Ab initio study of photodissociation of several small molecules.

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The mechanisms of photodissociation of several small molecules, including CH_3O, C_2H_2, and O_3^-, have been studied with ab initio calculations. The CASSCF-MRSDCI approach as well as the EOM-CCSD method has been applied to study the potential energy surfaces of ground and excited electronic states. Minima on the seam of crossing have been located and the reaction coordinates from them have been analyzed using the analytical gradient method, and their roles in the photodissociation process are discussed.