**Electronic Supplementary Information for:**

# Cyclo[18]carbon including Zero-Point Motion: Ground State, First Singlet and Triplet Excitations, and Hole Transfer

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## Additional Figures

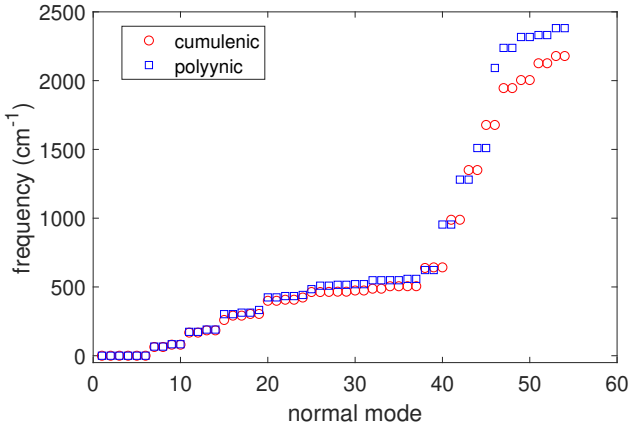


Figure S1: Vibrational analysis of cumulenic (empty red circles) and polyynic (empty blue squares) cyclo[18]carbon, with the cc-pVTZ basis set.

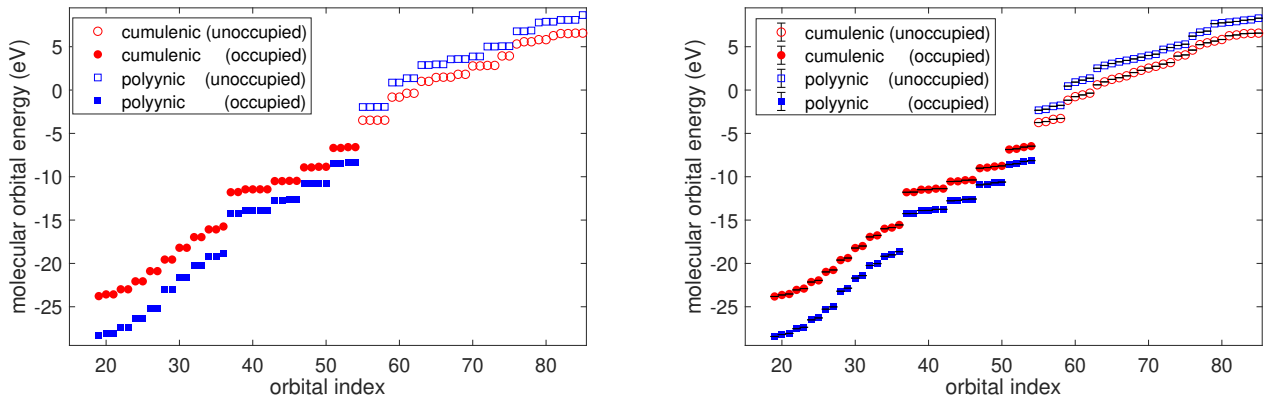


Figure S2: Energies of several occupied (filled shapes) and unoccupied (empty shapes) orbitals of cumulenic (red circles) and polyynic (blue squares) cyclo[18]carbon. (Left) Static conformations. (Right) Averaged values of the Monte Carlo sample, accounting for zero-point vibrations, including standard errors.

