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Spin transport properties of 3d transition metal (II) phthalocyanines in contact with single-walled carbon nanotube electrodes

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1. Spin transport properties of the FePc molecule connected to two semi-infinite (3,3) armchair singe-walled carbon nanotubes

In Fig. S1 we present the energy-dependent spin-resolved transmission spectrum of the FePc molecule connected to two semi-infinite (3,3) SWCNT electrodes. When compared to the transmission spectrum for the same junction but using (4,4) SWCNTs as the electrodes [see Fig. 4(b)], we note that the tube size does not affect the overall shape of the transmission curve too much. Around the Fermi level, the transmission for spin-down electrons is still dominated by the Fe 3d_{xz} atomic orbital and the transmission for spin-up electrons is still negligibly small, exhibiting nearly perfect spin filtering with a spin-polarization (approaching 100%).

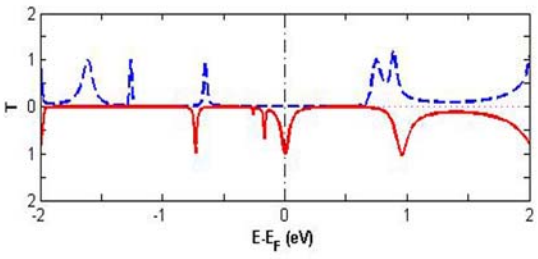

Fig. S1 Energy-dependent spin-resolved transmission spectrum of the FePc molecule attached to

two semi-infinite (3,3) armchair SWCNT electrodes with the dangling bonds at the open ends terminated by H: the blue (dashed) and red (solid) curves are respectively for the spin-up and spin-down electrons.

2. Effects of the chemisorption of one carbon monoxide molecule on the spin transport of the FePc molecule

Fig. S2 shows the energy-dependent spin-resolved transmission spectrum of the FePc molecule with one CO molecule adsorbed over the Fe atom, where two semi-infinite (4,4) armchair SWCNTs are used as the electrodes. As we can see, the adsorption of the CO molecule on the Fe atom drastically changes the spin transport properties of the SWCNT-FePc-SWCNT junction: the spin polarization is completely destroyed and the transmission around the Fermi level for both spin-up and spin-down electrons is negligibly small.

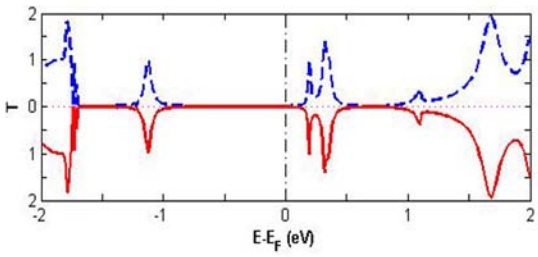

Fig. S2 Energy-dependent spin-resolved transmission spectrum of the SWCNT-FePc-SWCNT junction with one CO molecule adsorbed over the Fe atom: the blue (dashed) and red (solid) curves are respectively for the spin-up and spin-down electrons.

3. Atomic coordinates of isolated MPc molecules

3.1 MnPc in the gas phase

3.1.1 Atomic coordinates calculated using the PBE functional (Siesta)

Mn	0.000000	0.000000	0.000000
N	1.956850	1.956850	0.000000
N	0.000000	0.000000	0.000000
N	-1.956850	-1.956850	-0.000000
N	0.000000	0.000000	-0.000000
C	2.775300	2.775300	-0.000000
C	2.775300	2.775300	0.000000
C	4.170712	4.170712	0.000000
C	4.170712	4.170712	-0.000000

C	5.372635	5.372635	0.000000
C	5.372635	5.372635	-0.000000
C	6.571561	6.571561	0.000000
C	6.571561	6.571561	-0.000000
H	5.356265	5.356265	0.000000
H	5.356265	5.356265	-0.000000
H	7.525958	7.525958	0.000000
H	7.525958	7.525958	-0.000000
C	1.129871	1.129871	0.000000
C	-1.129871	-1.129871	-0.000000
C	0.708263	0.708263	0.000000
C	-0.708263	-0.708263	-0.000000
C	1.438605	1.438605	0.000000
C	-1.438605	-1.438605	-0.000000
C	0.709060	0.709060	0.000000
C	-0.709060	-0.709060	-0.000000
H	2.530452	2.530452	0.000000
H	-2.530452	-2.530452	-0.000000
H	1.240347	1.240347	0.000000
H	-1.240347	-1.240347	-0.000000
C	-2.775300	-2.775300	-0.000000
C	-2.775300	-2.775300	-0.000000
C	-4.170712	-4.170712	-0.000000
C	-4.170712	-4.170712	-0.000000
C	-5.372635	-5.372635	-0.000000
C	-5.372635	-5.372635	-0.000000
C	-6.571561	-6.571561	-0.000000
C	-6.571561	-6.571561	-0.000000
H	-5.356265	-5.356265	0.000000
H	-5.356265	-5.356265	-0.000000
H	-7.525958	-7.525958	-0.000000
H	-7.525958	-7.525958	-0.000000
C	-1.129871	-1.129871	-0.000000
C	1.129871	1.129871	-0.000000
C	-0.708263	-0.708263	-0.000000
C	0.708263	0.708263	-0.000000
C	-1.438605	-1.438605	-0.000000
C	1.438605	1.438605	-0.000000
C	-0.709060	-0.709060	-0.000000
C	0.709060	0.709060	-0.000000
H	-2.530452	-2.530452	-0.000000
H	2.530452	2.530452	-0.000000
H	-1.240347	-1.240347	-0.000000
H	1.240347	1.240347	-0.000000

N	2.402340	2.402340	0.000000
N	-2.402340	-2.402340	-0.000000
N	-2.402340	-2.402340	-0.000000
N	2.402340	2.402340	-0.000000

