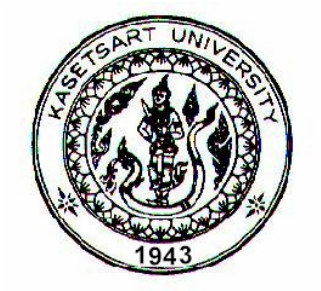

THESIS

THE 1,3-DIPOLAR CYCLOADDITIONS OF OZONE ON THE CAP OF TWO SERIES OF [5,5] ARMCHAIR AND [9,0] ZIGZAG SINGLE-WALLED CARBON NANOTUBES CAPPED WITH FULLERENE HEMISPHERES

MONTREE SAWANGPHRUK

GRADUATE SCHOOL, KASETSART UNIVERSITY

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The 1,3-dipolar cycloadditions of ozone on the caps of [5,5]- and [9,0]-single-walled carbon nanotubes capped with [60]-fullerene hemispheres (SWNTs) have been carried out using ONIOM(B3LYP/6-31G(d):AM1) and PBE/def-SV(P) methods. Increasing of the length of [5,5]-SWNTs (C_{60+10n}) where n starts from 1 to 14 and [9,0]-SWNTs (C_{60+18n}) where n starts from 1 to 8 leads to the change of the absolute chemical hardness (η) and the frontier molecular orbital (FMO) interaction energy. The absolute chemical hardness of [5,5]-SWNTs, calculated using the appropriate PBE approach, fluctuates and decreases from 0.83 eV to 0.15 eV when the size of the nanotube is increased from C_{60} to C_{200}. The absolute chemical hardness of [9,0]-SWNTs decreases without fluctuation from 0.72 eV to 0.28 eV for C_{78} to C_{204}. Also, the FMO interaction energy of [5,5]-SWNTs decreases with the fluctuation behavior from 0.05 eV to -1.05 eV. The FMO interaction energy of [9,0]-SWNTs decreases from -0.22 to -0.94 eV. While their activation and reaction energies are insensitive to the nanotube length. The basis set super position error corrected activation energies (E_a) are 2.8, 1.8-2.8, and 2.2 kcal/mol and the reaction energies are exothermic by 46.3, 45.9-49.4, and 48.4 kcal/mol for [60]-fullerene, [5,5]-SWNTs, and [9,0]-SWNTs, respectively.

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