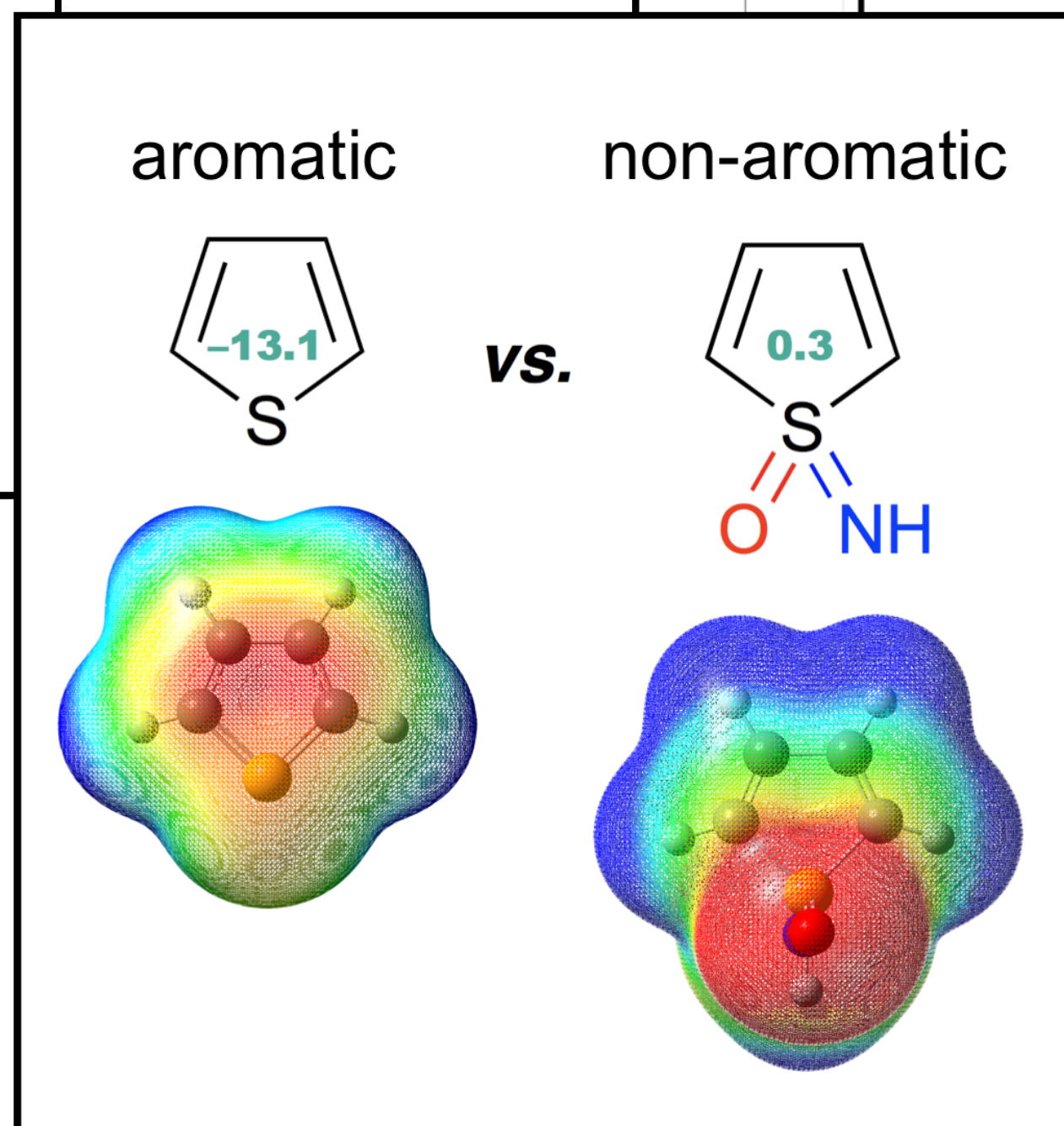
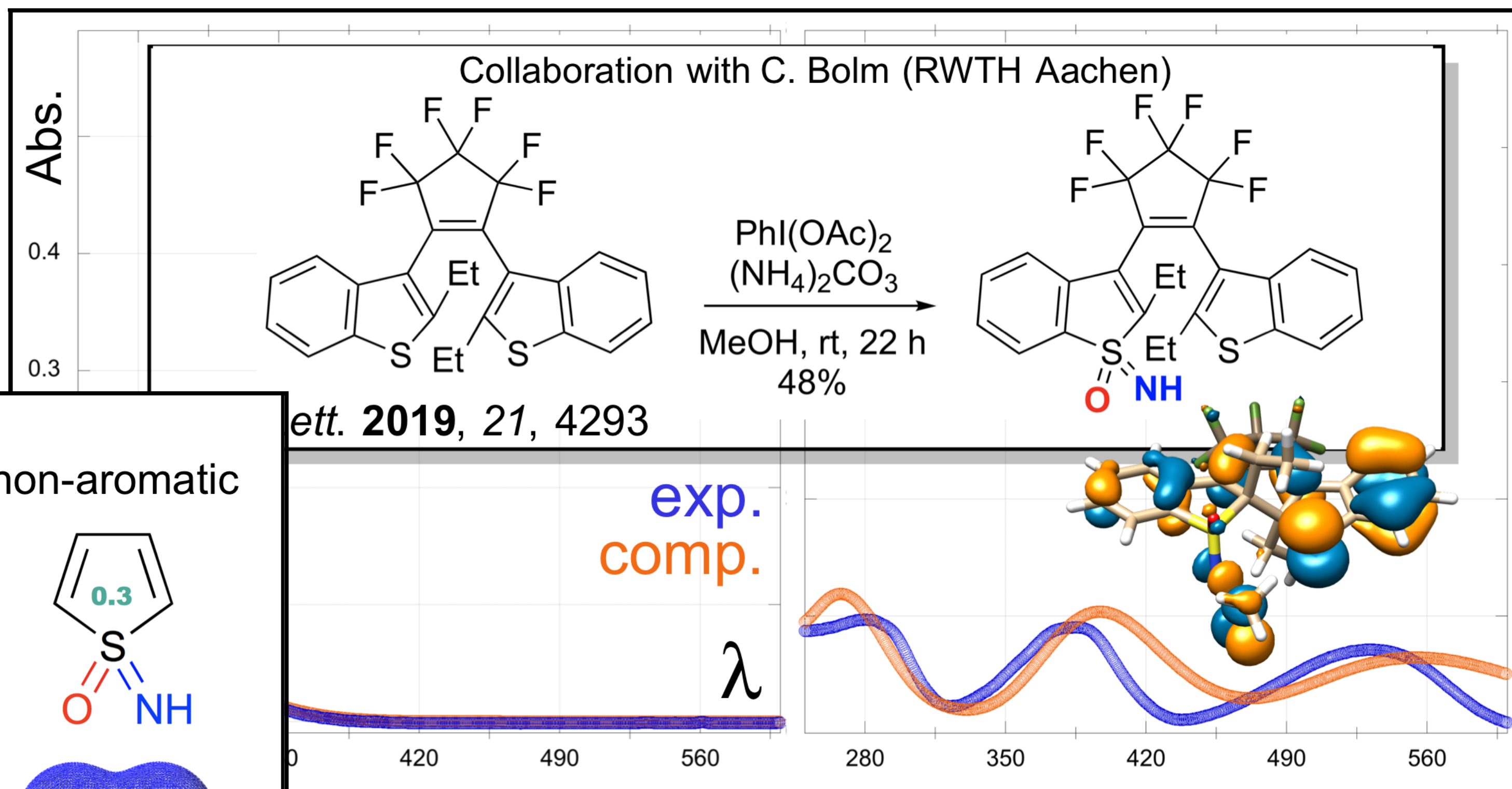
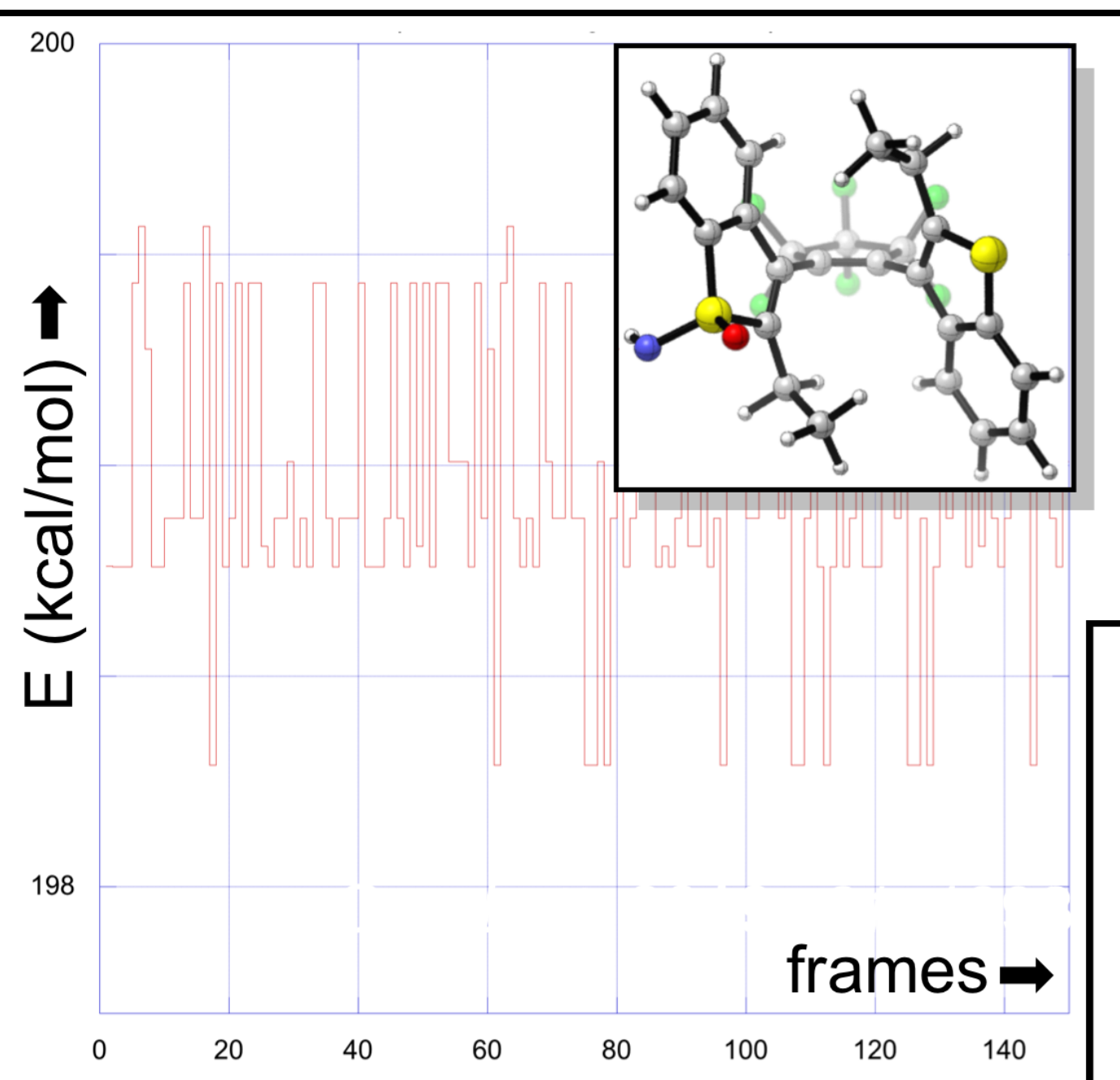


