GEOMETRIES AND VIBRATIONAL FREQUENCIES OF CALCIUM AND STRONTIUM RADICAL SALTS

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The equilibrium structures and vibrational frequencies of a variety of inorganic radicals containing Calcium and Strontium, CaX and SrX were computed using Density functional method B3LYP and double-zeta basis sets with polarization functions. Ligands X of the radical salts studied include: H, F, Cl, OH, SH, CN, NC, CCH, N_3, NCO, NCS, NH_2, CH_3, OCH_3, SCH_3, BH_4, HCOO, CH_3COO, HCONH, $HCONCH_3$, C_5H_5, C_4H_4N and $CH_3C_5H_4$. Discussion of vibration frequencies characteristic of the radical salts will focus on the stretching and bending of the metal-ligand bond across the series from monodendate, bidendate to half-sandwiched type of binding. Computational estimates of quantities that will aid future experimental measurements such as isotopic shift of vibrations will be presented. The radical salts are found to be ionic generally with the metal atom carrying a partial positive charge near unity.