3.1.2 Atomic coordinates calculated using the PBE functional (Gaussian 03)

Mn	0.000000	0.000000	0.000000
N	0.000000	1.951295	0.000000
N	1.951295	0.000000	0.000000
N	0.000000	-1.951295	0.000000
N	-1.951295	0.000000	0.000000
C	-1.126884	2.773820	0.000000
C	1.126884	2.773820	0.000000
C	-0.706232	4.164985	0.000000
C	0.706232	4.164985	0.000000
C	-1.430514	5.363830	0.000000
C	1.430514	5.363830	0.000000
C	-0.706335	6.559178	0.000000
C	0.706335	6.559178	0.000000
H	-2.522191	5.354122	0.000000
H	2.522191	5.354122	0.000000
H	-1.239189	7.513011	0.000000
H	1.239189	7.513011	0.000000
C	2.773820	1.126884	0.000000
C	2.773820	-1.126884	0.000000
C	4.164985	0.706232	0.000000
C	4.164985	-0.706232	0.000000
C	5.363830	1.430514	0.000000
C	5.363830	-1.430514	0.000000
C	6.559178	0.706335	0.000000
C	6.559178	-0.706335	0.000000
H	5.354122	2.522191	0.000000
H	5.354122	-2.522191	0.000000
H	7.513011	1.239189	0.000000
H	7.513011	-1.239189	0.000000
C	1.126884	-2.773820	0.000000
C	-1.126884	-2.773820	0.000000
C	0.706232	-4.164985	0.000000
C	-0.706232	-4.164985	0.000000
C	1.430514	-5.363830	0.000000
C	-1.430514	-5.363830	0.000000
C	0.706335	-6.559178	0.000000
C	-0.706335	-6.559178	0.000000

H	2.522191	-5.354122	0.000000
H	-2.522191	-5.354122	0.000000
H	1.239189	-7.513011	0.000000
H	-1.239189	-7.513011	0.000000
C	-2.773820	-1.126884	0.000000
C	-2.773820	1.126884	0.000000
C	-4.164985	-0.706232	0.000000
C	-4.164985	0.706232	0.000000
C	-5.363830	-1.430514	0.000000
C	-5.363830	1.430514	0.000000
C	-6.559178	-0.706335	0.000000
C	-6.559178	0.706335	0.000000
H	-5.354122	-2.522191	0.000000
H	-5.354122	2.522191	0.000000
H	-7.513011	-1.239189	0.000000
H	-7.513011	1.239189	0.000000
N	2.398157	2.398157	0.000000
N	2.398157	-2.398157	0.000000
N	-2.398157	-2.398157	0.000000
N	-2.398157	2.398157	0.000000

3.1.3 Atomic coordinates calculated using the PBEh functional (Gaussian 03)

Mn	0.000000	0.000000	0.000000
N	0.000000	1.945456	0.000000
N	1.945456	0.000000	0.000000
N	0.000000	-1.945456	0.000000
N	-1.945456	0.000000	0.000000
C	-1.116253	2.752865	0.000000
C	1.116253	2.752865	0.000000
C	-0.700016	4.138374	0.000000
C	0.700016	4.138374	0.000000
C	-1.421309	5.329001	0.000000
C	1.421309	5.329001	0.000000
C	-0.702204	6.514486	0.000000
C	0.702204	6.514486	0.000000
H	-2.505474	5.319162	0.000000
H	2.505474	5.319162	0.000000
H	-1.230494	7.462337	0.000000
H	1.230494	7.462337	0.000000
C	2.752865	1.116253	0.000000
C	2.752865	-1.116253	0.000000
C	4.138374	0.700016	0.000000
C	4.138374	-0.700016	0.000000

C	5.329001	1.421309	0.000000
C	5.329001	-1.421309	0.000000
C	6.514486	0.702204	0.000000
C	6.514486	-0.702204	0.000000
H	5.319162	2.505474	0.000000
H	5.319162	-2.505474	0.000000
H	7.462337	1.230494	0.000000
H	7.462337	-1.230494	0.000000
C	1.116253	-2.752865	0.000000
C	-1.116253	-2.752865	0.000000
C	0.700016	-4.138374	0.000000
C	-0.700016	-4.138374	0.000000
C	1.421309	-5.329001	0.000000
C	-1.421309	-5.329001	0.000000
C	0.702204	-6.514486	0.000000
C	-0.702204	-6.514486	0.000000
H	2.505474	-5.319162	0.000000
H	-2.505474	-5.319162	0.000000
H	1.230494	-7.462337	0.000000
H	-1.230494	-7.462337	0.000000
C	-2.752865	-1.116253	0.000000
C	-2.752865	1.116253	0.000000
C	-4.138374	-0.700016	0.000000
C	-4.138374	0.700016	0.000000
C	-5.329001	-1.421309	0.000000
C	-5.329001	1.421309	0.000000
C	-6.514486	-0.702204	0.000000
C	-6.514486	0.702204	0.000000
H	-5.319162	-2.505474	0.000000
H	-5.319162	2.505474	0.000000
H	-7.462337	-1.230494	0.000000
H	-7.462337	1.230494	0.000000
N	2.376988	2.376988	0.000000
N	2.376988	-2.376988	0.000000
N	-2.376988	-2.376988	0.000000
N	-2.376988	2.376988	0.000000

3.2 FePc in the gas phase

3.2.1 Atomic coordinates calculated using the PBE functional (Siesta)

Fe	0.000000	0.000000	0.000000
C	0.708382	6.563451	0.000000
C	-0.708382	6.563451	0.000000

