SUPPLEMENTARY MATERIAL

**Mechanistic, Energetic and Structural Studies of Carbon Nanotubes Functionalized with Penicillamine**

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Cartesian coordinates, sum of electronic and zero-point energies (E), sum of electronic and thermal enthalpies (H) and Gibbs free energies (G) for the calculated structures.

1- In water

NTCOOH

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C -1.229466000 -1.221036000 3.237048000

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C 1.217941000 2.599525000 1.865479000

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C 2.501168000 3.306701000 -0.121748000

C 3.730174000 3.187182000 -0.823237000

C 3.717802000 2.529042000 -2.105523000

C 4.912255000 2.021834000 -2.720980000

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1. \*Corresponding author. E-mail: almorsali@yahoo.com, morsali@mshdiau.ac.ir [↑](#footnote-ref-2)