Name of the Scholar: Nowsheenah Farooq Name of Supervisor: Prof. Athar Adil Hashmi Name of Department: Chemistry Topic of Research: Synthesis, Characterization and Iodine Capture Application of Porous Organic Polymers

Findings

The Ph.D. thesis entitled, "Synthesis, Characterization and Iodine Capture Application of Porous Organic Polymers" presents a comprehensive study on the synthesis and characterization of Porous Organic Polymers (POPs) tailored for capturing radioactive iodine. This research underscores the eco-friendly and cost-efficient attributes of these POPs, highlighting their promise for sustainable and economical iodine sequestration. The thesis is composed of five chapters. The first chapter provides an overview of Porous Organic Polymers (POPs), focusing on their synthesis, properties, and applications in iodine capture. The chapters describe the synthesis, characterization, and iodine adsorption capacities of several nitrogen-rich covalent organic frameworks (COFs) and porous organic polymers (POPs), all developed through Schiff base polycondensation reactions. These materials are designed to efficiently capture iodine, a key concern in nuclear fuel reprocessing and environmental safety.

In Chapter 2, NR_COF-C1 is synthesized using triazine trialdehyde and diamine monomers. This material demonstrates remarkable thermal stability, enduring up to 300 °C, and chemical stability, attributed to the strong C–N bonds within its polymeric structure. The crystalline nature of NR_COF-C1 is confirmed by PXRD, with a sharp peak observed at $2\theta = 4.90$, and the material exhibits significant microporosity, evidenced by a BET surface area of 175.477 m²/g and a pore volume of 0.407 cc/g. FTIR analysis further verifies the successful formation of imine linkages between the monomers. NR_COF-C1 is highly effective in iodine adsorption, showing impressive uptake in the vapor phase (5.45 g/g at 75 °C), at room temperature (2.15 g/g), and in aqueous solutions (4850.75 mg/g). Additionally, the material maintains high recyclability, with minimal

loss of efficiency, suggesting its potential as a robust and sustainable adsorbent for iodine containment.

Chapter 3 introduces MPOP-4, a melamine-based porous organic polymer synthesized by reacting melamine and uracil through a hydrothermal process. The material is characterized by various techniques including FTIR, solid-state NMR, PXRD, and TGA, which confirm its successful synthesis and high thermal stability, withstanding temperatures up to 483 °C. The mesoporous nature of MPOP-4 is revealed through a BET surface area of 195.48 m²/g and a pore volume of 0.612 cc/g. Iodine adsorption tests demonstrate that MPOP-4 captures iodine effectively, with capacities of 6.30 g/g in vapor at 80 °C, 1.98 g/g at 25 °C, and 4833.15 mg/g in aqueous solutions. The polymer's nitrogen-rich framework and robust porous structure contribute to its efficient iodine capture and recyclability, making it a promising green, metal-free material for iodine sequestration.

In Chapter 4, the synthesis of two nitrogen-rich porous organic polymers, NR_POP-C2 and NR_POP-C3, is detailed. These materials are produced through Schiff base polycondensation of triazine trialdehyde with diamines 4,4'-oxydianiline and naphthalene-1,5-diamine. Their structure and properties are confirmed by FTIR, NMR, PXRD, SEM, EDX, and nitrogen adsorption measurements. NR_POP-C2 has a lower BET surface area (64.1 m²/g), while NR_POP-C3 demonstrates a much higher surface area (699 m²/g), making it more suitable for iodine capture. Both materials exhibit excellent thermal stability, with NR_POP-C2 stable up to 340 °C and NR_POP-C3 up to 390 °C. The iodine adsorption capacities of both materials are impressive, with NR_POP-C2 adsorbing 7.16 g/g at 75 °C, 2.71 g/g at 25 °C, and 4680.6 mg/g in aqueous solutions, while NR_POP-C3 shows similar performance. The polymers maintain high adsorption efficiency after several cycles, confirming their recyclability and potential for long-term use in iodine capture applications.

Chapter 5 presents Ac_POP-5, a nitrogen-rich acridine-based porous organic polymer synthesized from 2,4,6-triformylresorcinol (TFR) and 3,6-diaminoacridine (DAA) via Schiff base polycondensation. This material is insoluble in various organic solvents, and its structure is confirmed by FTIR, PXRD, SEM, nitrogen adsorption, and TGA. Ac_POP-5 exhibits high thermal stability, withstanding temperatures up to 350 °C, and is chemically stable under acidic and basic conditions. The material demonstrates exceptional iodine adsorption capacities, including 8.11 g/g

at elevated temperatures, 3.02 g/g at room temperature, and 4975.39 mg/g in aqueous solutions. Furthermore, Ac_POP-5 retains its iodine capture efficiency across multiple cycles, even under extreme conditions. It's simple synthesis, coupled with its exceptional chemical and thermal stability and recyclability, makes it a promising material for iodine capture during nuclear fuel reprocessing.

Overall, these nitrogen-rich POPs exhibit outstanding potential for iodine sequestration due to their high thermal stability, robust chemical structure, and efficient iodine adsorption properties. Their ability to maintain performance across multiple cycles highlights their long-term applicability in environmental and safety-related applications. These materials, with their cost-effective synthesis, sustainability, and recyclability, are well-suited for use in the safe and effective capture of iodine, especially in industries dealing with nuclear waste and iodine-containing gases.