Helical Length Dependence in Molecular Spring Properties of Carbo[*n*]Helicenes

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Helically twisted π-conjugated molecules, such as helicenes, hold potential as molecular springs due to their helical ladder geometries and flexible mechanical properties.[1,2] In our previous work, we demonstrated that the mechanical property of helical π-conjugated molecules—i.e., molecular spring constant (k), derived from the Hooke's law $\Delta E = 1/2 \cdot k \cdot (\Delta r)^2$ where ΔE represents the change in potential energy and Δr denotes the strain upon elongation of the molecular springs—decreases with increasing the helical diameters (Figure 1 left).[3] However, a systematic evaluation of molecular spring properties, particularly in carbo[*n*]helicenes, remains unexplored.

In this work, the relationship between helical length and molecular spring properties of carbo[*n*]helicenes (n = 7–20) during the elongation of the helical framework was investigated by quantum chemical calculations at the B3LYP-GD3BJ/6-311G(2d,p) level (Figure 1 right). The helical length dependence of the molecular spring constants was found due to the influence of intramolecular π-π interactions between molecular layers and the position of the elongated carbon atoms.

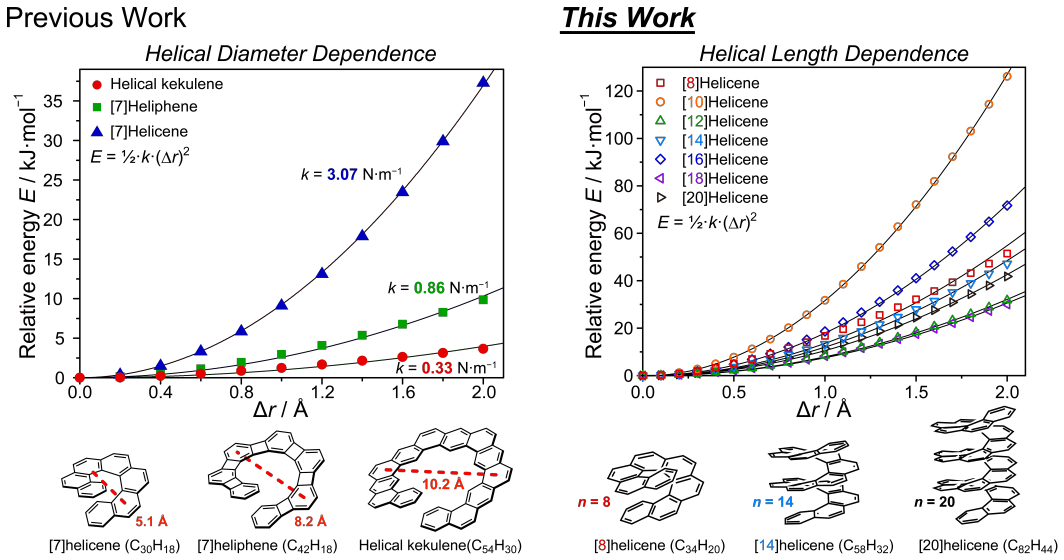

Figure 1. Concept of our previous work (left) and this work (right).

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