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Selenium or sulfur based aminofurazan *N*-hydroxyamidine materials as sorbents for removal of uranium from liquid media

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Synthesis of Se-derivative of *N*'-hydroxy-1,2,5-oxadiazole-3-carboximidamide (polymer P1). A mixture of *N*'-hydroxy-1,2,5-oxadiazole-3-carboximidamide **1** (1.43 g, 10 mmol) and SeO_2 (1.11 g, 10 mmol) was refluxed in acetic acid (30 ml) and violent stirring for 80-100 min. A dark purple precipitate was formed. In the end of the processing, the mixture was cooled to room temperature, and the precipitate was filtered off. The material was sequentially washed with cold distilled water (thrice), EtOH, and finally with dichloromethane to remove unreacted components of the initial mixture. The material was dried to a constant weight in a vacuum desiccator at 5-10 Torr over P_2O_5 at 20-25°C for 24 hours. The resulting material (yield 45%) appeared as dark purple granules of irregular shape and a grain size of 0.05-0.2 mm. **IR-spectrum**: 3454 cm^{-1} (O-H at the oxime group), 3311 cm^{-1} (N-H), 412 cm^{-1} (Se–Se), 489 cm^{-1} (N-Se), 1623 cm^{-1} (C=N), 1357 cm^{-1} (C-N), 1540 cm^{-1} (Se-C-N), 1150 cm^{-1} (C-NO). **X-ray photoelectron spectrum:** 533.6 eV and 531.2 eV (O 1s); 400.4 eV and 399.2 eV (N 1s); 288.5 eV, 286.9 eV and 285.0 eV (C 1s); 164.0 eV and 169.3 eV (Se 3p).

Synthesis of bis{5-[3-(4-{[amino(mercapto)methylidene]amino}-1,2,5-oxadiazol-3-yl)-1,2,4-thiadiazol-5-yl]-4-thioxo-4,5-dihydro-1,3,5-triazin-2-yl} disulfide (product P2). Dry *N*'-hydroxy-1,2,5-oxadiazole-3-carboximidamide **1** was mixed with thiourea (1.5 mol) at a ratio of 1:3, and then the mixture was slowly fused at 220-250°C for 60-80 minutes. When the homogeneous melt was formed and the gas evolution ceased, the melt was cooled to room temperature, ground and sequentially washed with distilled water (three times), EtOH (once), and dichloromethane (once). The material was dried to a constant weight in a vacuum desiccator at 5-10 Torr over P_2O_5 at 20-25°C for one day. The resulting material (yield of 36%) appeared as brown granules of irregular shape and a grain size of 0.05-0.2 mm. **IR-spectrum**: 3323 cm^{-1} (N-H), 2056 cm^{-1} (S-N), 1537 cm^{-1} (S=C-N), 1623 cm^{-1} (C= N), 3163 cm^{-1} (H-O-H), 532 cm^{-1} (S-S), 810 cm^{-1} (S-H), 476 cm^{-1} (N-S), 1369 cm^{-1} (C-N). **X-ray photoelectron spectrum:** 533.5 eV and 530.5 eV (O 1s); 399.7 eV and 388.3 eV (N 1s); 288.4 eV, 286.9 eV and 285.0 eV (C 1s); 165.0 eV and 163.0 eV (S 2p).

