Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Ab Initio Study of KCl and NaCl Clusters CLIFTON BROWN-RIGG, AJIT HIRA, JOSE PACHECO, JUSTIN SALAZAR, Northern New Mexico College — We continue our interest in the theoretical study of molecular clusters to examine the chemical properties of small K_nCl_n and Na_nCl_n clusters (n = 2 - 15). 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 have been performed to examine the interactions of these clusters with some atoms and molecules of biological interest, including O, O2, and Fe. The potential for design of new medicinal drugs is explored.

Ajit Hira
Northern New Mexico College

Date submitted: 27 Nov 2012 Electronic form version 1.4