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C	1.438952	5.363652	0.000000
C	-1.438952	5.363652	0.000000
C	0.706538	4.163671	0.000000
C	-0.706538	4.163671	0.000000
C	1.125039	2.764243	0.000000
C	-1.125039	2.764243	0.000000
H	1.239036	7.518338	0.000000
H	-1.239036	7.518338	0.000000
H	2.530916	5.348384	0.000000
H	-2.530916	5.348384	0.000000
N	0.000000	1.942897	0.000000
C	0.708382	-6.563451	0.000000
C	-0.708382	-6.563451	0.000000
C	1.438952	-5.363652	0.000000
C	-1.438952	-5.363652	0.000000
C	0.706538	-4.163671	0.000000
C	-0.706538	-4.163671	0.000000
C	1.125039	-2.764243	0.000000
C	-1.125039	-2.764243	0.000000
H	1.239036	-7.518338	0.000000
H	-1.239036	-7.518338	0.000000
H	2.530916	-5.348384	0.000000
H	-2.530916	-5.348384	0.000000
N	0.000000	-1.942897	0.000000
C	6.563451	0.708382	0.000000
C	6.563451	-0.708382	0.000000
C	5.363652	1.438952	0.000000
C	5.363652	-1.438952	0.000000
C	4.163671	0.706538	0.000000
C	4.163671	-0.706538	0.000000
C	2.764243	1.125039	0.000000
C	2.764243	-1.125039	0.000000
H	7.518338	1.239036	0.000000
H	7.518338	-1.239036	0.000000
H	5.348384	2.530916	0.000000
H	5.348384	-2.530916	0.000000
N	1.942897	0.000000	0.000000
C	-6.563451	0.708382	0.000000
C	-6.563451	-0.708382	0.000000
C	-5.363652	1.438952	0.000000
C	-5.363652	-1.438952	0.000000
C	-4.163671	0.706538	0.000000
C	-4.163671	-0.706538	0.000000
C	-2.764243	1.125039	0.000000

C	-2.764243	-1.125039	0.000000
H	-7.518338	1.239036	0.000000
H	-7.518338	-1.239036	0.000000
H	-5.348384	2.530916	0.000000
H	-5.348384	-2.530916	0.000000
N	-1.942897	0.000000	0.000000
N	2.396237	2.396237	0.000000
N	-2.396237	2.396237	0.000000
N	-2.396237	-2.396237	0.000000
N	2.396237	-2.396237	0.000000

3.2.2 Atomic coordinates calculated using the PBE functional with (Gaussian 03)

Fe	0.000000	0.000000	0.000000
N	0.000000	1.933900	0.000000
N	1.933900	0.000000	0.000000
N	0.000000	-1.933900	0.000000
N	-1.933900	0.000000	0.000000
C	-1.121111	2.761013	0.000000
C	1.121111	2.761013	0.000000
C	-0.704293	4.155032	0.000000
C	0.704293	4.155032	0.000000
C	-1.430308	5.351603	0.000000
C	1.430308	5.351603	0.000000
C	-0.705757	6.547776	0.000000
C	0.705757	6.547776	0.000000
H	-2.521962	5.341657	0.000000
H	2.521962	5.341657	0.000000
H	-1.239046	7.501389	0.000000
H	1.239046	7.501389	0.000000
C	2.761013	1.121111	0.000000
C	2.761013	-1.121111	0.000000
C	4.155032	0.704293	0.000000
C	4.155032	-0.704293	0.000000
C	5.351603	1.430308	0.000000
C	5.351603	-1.430308	0.000000
C	6.547776	0.705757	0.000000
C	6.547776	-0.705757	0.000000
H	5.341657	2.521962	0.000000
H	5.341657	-2.521962	0.000000
H	7.501389	1.239046	0.000000
H	7.501389	-1.239046	0.000000
C	1.121111	-2.761013	0.000000
C	-1.121111	-2.761013	0.000000

C	0.704293	-4.155032	0.000000
C	-0.704293	-4.155032	0.000000
C	1.430308	-5.351603	0.000000
C	-1.430308	-5.351603	0.000000
C	0.705757	-6.547776	0.000000
C	-0.705757	-6.547776	0.000000
H	2.521962	-5.341657	0.000000
H	-2.521962	-5.341657	0.000000
H	1.239046	-7.501389	0.000000
H	-1.239046	-7.501389	0.000000
C	-2.761013	-1.121111	0.000000
C	-2.761013	1.121111	0.000000
C	-4.155032	-0.704293	0.000000
C	-4.155032	0.704293	0.000000
C	-5.351603	-1.430308	0.000000
C	-5.351603	1.430308	0.000000
C	-6.547776	-0.705757	0.000000
C	-6.547776	0.705757	0.000000
H	-5.341657	-2.521962	0.000000
H	-5.341657	2.521962	0.000000
H	-7.501389	-1.239046	0.000000
H	-7.501389	1.239046	0.000000
N	2.390728	2.390728	0.000000
N	2.390728	-2.390728	0.000000
N	-2.390728	-2.390728	0.000000
N	-2.390728	2.390728	0.000000

3.2.3 Atomic coordinates calculated using the PBEh functional (Gaussian 03)

Fe	0.000000	0.000000	0.000000
N	0.000000	1.940800	0.000000
N	1.940800	0.000000	0.000000
N	0.000000	-1.940800	0.000000
N	-1.940800	0.000000	0.000000
C	-1.110298	2.744918	0.000000
C	1.110298	2.744918	0.000000
C	-0.699112	4.135394	0.000000
C	0.699112	4.135394	0.000000
C	-1.421424	5.323918	0.000000
C	1.421424	5.323918	0.000000
C	-0.701693	6.510149	0.000000
C	0.701693	6.510149	0.000000
H	-2.505579	5.313974	0.000000
H	2.505579	5.313974	0.000000

H	-1.230006	7.457950	0.000000
H	1.230006	7.457950	0.000000
C	2.744918	1.110298	0.000000
C	2.744918	-1.110298	0.000000
C	4.135394	0.699112	0.000000
C	4.135394	-0.699112	0.000000
C	5.323918	1.421424	0.000000
C	5.323918	-1.421424	0.000000
C	6.510149	0.701693	0.000000
C	6.510149	-0.701693	0.000000
H	5.313974	2.505579	0.000000
H	5.313974	-2.505579	0.000000
H	7.457950	1.230006	0.000000
H	7.457950	-1.230006	0.000000
C	1.110298	-2.744918	0.000000
C	-1.110298	-2.744918	0.000000
C	0.699112	-4.135394	0.000000
C	-0.699112	-4.135394	0.000000
C	1.421424	-5.323918	0.000000
C	-1.421424	-5.323918	0.000000
C	0.701693	-6.510149	0.000000
C	-0.701693	-6.510149	0.000000
H	2.505579	-5.313974	0.000000
H	-2.505579	-5.313974	0.000000
H	1.230006	-7.457950	0.000000
H	-1.230006	-7.457950	0.000000
C	-2.744918	-1.110298	0.000000
C	-2.744918	1.110298	0.000000
C	-4.135394	-0.699112	0.000000
C	-4.135394	0.699112	0.000000
C	-5.323918	-1.421424	0.000000
C	-5.323918	1.421424	0.000000
C	-6.510149	-0.701693	0.000000
C	-6.510149	0.701693	0.000000
H	-5.313974	-2.505579	0.000000
H	-5.313974	2.505579	0.000000
H	-7.457950	-1.230006	0.000000
H	-7.457950	1.230006	0.000000
N	2.372343	2.372343	0.000000
N	2.372343	-2.372343	0.000000
N	-2.372343	-2.372343	0.000000
N	-2.372343	2.372343	0.000000