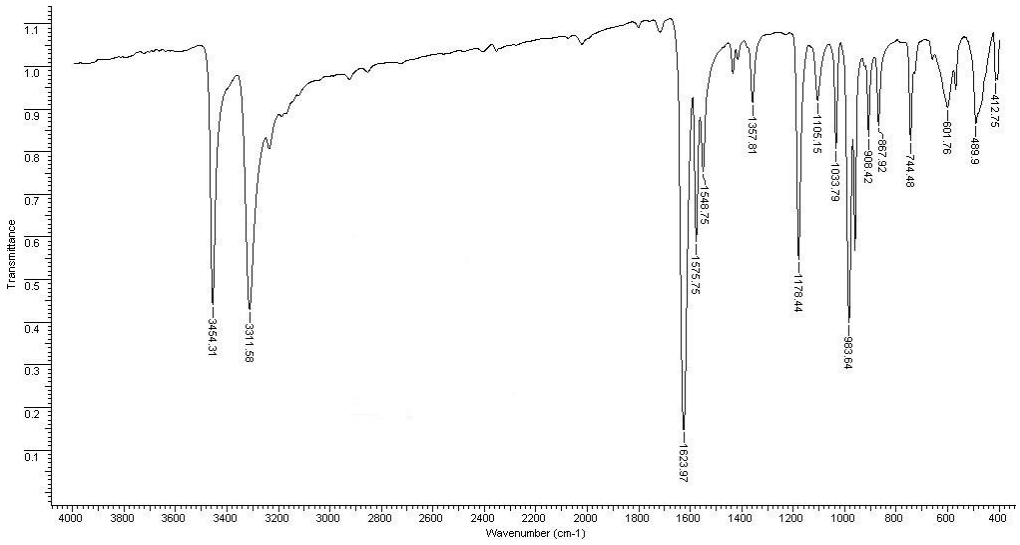

Figure S1 IR-spectroscopy of the P1

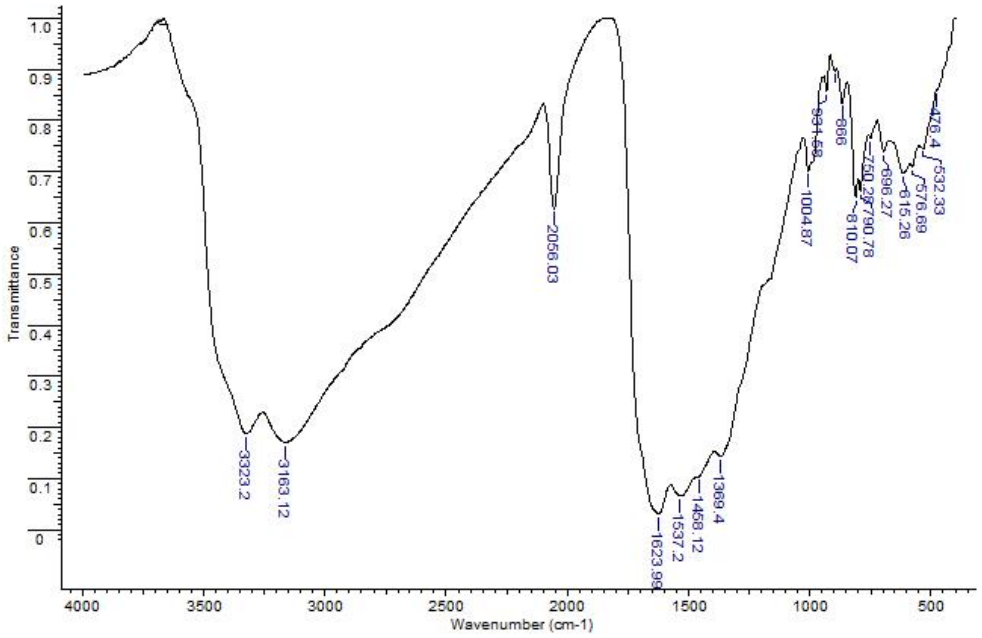

Figure S2 IR-spectroscopy of the P2

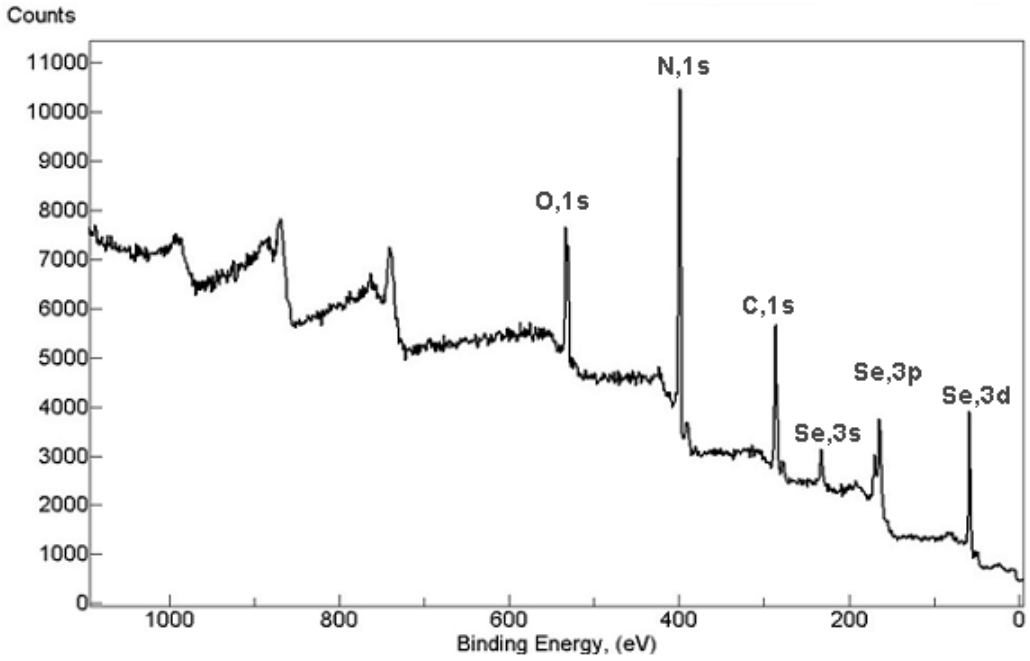

Figure S3 X-ray photoelectron spectroscopy of the P1