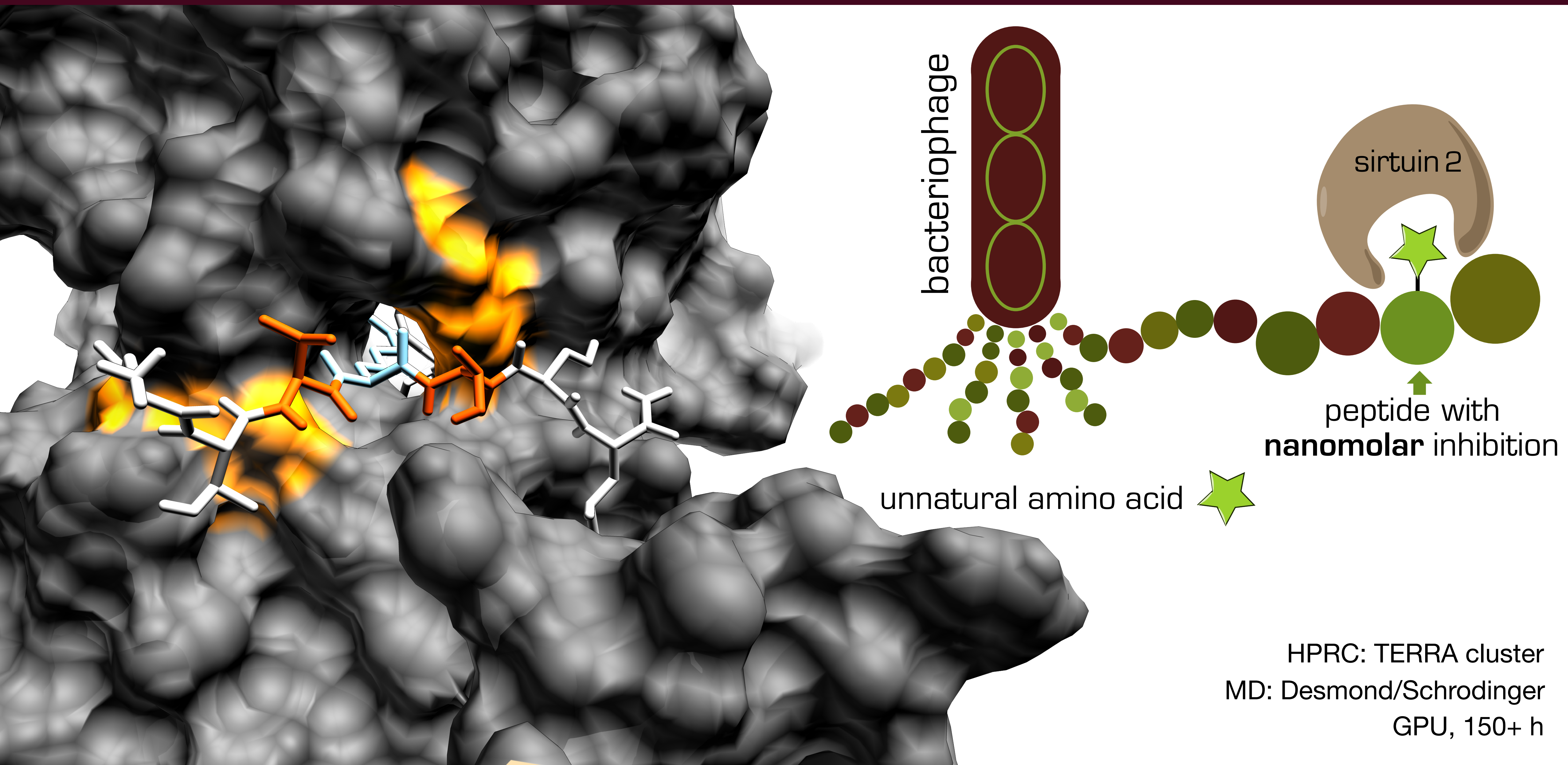
MD \longrightarrow conformational sampling

DFT \longrightarrow aromaticity index

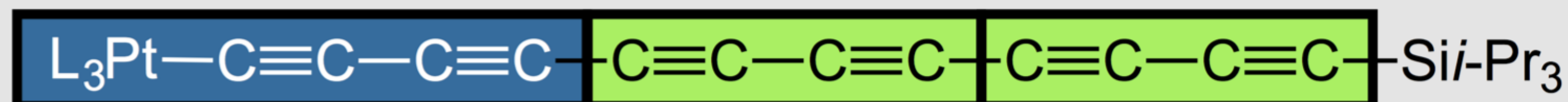
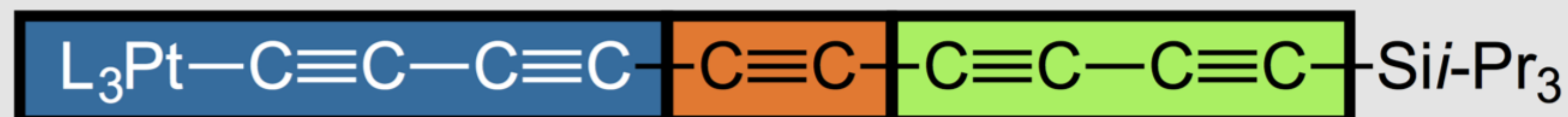
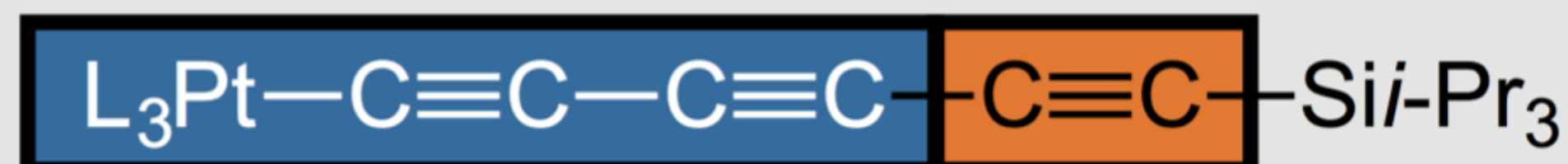
TDDFT \longrightarrow spectroscopy



HPRC: TERRA cluster
DFT and TDDFT: Gaussian 16
MD: Materials Studio
28 cores, 24h

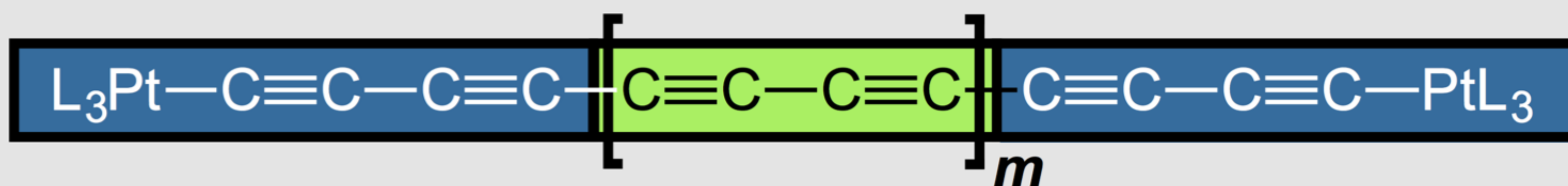
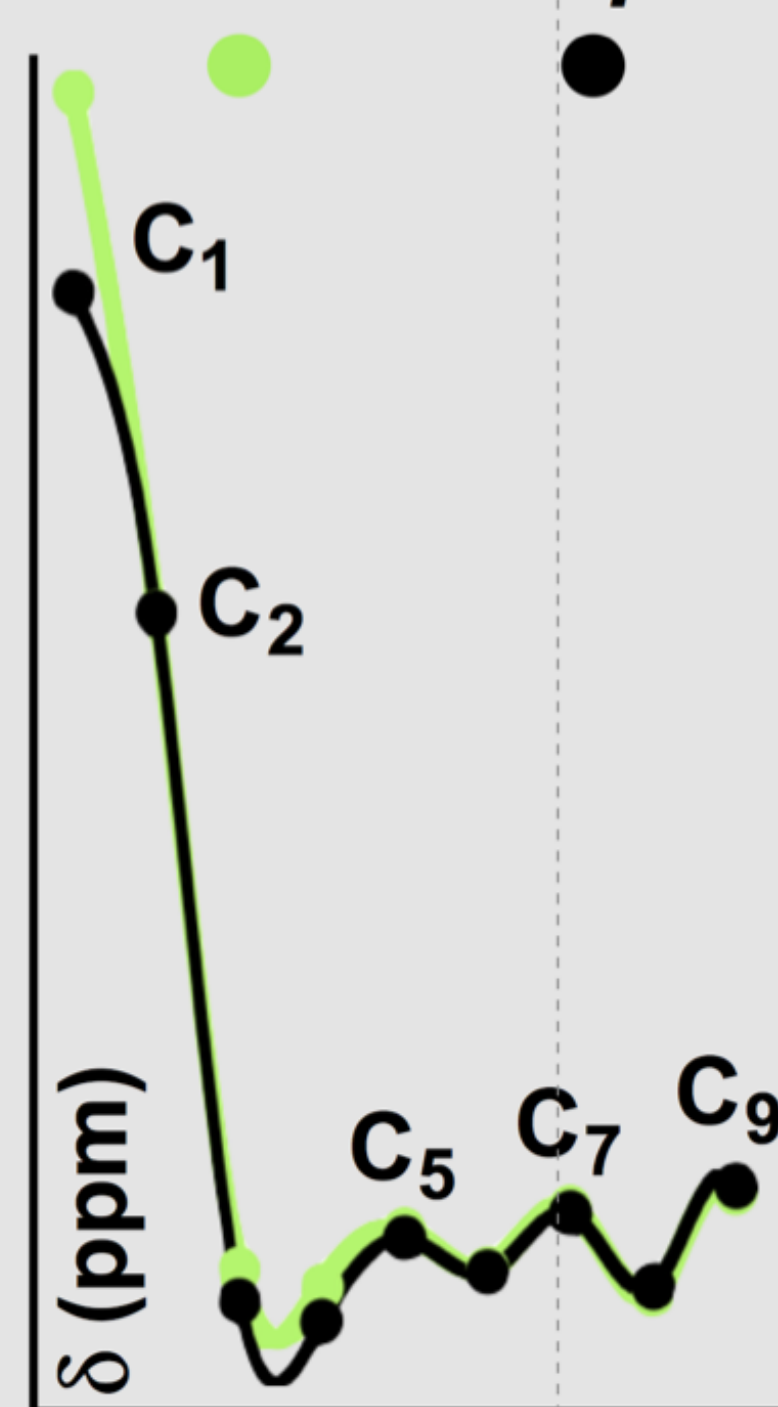


