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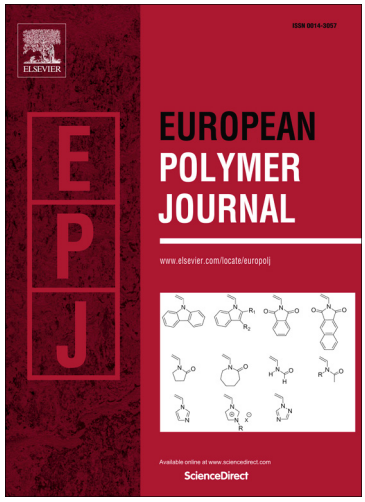

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Conjugated Polyphenols: Investigation of Structure-Property Relationships and Complexation with Zinc Ions

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ABSTRACT

Conjugated polymers with ion sensing groups have been synthesized and characterized for developing sensors for toxic and explosive chemicals in different media. In this study, three conjugated polyphenols (**P1(OH)$_n$** – **P3(OH)$_n$**) were synthesized using Sonogashira polymerization and structure-property relationships were established. The target conjugated polyphenols exhibited blue-shifts in absorption (up to 50 nm) and emission (up to 15 nm) maxima in THF, and red-shifts in absorption (up to 45 nm) and emission (up to 17 nm) maxima in DMF of the target polyphenols as compared to those of protected polymers (**P1** - **P3**). This is attributed to the disruption of polymer conformation owing to the formation of interchain hydrogen bonds between the trihydroxybenzene groups along the polymer backbone. **P1(OH)$_n$** showed strong interactions with Zn^{2+} ions with a red-shift in emission maximum from 475 nm to 535 nm and a high binding constant (K_{sv} = 3.73 x 10^5 M^{-1}). In contrast, **P2(OH)$_n$** and **P3(OH)$_n$** exhibited smaller changes in emission maximum upon addition of Zn^{2+} ions (K_{sv} = 0.69 x 10^5 M^{-1} for **P2(OH)$_n$** and 0.32 x 10^5 M^{-1} for **P3(OH)$_n$**). The understanding of the structure-property relationships of such polymers helps to develop metal ion sensors with better selectivity and sensitivity in the future.

Keywords: conjugated polyphenols; trihydroxybezene; metal ions; sensing