3.3 CoPc in the gas phase

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3.3.1 Atomic coordinates calculated using the PBE functional (Siesta)

Co	0.000000	0.000000	0.000000
N	1.931263	0.000000	0.000000
N	0.000000	1.931263	0.000000
N	-1.931263	0.000000	0.000000
N	0.000000	-1.931263	0.000000
C	2.752012	-1.119031	0.000000
C	2.752012	1.119031	0.000000
C	4.153020	-0.705957	0.000000
C	4.153020	0.705957	0.000000
C	5.351351	-1.439444	0.000000
C	5.351351	1.439444	0.000000
C	6.550905	-0.708623	0.000000
C	6.550905	0.708623	0.000000
H	5.333590	-2.531258	0.000000
H	5.333590	2.531258	0.000000
H	7.505543	-1.239727	0.000000
H	7.505543	1.239727	0.000000
C	1.119031	2.752012	0.000000
C	-1.119031	2.752012	0.000000
C	0.705957	4.153020	0.000000
C	-0.705957	4.153020	0.000000
C	1.439444	5.351351	0.000000
C	-1.439444	5.351351	0.000000
C	0.708623	6.550905	0.000000
C	-0.708623	6.550905	0.000000
H	2.531258	5.333590	0.000000
H	-2.531258	5.333590	0.000000
H	1.239727	7.505543	0.000000
H	-1.239727	7.505543	0.000000
C	-2.752012	1.119031	0.000000
C	-2.752012	-1.119031	0.000000
C	-4.153020	0.705957	0.000000
C	-4.153020	-0.705957	0.000000
C	-5.351351	1.439444	0.000000
C	-5.351351	-1.439444	0.000000
C	-6.550905	0.708623	0.000000
C	-6.550905	-0.708623	0.000000
H	-5.333590	2.531258	0.000000
H	-5.333590	-2.531258	0.000000
H	-7.505543	1.239727	0.000000
H	-7.505543	-1.239727	0.000000
C	-1.119031	-2.752012	0.000000

C	1.119031	-2.752012	0.000000
C	-0.705957	-4.153020	0.000000
C	0.705957	-4.153020	0.000000
C	-1.439444	-5.351351	0.000000
C	1.439444	-5.351351	0.000000
C	-0.708623	-6.550905	0.000000
C	0.708623	-6.550905	0.000000
H	-2.531258	-5.333590	0.000000
H	2.531258	-5.333590	0.000000
H	-1.239727	-7.505543	0.000000
H	1.239727	-7.505543	0.000000
N	2.394098	2.394098	0.000000
N	-2.394098	2.394098	0.000000
N	-2.394098	-2.394098	0.000000
N	2.394098	-2.394098	0.000000

3.3.2 Atomic coordinates calculated using the PBE functional (Gaussian 03)

Co	0.000000	0.000000	0.000000
C	0.707483	6.566877	0.000000
C	-0.707483	6.566877	0.000000
C	1.433004	5.366122	0.000000
C	-1.433004	5.366122	0.000000
C	0.707302	4.167858	0.000000
C	-0.707302	4.167858	0.000000
C	1.125907	2.774812	0.000000
C	-1.125907	2.774812	0.000000
H	1.240298	7.518382	0.000000
H	-1.240298	7.518382	0.000000
H	2.522418	5.354015	0.000000
H	-2.522418	5.354015	0.000000
N	0.000000	1.934044	0.000000
C	0.707483	-6.566877	0.000000
C	-0.707483	-6.566877	0.000000
C	1.433004	-5.366122	0.000000
C	-1.433004	-5.366122	0.000000
C	0.707302	-4.167858	0.000000
C	-0.707302	-4.167858	0.000000
C	1.125907	-2.774812	0.000000
C	-1.125907	-2.774812	0.000000
H	1.240298	-7.518382	0.000000
H	-1.240298	-7.518382	0.000000
H	2.522418	-5.354015	0.000000
H	-2.522418	-5.354015	0.000000

N	0.000000	-1.934044	0.000000
C	6.566877	0.707483	0.000000
C	6.566877	-0.707483	0.000000
C	5.366122	1.433004	0.000000
C	5.366122	-1.433004	0.000000
C	4.167858	0.707302	0.000000
C	4.167858	-0.707302	0.000000
C	2.774812	1.125907	0.000000
C	2.774812	-1.125907	0.000000
H	7.518382	1.240298	0.000000
H	7.518382	-1.240298	0.000000
H	5.354015	2.522418	0.000000
H	5.354015	-2.522418	0.000000
N	1.934044	0.000000	0.000000
C	-6.566877	0.707483	0.000000
C	-6.566877	-0.707483	0.000000
C	-5.366122	1.433004	0.000000
C	-5.366122	-1.433004	0.000000
C	-4.167858	0.707302	0.000000
C	-4.167858	-0.707302	0.000000
C	-2.774812	1.125907	0.000000
C	-2.774812	-1.125907	0.000000
H	-7.518382	1.240298	0.000000
H	-7.518382	-1.240298	0.000000
H	-5.354015	2.522418	0.000000
H	-5.354015	-2.522418	0.000000
N	-1.934044	0.000000	0.000000
N	2.405679	2.405679	0.000000
N	-2.405679	2.405679	0.000000
N	-2.405679	-2.405679	0.000000
N	2.405679	-2.405679	0.000000

