wavelength, λ (Å)	0.71073
Crystal system, space group	Monoclinic, $P2_1/n$
a (Å)	12.726(1)
b (Å)	12.8303(10)
c (Å)	13.457(2)
β (°)	107.030(9)
Unit-cell volume, V (Å^3)	2101.0(6)
Formula per unit cell, Z	4
Density, D_{calcd} (g cm^{-3})	1.324
Absorption coefficient, μ (mm^{-1})	0.213
F(000)	888
Crystal size (mm)	0.2 × 0.2 × 0.3
θ range for data collection (°)	2.51–30.67
Index ranges	$-16 \leq h \leq 18$ $-18 \leq k \leq 18$ $-19 \leq l \leq 19$
Reflections collected	6431
Independent reflections (R_{int})	4006 (0.0677)
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4006/0/266
Goodness-of-fit on F^2	1.043
R indices [$I > 2\sigma(I)$]	$R_1 = 0.0622$, $wR_2 = 0.1856$
Largest difference peak and hole (e Å^{-3})	0.394 and −0.406

a) Standard deviations in parentheses.

IP detector. Graphite-monochromatized Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å), and oscillation scan technique with $\Delta\omega = 5°$ for one image were used for data collection. Images of the compound were taken successfully by varying ω with three sets of different χ and ϕ values. For each compound, 108 images were performed in six different runs, covering about 99.0 % of the Ewald spheres. Lattice parameters were determined by the least-squares method considering all reflections with $F^2 > 2\sigma(F^2)$. Integration of the intensities, correction for the Lorentz and polarization effects and cell refinement were performed using the CrystalClear software (Rigaku/MSC, 2005). Structure was solved by the SHELXS-97 (Sheldrick, 1997a) and refined by the SHELXL-97 (Sheldrick, 1997b) software package. All non-H atoms were anisotropically refined. Hydrogen atoms were introduced in calculated positions, with C—H distances of 0.93 Å, 0.96 Å, and 0.97 Å for aromatic, methyl, and methylene H atoms, respectively, and refined using the riding model with $U_{\text{iso}}(\text{H}) = 1.5\,U_{\text{eq}}(\text{C})$ for methyl H atoms and $U_{\text{iso}}(\text{H}) = 1.2\,U_{\text{eq}}(\text{C})$ for other H atoms. H atoms on O4 and N1 were located in difference maps and their coordinates were refined freely. Final cycle of the refinement included 266 variable parameters, $R_1 = 0.0622$, $wR_2 = 0.1856$, where $w = 1/[\,\sigma^2(F_o^2) + (0.0779P)^2 + 0.4657P]$ with $P = (F_o^2 + 2F_c^2)/3$ were obtained. Details on the X-ray data collection, structure solution and refinement are given in Table 1. Atomic scattering factors were taken from the International Tables for X-ray Crystallography (Wilson, 1995). Further experimental details have been deposited as supplementary material with the Cambridge Crystallographic Data Centre, CCDC No. 673849.

Results and discussion

Dyes *II* and *III* were synthesized starting from 1-aminoanthraquinone (*I*) as described in Fig. 1. Their structures were confirmed by FTIR and ^{1}H NMR spectrometry, and elemental analysis. All relevant spectral data as well as the melting points and elemental analysis data were in accordance with those already published (Ma et al., 2003; Martelli et al., 1988; Sun & Ma, 2005; Berghot & Moawad, 1995).

ORTEP (Farrugia, 1997) diagram of the molecule, indicating the atomic numbering scheme with thermal ellipsoids at the 50 % probability level is illustrated in Fig. 2. The studied dye could be used under either acidic or basic conditions, particularly in the coloration of acrylics, nylon, and wool (Liu & Sun, 2008). Crystal packing in the unit cell is shown in Fig. 3. Selected bond lengths, bond angles, and torsion angles are listed in Table 2. Hydrogen bonding geometry is presented in Table 3. PARST (Nardelli, 1995) and PLATON (Spek, 2003) programs were used for the calculation of geometrical properties of the molecule of *III*. Molecule *III* consists of an anthraquinone ring, amide group, and a quaternary dimethylbutylamine system. The X-ray analysis revealed that the anthraquinone ring system in *III* is essentially of planar conformation within ± 0.039(2) Å (Fig. 2). Six-membered benzene rings of the anthraquinone system are all nearly planar with small distortions. C8 and

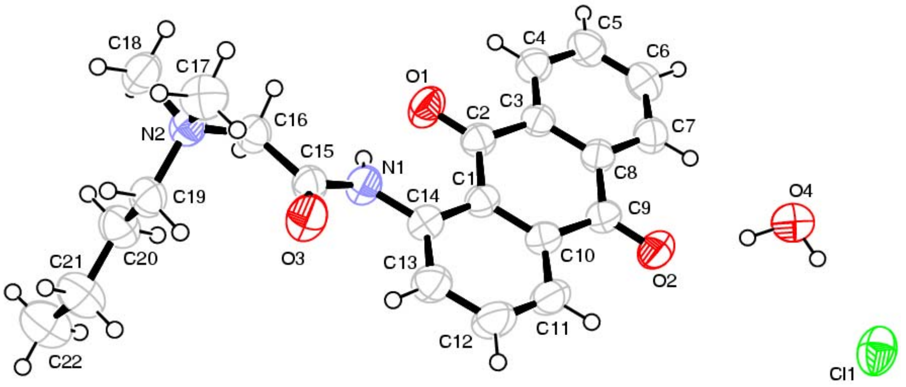

Fig. 2. Molecular structure of *III* with the atomic numbering scheme. Thermal ellipsoids were drawn at the 50 % probability level.

