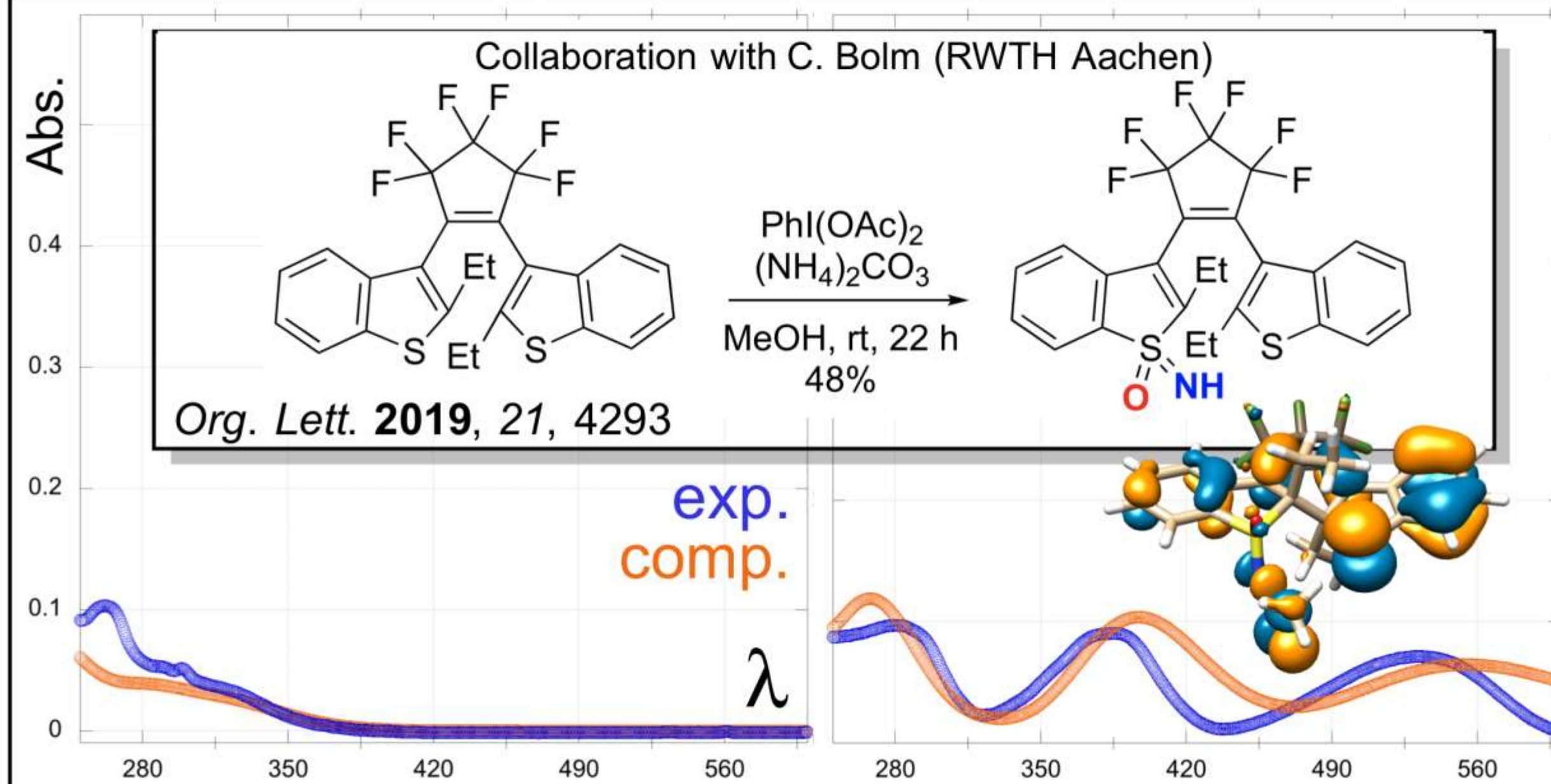
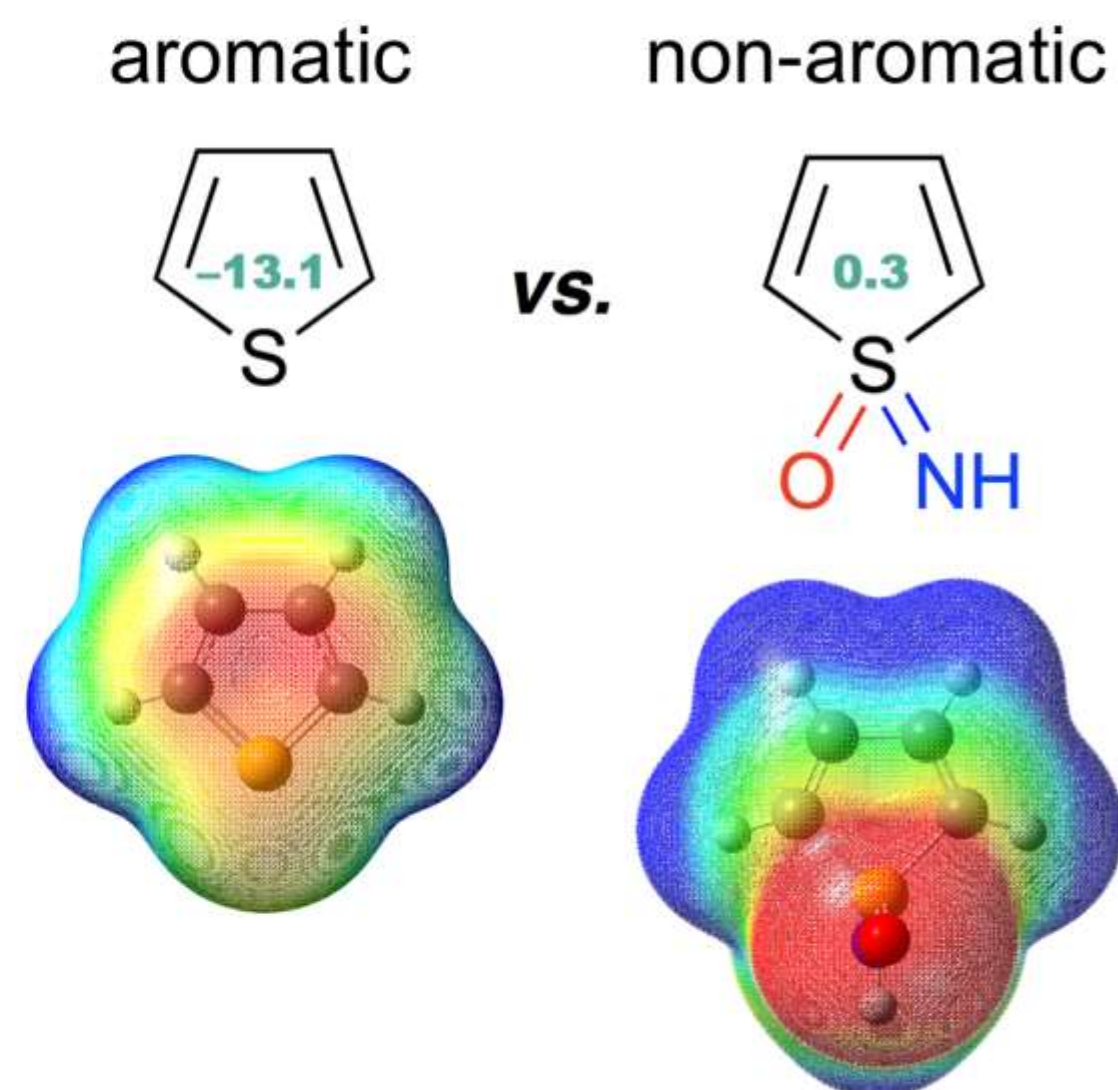