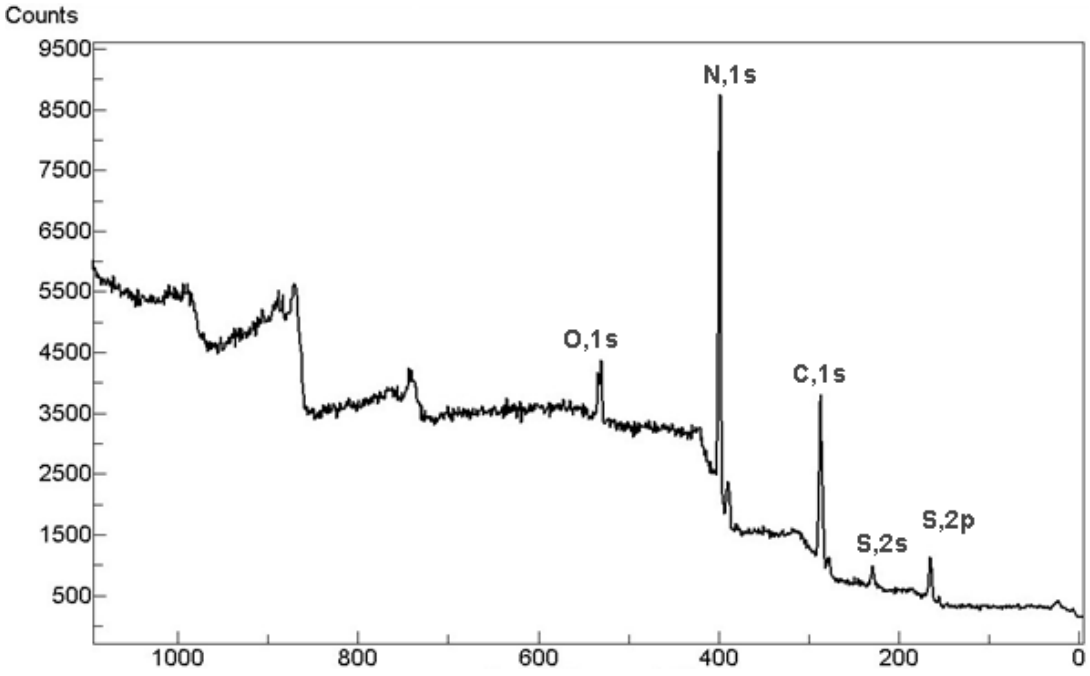

Figure S4 X-ray photoelectron spectroscopy of the P2

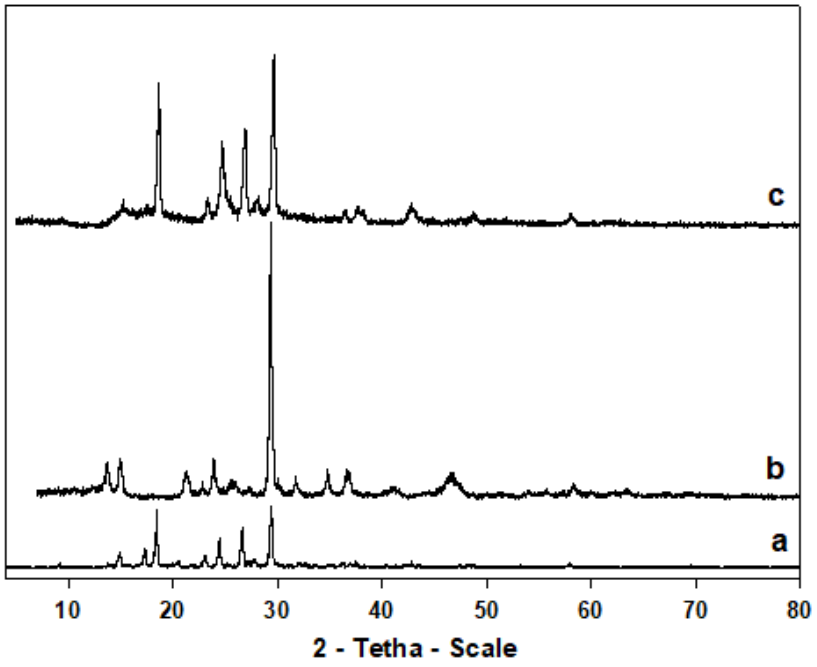

Figure S5 XRD image: **a** - compound 1, **b** – P1, **c** – P2