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Relativistic calculations of eka-francium and its homologues hydrides.

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This work presents calculations of the bond distances and dissociation energies of LiH, NaH, KH, RbH, CsH, FrH and 119H. The electron configuration of alkali metals contains one open s-orbital, therefore the molecular shells of alkali metal hydrides are closed, which simplifies the study of these molecules'chemical properties. To take into account electronic structure we use coupled cluster theory including single, double and perturbative triple cluster amplitudes (CCSD(T)). The calculations are performed within the framework of the relativistic Dirac-Coulomb Hamiltonian, employing the computational software package DIRAC. Based on the obtained results we can make a conclusion that relativistic effects related to contraction of the valence s-orbital are of a high importance for large Z.

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