Shibl, M.F.[a] , Hameed, S.A.[b] , Elroby, S.A.K.[b c]
A DFT study of the complexation behavior of hemispherands toward alkali metal cations
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[a] Chemistry Department, Faculty of Science, Cairo University, Cairo, Egypt
[b] Chemistry Department, Faculty of Science, King Abdul-Aziz University, Jeddah, Saudi Arabia
[c] Chemistry Department, Faculty of Science, Beni-Suief University, Beni-Suief, Egypt

Abstract
A density functional theory study of the behavior of hemispherands toward alkali metal ions (Li+, Na+, and K+) is performed. The effect of the replacement of the rigid anisyl group(s) by the mobile ether group(s) on the binding energy of hemispherands with alkali metal ions is investigated. The results indicated that the binding energies are inversely proportional to the ionic radius of the cations. Moreover, increasing the flexibility of the ligand results in decreasing the binding toward small ions. The structures of the hosts and the guests are correlated to the binding energies, and the correlations are interpreted in terms of the principle of preorganization. © 2010 Wiley Periodicals, Inc.

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Binding energy; DFT; Hemispherand; Host-guest

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