P5319: 2-PROPIONYLTHIOPHENE: PLANAR, OR NOT PLANAR, THAT IS THE QUESTION

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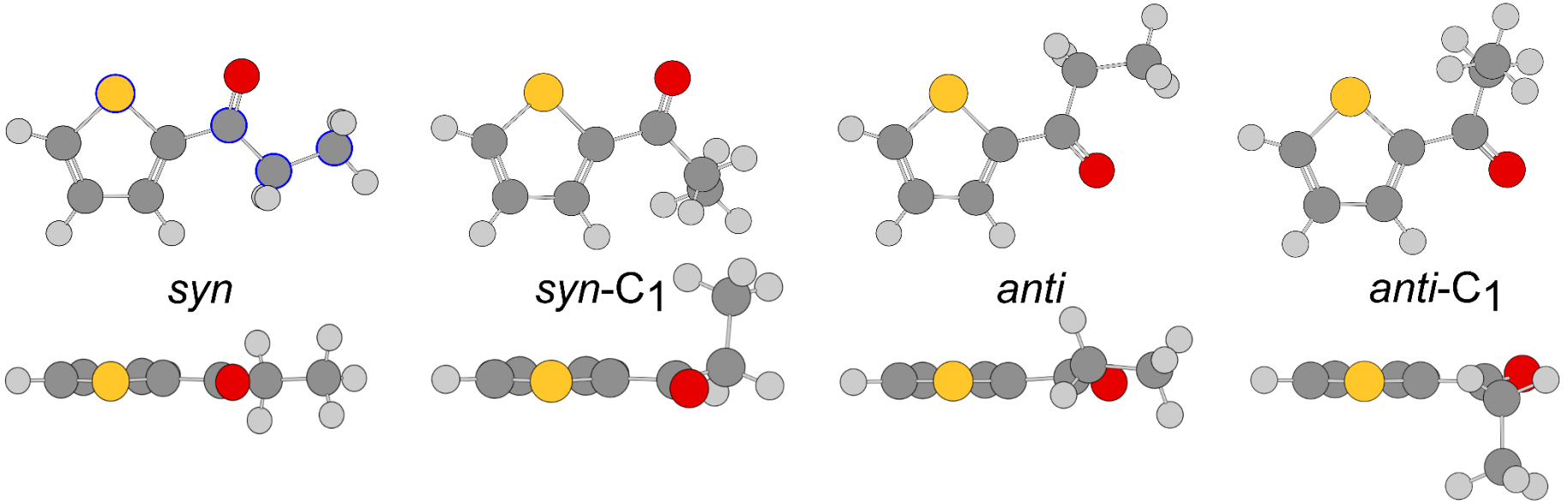

Energetic stability and structure are method-dependent in ab initio calculations

→ problem often encountered in ketones

① Which conformers are more stable? → Only *syn*- and *anti*-conformers found in MW spectrum

② Are *syn*- and *anti*-2PT planar? → Partial structure determination via isotopic substitution

→ r_s structure and inertial defects agree: not planar!

Internal rotation resolved for both *syn*- and *anti*-2PT → 806.94(54) and 864.5(88) cm^{-1}