Patraporn Luksirikul 2006: Hydroboration Reaction: The Effect of B and N Atoms Doping onto the (5,5) Armchair Sidewalls of Single-Wall Carbon Nanotubes (SWNTs). Master of Science (Chemistry),
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Hydroboration of the perfect structure and the defective structure which doped B,N atoms onto the sidewall of (5,5) armchair single-wall carbon nanotubes with borane (BH_3) has been investigated within the framework of our-Own-N-layered-Integrated molecular Orbital and molecular Mechanics (ONIOM) approaches utilizing the two layered ONIOM scheme. Three different systems of hydroboration reaction: (1) perfect sidewall of SWNT; (2) BN-doped SWNT; (3) NB-doped SWNT, respectively were studied and found to occur through a concerted mechanism of the electrophilic attack of borane to carbon nanotubes. The transition states and products of doped systems onto hydroboration were stabilized by electron transfer from B and N atoms substituted nearby the reactive site to C reactive center (demonstrated by NPA analysis). The BN-doped and NB-doped activation energies of hydroboration with could enhance reactivity of (5,5) armchair single-wall carbon nanotubes decreased by 4.43 and 2.32 kcal/mol, respectively such their reaction energies

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