DFT \longrightarrow Predict and assign $^{13}\text{C}\{^1\text{H}\}$ signals in platinum end-capped polyynes



C_{sp} chain extension

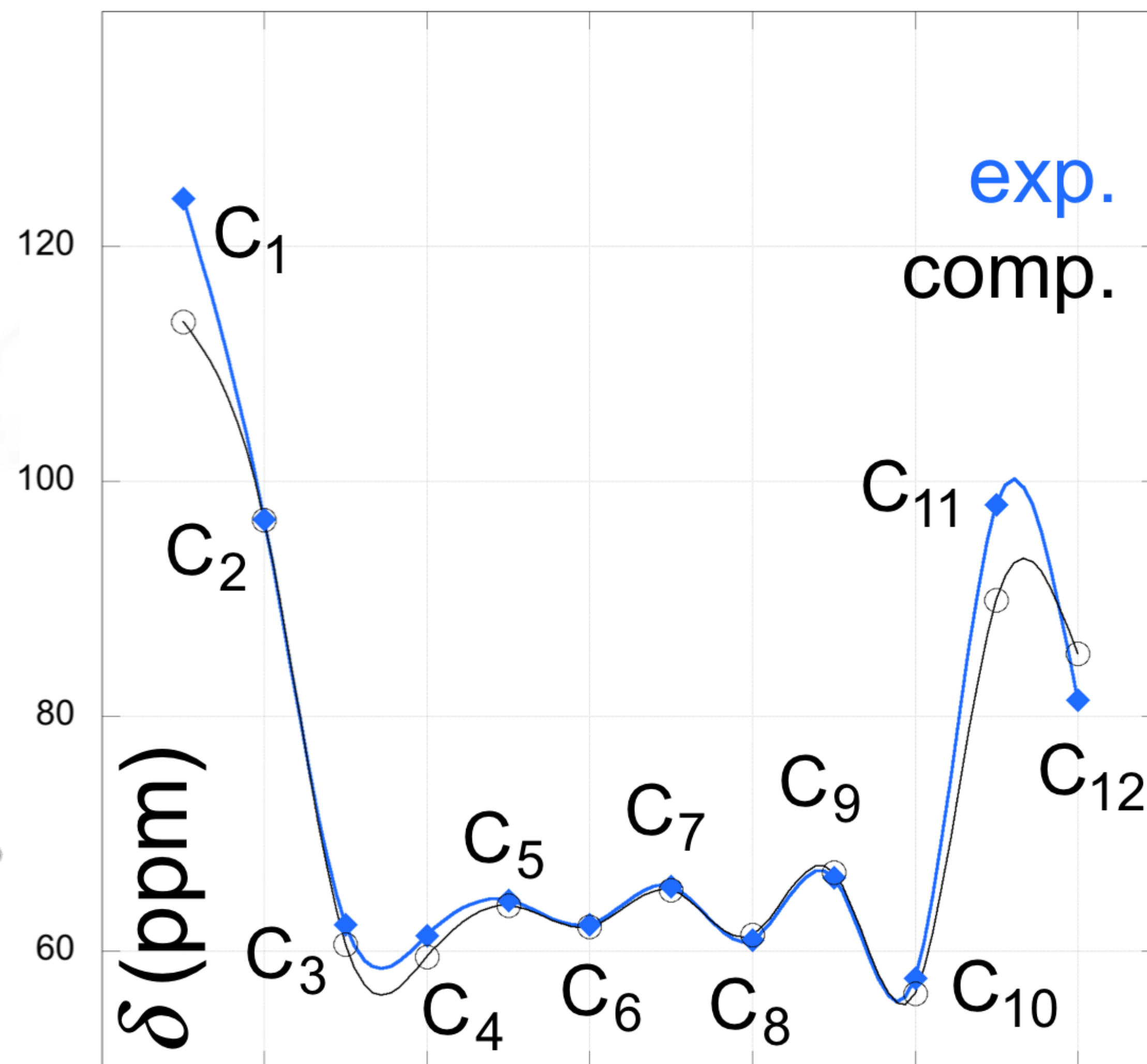
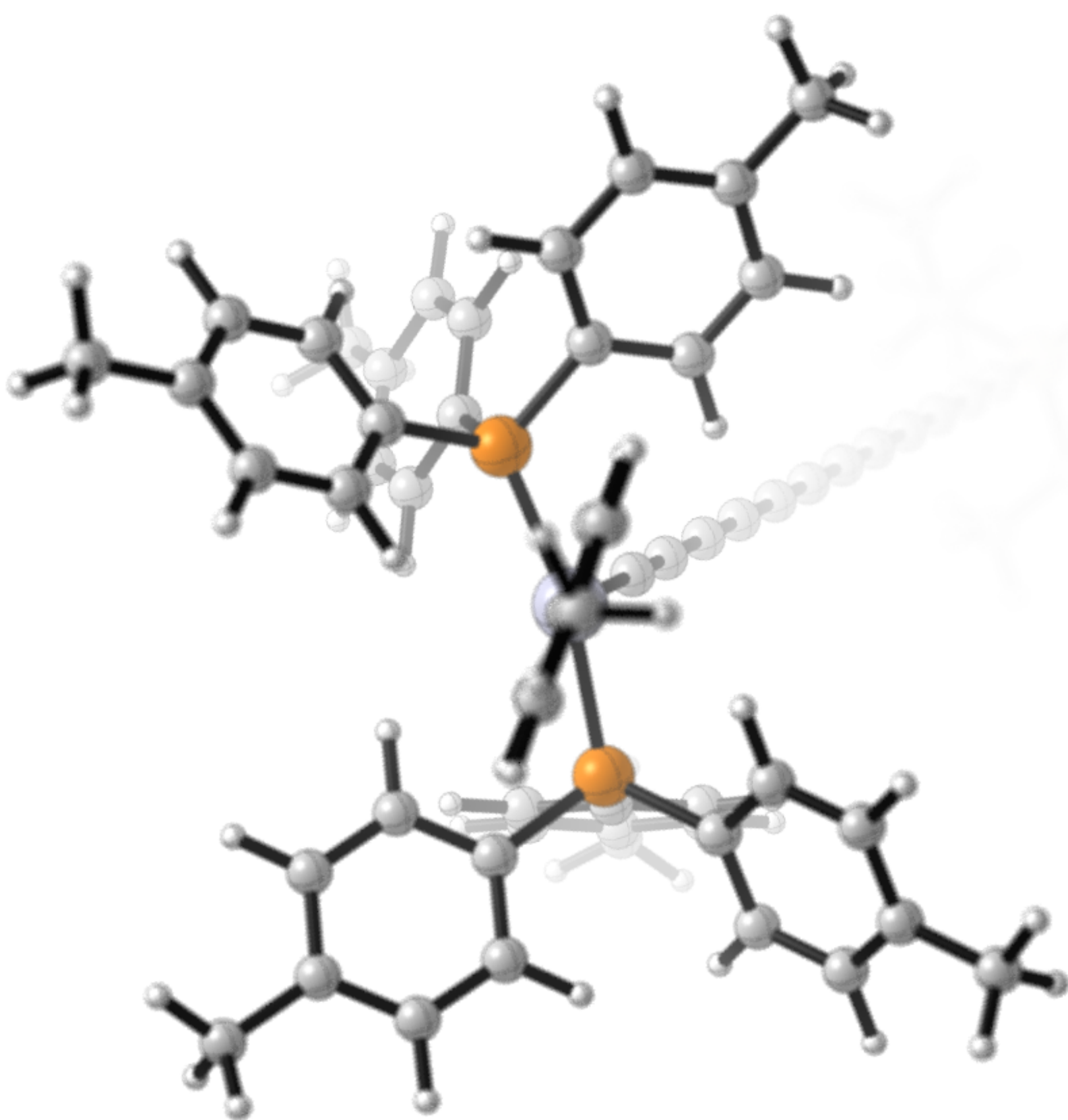
DFT vs. exp.



$m = 1 - 4$

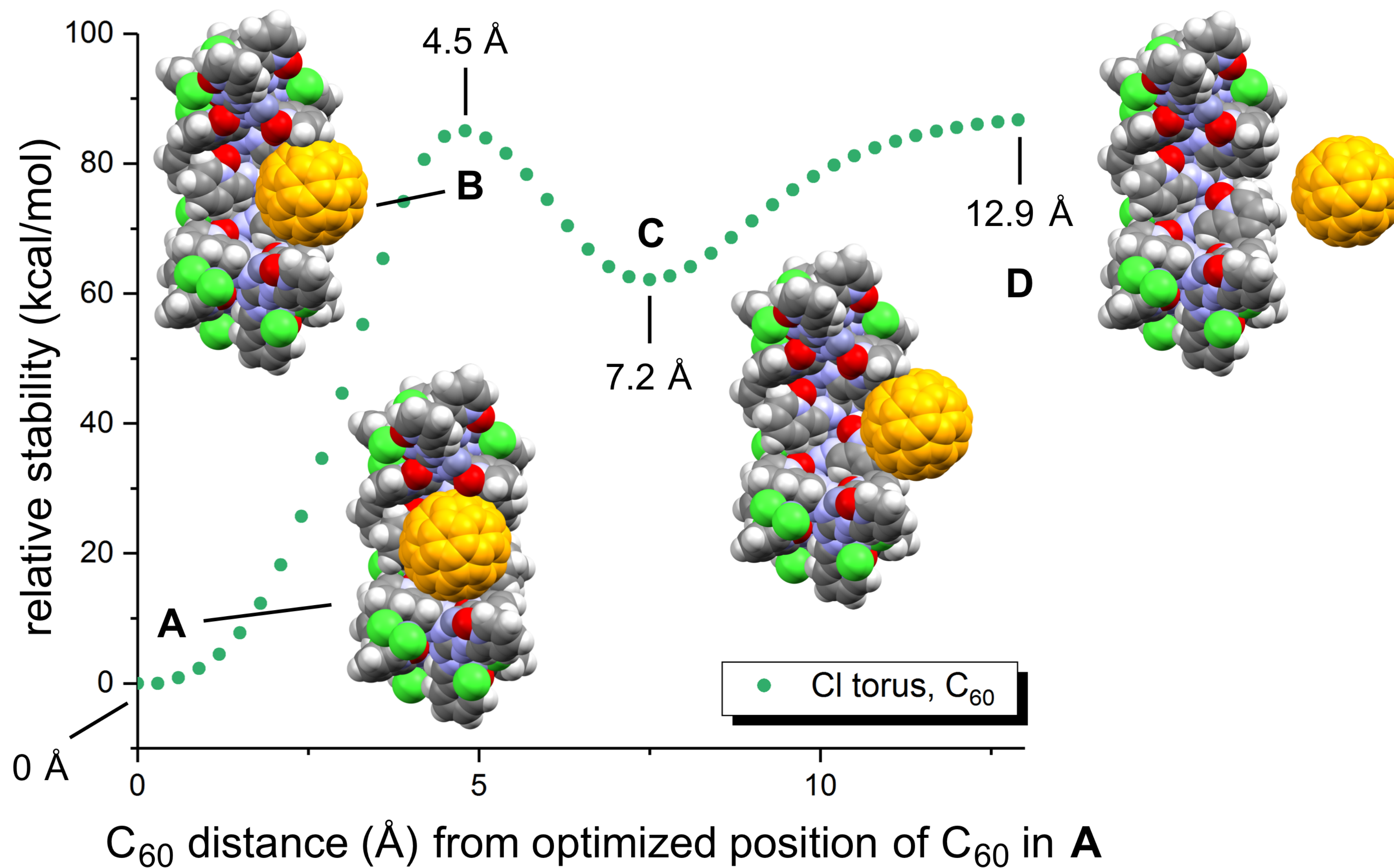
oxidative
homocoupling

DFT \longrightarrow Predict and assign $^{13}\text{C}\{^1\text{H}\}$ signals in platinum end-capped polyynes



