Title:	Ab Initio Potential Energy Curves for the Ground and Low-Lying Excited States of OH and OH– and a Study of Rotational Fine Structure in Photodetachment
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Abstract:	Complete basis set extrapolated ab initio potential energy curves obtained from multireference configuration interaction (MRCI) level calculations for the ground state (X1Σ+) of OH–, and the ground state (X2Π) and the first excited state (A2Σ+) of OH are reported. The potential energy curves for the excited states A1Π, a3Π, and b3Π of OH– have been computed using the V6Z basis set at the MRCI level. Λ-doubling parameters p and q were calculated for the ground and the first excited vibrational states of the ground electronic state of OH using second-order perturbation theory. Using the computed potential energy curves and the rovibrational spectra for photodetachment including the fine splitting, the threshold for electron detachment has been computed. The result is in agreement with the experimental results of Goldfarb et al.
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