Structure and Spectra modeling of CsRg (Rg=Ar, Xe, Kr) van der Waals Complexes

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The potential energy interactions of the ground state and many excited states of the CsRg van der Waals complexe have been determined using [Cs^+] and [e-Rg] pseudopotentials [1-3] with the inclusion of core polarization operators on atoms. This has reduced the number of active electrons of the CsRg dimer to only one valence electron, permitting the use of large basis sets for the Cs and Xe atoms. Potential energy curves of the ground state and many excited states have been performed at the SCF level. The core-core interactions for Cs^+Rg are included using the accurate CCSD potential of Hickling et al [4]. Spectroscopic constants for the ground and excited states of CsRg are derived and compared with the available theoretical and experimental results. In addition, the transition dipole moment have been evaluated in order to simulate the $X^2\Sigma^+$---$A^2\prod_{1/2}$, $X^2\Sigma^+$---$A\prod_{3/2}$ and $X^2\Sigma^+$--$B^2\Sigma_{1/2}^+$ absorption spectra and to predict molecular transition shift and the Cs atomic spectrum broadening requested for development of powerful Alkali metal vapor lasers that are pumped by diode lasers [5-6].

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