

Theoretical study of the thermodynamic stability of the alkali metal complexes with ammonia as a ligand

Hamed Mahmoodpour,^a Shima Saberifar^a and Zahra Mardani^{*a}

^aInorganic Chemistry Department, Faculty of Chemistry, Urmia University, Urmia, Iran

* E-mail: z.mardani@urmia.ac.ir

The thermodynamic stability of the alkali metals complexes was investigated using theoretical studies, based on DFT by the lanl2DZ/B3LYP level of theory [1,2]. In this research, the Gibbs free energy caused by the interaction of the ligand with the metal has been considered as a component of the theoretical stability of the complex, even in cases where the complex did not exist. Optimization and frequency calculations of metals, ligands and complexes were separately performed. To find the most stable of the $M(NH_3)_n$ complexes the ΔG_f /coordination number diagram has been drawn. After finding the most stable structure of each metal, the metal/energy diagram of the complexes was drawn to investigate the thermodynamic stability of the $M(NH_3)_{1-6}$ complexes (Fig.1-a) [3-4]. The results showed that the most stable form of these metals according to the coordination number will be $Li(NH_3)_4$, $NaNH_3$, KNH_3 , $RbNH_3$ and $CsNH_3$ complexes (Fig.1-b). Also, the comparison of the stability of these complexes showed the following order: $KNH_3 \gg Li(NH_3)_4 > RbNH_3 > CsNH_3 > NaNH_3$

Keyword: Alkali Metal, Theoretical study, Thermodynamic stability, Gibbs free energy

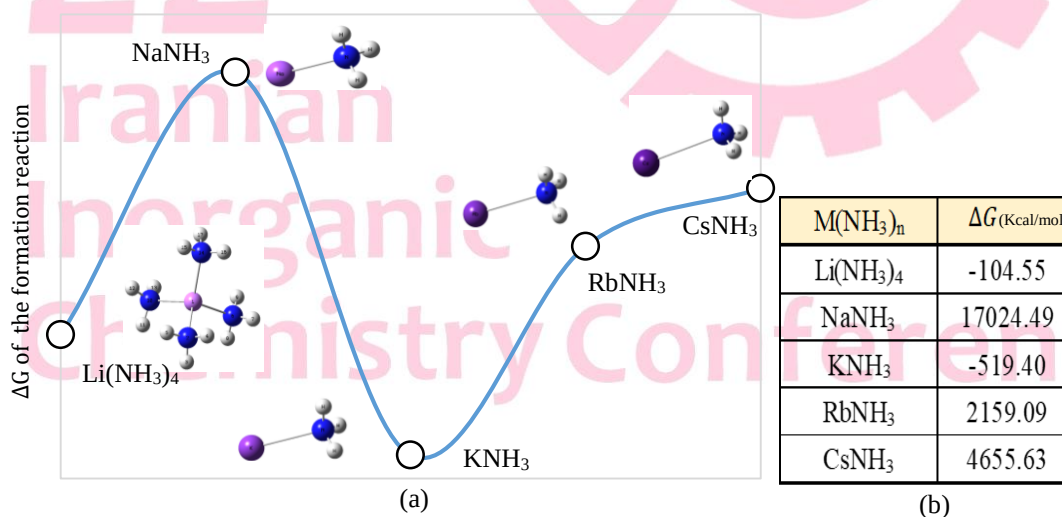


Fig.1. (a) Comparison of relative thermodynamic stability of alkali metal complexes. (b) The value of the theoretical Gibbs free energy of the formation reaction

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