

# STUDY OF BTPHEN AND ITS DERIVATIVES COMPLEXATION WITH LANTHANIDES AND ACTINIDES

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Nuclear power programs are considered by many countries in order to meet the rising energy demands. Although, nuclear energy is carbon neutral, the spent fuel is highly radiotoxic and must be therefore stored in a secure way to avoid environmental hazards. Lots of research has been carried out in “Partitioning and Transmutation” of spent fuel to reduce its radiotoxicity and therefore also decrease the storage time. [1]

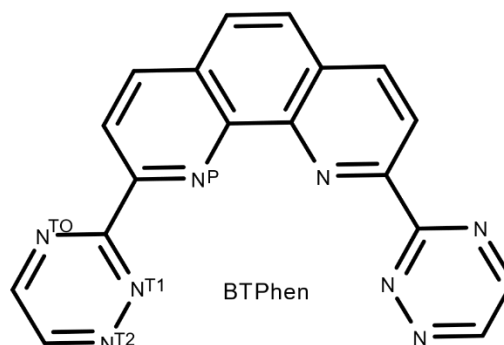


Figure 1. BTPhen ligand, where different nitrogens are described. [2]

The focus of the current work was to address modifications in the BTPhen ligand to increase its selectivity towards separation of actinides and lanthanides. As a first step [2] we started by gradually replacing nitrogens that were not directly connected to lanthanide with CH groups. This helped us to understand how these substitutions change the complex stability in the lanthanide series. Next we carried out the same analysis with only Am<sup>3+</sup> and Eu<sup>3+</sup> to further our understanding of lanthanide/actinide separation.

As a result we found that substituting N<sup>T0</sup> with CH group increases the complex stability while substituting N<sup>T2</sup> has the opposite effect. All of the complexation reactions were found to be exothermic in gas phase. The energetic parameters rise in lanthanide series from left to right. When carrying out the lanthanide/actinide separation analysis it was found that in gas phase and organic media Eu<sup>3+</sup> complexes are more stable in gas phase and organic media, while Am<sup>3+</sup> complexes are more stable in water media.

## References

1. J.N.Mathur, M.S.Murali, K.L.Nash, 2001, *Solvent Extr. Ion Exch.*, 19, 357.
2. J.Burk, A.Adamson, L.Sikk, K.Tämm, A.Pupart, P.Burk, 2020, *Comput. Theor. Chem*, 1175, 112729.



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