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Ab Initio Study of KCl and AgCl Clusters.[1] JAMES MCKEOUGH, AJIT HIRA, Northern New Mexico College, TOMMY CATHEY, Lockheed Martin , ALEXANDRA VALDEZ, Northern New Mexico College — This paper presents a theoretical study of molecular clusters that examines the chemical and physical properties of small K_nCl_n and Ag_nCl_n clusters (n = 2 - 24). Due to combinations of attractive and repulsive long-range forces, such clusters exhibit structural and dynamical behavior different from that of homogeneous clusters. The potentially important role of these molecular species in biochemical and medicinal processes is widely known. This work applies the hybrid ab initio methods 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. We will also investigate model and material dependence of the results.

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