

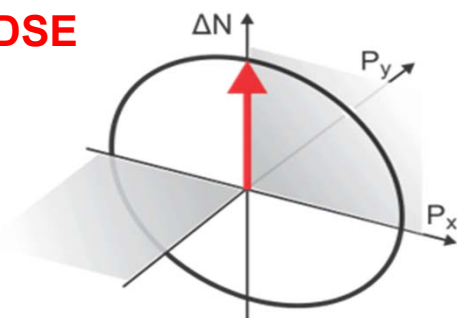
# P4290 USING COMPUTATIONAL TOOLS TO ENHANCE LEARNING IN AN UNDERGRADUATE MOLECULAR SPECTROSCOPY COURSE

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*Introduction to molecular spectroscopy; Nuclear magnetic resonance; Rotational spectroscopy of linear molecules  
Molecular symmetry; Vibrational spectroscopy (IR and Raman spectroscopy); Electronic spectroscopy*

**TDSE**



Molecular symmetry:  
Point groups of molecules

Rotational spectroscopy:  
Difference in equilibrium,  
effective, and substitution  
structures

Vibrational spectroscopy:  
Vibrational motions;  
Selection rules

NMR:  
Electron density ~~→~~ Chemical shifts

$$\sigma = \sigma_d + \sigma_p$$