EQUATION-OF-MOTION COUPLED-CLUSTER CALCULATIONS OF PHOTODETACHMENT CROSS SECTIONS FOR ATOMIC NEGATIVE IONS ACROSS THE PERIODIC TABLE

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The innovative application of the ion-trap technique by Wester and coworkers has yielded definitive experimental values of photodetachment cross sections for the atomic oxygen radical anion ($O^{\bullet -}$) [Hlavenka et al., J. Chem. Phys. **130**, 061105 (2009)]. In the present study, equation-of-motion coupled-cluster (EOM-CC) calculations have been performed to derive theoretical values of photodetachment cross sections for the negative ions of atoms in the first two periods of the periodic table as well as of those which belong to the alkali metal and halogen groups. Two methods have been employed to derive the cross sections. One involves the Dyson orbitals obtained from EOM-CC calculations and plane wave functions for the detached electron in the transition dipole moment integrals. The other method utilizes the moment theory following EOM-CC calculations of transition dipole moments for a large number of pseudo-states. The cross sections so evaluated for $O^{\bullet -}$ match the experimental values very well. Generally good agreement has been found between the theoretical and experimental values of the cross sections for the atoms in the first two periods, while the present calculations cast some doubt on reported experimental values for some atoms beyond the second period. Substantial relativistic effects on the cross section have been observed for heavy elements in the alkali metal and halogen groups.