Table 2. Selected bond lengths, bond angles, and torsion angles for *III*[a]

Bond	Bond length (Å)	Bond	Bond angle (°)	Bond	Torsion angle (°)
O1—C2	1.228(2)	C15—N1—C14	127.95(18)	C14—C1—C2—O1	−3.1
O2—C9	1.229(2)	C17—N2—C18	106.53(3)	C15—N1—C14—C1	−158.7
O3—C15	1.212(2)	N2—C16—C15	115.51(15)	C18—N2—C16—C15	177.28(3)
N1—C15	1.354(2)	C16—N2—C19	112.76(15)	N2—C16—C15—N1	−179.97
N1—C14	1.402(2)	N1—C15—C16	110.25(16)	C17—N2—C19—C20	171.41(19)
N2—C16	1.504(2)	C14—C1—C2	122.00(16)	C9—C10—C1—C14	−177.84
N2—C17	1.508(1)	C17—N2—C19	108.30(16)	C3—C2—C1—C14	177.43(3)
N2—C18	1.511(1)	O3—C15—N1	124.95(19)	C17—N2—C16—C15	61.1(2)
N2—C19	1.525(1)	–	–	C14—N1—C15—C16	178.31(19)
–	–	–	–	C16—N2—C19—C20	−64.9
–	–	–	–	C19—C20—C21—C22	174.3(2)

a) Standard deviations in parentheses.

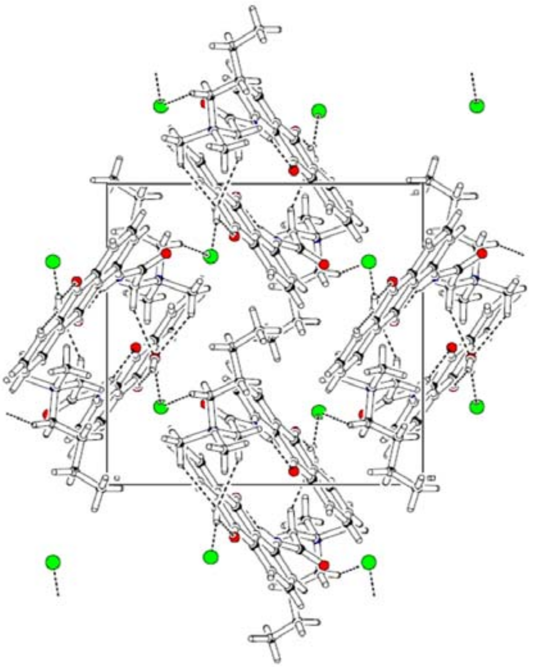

Fig. 3. Crystal packing of *III* along the *a*-axis. Dashed lines indicate hydrogen bonds.

C14 atoms deviate from the benzenes best plane by −0.0026(2) Å and 0.008(2) Å, respectively, and the dihedral angle between the two benzene rings of anthraquinone is 1.64(6)°. Non-H atoms of the amide and the quaternary groups (N1/N2/C15—C16/C18) in the molecule are in an antiperiplanar conformation with respect to the anthraquinone system with a torsion angle of C15—N1—C14—C1 (−158.7(2)°). All bond lengths and angles in the molecule have normal values (Allen et al, 1987) except for the C1—C14 (1.416(1) Å) bond length which is slightly longer than the average C—C bond length of benzene rings. All geometric parameters are comparable with those reported in literature, with some structures containing the anthraquinone ring system (Boonnak et al., 2005; Zhu et al, 2007). All C—N and C—O bond lengths lay within the range of 1.354(2)–1.525(1) Å and 1.212(2)–1.229(2) Å, confirming single and double-bond character, respectively.

In the crystal, the Cl^- anion and all O atoms are involved in hydrogen bonding. A number of strong intramolecular O—H· · ·Cl, C—H· · ·Cl, N—H· · ·O, and C—H· · ·O, as well as intermolecular O—H· · ·O, C—H· · ·O, and C—H· · ·Cl hydrogen bonds were found (Table 3), in particular the N1—H14· · ·O1 and O4—H1A· · ·O2 hydrogen bonds are quite short. In the molecular structure, the Cl^- anion plays a role in the formation of dimeric units as a result of the C—H· · ·Cl interactions which predominantly con-

Table 3. Hydrogen bonding geometry for *III*[a]

