THEORETICAL INVESTIGATION OF THE M^+-RG_2 (M = ALKALINE EARTH METAL; RG = RARE GAS) COMPLEXES

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Metal cation rare gas complexes provide an expectedly simple system with which to investigate intermolecular interactions. Despite this, we have previously found the M^+-RG (M = alkaline earth metal) complexes to very complicated systems, with the complexes of the heavier rare gases displaying surprisingly large degrees of chemical character.[a,b,c] Here we extend these studies by examining the nature of these interactions with increasing degrees of solvation through investigating the M^+-RG_2 complexes using high level *ab initio* techniques. Intriguing trends in the geometries and dissociation energies of these complexes have been observed and are rationalized.

[a] A. M. Gardner, C. D. Withers, J. B. Graneek, T. G. Wright, L. A. Viehland and W. H. Breckenridge, *J. Phys. Chem. A*, **2000**, *114*, 7631.

[b] A. M. Gardner, C. D. Withers, T. G. Wright, K. I. Kaplan, C. Y. N. Chapman, L. A. Viehland, E. P. F. Lee and W. H. Breckenridge, *J. Chem. Phys.*, **2010**, *132*, 054302.

[c] M. F. McGuirk, L. A. Viehland, E. P. F. Lee, W. H. Breckenridge, C. D. Withers, A. M. Gardner, R. J. Plowright and T. G. Wright, *J. Chem. Phys.*, **2009**, *130*, 194305.