Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Quantum Theoretical Study of KCl and LiCl Clusters TED KOETTER, AJIT HIRA, JUSTIN SALAZAR, DANELLE JARAMILLO, Northern New Mexico College — This research focuses on the theoretical study of molecular clusters to examine the chemical properties of small K_nCl_n and Li_nCl_n clusters (n = 2 - 20). The potentially important role of these molecular species in biochemical and medicinal processes is well known. This work applies the hybrid ab initio methods of quantum chemistry to derive the different alkali-halide (M_nH_n) geometries. Of particular interest is the competition between hexagonal ring geometries and rock salt structures. Electronic energies, rotational constants, dipole moments, and vibrational frequencies for these geometries are calculated. Magic numbers for cluster stability are identified and are related to the property of cluster compactness. Mapping of the singlet, triplet, and quintet, potential energy surfaces is performed. Calculations were performed to examine the interactions of these clusters with some atoms and molecules of biological interest, including O, O2, and Fe. Potential design of new medicinal drugs is explored.

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Date submitted: 14 Nov 2013 Electronic form version 1.4