



An ab initio molecular orbital study of the electronically excited and cationic states of the ozone molecule, and a comparison with spectral data

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The valence and Rydberg, singlet and triplet, excited states for ozone in the excitation energy range 1-12eV, have been calculated by large scale CI methods. A comparison of the theoretical intensity envelope with the VUV+EELS spectrum has been made. The present work supports the assignments for the Huggins+Hartley bands as having two electronic origins, 1A1 and 1B2. A Huggins+number of new valence and Rydberg states have been calculated, and these lead to the conclusion that the experimental 9 - 11 eV VUV spectral range in particular must yield more experimental states than the few so far identified. The experimental 9.3 and 10.2 eV bands of the VUV spectrum must have adventitious superposition of valence states on Rydberg transitions, because the high oscillator strengths of the valence states cannot be attributed to the 8.8 eV broad band. This suggests a major need for more sophisticated methods of experimental study for the excited state manifolds. These studies of the vertical cationic states, support the IP order as $2A1 < 2B2 < 2A2$.