Spin-orbit coupling from multistate CASPT2

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We report an approach to compute spin–orbit coupling within the extended multistate second-order multiconfigurational perturbation theory (XMS-CASPT2). Our approach is based on the state interaction method, in which both diagonal and off-diagonal elements of the spin–orbit matrix are computed at the CASPT2 level. It enables analysis of chemical processes that occur as a result of a change in spin multiplicity, such as photocatalysis and those involving intersystem crossing. The algorithm for this approach is being implemented in the BAGEL program package.