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From Six to Eight Π-electron Bare Rings of Group-XIV Elements and Beyond: Can Planarity be Deciphered from the "Quasi-molecules" They Embed?

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SUPPLEMENTARY INFORMATION

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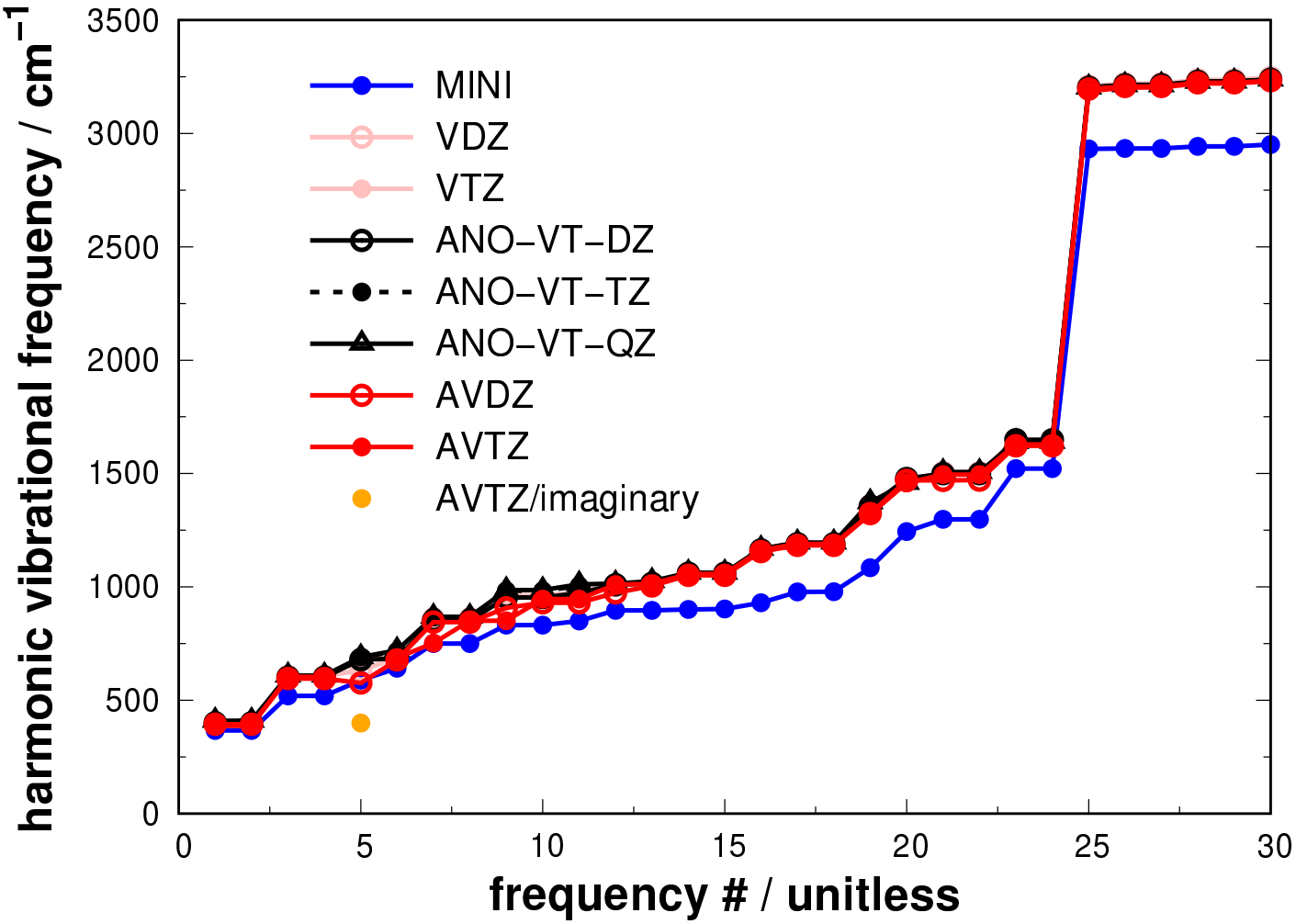

Fig. 1 Harmonic vibrational frquencies calculated in the present work for benzene at the MP2 level with MINI, VXZ, AVXZ, and ANO-VT-XZ basis sets (see the text).