D—H···A	Bond length (Å)			Bond angle (°)
	D—H	H···A	D···A	D—H···A
O4—H1B···Cl1	0.86(2)	2.20(1)	3.057(2)	175
N1—H14···O1	0.86(1)	1.92(1)	2.619(2)	138
C13—H13···O3	0.93	2.31	2.870(1)	118
C16—H16B···Cl1	0.97	2.58	3.473(2)	153
C17—H17C···O3	0.96	2.34	2.993(1)	125
C19—H19A···O3	0.97	2.38	3.043(1)	125
O4—H1A···O2^{i}	0.96	1.96	2.902(2)	165
C7—H7···O4^{ii}	0.93	2.55	3.446(1)	161
C16—H16A···O4^{iii}	0.97	2.33	3.231(1)	154
C17—H17B···O4^{iii}	0.96	2.57	3.393(1)	144
C19—H19B···Cl1^{iv}	0.97	2.60	3.496(2)	154

a) Standard deviations in parentheses. Symmetry codes: (*i*) 1 + *x*, *y*, *z*; (*ii*) –1 + *x*, *y*, *z*; (*iii*) 1 – *x*, – *y*, 1 – *z*; (*iv*) ½ + *x*, ½ – *y*, ½ + *z*.

Table 4. Photoluminescence data for compounds *I–III*

Dyes	$\lambda_{\max}$ (nm)^{a}	Intensity^{b}	$\lambda_{\max}$ (nm)^{c}	Intensity^{d}	$\phi_{\rm f}$ (%)^{e}	$\tau_{\rm f}$ (ns)^{f}
I	283	885	341	884	73	6.87
II	284	822	337	818	66	6.14
III	284	779	336	776	61	5.69

a) Maximum excitation wavelength, *b*) maximum excitation intensity, *c*) maximum emission wavelength, *d*) maximum emission intensity, *e*) quantum yield, *f*) excited-state lifetime.

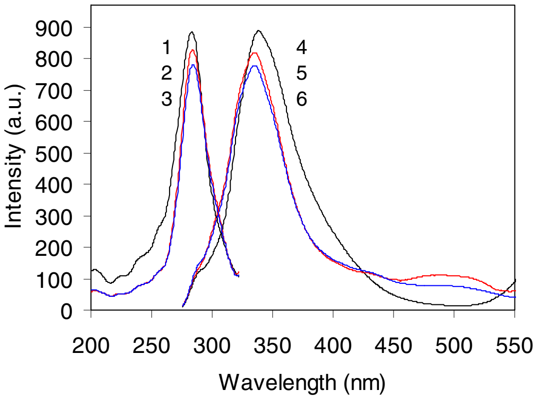

Fig. 4. Photoluminescence spectra of *I–III* in MeOH; excitation of: *I* (1), *II* (2), *III* (1); emission of: *I* (4), *II* (5), *III* (6); samples were excited at 283 nm.

tribute to the stability of the overall structure.

Absorption and photoluminescence spectra of *I* were measured in methanol and they are shown in Fig. 4. The most striking feature of the absorption/emission spectrum of *I* was the appearance of an intense emission band upon its irradiation by UV light. Maximum luminescence intensity was observed at 341 nm, and the half-band width was 59 nm. Compound *I* exhibited a photoluminescence quantum yield of 73 % and a long excited-state lifetime of 6.87 ns.

Fig. 4 also shows the comparison of emission spectra of *I–III* in methanol. Compound *II* showed maximum luminescence intensity at 337 nm, and the half-band width was 48 nm; *III* showed maximum luminescence intensity at 336 nm and the half-band width was 47 nm. It can be seen that upon derivatization of *I*, the luminescence is shifted from 341 nm to 336 nm. For these compounds, quantum efficiencies and intensities could be correlated with the presence of electron donating groups. Since *II* and *III* have weaker electron donating groups in comparison with *I*, a shift in their luminescence values to lower wavelengths was observed, and thus, lower intensity and quantum efficiency were found; this emission wavelength difference could be used for tuning in photoluminescent devices. Dyes *II* and *III* were excited at 283 nm and they showed strong luminescence. Compounds *II* and *III* gave photoluminescence quantum yields of 66 % and 61 %, respectively, and long excited-state lifetimes of 6.14 ns and 5.69 ns, respectively. Photoluminescence data of compounds *I–III* are summarized in Table 4. Photoluminescent properties of dyes *I–III* allow these to be used for optical and electronic applications.

Conclusions

X-ray structural analysis showed that the anthraquinone ring system in *III* is essentially planar. In the molecular structure of *III*, the $\mathrm{Cl^-}$ anion contributes to the stability of the overall structure. Compound *I* was found to exhibit intense photoluminescence at 341 nm, while *II* and *III* showed maximum luminescence intensity at 337 nm and 336 nm, respectively. Upon derivatization, the luminescence peak shifted from 341 nm to 336 nm. These dyes are interesting materials for their applications in electroluminescent devices.

Acknowledgements. The authors wish to thank TUBITAK for financial support (Project No.: 104M316), the Department of Chemistry and the Department of Textile Engineering at Kahramanmaras Sutcu Imam University. The authors also wish to thank the Department of Chemistry at Atatürk University, Turkey, for the access to the X-ray diffractometer.

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