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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 Zn²⁺ ions with a red-shift in emission maximum from 475 nm to 535 nm and a high binding constant ($K_{sv} = 3.73 \times 10^5 \text{ M}^{-1}$). In contrast, **P2(OH)_n** and **P3(OH)_n** exhibited smaller changes in emission maximum upon addition of Zn²⁺ ions ($K_{sv} = 0.69 \times 10^5 \text{ M}^{-1}$ for **P2(OH)_n** and $0.32 \times 10^5 \text{ M}^{-1}$ 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; trihydroxybenzene; metal ions; sensing

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