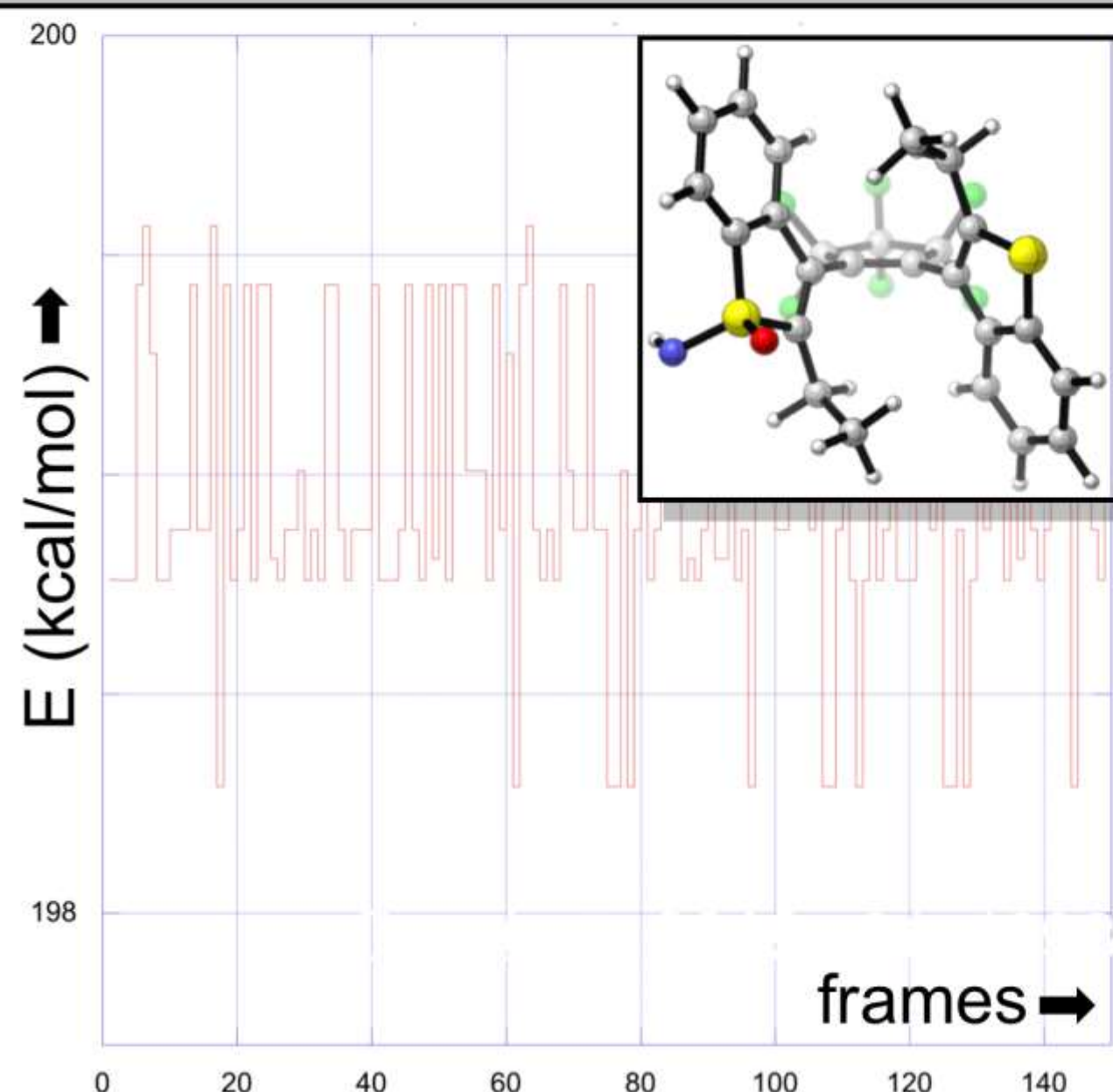


MD → conformational sampling

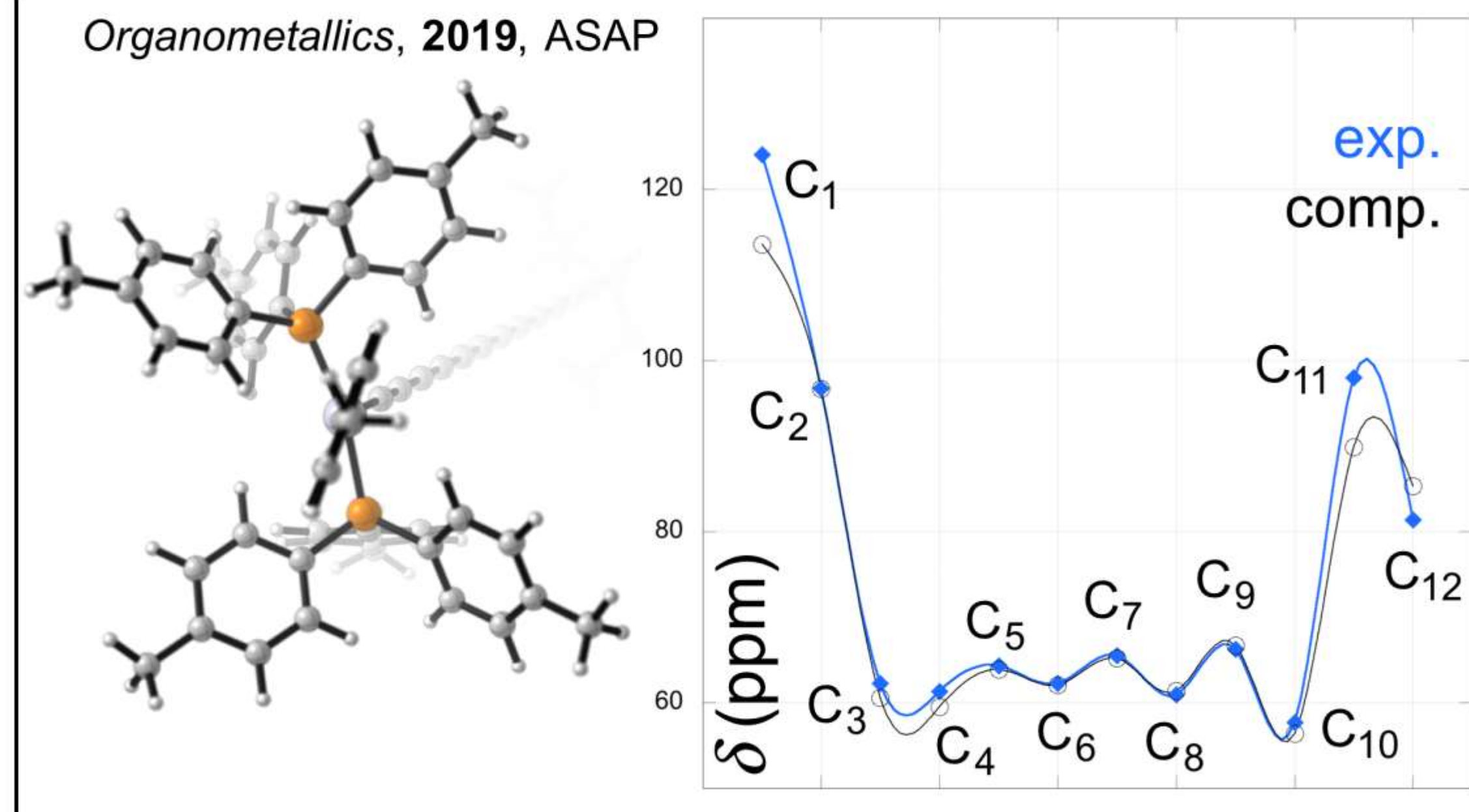
