## Design and Synthesis of Efficient Initiator for Photoinduced Radical Polymerisation Utilizing the Anomeric Effect of Five-Membered Ring Molecules

Asrar Ahmad, Ajay Shelke and Ajoy Kapat\*

Department of Chemistry, School of Natural Sciences, Shiv Nadar (Institution of Eminence Deemed to be University), Delhi-NCR, Gautam Buddha Nagar, Uttar Pradesh 201314, India; Email\*- <u>ajoy.kapat@snu.edu.in</u>

**Abstract:** Photochemical reactions are becoming essential tools both in academia and industry due to it's operational simplicity, environmentally friendly and economically sustainable nature in comparison to thermochemistry.<sup>[1]</sup> Particularly scientific community are attracted towards photoinduced radical polymerization (PRP) reaction due to it's various applications in the areas of dental restoration process, tissue engineering, artificial bone generation and 3D-Printing.<sup>[2]</sup> Herein we report the design of new initiator for PRP reaction via intramolecular hydrogen atom transfer reaction utilizing the inherent anomeric effect of five membered ring containing molecules. We have synthesized new efficient photoinitiator via barrierless sequential conjugate addition reaction.



Figure: Design, synthesis of initiator and application in PRP reaction.

Polymerization of diurethane dimethacrylate (UDMA, 70%) and triethylene glycol dimethacrylate (TEGDMA, 30%) in presence of 450 nm LED (15 W) under the aerobic conditions turned out to be very efficient (71 seconds) using our newly synthesized 1,2-benzenedithiol (DTH) based initiator and the resultant polymeric material has excellent physical properties.<sup>[3, 4]</sup> Higher efficiency of this initiator is due to the low bond dissociation energy of C-H bond adjacent to the two heteroatoms and puckered ring structure of the five membered rings. This hypothesis was further supported by X-Crystal structure of the initiator, NMR and computational data.

- [1] S. Dadashi-Silab, S. Doran and Y. Yagci, Chem. Rev. 2016, 116, 10212.
- [2] A. Bagheri, J. Jin, ACS Appl. Polym. Mater. 2019, 1, 593.
- [3] A. Ahmad, S. A. Siddiqui, G. Mittal, N. Sukumar, K. D. Dubey, A. Kapat *Chem. Eur. J.* **2023**, *29*, e2023018.
- [4] A. Ahmad, S. Ajay, A. Kapat manuscript under preparation.