

Binding of radionuclides to crown ether by density function theory

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Experimental research^[1] had reported that crown ether can chelate cerium nitride. We used the density functional theory to model this complex and found that the structure shows good agreement with experimental data. The binding energy between the crown ether and cerium nitride is -2.5 eV, indicating strong bond between these two species. In addition, we consider the formation of complexes between actinides systems (U, Am and Cm) and the crown ether. Hadisaputra *et al* ^[2]reported that the increasing number of oxygen which are substituted by nitrogen in crown ether increase the binding energy and increases the amount of the charge transfer. We explore the effects of substitution of nitrogen for oxygen also consider crown ethers containing sulfur and phosphorus.

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Key words: crown ether, radionuclides, density functional theory

Reference:

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- [2] S. Hadisaputra, A. A. Purwoko, R. Armunanto, H. D. Pranowo, *Acta Chim. Asiana* **2020**, 3, 147–156.