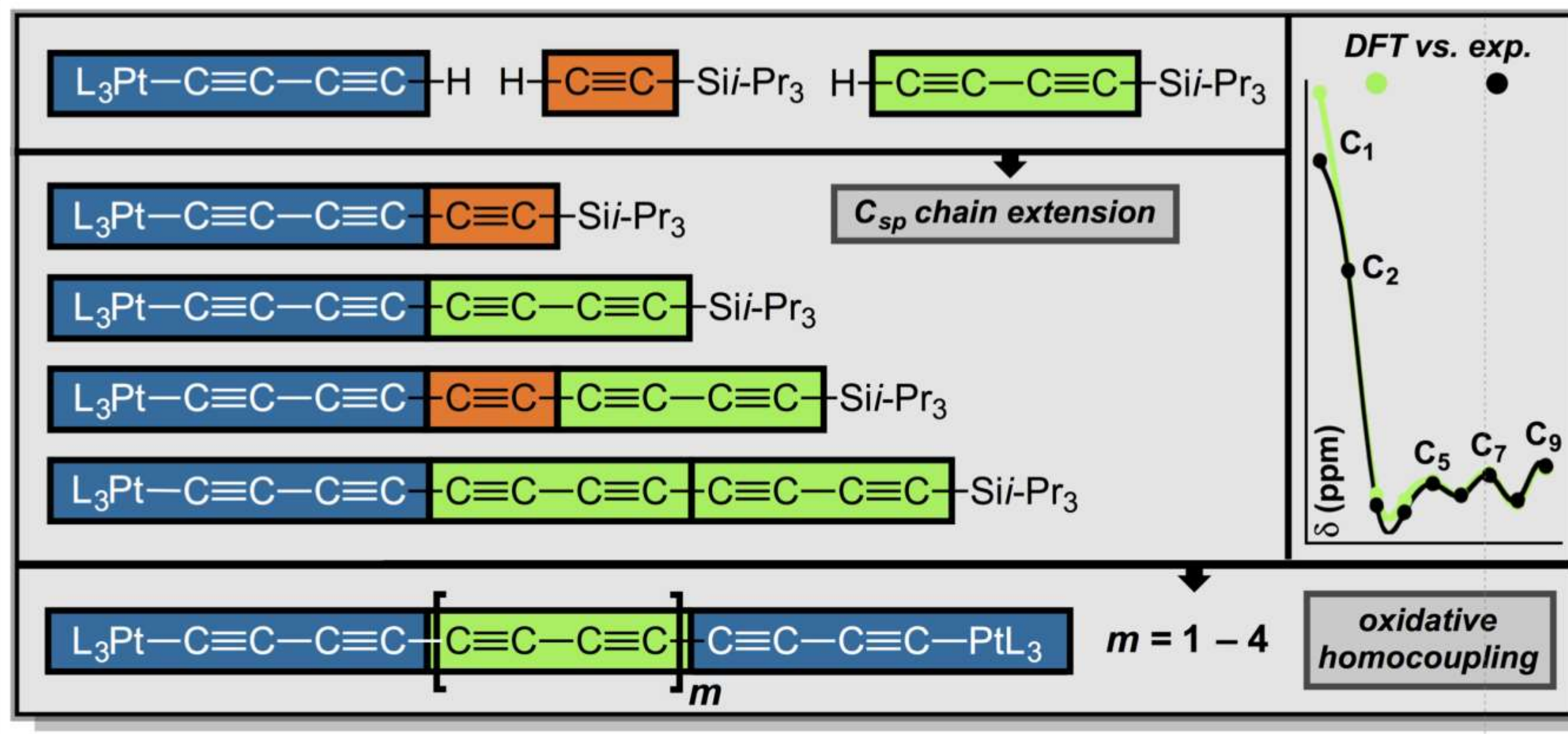
DFT → aromaticity index

TDDFT → spectroscopy



