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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C 7.596334000 0.571594000 -2.348640000

C 6.844128000 -0.680018000 -0.209594000

O 6.667953000 0.558774000 -3.320468000

N 9.070997000 -1.068412000 -1.439273000

S 5.048143000 -0.444493000 -0.758958000

O 8.315570000 1.524747000 -2.125967000

C 7.324018000 0.466972000 0.689197000

C 6.965365000 -2.037213000 0.502705000

H 7.187547000 -1.518951000 -2.190932000

H 6.671728000 1.436114000 -3.744008000

H 9.205765000 -1.922309000 -0.907593000

H 9.562265000 -0.314292000 -0.967127000

H 5.373298000 -0.276717000 3.471286000

H 6.929175000 0.364367000 1.699477000

H 7.053838000 1.447711000 0.293446000

H 8.415584000 0.422562000 0.766662000

H 6.310292000 -2.077984000 1.373174000

H 7.989738000 -2.178382000 0.862180000

H 6.713299000 -2.864838000 -0.166541000

Cl 5.966697000 -0.162046000 4.625709000

E=-4814,937351000,H=-4814,87657300 ,G=-4815,02316000a.u.

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