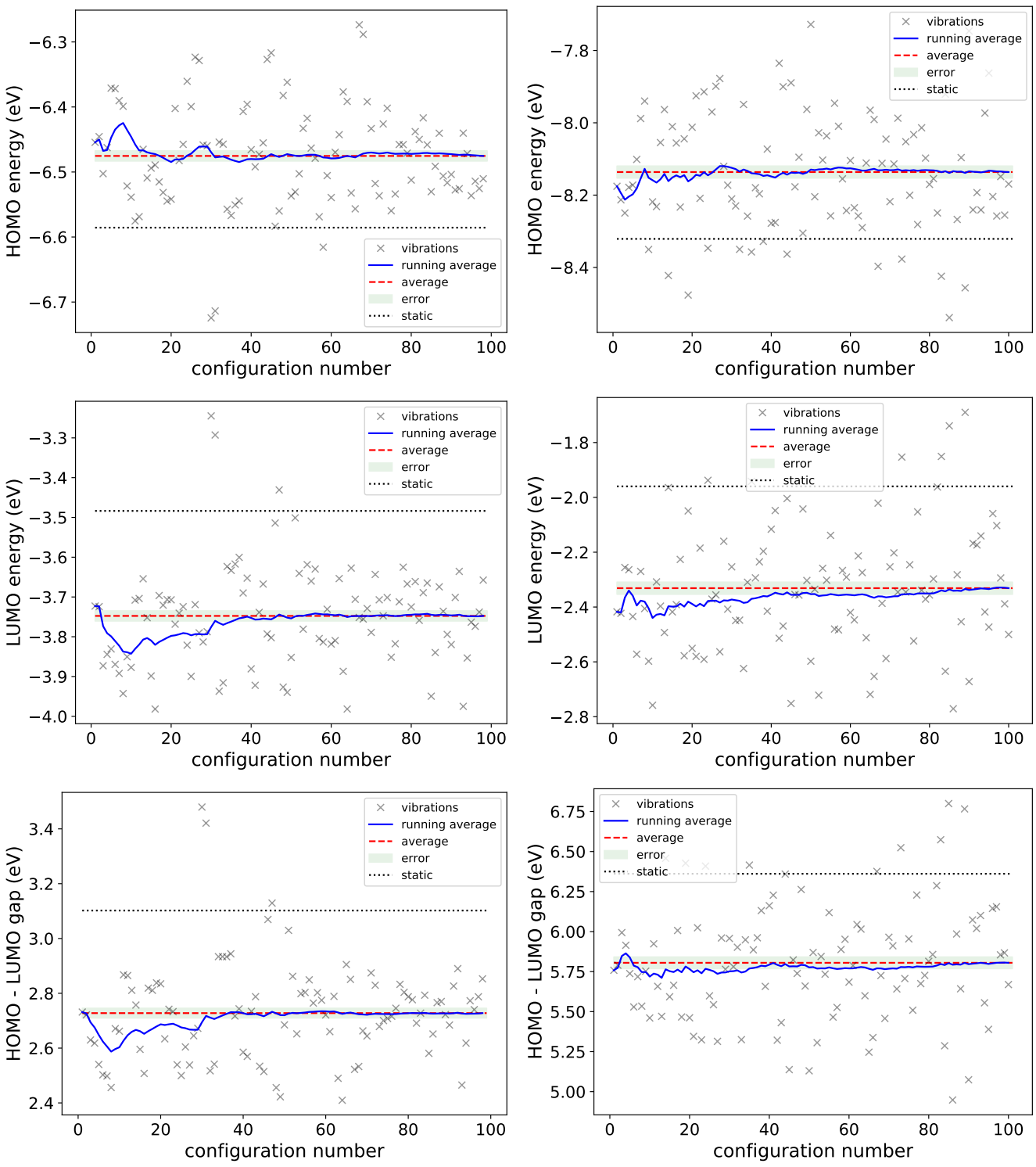


Figure S3: Comparison of the HOMO energy (first row), LUMO energy (second row), and HOMO-LUMO gap (third row) of static cumulenic (left column) and polyynic (right column) cyclo[18]carbon with their corresponding renormalized values due to zero-point vibrations, using the Monte Carlo method. The values for each Monte Carlo configuration and the running averages are also shown.

