DYNAMICS OF NeI_2 SYSTEM IN THE "INFINITE ORDER SUDDEN APPROXIMATION" (IOSA): A QUANTUM MECHANICAL CLOSE-COUPLED TREATMENT.

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Taking advantage of fast vibrational and low rotational motions within the NeI_2 molecule, we solve "exactly" the vibrations in the "close-coupled equations" formalism for each atom-diatom orientation γ . In the IOSA frame we start with the excited electronic state of I_2 subunit. As a consequence, we obtain an effective potential for the bending motion and calculate the energies and vibrational predissociation (VP) linewidths of the resonances as functions of the angular configuration of the triatomic system. This may be performed by some of the currently available numerical integration methods. So, bending motion is considered in an approximate way and three-dimensional rates for VP are reached by averaging on the configurations. We do this for the region of intermediate vibrational excitation of the I_2 diatom obtaining then the behaviour of the VP rates as a function of the vibrational quantum number of I_2 . Final rotational and vibrational distributions of the diatomic fragment are also calculated.