Investigating Piezochromic Properties of π-conjugated Materials: a combined Raman and DFT Study

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Π-conjugated materials have been studied for decades due to their great interest in organic electronics. Among them, piezochromic materials, which exhibit color changes resulting from external pressure or mechanical grinding, become very attractive from a scientific viewpoint owing to their potential applications as pressure-sensing and optical-recording systems[1]. The main target of the present work is to develop a joint experimental and theoretical approach able to deliver crucial information for the understanding of the structural effects causing piezochromic changes. To this end, we will focus our attention on two families of π-conjugated materials with potential application as sensors. The first one is a family of 9,10-Bis((E)-n-(pyrid-2-yl)vinyl) anthracene, BPnVA (n=2 orto-,3 metha- and 4 para-) compounds, see Figure 1. Interestingly, these three compounds with varying position of the nitrogen on the external pyridyl group exhibit different molecular packing modes. Grinding and the application of external pressure on the powder also led to a strong change in their photoluminescence color.[2] The second familiy is based on the N,N'-Bis-Boc-3,3'-di(pyren-1-yl)-2,2'-biindole compound (compound 1c in Figure 1) which also shows photoluminescence under pressure application. However, the molecular packing induced by this phenomenon is still under study [3]. In both cases, it will be also very interesting to determine how temperature affects the vibrational structure of these systems.

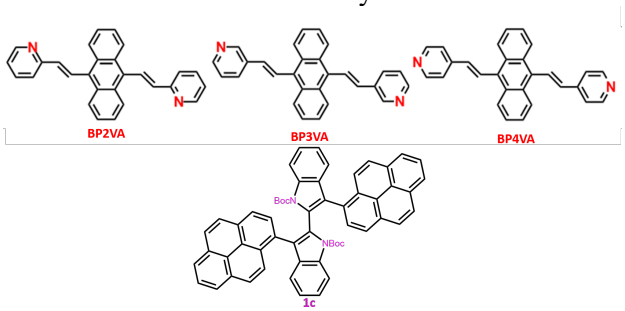

Figure 1. Chemical structures under study.

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