UNDULATING POTENTIAL ENERGY SURFACES FOR THE RYDBERG STATES OF SMALL MOLECULES CONTAINING A METAL ATOM

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The undulating potential curves originating from the atomic orbital structure of the Rydberg metal atom in diatomic molecules reported before [a] are generally present in all Rydberg states of Σ symetry in diatomic molecules. These undulations are not related with any avoided crossing between adiabatic electronic states, but they come from steric interaction between the Rydberg electron and the compact atom or ligand. As the Rydberg electron distribution occupies a large volume, these undulations are present at long internuclear distances. The Rydberg states of triatomic and quadratomic molecules containing a metal atom also show undulating potential surfaces. We present here several cases to prove the generality of this peculiar spectroscopic property.