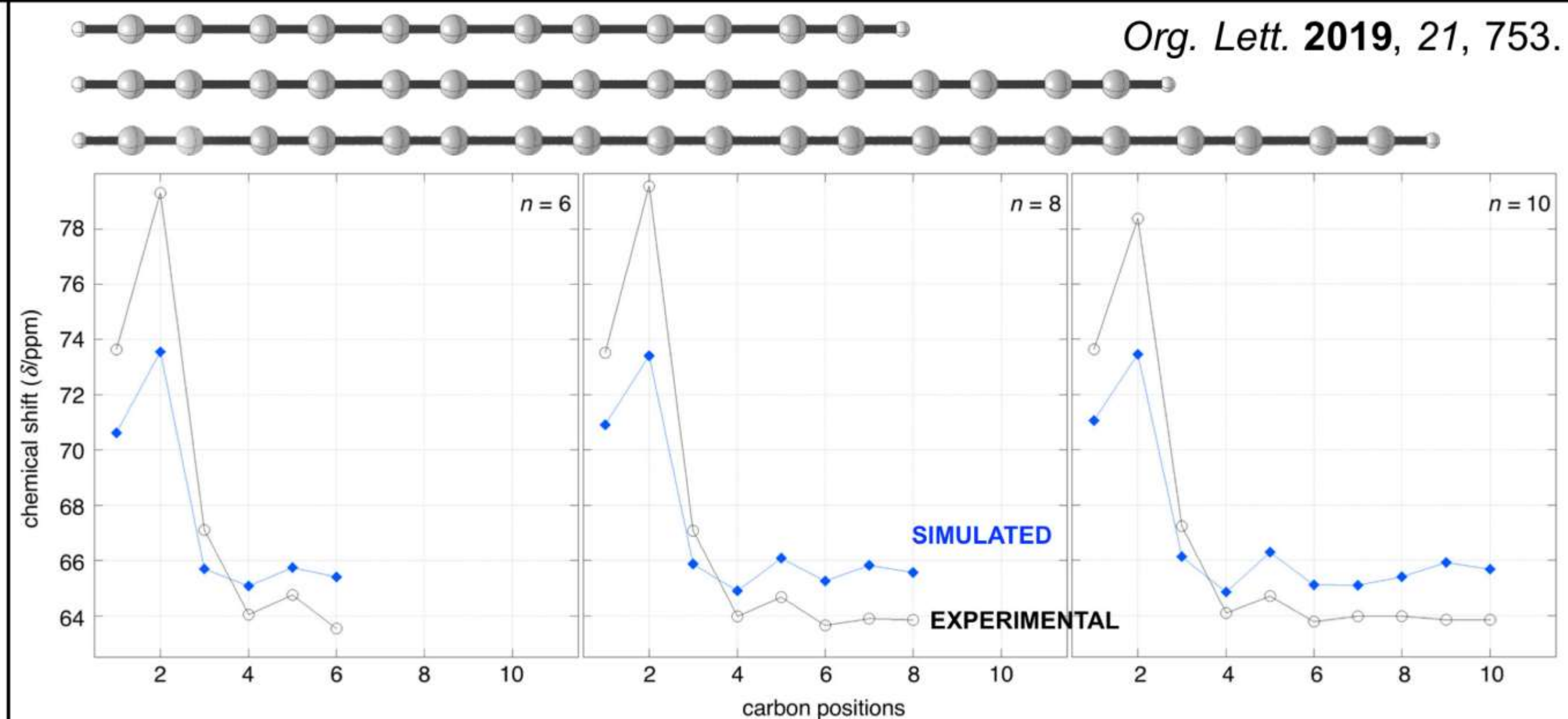
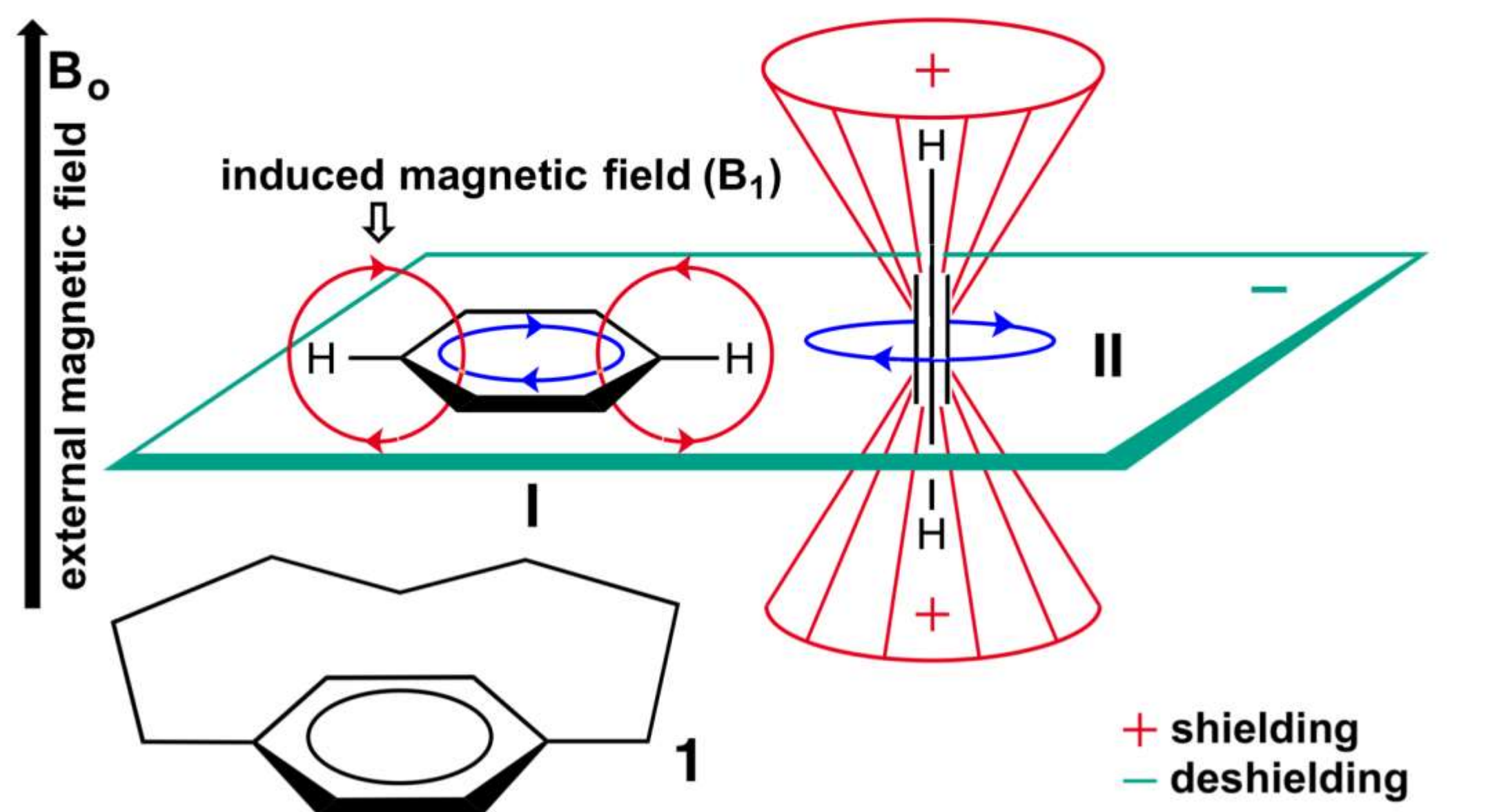
HPRC: TERRA cluster