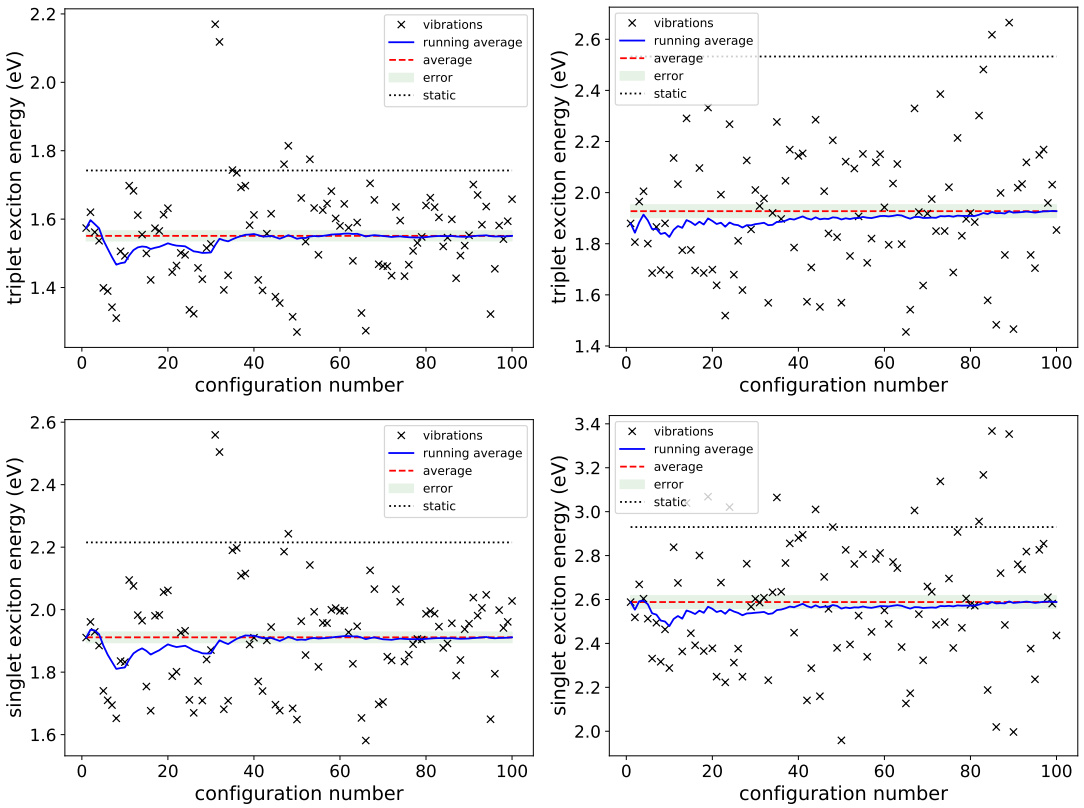


Figure S4: Comparison of the first triplet (first row) and first singlet (second row) excitation energies of static cumulenic (left column) and polyynic (right column) cyclo[18]carbon with their corresponding renormalized values due to zero-point vibrations, using the Monte Carlo method. The values for each Monte Carlo sample and the running averages are also shown.

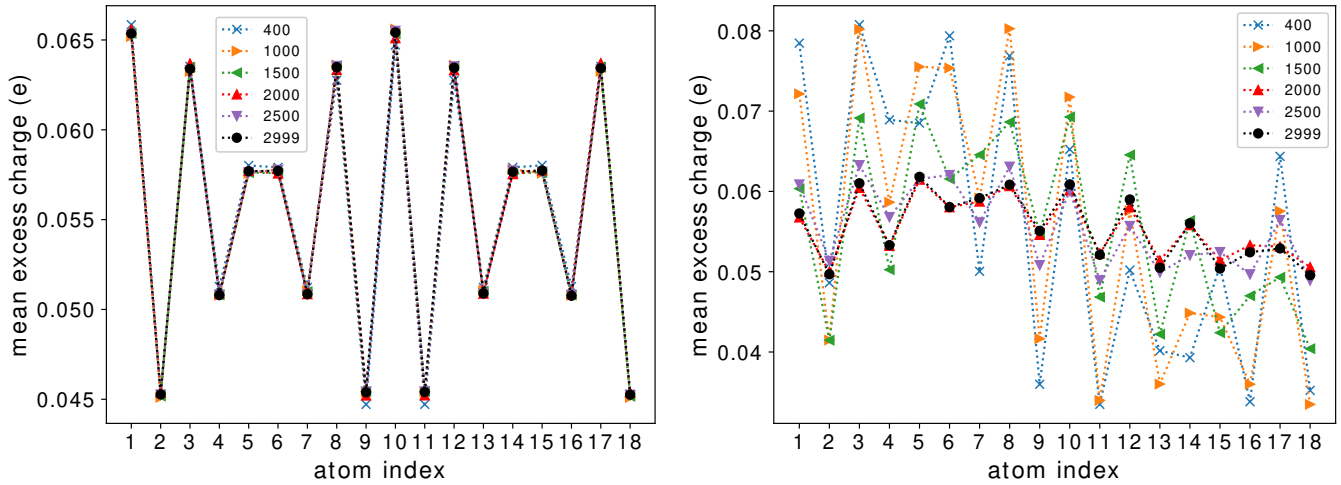


Figure S5: Time-convergence of the mean excess charge distribution of static cumulenic (left) and polyynic (right) cyclo[18]carbon. Time intervals are specified in the legend, in atomic units. Dotted lines are guide for the eye.