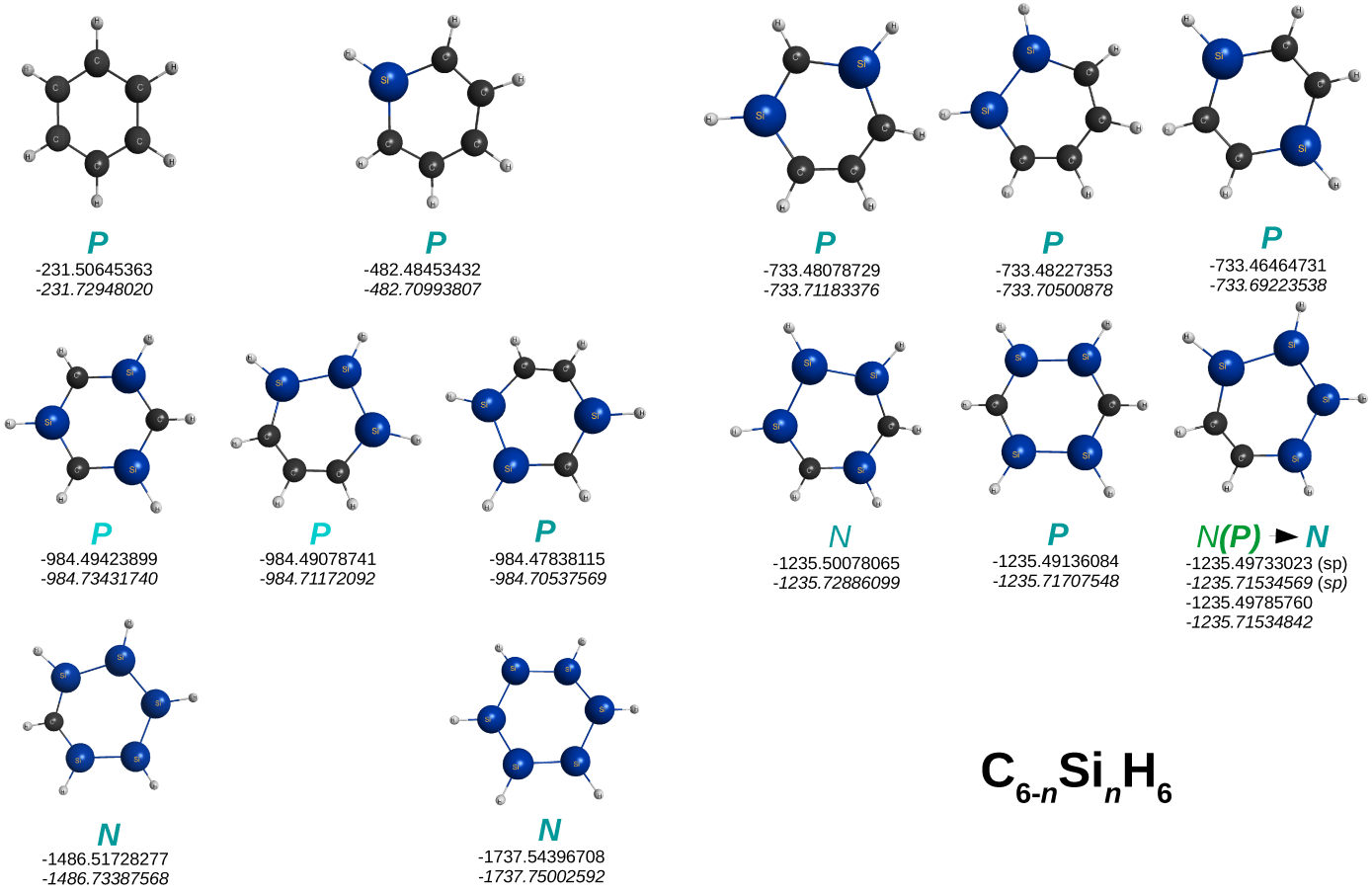

Fig. 2 Actual optimized structures for benzene and its E-derivatives. The optimized energies (in hartree, $\mathrm{E_h}$) here calculated at the MP2/VDZ level of theory are in roman, the MP2/VTZ ones in italic. Signaled by N***(P)*** $\rightarrow$ ***N*** is the fact that the indicated structure varies from weakly nonplanar (light-italic N) to nonplanar at MP2/VDZ level of theory when transiting from the saddle point to the nearby minimum structure. Note that the saddle point structure is perfectly planar even when MP2/V(T+d)Z optimized. Notation as in Figure 1 of the text.

