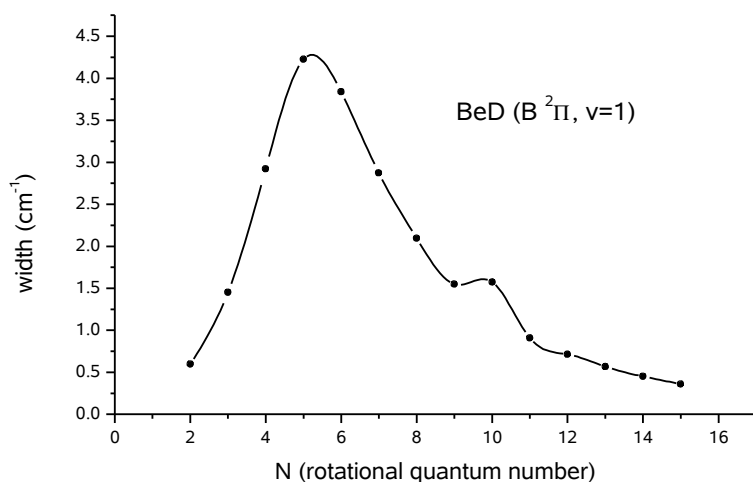
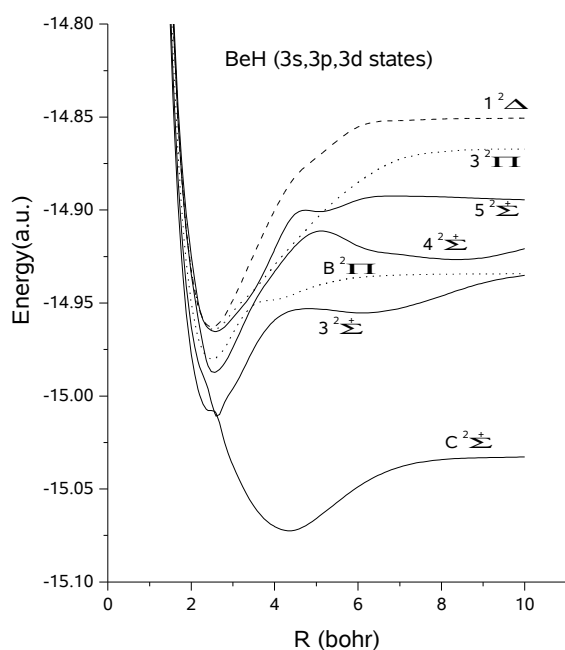


## Multi-state calculations by solution of the complex eigenvalue Schroedinger equation

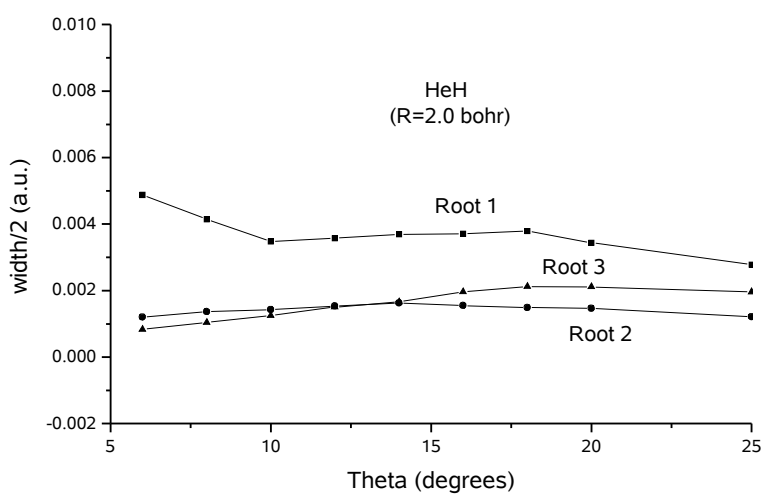
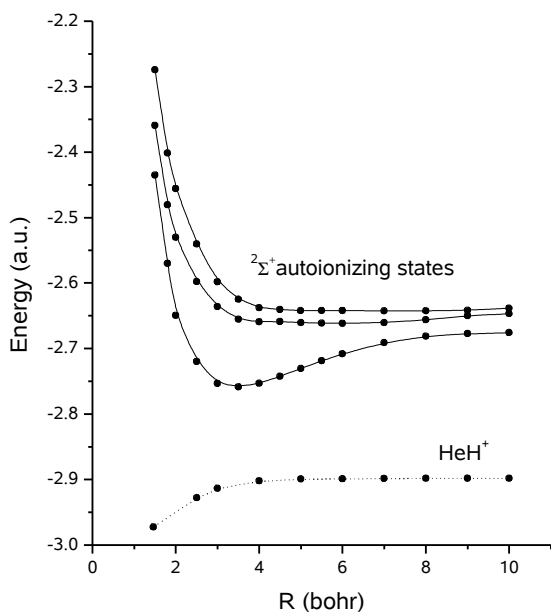
Different types of coupling interactions, not accounted for by Born – Oppenheimer calculations exist between the excited electronic states of a molecule, which may lead to spectral perturbation and predissociation phenomena. In TPCI a multi-state complex scaling method is employed for the calculation of spectral perturbations and predissociation resonances, where all the interactions between the different states are included in the same complex eigenvalue Schroedinger equation [1-3]

### Excited electronic states of BeH, width of the $v=1$ $B^2\Pi$ state



Molecular electronic states lying above the first ionization limit autoionize. A CCR (complex coordinate rotation) configuration interaction calculation can determine the resonance [4].

### Autoionizing electronic states of HeH, stabilization of the calculated width



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[doi:10.1016/S0009-2614\(99\)00408-X](https://doi.org/10.1016/S0009-2614(99)00408-X)