ANOMALOUS ISOTOPIC EFFECT IN THE H-Xe STRETCHING FREQUENCY OF HXeOH

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The rovibrational energy levels of HXeOH and its isotopomers have been calculated using a two-layer Lanczos algorithm in Radau-diatom-Jacobi coordinates based on a high level *ab initio* potential energy surface. The surface is obtained by fitting to 1229 RCCSD(T)/SDB-cc-pVQZ energy points. The equilibrium geometry of HXeOH is determined to have a trans configuration with a nearly collinear HXeO bond angle of 177.32 degrees. The well depth of this minimum is only 0.6123 eV with respect to the OH + Xe + H dissociation limit. The results show that the H-Xe stretching frequency of HXeOH and HXeOD has an anomalous isotopic shift upon ^{18}O isotope substitution, whereas the D-Xe stretch in DXeOH and DXeOD displays a normal isotopic shift. This trend is consistent with the experimental observations in a Xe solid matrix. The present results predict a lower frequency for the H-Xe stretch than was observed in the solid matrix expriment. Either these results are too low or there is a strong blue shift due to the matrix in the experimental values.