3.3.3 Atomic coordinates calculated using the PBEh functional (Gaussian 03)

Co	0.000000	0.000000	0.000000
C	0.702787	6.522825	0.000000
C	-0.702787	6.522825	0.000000
C	1.422971	5.331815	0.000000
C	-1.422971	5.331815	0.000000
C	0.701177	4.142562	0.000000
C	-0.701177	4.142562	0.000000
C	1.113332	2.754682	0.000000
C	-1.113332	2.754682	0.000000
H	1.230788	7.467589	0.000000

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H	-1.230788	7.467589	0.000000
H	2.504162	5.319695	0.000000
H	-2.504162	5.319695	0.000000
N	0.000000	1.931507	0.000000
C	0.702787	-6.522825	0.000000
C	-0.702787	-6.522825	0.000000
C	1.422971	-5.331815	0.000000
C	-1.422971	-5.331815	0.000000
C	0.701177	-4.142562	0.000000
C	-0.701177	-4.142562	0.000000
C	1.113332	-2.754682	0.000000
C	-1.113332	-2.754682	0.000000
H	1.230788	-7.467589	0.000000
H	-1.230788	-7.467589	0.000000
H	2.504162	-5.319695	0.000000
H	-2.504162	-5.319695	0.000000
N	0.000000	-1.931507	0.000000
C	6.522825	0.702787	0.000000
C	6.522825	-0.702787	0.000000
C	5.331815	1.422971	0.000000
C	5.331815	-1.422971	0.000000
C	4.142562	0.701177	0.000000
C	4.142562	-0.701177	0.000000
C	2.754682	1.113332	0.000000
C	2.754682	-1.113332	0.000000
H	7.467589	1.230788	0.000000
H	7.467589	-1.230788	0.000000
H	5.319695	2.504162	0.000000
H	5.319695	-2.504162	0.000000
N	1.931507	0.000000	0.000000
C	-6.522825	0.702787	0.000000
C	-6.522825	-0.702787	0.000000
C	-5.331815	1.422971	0.000000
C	-5.331815	-1.422971	0.000000
C	-4.142562	0.701177	0.000000
C	-4.142562	-0.701177	0.000000
C	-2.754682	1.113332	0.000000
C	-2.754682	-1.113332	0.000000
H	-7.467589	1.230788	0.000000
H	-7.467589	-1.230788	0.000000
H	-5.319695	2.504162	0.000000
H	-5.319695	-2.504162	0.000000
N	-1.931507	0.000000	0.000000
N	2.381081	2.381081	0.000000

N	-2.381081	2.381081	0.000000
N	-2.381081	-2.381081	0.000000
N	2.381081	-2.381081	0.000000

3.4 NiPc in the gas phase

3.4.1 Atomic coordinates calculated using the PBE functional (Siesta)

Ni	0.000000	0.000000	0.000000
N	1.918966	0.000000	0.000000
N	0.000000	1.918966	0.000000
N	-1.918966	0.000000	0.000000
N	0.000000	-1.918966	0.000000
C	2.742513	-1.116914	0.000000
C	2.742513	1.116914	0.000000
C	4.143071	-0.705263	0.000000
C	4.143071	0.705263	0.000000
C	5.340820	-1.440002	0.000000
C	5.340820	1.440002	0.000000
C	6.540024	-0.708811	0.000000
C	6.540024	0.708811	0.000000
H	5.322792	-2.531668	0.000000
H	5.322792	2.531668	0.000000
H	7.494779	-1.239683	0.000000
H	7.494779	1.239683	0.000000
C	1.116914	2.742513	0.000000
C	-1.116914	2.742513	0.000000
C	0.705263	4.143071	0.000000
C	-0.705263	4.143071	0.000000
C	1.440002	5.340820	0.000000
C	-1.440002	5.340820	0.000000
C	0.708811	6.540024	0.000000
C	-0.708811	6.540024	0.000000
H	2.531668	5.322792	0.000000
H	-2.531668	5.322792	0.000000
H	1.239683	7.494779	0.000000
H	-1.239683	7.494779	0.000000
C	-2.742513	1.116914	0.000000
C	-2.742513	-1.116914	0.000000
C	-4.143071	0.705263	0.000000
C	-4.143071	-0.705263	0.000000
C	-5.340820	1.440002	0.000000
C	-5.340820	-1.440002	0.000000
C	-6.540024	0.708811	0.000000

C	-6.540024	-0.708811	0.000000
H	-5.322792	2.531668	0.000000
H	-5.322792	-2.531668	0.000000
H	-7.494779	1.239683	0.000000
H	-7.494779	-1.239683	0.000000
C	-1.116914	-2.742513	0.000000
C	1.116914	-2.742513	0.000000
C	-0.705263	-4.143071	0.000000
C	0.705263	-4.143071	0.000000
C	-1.440002	-5.340820	0.000000
C	1.440002	-5.340820	0.000000
C	-0.708811	-6.540024	0.000000
C	0.708811	-6.540024	0.000000
H	-2.531668	-5.322792	0.000000
H	2.531668	-5.322792	0.000000
H	-1.239683	-7.494779	0.000000
H	1.239683	-7.494779	0.000000
N	2.391737	2.391737	0.000000
N	-2.391737	2.391737	0.000000
N	-2.391737	-2.391737	0.000000
N	2.391737	-2.391737	0.000000

3.4.2 Atomic coordinates calculated using the PBE functional (Gaussian 03)

Ni	0.000000	0.000000	0.000000
C	0.706073	6.527270	0.000000
C	-0.706073	6.527270	0.000000
C	1.431381	5.331916	0.000000
C	-1.431381	5.331916	0.000000
C	0.703055	4.136758	0.000000
C	-0.703055	4.136758	0.000000
C	1.113688	2.741069	0.000000
C	-1.113688	2.741069	0.000000
H	1.238401	7.481366	0.000000
H	-1.238401	7.481366	0.000000
H	2.522905	5.321076	0.000000
H	-2.522905	5.321076	0.000000
N	0.000000	1.913424	0.000000
C	0.706073	-6.527270	0.000000
C	-0.706073	-6.527270	0.000000
C	1.431381	-5.331916	0.000000
C	-1.431381	-5.331916	0.000000
C	0.703055	-4.136758	0.000000
C	-0.703055	-4.136758	0.000000

