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Molecular vibrations and the rotating Eckart frame of the ArHCl van der Waals complex FLORENCE J. LIN, University of Southern California — By changing its shape while conserving angular momentum, a polyatomic molecule can return to its initial shape with a different orientation (as a "falling cat" or a diver can do). Floppy atom-diatomic molecule van der Waals complexes are excellent candidates in which to observe this. It is shown that large-amplitude "internal" motions of an atom-diatomic molecule van der Waals complex with zero total angular momentum can lead to overall rotation of the complex in the center-of- mass frame, i.e., the internal motion and overall rotation are coupled. Using geometric mechanics, the net angle of overall rotation is explicitly described in terms of Jacobi coordinates. The net angle of overall rotation is the sum of a dynamic phase plus a geometric phase; the latter is also described in terms of a gauge potential and, alternatively, molecular rotational constants. This is demonstrated by numerically integrating Hamilton's equations using a potential energy surface determined by fitting to experimental data for the ArHCl van der Waals complex.

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