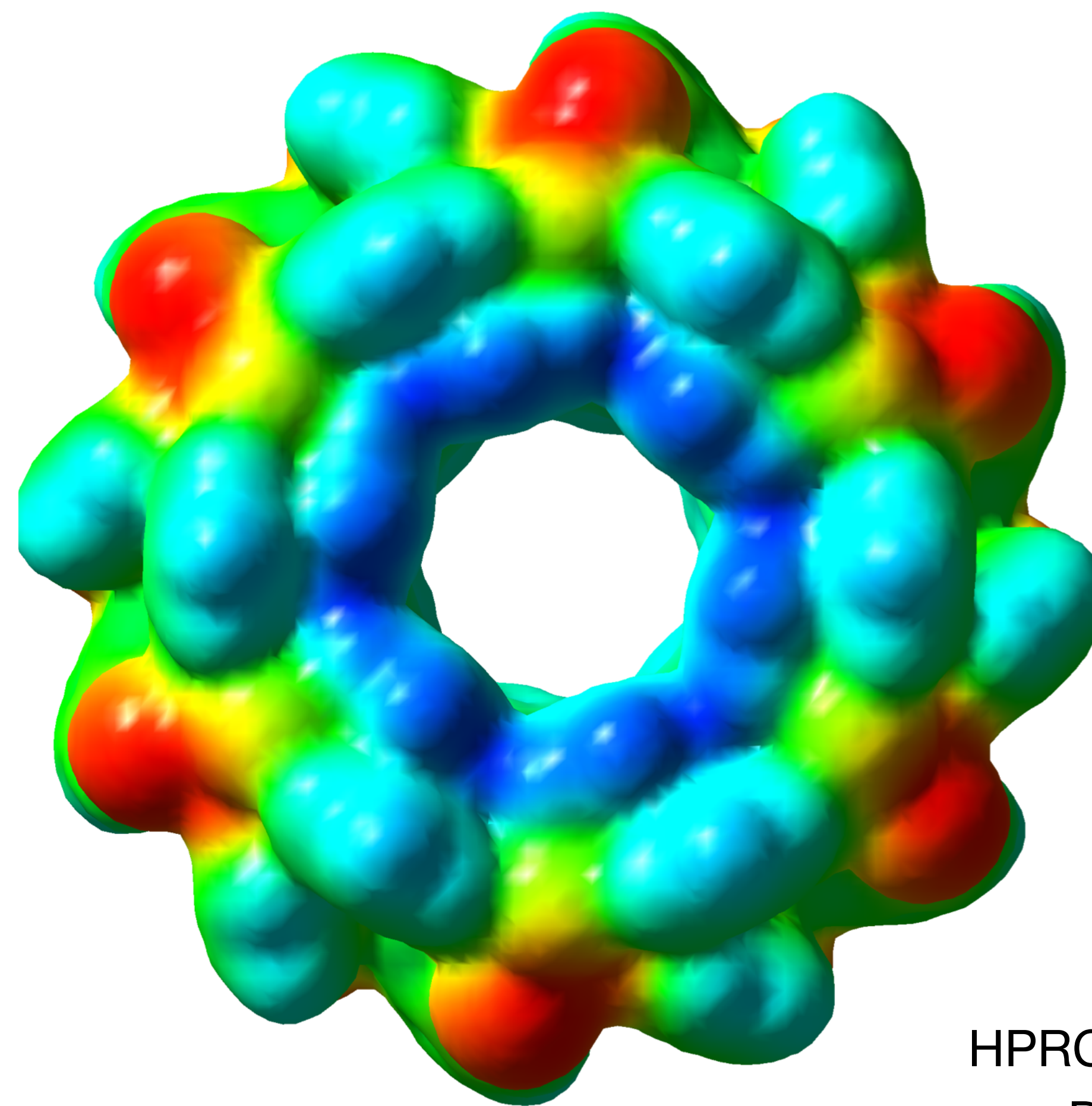
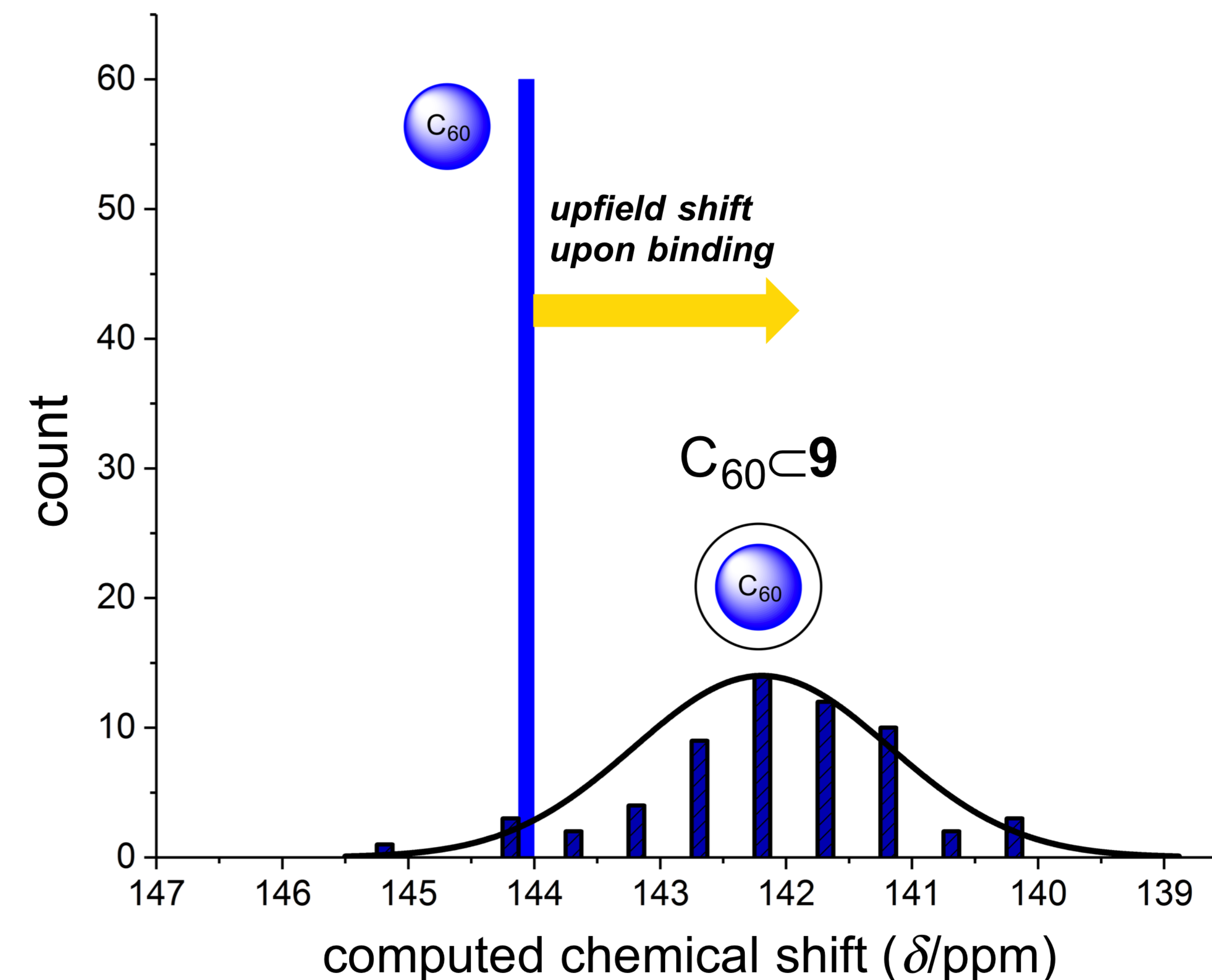
HPRC: TERRA cluster
DFT: Gaussian 09
28 cores, 96 h

