AB INITIO CALCULATION OF THE INFRARED SPECTRUM FOR XeF6 MOLECULE

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Scalar relativistic coupled cluster calculations are presented for the infrared spectrum of the xenon hexafluoride (XeF6) molecule in its Oh and C3v structures. Anharmonic contributions to vibrational frequencies and infrared intensities of the C3v structure are taken into account using second order vibrational perturbation theory (VPT2). The effect due to Fermi resonances in the VPT2 calculations is analyzed. A transition state linking the C3v and Oh structures has also been located in the potential energy surface. The fluxional character of the molecule is discussed.