PIECES OF THE PROPELLANE PUZZLE: AN INVESTIGATION OF ROVIBRATIONAL COUPLING

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[1.1.1]Propellane (C₅H₆) is a small ring D_{3h} molecule with an axial bond that continues to be a topic of debate. Recently propellane was subjected to high resolution spectroscopic scrutiny for the first time, and its ν ,l,J,K structure is being determined. It was found that ν_{15} , the axial antisymmetric C-C stretching mode that has a remarkably high dipole derivative, and the ν_{12} H wagging modes are rotationally coupled.