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Vibrational Conical Intersections: Implications for Ultrafast Vibrational Dynamics[1] MAHESH DAWADI, BISHNU PRASAD THAPALIYA, Department of Chemistry, The University of Akron, RAM BHATTA, Department of Polymer Science, The University of Akron, DAVID PERRY, Department of Chemistry, The University of Akron — The presence of conical intersections (CIs) between electronic potential energy surfaces is known to play a key role in ultrafast electronic relaxation in diverse circumstances. Recent reports have documented the existence of vibrational CIs connecting vibrationally adiabatic surfaces. Just as electronic CIs are now appreciated to be ubiquitous, controlling the rates of many photochemical processes, the present work on methanol and methyl mercaptan suggests that vibrational CIs may also be widespread, possibly controlling the outcome of some high-energy processes where vibrationally excited species are present. Other examples of vibrational CIs include the vibrational Jahn-Teller effect in C_{3V} organic molecules and transition metal complexes. While the present work addresses only the couplings within bound molecules, the concept of vibrational CIs providing pathways for ultrafast relaxation also applies to molecular collisions.

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