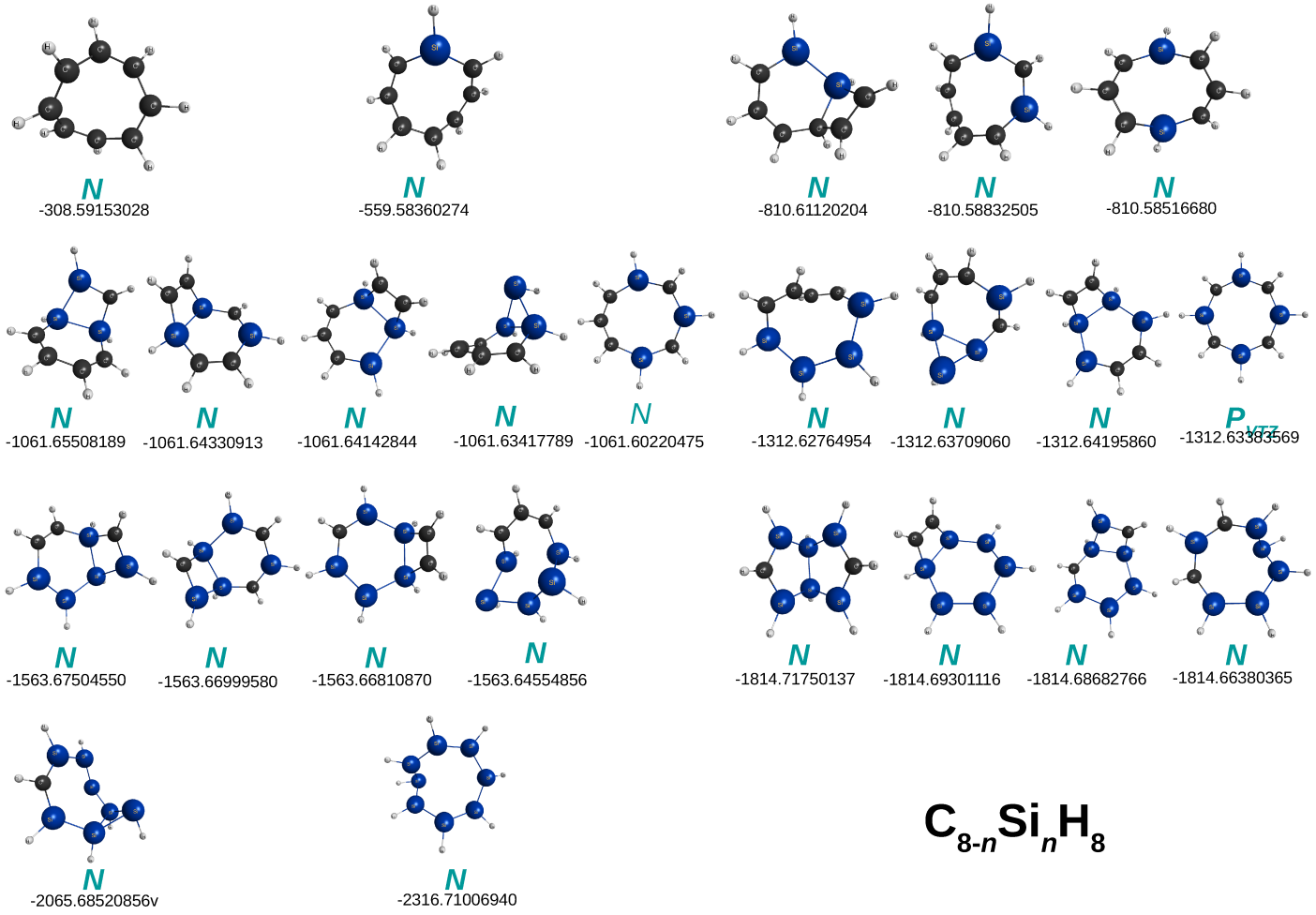

Fig. 3 Actual optimized structures for COT and its E-derivatives. The optimized energies (in $\mathrm{E_h}$) here calculated at the MP2/VTZ level of theory are also indicated. Notation as in Figure 1 of the text.