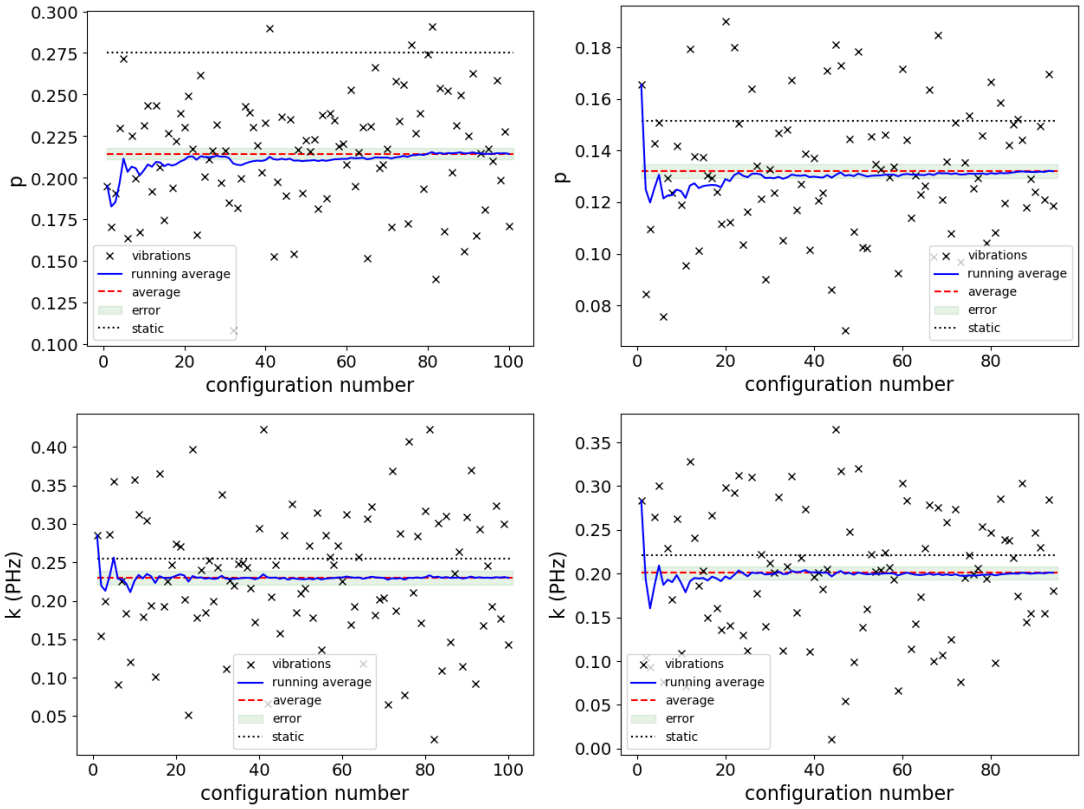


Figure S6: Comparison of the maximum value of excess charge, $p$, at the diametrically opposed atom to the one the hole was initially placed (first row) and the mean transfer rate, $k$, (second row) of static cumulenic (left column) and polyynic (right column) cyclo[18]carbon with their corresponding renormalized values due to zero-point vibrations, using the Monte Carlo method. The values for each sample and the running averages are also shown.

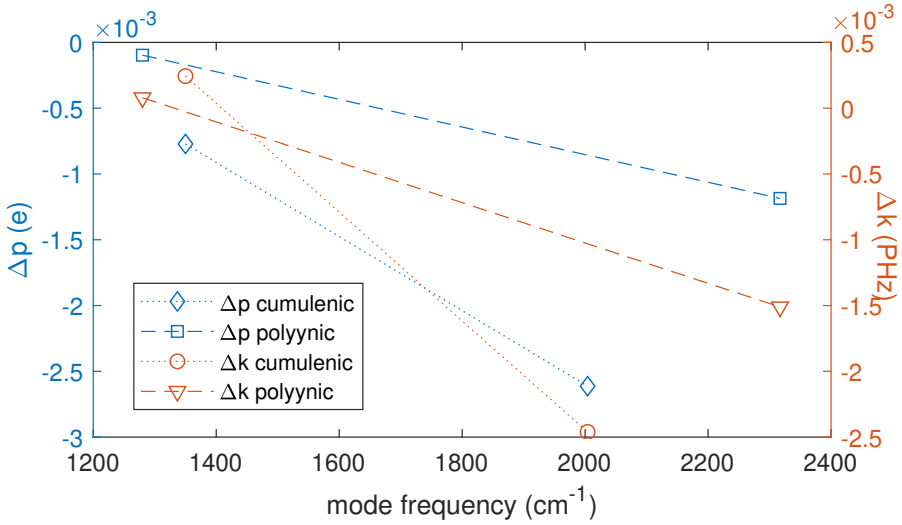


Figure S7: Contribution of the modes at $\approx$ 2004 cm$^{-1}$ ($\approx$ 2317 cm$^{-1}$) and $\approx$ 1350 cm$^{-1}$ ($\approx$ 1280 cm$^{-1}$) which display major and minor contributions, respectively, on the HOMO-LUMO gaps, and $T_1$ and $S_1$ excitation energies [cf, Fig. 2(d)-(e) of the main text], for cumulenic (polyynic) cyclo[18]carbon, within the quadratic method.