APPLICATION OF EQUATION-OF-MOTION COUPLED-CLUSTER THEORY TO PHOTODETACHMENT CROSS SECTION CALCULATIONS

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Photodetachment cross sections of atomic anions have been calculated with equation-of-motion coupled-cluster (EOM-CC) theory. Two techniques have been examined. One of them treats the photodetached electron as a plane wave, and the transition moment integral is evaluated with the Dyson orbital obtained from EOMIP-CC calculations. In the other technique, the EOM-EE method is utilized to calculate the oscillator strengths for photodetachment processes within the framework of moment theory. The results of these calculations are compared with experimental results, and the pros and cons of the two techniques are discussed.