C	1.113688	-2.741069	0.000000
C	-1.113688	-2.741069	0.000000
H	1.238401	-7.481366	0.000000
H	-1.238401	-7.481366	0.000000
H	2.522905	-5.321076	0.000000
H	-2.522905	-5.321076	0.000000
N	0.000000	-1.913424	0.000000
C	6.527270	0.706073	0.000000
C	6.527270	-0.706073	0.000000
C	5.331916	1.431381	0.000000
C	5.331916	-1.431381	0.000000
C	4.136758	0.703055	0.000000
C	4.136758	-0.703055	0.000000
C	2.741069	1.113688	0.000000
C	2.741069	-1.113688	0.000000
H	7.481366	1.238401	0.000000
H	7.481366	-1.238401	0.000000
H	5.321076	2.522905	0.000000
H	5.321076	-2.522905	0.000000
N	1.913424	0.000000	0.000000
C	-6.527270	0.706073	0.000000
C	-6.527270	-0.706073	0.000000
C	-5.331916	1.431381	0.000000
C	-5.331916	-1.431381	0.000000
C	-4.136758	0.703055	0.000000
C	-4.136758	-0.703055	0.000000
C	-2.741069	1.113688	0.000000
C	-2.741069	-1.113688	0.000000
H	-7.481366	1.238401	0.000000
H	-7.481366	-1.238401	0.000000
H	-5.321076	2.522905	0.000000
H	-5.321076	-2.522905	0.000000
N	-1.913424	0.000000	0.000000
N	2.387900	2.387900	0.000000
N	-2.387900	2.387900	0.000000
N	-2.387900	-2.387900	0.000000
N	2.387900	-2.387900	0.000000

3.4.3 Atomic coordinates calculated using the PBEh functional (Gaussian 03)

Ni	0.000000	0.000000	0.000000
C	0.701972	6.483617	0.000000
C	-0.701972	6.483617	0.000000
C	1.422146	5.298028	0.000000

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C	-1.422146	5.298028	0.000000
C	0.697073	4.111012	0.000000
C	-0.697073	4.111012	0.000000
C	1.101805	2.720441	0.000000
C	-1.101805	2.720441	0.000000
H	1.229756	7.431733	0.000000
H	-1.229756	7.431733	0.000000
H	2.506193	5.287309	0.000000
H	-2.506193	5.287309	0.000000
N	0.000000	1.905993	0.000000
C	0.701972	-6.483617	0.000000
C	-0.701972	-6.483617	0.000000
C	1.422146	-5.298028	0.000000
C	-1.422146	-5.298028	0.000000
C	0.697073	-4.111012	0.000000
C	-0.697073	-4.111012	0.000000
C	1.101805	-2.720441	0.000000
C	-1.101805	-2.720441	0.000000
H	1.229756	-7.431733	0.000000
H	-1.229756	-7.431733	0.000000
H	2.506193	-5.287309	0.000000
H	-2.506193	-5.287309	0.000000
N	0.000000	-1.905993	0.000000
C	6.483617	0.701972	0.000000
C	6.483617	-0.701972	0.000000
C	5.298028	1.422146	0.000000
C	5.298028	-1.422146	0.000000
C	4.111012	0.697073	0.000000
C	4.111012	-0.697073	0.000000
C	2.720441	1.101805	0.000000
C	2.720441	-1.101805	0.000000
H	7.431733	1.229756	0.000000
H	7.431733	-1.229756	0.000000
H	5.287309	2.506193	0.000000
H	5.287309	-2.506193	0.000000
N	1.905993	0.000000	0.000000
C	-6.483617	0.701972	0.000000
C	-6.483617	-0.701972	0.000000
C	-5.298028	1.422146	0.000000
C	-5.298028	-1.422146	0.000000
C	-4.111012	0.697073	0.000000
C	-4.111012	-0.697073	0.000000
C	-2.720441	1.101805	0.000000
C	-2.720441	-1.101805	0.000000

H	-7.431733	1.229756	0.000000
H	-7.431733	-1.229756	0.000000
H	-5.287309	2.506193	0.000000
H	-5.287309	-2.506193	0.000000
N	-1.905993	0.000000	0.000000
N	2.365378	2.365378	0.000000
N	-2.365378	2.365378	0.000000
N	-2.365378	-2.365378	0.000000
N	2.365378	-2.365378	0.000000

3.5 CuPc in the gas phase

3.5.1 Atomic coordinates calculated using the PBE functional (Siesta)

Cu	0.000000	0.000000	0.000000
N	1.956850	0.000000	0.000000
N	0.000000	1.977704	0.000000
N	-1.956850	0.000000	-0.000000
N	0.000000	-1.977704	-0.000000
C	2.775300	-1.125118	-0.000000
C	2.775300	1.125118	0.000000
C	4.170712	-0.708402	0.000000
C	4.170712	0.708402	-0.000000
C	5.372635	-1.437856	0.000000
C	5.372635	1.437856	-0.000000
C	6.571561	-0.708181	0.000000
C	6.571561	0.708181	-0.000000
H	5.356265	-2.529774	0.000000
H	5.356265	2.529774	-0.000000
H	7.525958	-1.239970	0.000000
H	7.525958	1.239970	-0.000000
C	1.129871	2.778435	0.000000
C	-1.129871	2.778435	-0.000000
C	0.708263	4.184068	0.000000
C	-0.708263	4.184068	-0.000000
C	1.438605	5.384856	0.000000
C	-1.438605	5.384856	-0.000000
C	0.709060	6.585297	0.000000
C	-0.709060	6.585297	-0.000000
H	2.530452	5.370423	0.000000
H	-2.530452	5.370423	-0.000000
H	1.240347	7.539468	0.000000
H	-1.240347	7.539468	-0.000000
C	-2.775300	1.125118	-0.000000

