

# Geometric Mechanics and Internal Rotation in van der Waals Complexes

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## Abstract

Geometric mechanics and the geometric phase use differential geometry to describe Hamiltonian dynamical systems and Berry's phase. Here the more general and more accessible Poisson formulation is applied to the classical dynamics of atom-diatom molecule van der Waals complexes exhibiting unhindered internal rotation, such as NeHCl. A differential geometric result of Guichardet for classical molecular dynamics states that a purely vibrational motion can take a molecule to a final configuration related to the original configuration by a pure rotation. This paper provides three related results for atom-diatom molecule van der Waals complexes: (1) The internal rotational motion can not be separated from the overall rotational motion. (2) An explicit expression for the angular velocity of overall rotation is obtained by using Jacobi coordinates. (3) In the case of zero total angular momentum, the net angle of overall rotation is explicitly related to the angle of internal rotation of the diatomic molecule in the van der Waals complex and is a classical geometric phase.