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Multiconfigurational Study of $X^2\Sigma^+$ and $A^2\Pi$ States of BeF, MgF and CaF molecules

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Alkaline-earth monofluorides have applications in several areas such as industrial chemistry and astrophysics. Recently, the diatomic molecules BeF, MgF and CaF have been used in laser deceleration and cooling processes [1]. These processes allow more accurate measurements of the properties of these systems. The objective of this work is to perform a qualitative and quantitative description of the BeF, MgF and CaF potential energy curves of the two low-lying states $X^2\Sigma^+$ and $A^2\Pi$. The qualitative analysis of the chemical bond between halogens and alkaline-earth metals was carried out from the information of the separated atoms, using a simple model to describe the ionic and covalent character of this bond and predicting the behavior of the potential energy curves. The quantitative analysis of the electronic states was performed employing MRCI and CASPT2 correlation methods assigning dynamic weight to the involved states in the average orbital during the CASSCF method. Calculations were performed using the cc-pV5Z basis set for the metals and aug-cc-pV5Z for the fluorine. Potential energy curves show interaction between states of the same symmetry at the internuclear distance where there is charge transfer. At these distances, avoided crossings arise and the change of ionic character to covalent occurs. Spectroscopic constants of these diatomic molecules were calculated and compared to the experimental data [2]. Analyzing the results was possible to observe that the choice of multiconfiguration methods allows the wave function to correctly describe the change of character of the chemical bond. The obtained molecular constants are in agreement with the experimental data. The calcium monofluoride exhibits the lowest excitation energy among the studied molecules, being the transition $A^2\Pi \rightarrow X^2\Sigma^+$ more favorable for that molecule.

Key-words: Eletronic structure, Diatomics, Qualitative analysis
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