AB INITIO STUDY OF $MgAr^+$ AND $MgXe^+$

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Potential curves for the four lowest lying states of the $MgRG^+$ type complexes (where RG: Ar, Xe) were generated using relativistic spin-orbit configuration interaction calculations based on effective core potentials. The weak interaction forces between Mg^+ and RG atoms, ion-induced dipole forces, dispersion forces, etc. require a more extensive correlation energy description than we could use, so this work gives law dissociation energies and high internuclear distances compared to experimental values. But the most important aspect of this theoretical study is that we are able to give an explanation for the unexpectedly large spin-orbit splitting between the $^2\Pi_{1/2}$-$^2\Pi_{1/2}$ excited states of these systems.