UV excitation and radiationless deactivation of imidazole

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The vertical spectrum and the radiationless decay of imidazole have been investigated theoretically. Benchmark calculations were performed employing different methods and levels. Four different conical intersections were characterized and the reaction paths connecting the Franck–Condon region to them were computed. Two of the conical intersections show puckered structures while the other two show NH and ring dissociation patterns. The $\pi\pi^*$/$S_0$ N1-puckered conical intersection is connected to the planar $\pi\pi^*$/$S_0$ ring-opened conical intersection by a branch of the crossing seam. After excitation into the first $^1\pi\pi^*$ state, the internal conversion can occur either in this branch of crossing seam or along the NH-dissociation path. © 2009 American Institute of Physics.

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