 DFT and TDDFT: Gaussian 16
 MD: Materials Studio
 28 cores, 24h

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

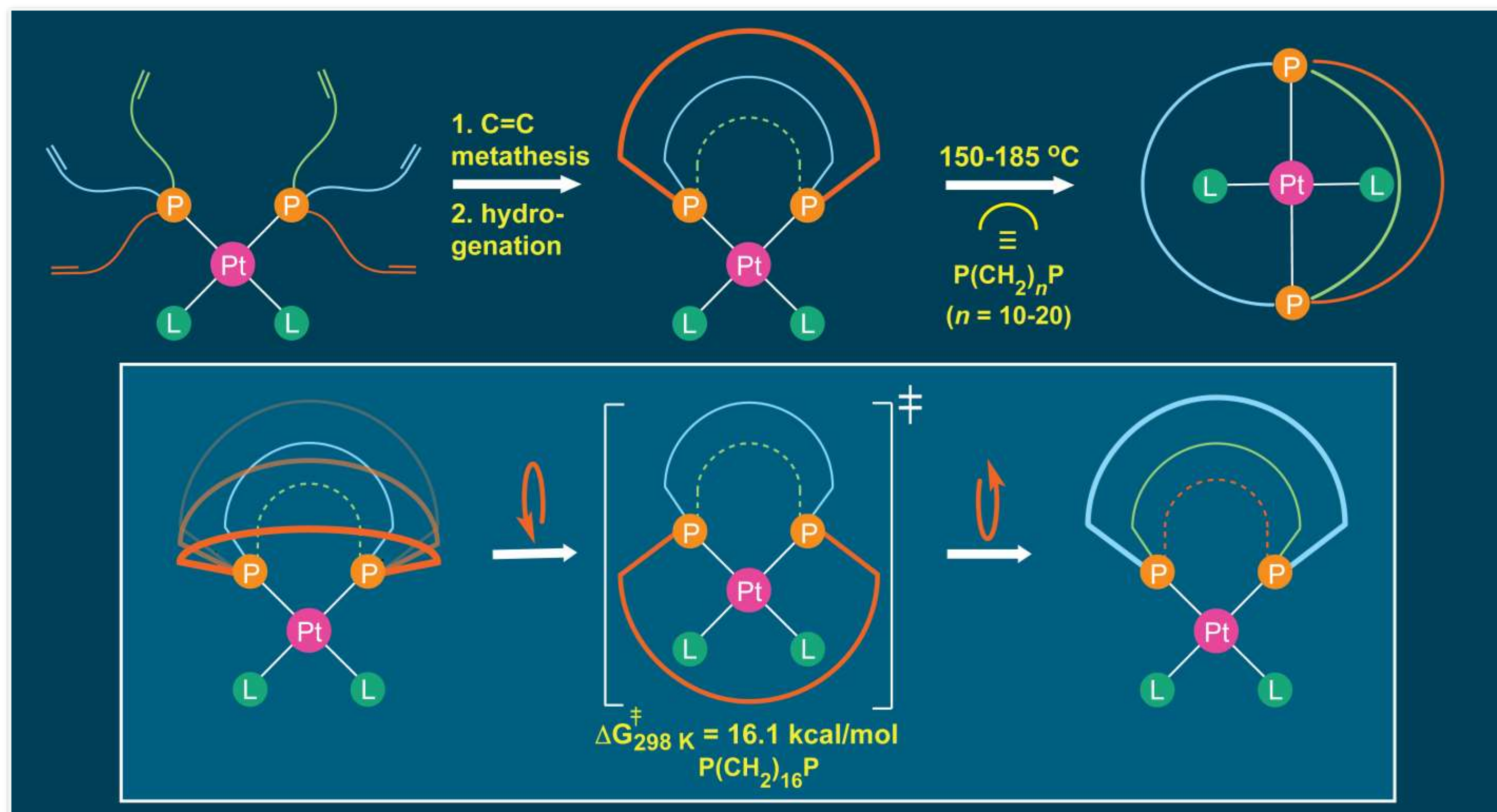


HPRC: TERRA cluster
 Gaussian 16 computational software
 28 cores, 150 h

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



HPRC: ADA cluster
DFT: Gaussian 16
20 cores, 6 h



HPRC: ADA cluster

DFT: Gaussian 16

20 cores, 150+ h

