Supporting Information: A natural helical crystal lattice model for carbon nanotubes

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Comparison between the natural helical lattice model and the Clar VB model

In most cases, including all achiral CNTs and the chiral CNTs when $r = \mathrm{mod}(n-m, 3) = 0$ or 2, it is possible to define a unit cell in the Clar VB model that coincides with the unit cell in natural helical lattice model. However when $r = 1$, the unit cell defined by the Clar model contains $(2m + n - 1)/3$ aromatic sextets and one double bond. The helical vector, $\mathbf{T_R}$ (the seam of the double bonds), parallel to $2\mathbf{a_1} - \mathbf{a_2}$[1], is different from the helical vector defined in the natural helical lattice model, $\mathbf{T_R} = \mathbf{a_1} - 2\mathbf{a_2}$, as shown in the case of (6,5)-CNT in Figure S1.

References

[1] J. L. Ormsby and B. T. King, J. Org. Chem.,**69**, 4287-4291 (2004)

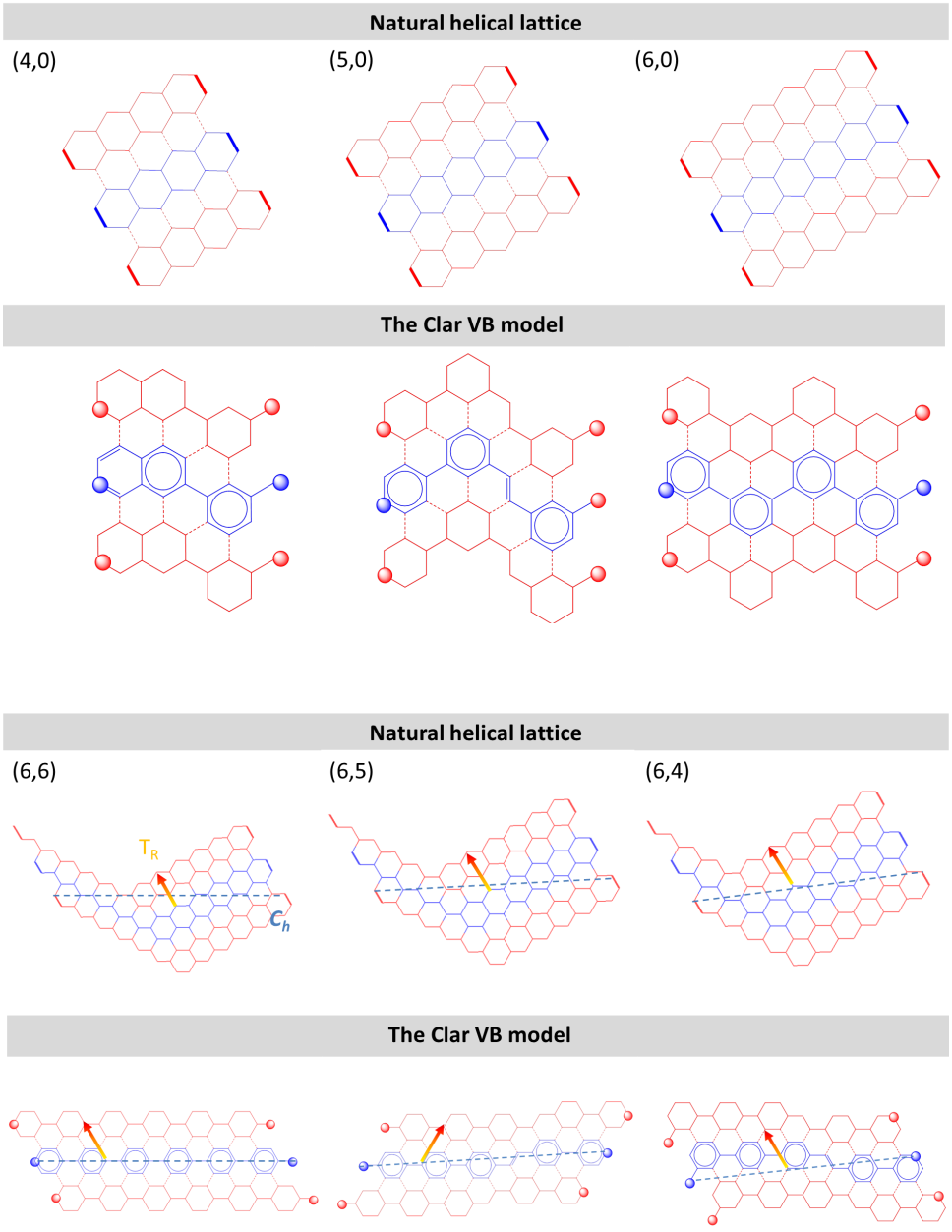

Figure S1: The unit cell for some chiral and achiral CNTs defined by the natural helical crystal lattice model and the Clar VB model. 3 unit cells are plotted in each graph and the central cell is marked in blue. The overlapping C-C bonds or C atoms are marked in bold. The circumference vector $\mathbf{C_h}$ and the helical vector $\mathbf{T_R}$ are also marked for chiral CNTs.