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New anthracene-based Schiff bases: theoretical and experimental investigations of photophysical and electrochemical properties

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Abstract: The new Schiff bases bearing anthracene unit were synthesized from 2-aminoanthracene and various aldehydes such as: benzaldehyde, 4-(diphenylamino)benzaldehyde, 9-phenanthrenecarboxaldehyde, 9-anthracenecarboxaldehyde, and biphenyl-4-carboxaldehyde, 2-naphthaldehyde. Resulted azomethines were characterized by IR, NMR (^{1}H and ^{13}C), elemental analysis and UV-Vis spectroscopy. The imine consists of anthracene and biphenyl moieties exhibited liquid crystal properties and their nematic phase showed Schlieren texture. The photoluminescence measurements carried out in solution and in solid state as blend with PMMA revealed the ability of the imines to emission of the blue light with quantum yield efficiency in the range of 2.18–6.03% in blend. Based on the electrochemical experiment they showed value of energy gap (E_g) in the range of 2.5 - 2.7 eV. Additionally, density functional theory (DFT) was applied for calculations of both electronic structure and spectroscopic properties of synthesized Schiff bases. Moreover, the results obtained from preliminary tests of application of the azomethines in organic photovoltaic (OPV) devices confirmed their electron acceptor character.