SUPRAMOLECULAR METALLACYCLES AND THEIR BINDING OF FULLERENES



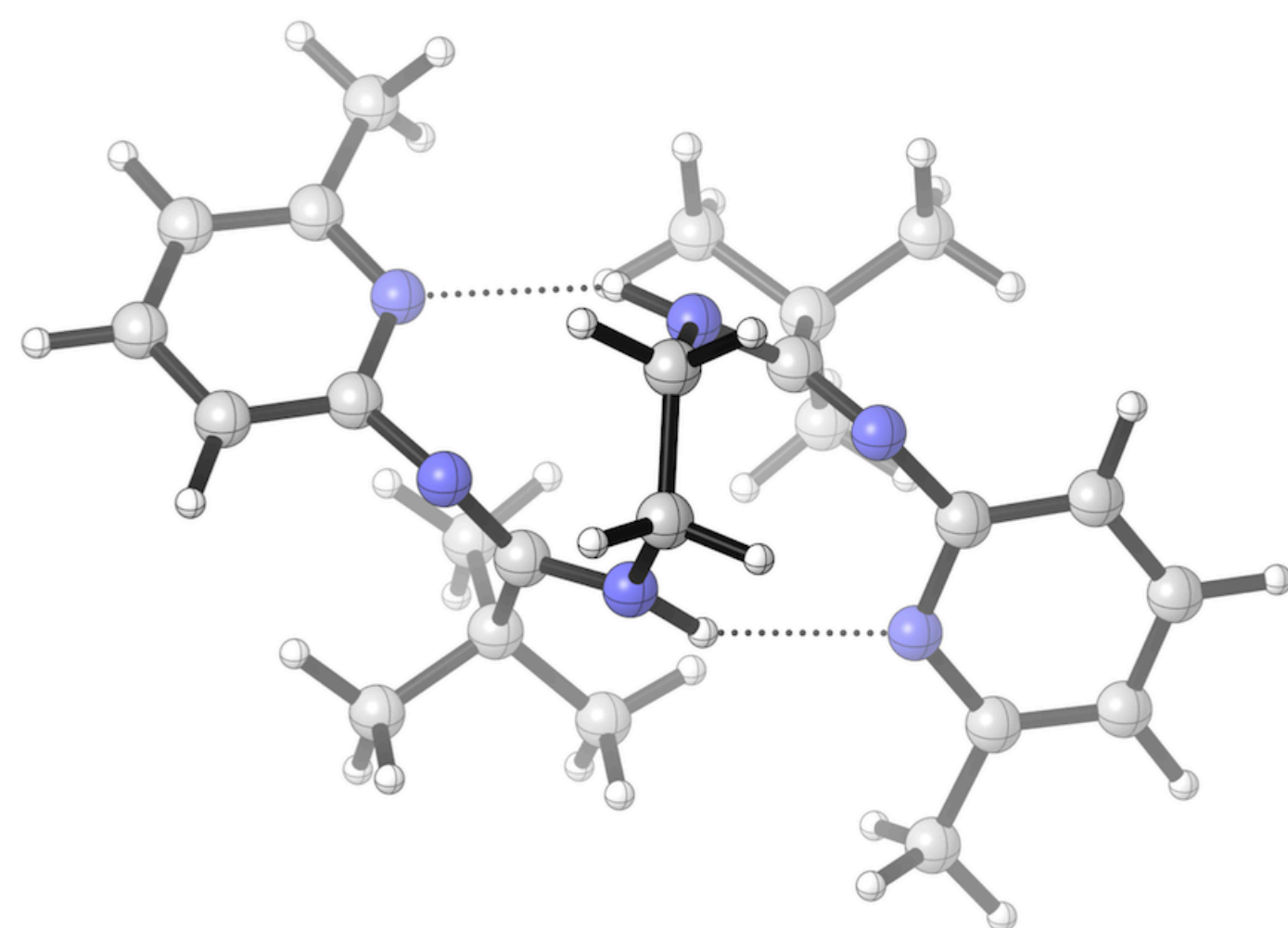
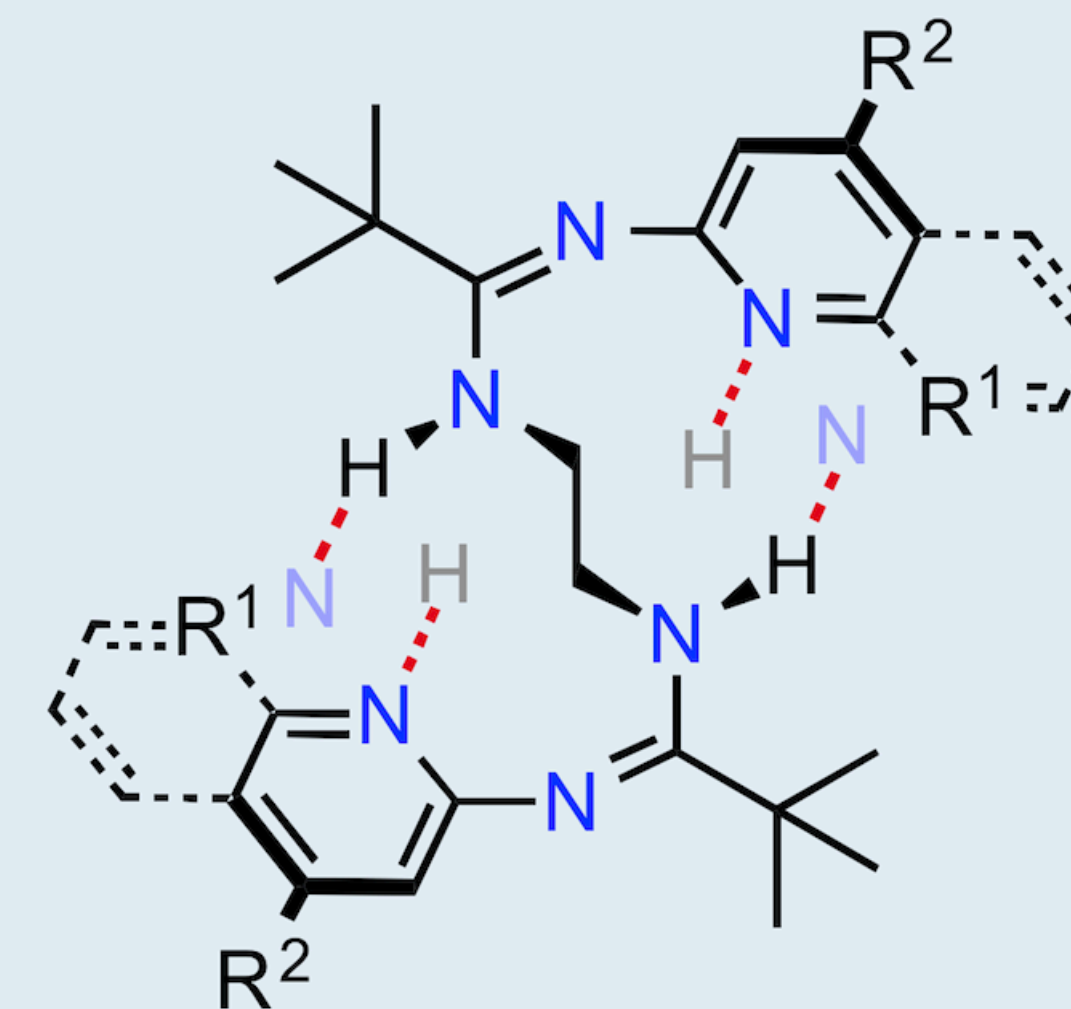
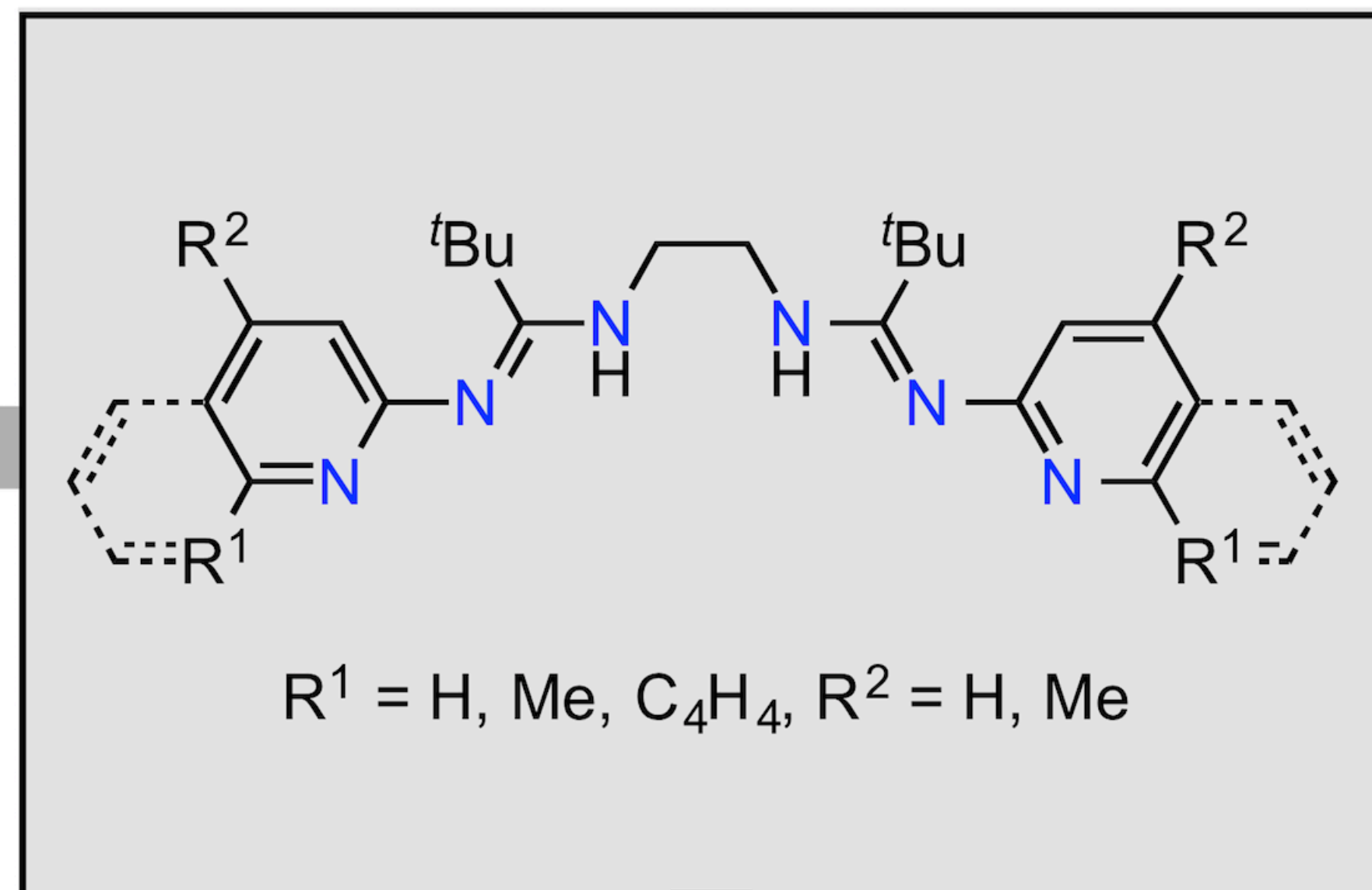
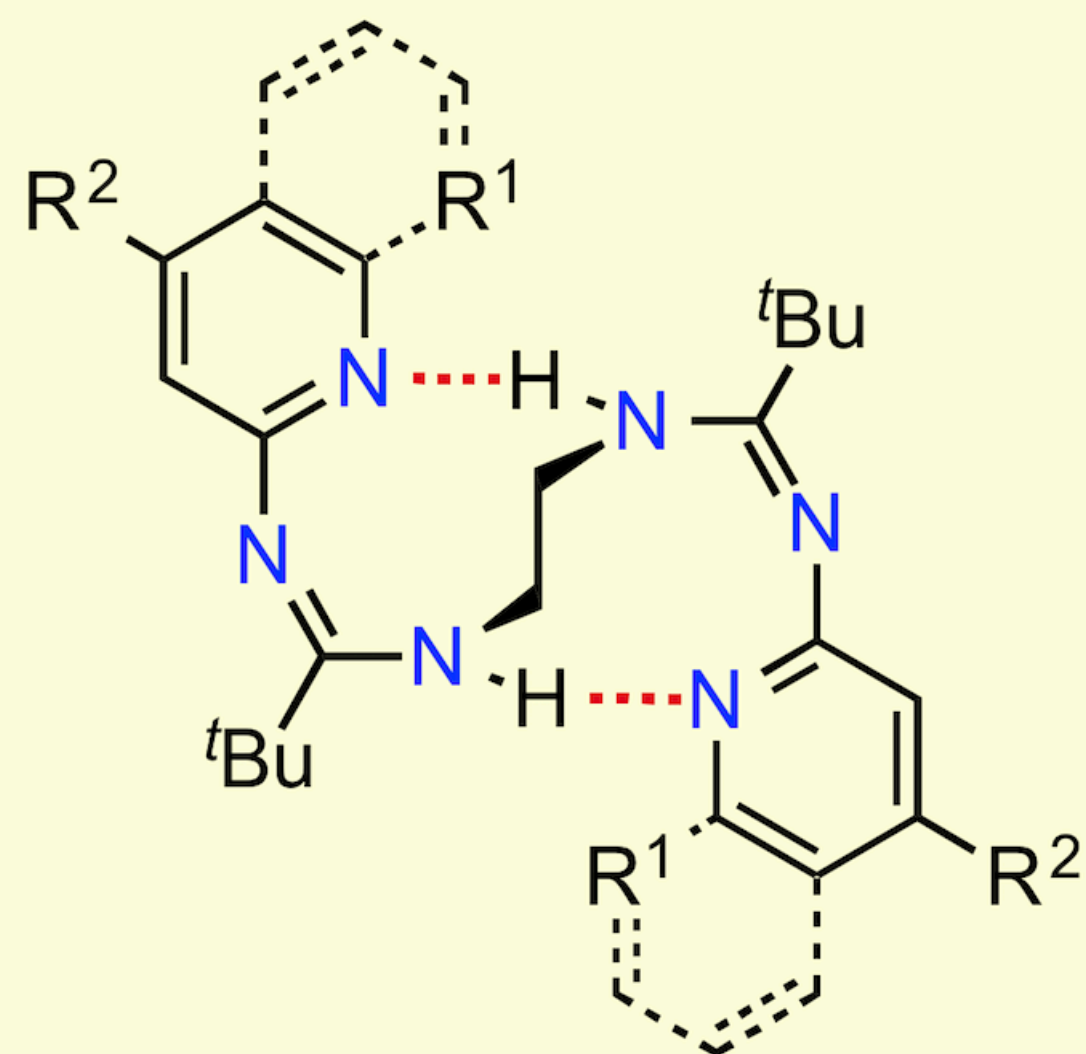
HPRC: TERRA cluster
DFT: Gaussian 16
28 cores, 300 h

