PHYS 508: **Ratio of the number of states in asymmetric and symmetric ozone molecules deviates from the symmetry driven value of 2**

Abstract: Calculations of the vibrational states up to dissociation threshold are carried out in the singly and doubly substituted molecules of ozone: $^{16}O^{18}O^{16}O$, $^{18}O^{16}O^{18}O$, $^{18}O^{16}O^{16}O$ and $^{16}O^{18}O^{18}O$. This includes the usual vibrational states of ozone bound in a deep covalent well, but also the weakly bound floppy OO_2 complexes delocalized over the shallow van der Waals interaction region of the potential energy surface near dissociation threshold. Accurate variational approach is employed that uses the APH hyper-spherical coordinates and an accurate potential energy surface. Analysis of these spectra reveals noticeable deviations from the statistical factor of 2 for the ratio between the number of states in asymmetric and symmetric ozone molecules. It is found that, for the lower energy parts of spectra, the ratio is below 2 in the singly substituted ozone molecules, but it is above 2 in the doubly substituted ozone molecules. However, the upper parts of spectra, just below dissociation thresholds, exhibit a different behavior. In this energy range the singly and doubly substituted ozone molecules behave similar, with the ratio of states in asymmetric and symmetric ozone molecules being above 2 in both cases. This property may contribute to explanation of the mysterious eta-effect in the ozone forming reaction that favors formation of the asymmetric ozone molecules.

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