

Abstract Submitted
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Theoretical study of photodetachment of HOCO^- near threshold¹

SHUNGO MIYABE, U. C. Davis, C. WILLIAM MCCURDY, U. C. Davis, THOMAS N. RESCIGNO, Lawrence Berkeley National Laboratory — Continetti and Lu (Phys. Rev. Lett. 99, 113005 (2007)) have shown that the photoelectron kinetic energy distribution from HOCO^- exhibits two sharp peaks near threshold accompanied by a broader feature ranging from 0.4 to 1.9 eV. They have argued that the threshold peaks are s- and p- wave shape resonances. In contrast, here we show that these resonances can be attributed to the vibrational levels of a dipole-bound state of trans- HOCO^- . Our MP2 calculations give a value of 2.50 Debye for the dipole moment of trans- HOCO^- . The electron binding energy for the dipole-bound anion was found to be 0.0012 eV at the configuration-interaction level of theory with single and double excitations. We have also calculated the fixed-nuclei photodetachment amplitudes using variationally obtained electron-molecule scattering wavefunctions, which identifies the broad feature as an A'' -shape resonance.

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