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Spectroscopic Constant Calculation of the BeF Molecule

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Abstract : Ab-initio calculations have been performed to investigate the spectroscopic constants for the diatomic compound BeF. Values of the internuclear distance Re, the harmonic frequency ωe, the rotational constants Be, the electronic transition energy with respect to the ground state Te, the eignvalues Ev, the abscissas of the turning points Rmin, Rmax, the rotational constants Bv and the centrifugal distortion constants Dv have been calculated for the molecule's ground and excited electronic states. Results are in agreement with experimental data.

Keywords : spectroscopic constant, potential energy curve, diatomic molecule, spectral analysis
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