C	-2.775300	-1.125118	-0.000000
C	-4.170712	0.708402	-0.000000
C	-4.170712	-0.708402	-0.000000
C	-5.372635	1.437856	-0.000000
C	-5.372635	-1.437856	-0.000000
C	-6.571561	0.708181	-0.000000
C	-6.571561	-0.708181	-0.000000
H	-5.356265	2.529774	0.000000
H	-5.356265	-2.529774	-0.000000
H	-7.525958	1.239970	-0.000000
H	-7.525958	-1.239970	-0.000000
C	-1.129871	-2.778435	-0.000000
C	1.129871	-2.778435	-0.000000
C	-0.708263	-4.184068	-0.000000
C	0.708263	-4.184068	-0.000000
C	-1.438605	-5.384856	-0.000000
C	1.438605	-5.384856	-0.000000
C	-0.709060	-6.585297	-0.000000
C	0.709060	-6.585297	-0.000000
H	-2.530452	-5.370423	-0.000000
H	2.530452	-5.370423	-0.000000
H	-1.240347	-7.539468	-0.000000
H	1.240347	-7.539468	-0.000000
N	2.402340	2.401872	0.000000
N	-2.402340	2.401872	-0.000000
N	-2.402340	-2.401872	-0.000000
N	2.402340	-2.401872	-0.000000

3.5.2 Atomic coordinates calculated using the PBE functional (Gaussian 03)

Cu	0.000000	0.000000	0.000000
C	0.705601	6.566700	0.000000
C	-0.705601	6.566700	0.000000
C	1.430391	5.370369	0.000000
C	-1.430391	5.370369	0.000000
C	0.706092	4.173415	0.000000
C	-0.706092	4.173415	0.000000
C	1.121067	2.773231	0.000000
C	-1.121067	2.773231	0.000000
H	1.238475	7.520533	0.000000
H	-1.238475	7.520533	0.000000
H	2.522080	5.360701	0.000000
H	-2.522080	5.360701	0.000000
N	0.000000	1.967354	0.000000

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C	0.705601	-6.566700	0.000000
C	-0.705601	-6.566700	0.000000
C	1.430391	-5.370369	0.000000
C	-1.430391	-5.370369	0.000000
C	0.706092	-4.173415	0.000000
C	-0.706092	-4.173415	0.000000
C	1.121067	-2.773231	0.000000
C	-1.121067	-2.773231	0.000000
H	1.238475	-7.520533	0.000000
H	-1.238475	-7.520533	0.000000
H	2.522080	-5.360701	0.000000
H	-2.522080	-5.360701	0.000000
N	0.000000	-1.967354	0.000000
C	6.566700	0.705601	0.000000
C	6.566700	-0.705601	0.000000
C	5.370369	1.430391	0.000000
C	5.370369	-1.430391	0.000000
C	4.173415	0.706092	0.000000
C	4.173415	-0.706092	0.000000
C	2.773231	1.121067	0.000000
C	2.773231	-1.121067	0.000000
H	7.520533	1.238475	0.000000
H	7.520533	-1.238475	0.000000
H	5.360701	2.522080	0.000000
H	5.360701	-2.522080	0.000000
N	1.967354	0.000000	0.000000
C	-6.566700	0.705601	0.000000
C	-6.566700	-0.705601	0.000000
C	-5.370369	1.430391	0.000000
C	-5.370369	-1.430391	0.000000
C	-4.173415	0.706092	0.000000
C	-4.173415	-0.706092	0.000000
C	-2.773231	1.121067	0.000000
C	-2.773231	-1.121067	0.000000
H	-7.520533	1.238475	0.000000
H	-7.520533	-1.238475	0.000000
H	-5.360701	2.522080	0.000000
H	-5.360701	-2.522080	0.000000
N	-1.967354	0.000000	0.000000
N	2.396643	2.396643	0.000000
N	-2.396643	2.396643	0.000000
N	-2.396643	-2.396643	0.000000
N	2.396643	-2.396643	0.000000

3.5.3 Atomic coordinates calculated using the PBEh functional (Gaussian 03)

Cu	0.000000	0.000000	0.000000
C	0.701514	6.519092	0.000000
C	-0.701514	6.519092	0.000000
C	1.421303	5.332503	0.000000
C	-1.421303	5.332503	0.000000
C	0.699840	4.143837	0.000000
C	-0.699840	4.143837	0.000000
C	1.109667	2.750100	0.000000
C	-1.109667	2.750100	0.000000
H	1.229924	7.466921	0.000000
H	-1.229924	7.466921	0.000000
H	2.505509	5.322691	0.000000
H	-2.505509	5.322691	0.000000
N	0.000000	1.954060	0.000000
C	0.701514	-6.519092	0.000000
C	-0.701514	-6.519092	0.000000
C	1.421303	-5.332503	0.000000
C	-1.421303	-5.332503	0.000000
C	0.699840	-4.143837	0.000000
C	-0.699840	-4.143837	0.000000
C	1.109667	-2.750100	0.000000
C	-1.109667	-2.750100	0.000000
H	1.229924	-7.466921	0.000000
H	-1.229924	-7.466921	0.000000
H	2.505509	-5.322691	0.000000
H	-2.505509	-5.322691	0.000000
N	0.000000	-1.954060	0.000000
C	6.519092	0.701514	0.000000
C	6.519092	-0.701514	0.000000
C	5.332503	1.421303	0.000000
C	5.332503	-1.421303	0.000000
C	4.143837	0.699840	0.000000
C	4.143837	-0.699840	0.000000
C	2.750100	1.109667	0.000000
C	2.750100	-1.109667	0.000000
H	7.466921	1.229924	0.000000
H	7.466921	-1.229924	0.000000
H	5.322691	2.505509	0.000000
H	5.322691	-2.505509	0.000000
N	1.954060	0.000000	0.000000
C	-6.519092	0.701514	0.000000
C	-6.519092	-0.701514	0.000000

C	-5.332503	1.421303	0.000000
C	-5.332503	-1.421303	0.000000
C	-4.143837	0.699840	0.000000
C	-4.143837	-0.699840	0.000000
C	-2.750100	1.109667	0.000000
C	-2.750100	-1.109667	0.000000
H	-7.466921	1.229924	0.000000
H	-7.466921	-1.229924	0.000000
H	-5.322691	2.505509	0.000000
H	-5.322691	-2.505509	0.000000
N	-1.954060	0.000000	0.000000
N	2.373851	2.373851	0.000000
N	-2.373851	2.373851	0.000000
N	-2.373851	-2.373851	0.000000
N	2.373851	-2.373851	0.000000