SUPRAMOLECULAR METALLACYCLES AND THEIR BINDING OF FULLERENES

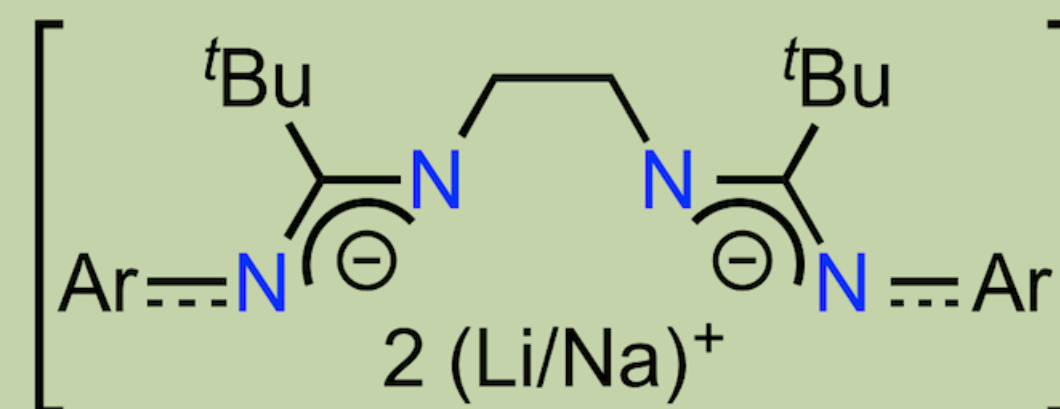


> 4000 electron system

HPRC: TERRA cluster
DFT: Gaussian 16
28 cores, 300 h

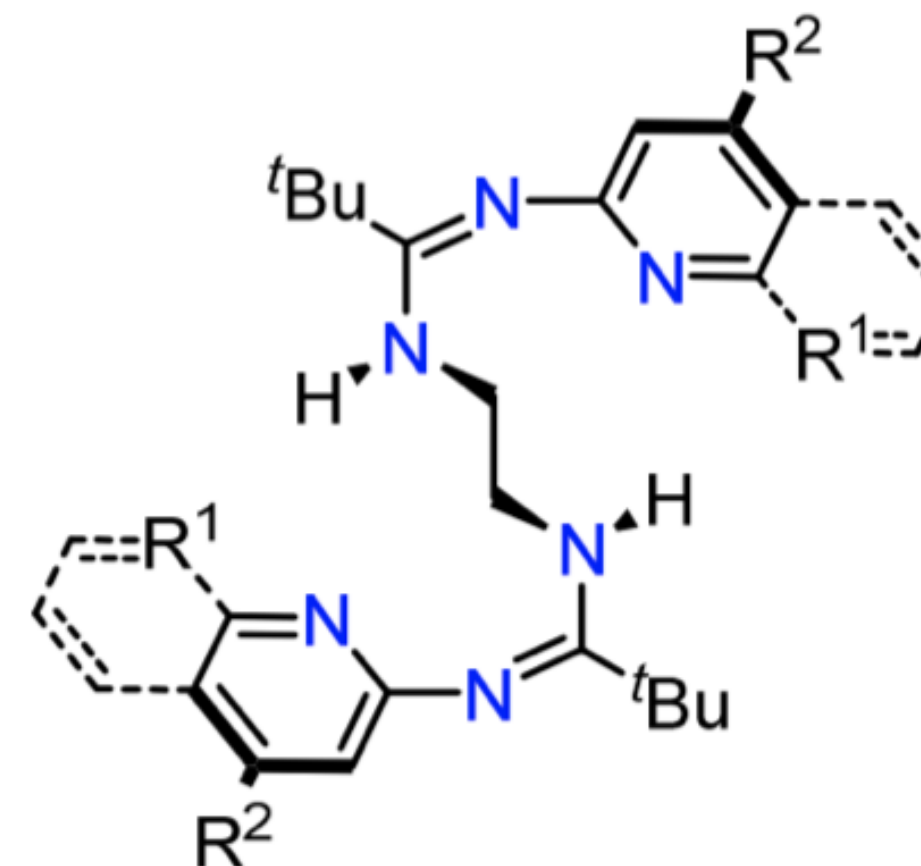
