

PHOTOPHYSICAL STUDY OF PURINE BASED METAL ION SENSORS

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The purine heterocyclic system holds a significant role in biological and medicinal chemistry, primarily attributed to its intrinsic involvement in genetic information transcription and translation processes. These materials show potential applications as efficient chemical sensors, fluorescence imaging agents, photocatalysts, and sensitizers for photodynamic therapy (PDT) activated by light, including solar illumination.

The purine core proves highly advantageous for chemical modification due to well-established synthetic methods and its chemical structure, allowing to incorporate electron-donating functional groups at the C2, C6, or C8 positions of the purine core. Expanding the functionality of purine derivatives can be achieved by capitalizing on long-lived excited triplet and/or radical states. Additionally, there is the opportunity for a steady-state absorption shift towards the visible or even near-infrared range, aligning with the therapeutic window. Alternatively, derivatives featuring an external C8-complexing arm, working in conjunction with the purine N7, have been developed. Notably, there are only a limited number of recent examples showcasing purine-based metal ion sensors that leverage both the C6-substituent and the purine N7.

Here we present a detailed photophysical study of purine-based derivatives complexation processes in polar solvents and aqueous media in the field of chemical sensors. Several chemical sensor prototypes have been demonstrated for the detection of metal ions of different nature: alkali, alkaline earth, heavy and transition metals, which can be used in industry (acetonitrile as a solvent) as well as in biology and the environment (water). The synthesized compounds were able to detect traces of transition and heavy metal ions at ppb level. The new water-soluble compounds were found to exhibit high sensitivity to mercury (II) ions in water.

[1] J. Jovaisaite et al., Proof of principle of a purine D-A-D ligand based ratiometric chemical sensor harnessing complexation induced intermolecular PET, *Phys. Chem. Chem. Phys.*, 2020.