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Polydentate phosphinoxide-bearing N-heterocycles as extractants for f-elements

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A new type of heterocyclic "hard-and-soft"phosphinoxide-bearing N-heterocycles for f-elements binding was proposed from the basis of DFT simulation (PBE, B3LYP, cc-pVDZ and cc-pVTZ basis sets). The efficient method for the scalable preparation of the reagents by cross-coupling reactions was developed. As a N-donor scaffold the pyridine, 2,2'-bipyridine and phenanthroline were used and their combination with different dialkyl-, diaryl- or alkylarylphosphinoxides were applied. The structures of the ligands were estimated by X-Ray. All of the synthesized reagents demonstrate selectivity to Am over Eu on extraction from 0.5-5M nitric acid to polar diluents. For the first time the significant affect of P,P-diasteriomers on extraction was observed for phenanthroline-based reagent. Solvate numbers for the extractants strongly depends on the number of donating atoms and less on their nature. The model Eu complexes were prepared and structurally characterized for the extractants based on 2,2'-bipyridine and phenanthroline scaffolds. Phosphinoxides based on 2,6-disubstituted pyridine possess the better among investigated compounds efficiency in Am/Cm separation (SFAm/Cm 2.9-3.5 from 0.1-3M HNO3) which was estimated based on three methods γ-, α- and liquid-scintillation spectrometry. The DTF modeling of the extracting species show that the better fitting of the spatial requirements of the ligand was observed for Am than Cm or Eu . The reagents demonstrate excellent radiation stability: the γ-radiolysis up to 350kGr doesn't decrease the Am, Eu and Cm distribution coefficients. So the new generation of neutral organophosphorous reagents are promising for application in minor actinide separation technology.
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