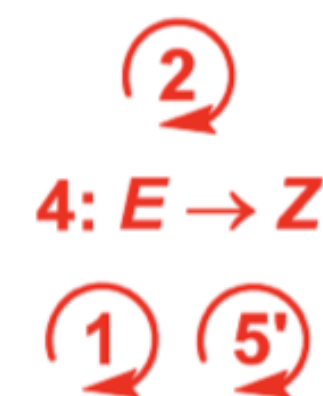
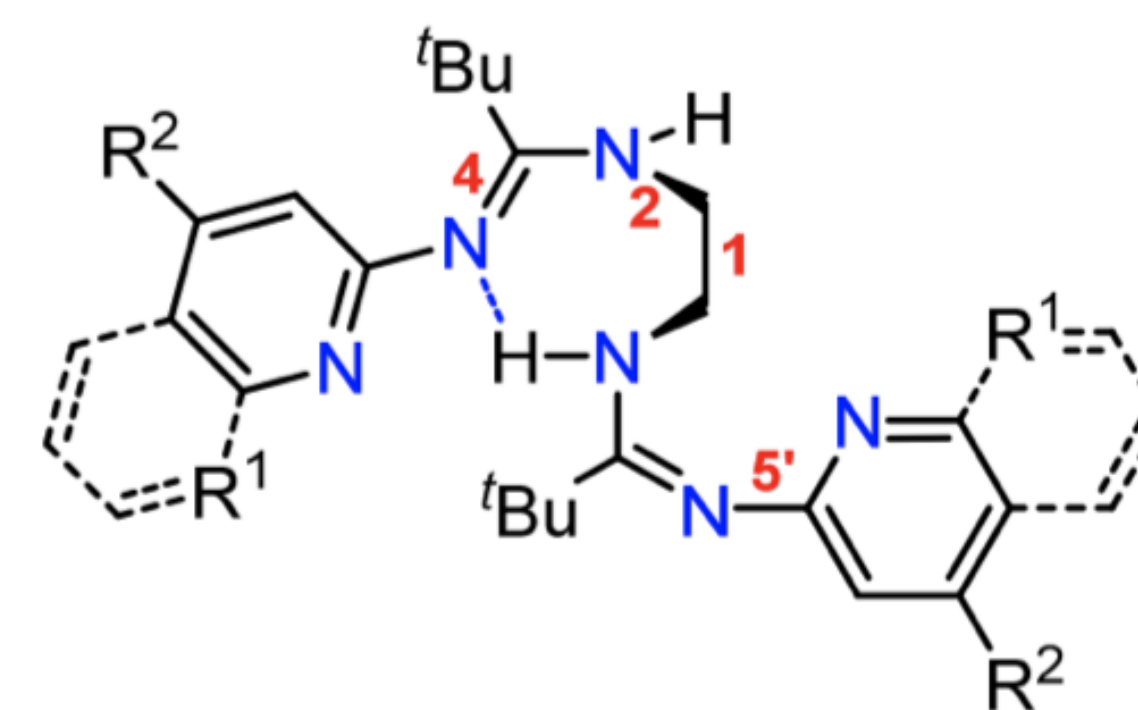
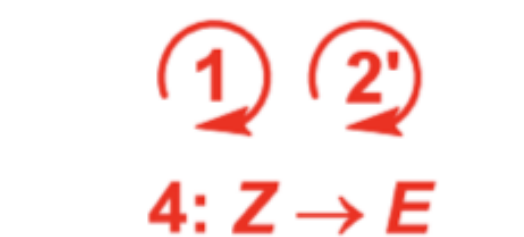
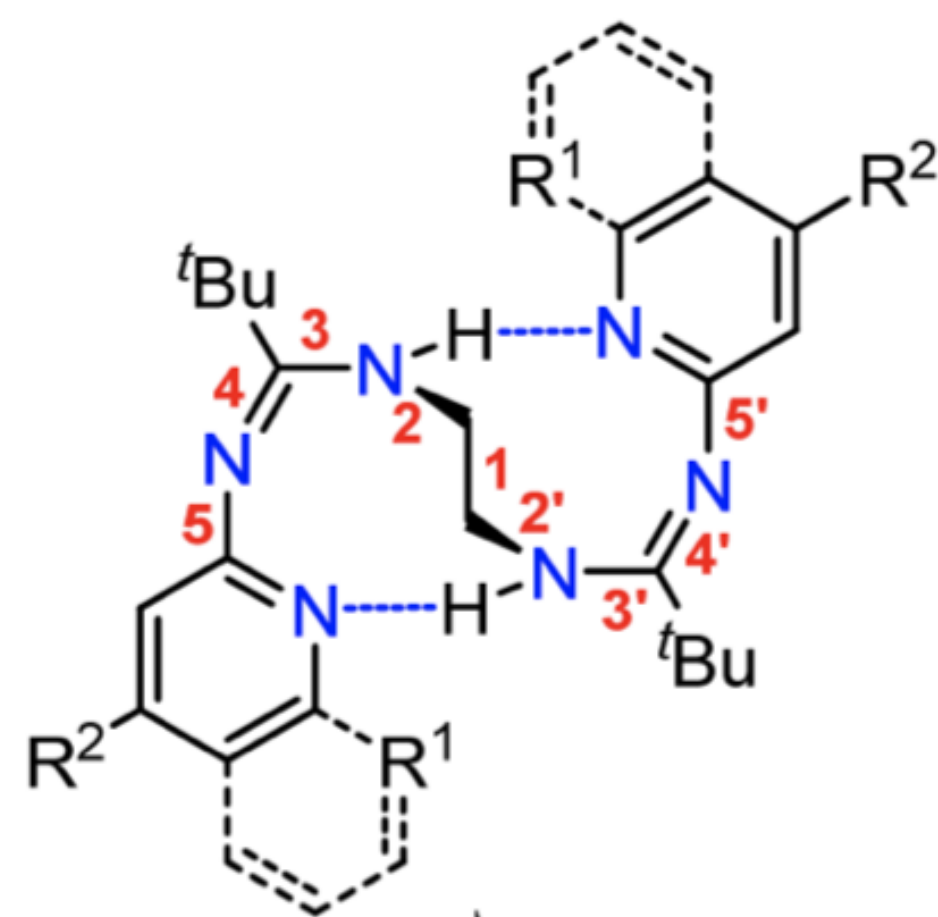
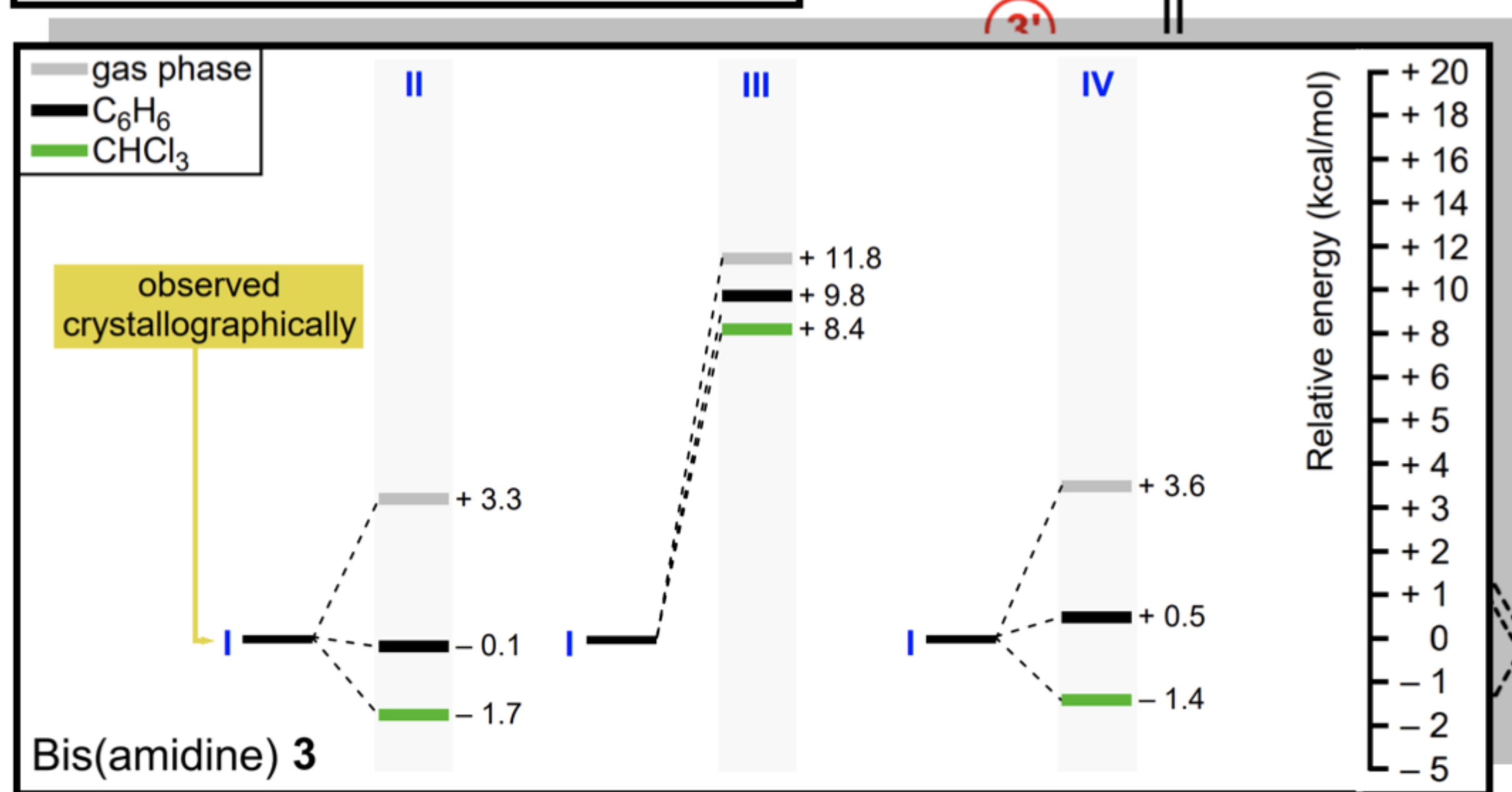
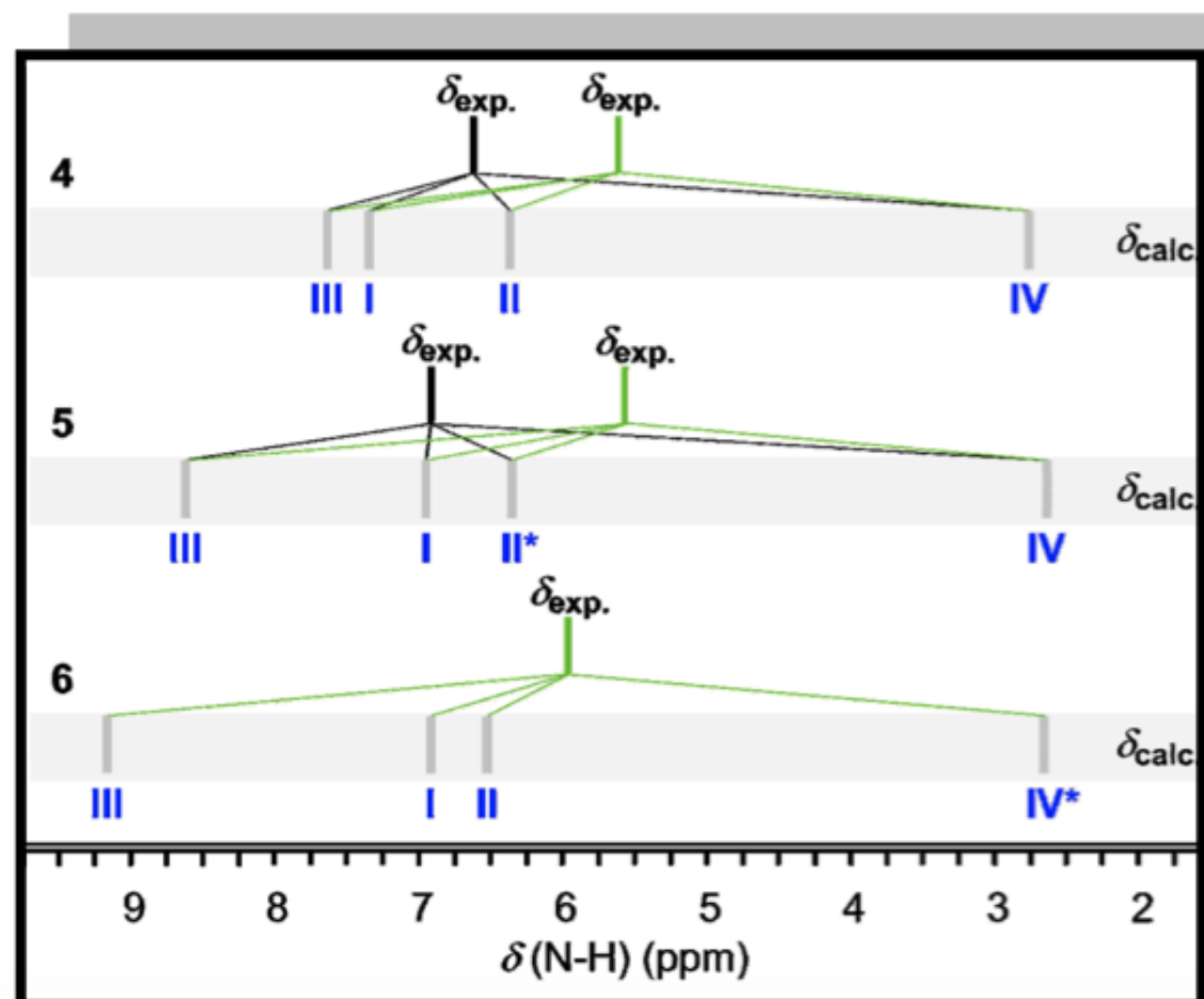


