Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Nanotubols under H_2O_2 Exposure: Is It Possible to Poly-Hydroxylate Carbon Nanotubes?

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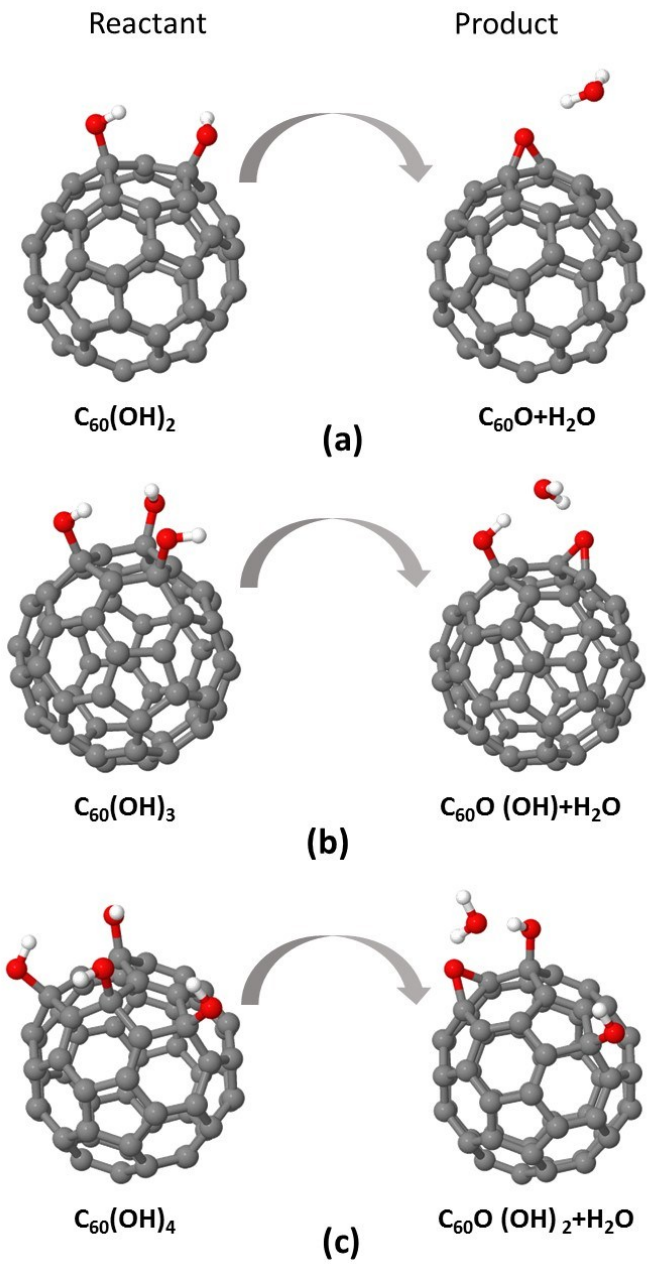

Figure S1. *(left column) Low-energy atomic configurations for two, three, and four OH's chemisorbed on C_{60} forming small molecular islands, labelled as $C_{60}(OH)_2$ [(a)-left], $C_{60}(OH)_3$ [(b)-left], and $C_{60}(OH)_4$ [(c)-left]. In the right column, we show the low energy structures of our so called "products", obtained by assuming the reaction of two neighboring hydroxyl groups (see text) to yield a physisorbed water and fullerenes with the following chemical composition: $C_{60}H_20O$ [(a)-right], $C_{60}H_20O(OH)$ [(b)-right], and $C_{60}H_20O(OH)_2$ [(c)-right].*

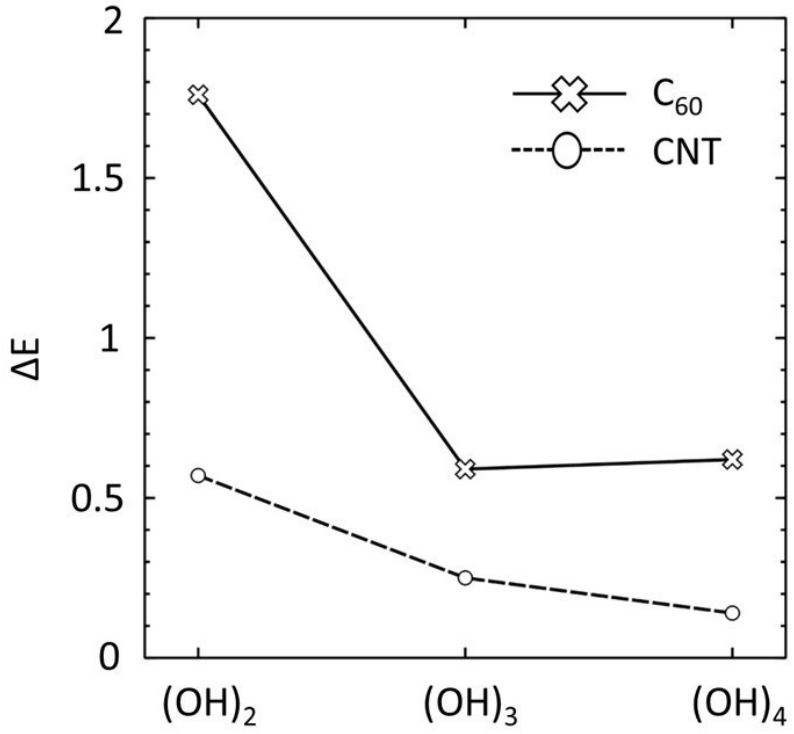

Figure S2. *Calculated energy barriers* ΔE *for the OH+OH→O+H_2O reaction on the C_{60} fullerene (continuous line) and on the CNT surface (dashed line) shown in Fig. 10.*