Theoretical study of the FrLi molecule: Potential energy curves, Spectroscopic constants, Dipole moment, Radiative lifetime and Spectrum absorption

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Abstract

The FrLi molecule has not yet been well reported. In this paper, potential energy curves, as well as relevant permanent and transition dipole moments, for X1Σ+-101Σ+, 13Σ+-103Σ+, 11,3Π - 61,3Π and 11,3[?]-21,3[?] of FrLi are obtained using a standard quantum chemistry approach based on pseudopotential for Fr+ and Li+ cores, Gaussian basis sets, effective core polarization potentials and full configuration interaction calculations. We present extensive predictions for the electronic structure of FrLi for which numerical data have been listed in a data base available as supplementary data. Based on the Effective Hamiltonian Theory and an effective metric, a diabatisation procedure was used to produce the quasi-diabatic potential energy. We have determined the adiabatic and quasi-diabatic potential energy curves. Spectroscopic constants (Re, De, Te, ωe, ωeχe and Be) are also determined. In addition, we have localized and analyzed numerous avoided crossings between electronic states of 1,3Σ+, 1,3Π and 1,3Δ symmetries. For the FrLi molecule, these avoided crossings can be explained by the ionic interaction between Fr+ and Li-, and Fr- and Li+. The permanent dipole moment of FrLi has revealed both ionic characters relating to electron transfer and yielding Fr+Li- and Fr-Li+ arrangements. These transition dipole moments is used to evaluate the radiative lifetimes of the vibrational levels trapped in the two excited states. In addition to the bound–bound contribution, the bound-free term calculated using two different methods the Franck–Condon (FC) approximation, the sum role approximation and added to the total radiative lifetime. On the other hand we have presented the absorption spectrum.

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