+ $n\text{BuLi}$ or
 $\text{Na}(\text{N}(\text{SiMe}_3)_2)$



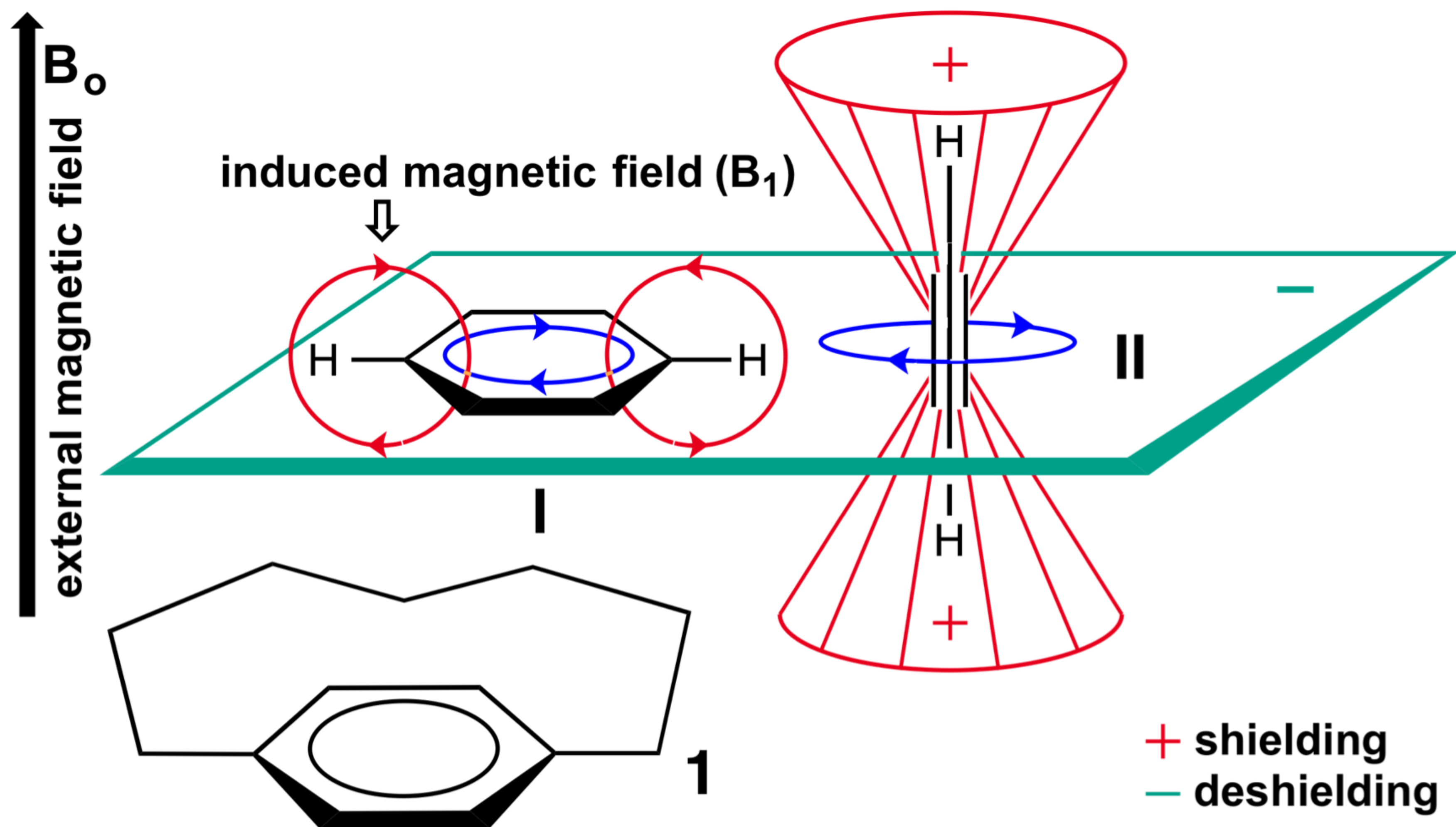
Hydrogen bonding
in the solid state *and* in solution

Photoluminescence
upon deprotonation

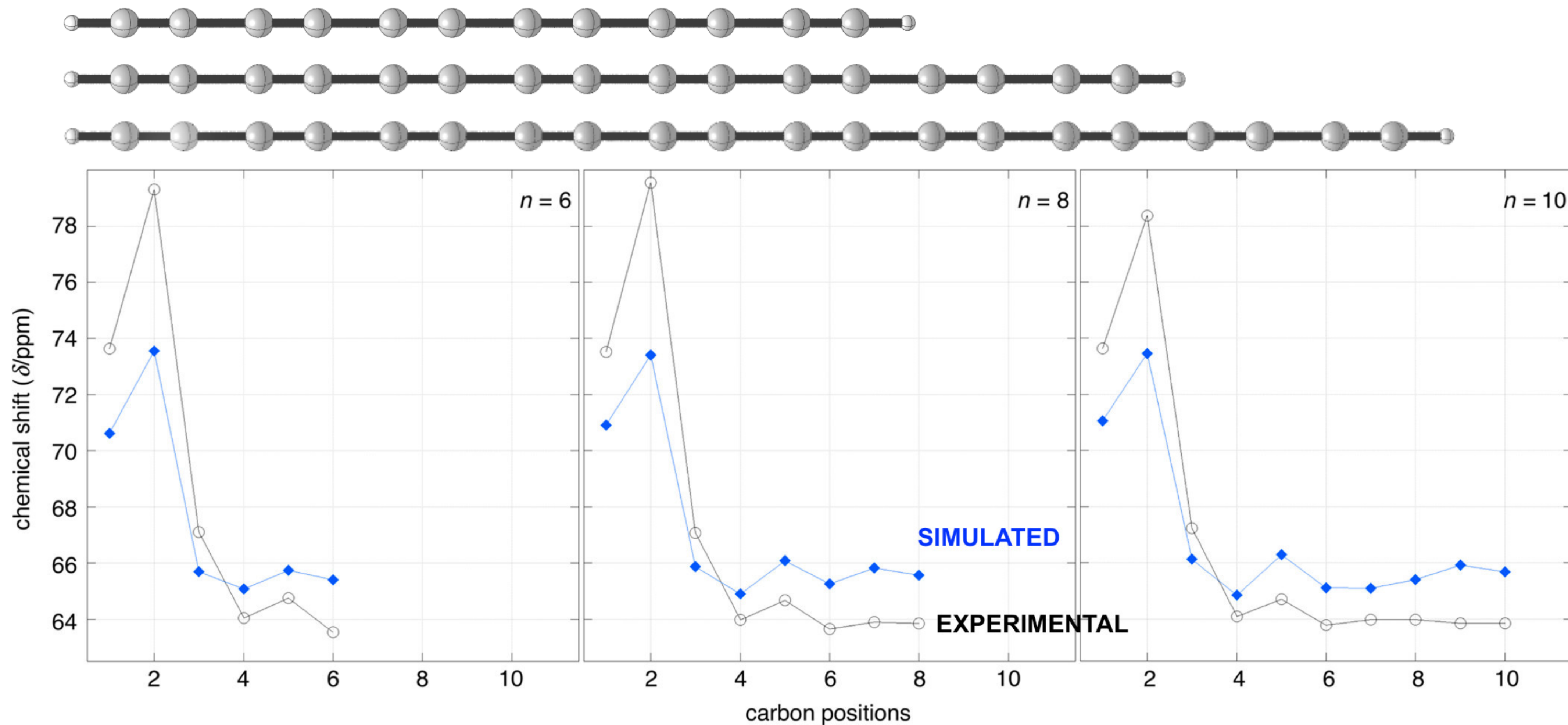


HPRC: ADA cluster
DFT: Gaussian 09
20 cores, 48 h

DFT → Origin of Shielding and Deshielding Effects in NMR Spectra of Organic Conjugated Polyynes



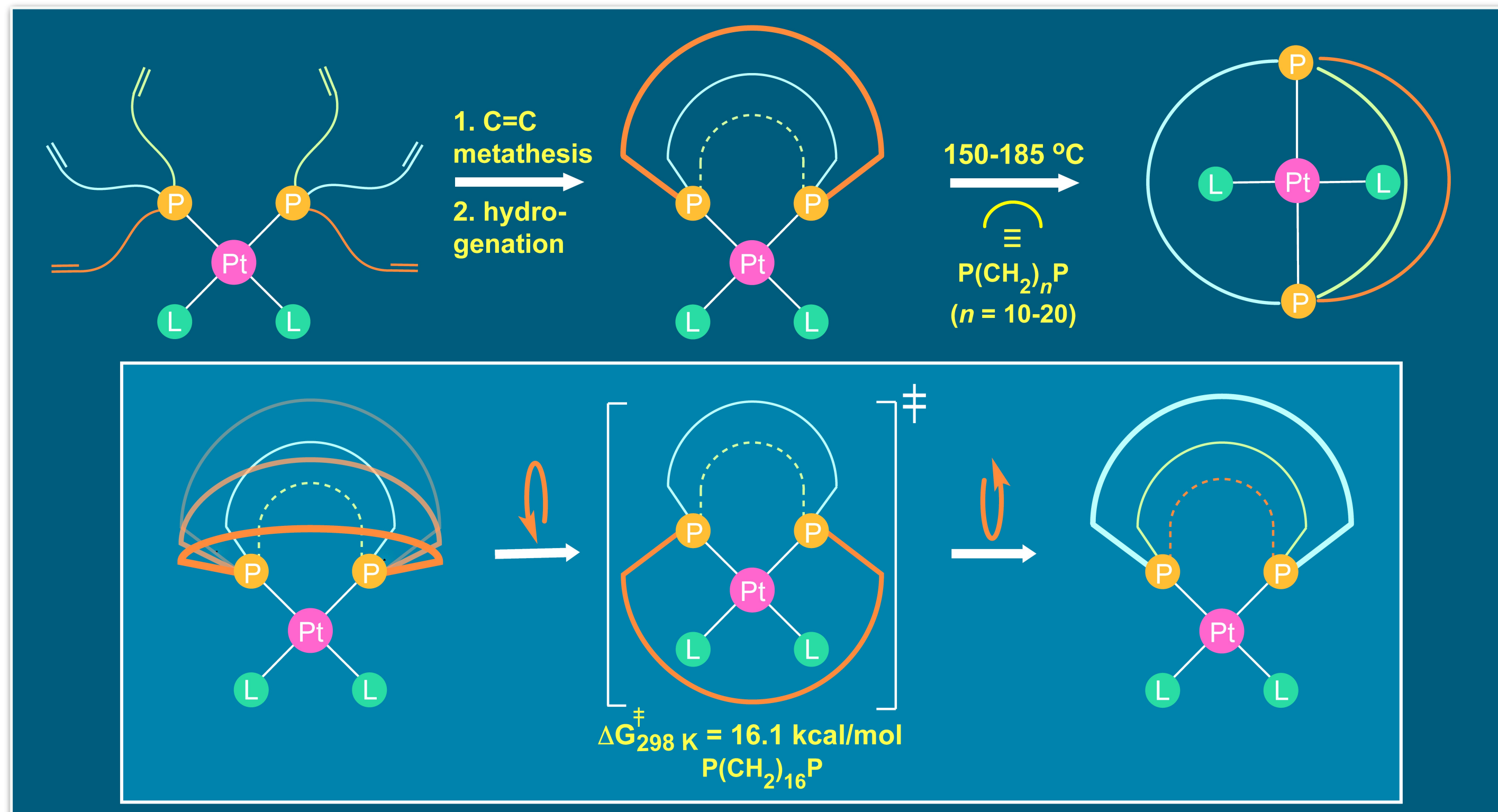
HPRC: ADA cluster
DFT: Gaussian 09
4 cores, 1 h <



HPRC: ADA cluster

DFT: Gaussian 09

4 cores, 1 h <



HPRC: ADA cluster

DFT: Gaussian 16

20 cores, 150+ h

