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Title:	The Effect of Hydration on the Cation- π Interaction Between Benzene and Various Cations
Authors:	Dhindhwal, V. (/jspui/browse?type=author&value=Dhindhwal%2C+V.) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Hydration Cation- π interaction Qualitative
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Citation:	Journal of Chemical Sciences, 128(10),pp.1597–1606.
Abstract:	The effect of hydration on cation- π interaction in $M^+ \cdots B \cdots W_n$ (B = benzene; W = water; M^+ = Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Al^{3+} , $0 \leq n, m \leq 4, 1 \leq m + n \leq 4$) complexes has been investigated using ab initio quantum chemical methods. Interaction energy values computed at the MP2 level of theory using the 6-31G(d,p) basis set reveal a qualitative trend in the relative affinity of different cations for benzene and water in these complexes. The π -cloud thickness values for benzene have also been estimated for these systems.
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