

SYNTHESIS AND CHARACTERIZATION OF SERS-ACTIVE HETEROAROMATIC MOLECULES

Francesca Fontana^a, Matteo Tommasini^b, Chiara Zanchi^b, Paolo Ossi^c, Simona Rizzo^d and Sebastiano Trusso^e

^aDept. of Engineering and Applied Sciences, University of Bergamo, Italy

^bDept. of Chemistry, Materials and Chemical Engineering, Politecnico di Milano, Italy

^cDept. of Energy, Politecnico di Milano, Italy

^dCNR-ISTM, Istituto di Scienze e Tecnologie Molecolari CNR, Milano, Italy

^eCNR-IPCF, Istituto per i Processi Chimico-Fisici del CNR, Messina, Italy

Azahelicenes are extensively conjugated, intrinsically chiral molecules with interesting optical and optoelectronic properties [1]. They show interesting SERS activity as well as fluorescence [2]. We synthesized and characterized 5-aza[6]helicene (**1**, Fig.1). In the last step of the synthesis, represented by the photocyclization of precursor (**3**) (Fig.2), we observed concurrent formation of derivative (**2**) indicated in Fig. 1. Since it was formed in non-negligible amount, we decided to characterize it as well respect to its spectroscopic and emission properties.

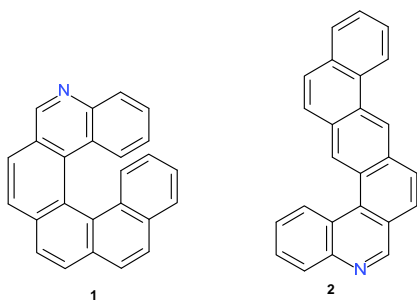


Figure 1. 5-aza[6]helicene (**1**) and its isomer (**2**).

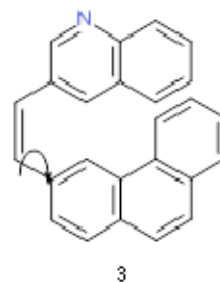


Figure 2. Precursor (**3**). Rotation around the indicated bond brings to formation of isomer (**2**).

We recorded UV-Vis absorption and concentration-dependent fluorescence spectra of (**2**) excited at 314 nm. We observed an excellent linear dependence of the emission maximum (429 nm) vs. concentration in diluted MeOH solutions (5×10^{-5} - 3×10^{-4} mM). We also carried out density functional theory calculations, aiming at the interpretation of the observed SERS features of the molecule once adsorbed on gold substrates produced by PLD with a plasmon resonance close to 785 nm.

[1] S.Abbate et al. *Phys. Chem. C*, **2014**, *118* (3), 1682-1695.

[2] C.Zanchi et al. *Chirality* **2018**, 1-8