3.6 ZnPc in the gas phase

3.6.1 Atomic coordinates calculated using the PBE functional (Siesta)

Zn	0.000000	0.000000	0.000000
N	2.009693	0.000000	0.000000
N	0.000000	2.009693	0.000000
N	-2.009693	0.000000	0.000000
N	0.000000	-2.009693	0.000000
C	2.801167	-1.130354	0.000000
C	2.801167	1.130354	0.000000
C	4.208719	-0.710238	0.000000
C	4.208719	0.710238	0.000000
C	5.410937	-1.436939	0.000000
C	5.410937	1.436939	0.000000
C	6.612243	-0.707986	0.000000
C	6.612243	0.707986	0.000000
H	5.395936	-2.528933	0.000000
H	5.395936	2.528933	0.000000
H	7.566257	-1.240005	0.000000
H	7.566257	1.240005	0.000000
C	1.130354	2.801167	0.000000
C	-1.130354	2.801167	0.000000
C	0.710238	4.208719	0.000000
C	-0.710238	4.208719	0.000000
C	1.436939	5.410937	0.000000
C	-1.436939	5.410937	0.000000
C	0.707986	6.612243	0.000000

C	-0.707986	6.612243	0.000000
H	2.528933	5.395936	0.000000
H	-2.528933	5.395936	0.000000
H	1.240005	7.566257	0.000000
H	-1.240005	7.566257	0.000000
C	-2.801167	1.130354	0.000000
C	-2.801167	-1.130354	0.000000
C	-4.208719	0.710238	0.000000
C	-4.208719	-0.710238	0.000000
C	-5.410937	1.436939	0.000000
C	-5.410937	-1.436939	0.000000
C	-6.612243	0.707986	0.000000
C	-6.612243	-0.707986	0.000000
H	-5.395936	2.528933	0.000000
H	-5.395936	-2.528933	0.000000
H	-7.566257	1.240005	0.000000
H	-7.566257	-1.240005	0.000000
C	-1.130354	-2.801167	0.000000
C	1.130354	-2.801167	0.000000
C	-0.710238	-4.208719	0.000000
C	0.710238	-4.208719	0.000000
C	-1.436939	-5.410937	0.000000
C	1.436939	-5.410937	0.000000
C	-0.707986	-6.612243	0.000000
C	0.707986	-6.612243	0.000000
H	-2.528933	-5.395936	0.000000
H	2.528933	-5.395936	0.000000
H	-1.240005	-7.566257	0.000000
H	1.240005	-7.566257	0.000000
N	2.407493	2.407493	0.000000
N	-2.407493	2.407493	0.000000
N	-2.407493	-2.407493	0.000000
N	2.407493	-2.407493	0.000000

3.6.2 Atomic coordinates calculated using the PBE functional (Gaussian 03)

Zn	0.000000	0.000000	0.000000
C	0.705353	6.595435	0.000000
C	-0.705353	6.595435	0.000000
C	1.429518	5.398500	0.000000
C	-1.429518	5.398500	0.000000
C	0.708353	4.199782	0.000000
C	-0.708353	4.199782	0.000000
C	1.126727	2.797540	0.000000

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C	-1.126727	2.797540	0.000000
H	1.238483	7.549141	0.000000
H	-1.238483	7.549141	0.000000
H	2.521323	5.389543	0.000000
H	-2.521323	5.389543	0.000000
N	0.000000	2.002314	0.000000
C	0.705353	-6.595435	0.000000
C	-0.705353	-6.595435	0.000000
C	1.429518	-5.398500	0.000000
C	-1.429518	-5.398500	0.000000
C	0.708353	-4.199782	0.000000
C	-0.708353	-4.199782	0.000000
C	1.126727	-2.797540	0.000000
C	-1.126727	-2.797540	0.000000
H	1.238483	-7.549141	0.000000
H	-1.238483	-7.549141	0.000000
H	2.521323	-5.389543	0.000000
H	-2.521323	-5.389543	0.000000
N	0.000000	-2.002314	0.000000
C	6.595435	0.705353	0.000000
C	6.595435	-0.705353	0.000000
C	5.398500	1.429518	0.000000
C	5.398500	-1.429518	0.000000
C	4.199782	0.708353	0.000000
C	4.199782	-0.708353	0.000000
C	2.797540	1.126727	0.000000
C	2.797540	-1.126727	0.000000
H	7.549141	1.238483	0.000000
H	7.549141	-1.238483	0.000000
H	5.389543	2.521323	0.000000
H	5.389543	-2.521323	0.000000
N	2.002314	0.000000	0.000000
C	-6.595435	0.705353	0.000000
C	-6.595435	-0.705353	0.000000
C	-5.398500	1.429518	0.000000
C	-5.398500	-1.429518	0.000000
C	-4.199782	0.708353	0.000000
C	-4.199782	-0.708353	0.000000
C	-2.797540	1.126727	0.000000
C	-2.797540	-1.126727	0.000000
H	-7.549141	1.238483	0.000000
H	-7.549141	-1.238483	0.000000
H	-5.389543	2.521323	0.000000
H	-5.389543	-2.521323	0.000000

N	-2.002314	0.000000	0.000000
N	2.402806	2.402806	0.000000
N	-2.402806	2.402806	0.000000
N	-2.402806	-2.402806	0.000000
N	2.402806	-2.402806	0.000000

3.6.3 Atomic coordinates calculated using the PBEh functional (Gaussian 03)

Zn	0.000000	0.000000	0.000000
C	0.701143	6.546236	0.000000
C	-0.701143	6.546236	0.000000
C	1.420463	5.358979	0.000000
C	-1.420463	5.358979	0.000000
C	0.701910	4.168932	0.000000
C	-0.701910	4.168932	0.000000
C	1.115691	2.773148	0.000000
C	-1.115691	2.773148	0.000000
H	1.229930	7.493828	0.000000
H	-1.229930	7.493828	0.000000
H	2.504741	5.350015	0.000000
H	-2.504741	5.350015	0.000000
N	0.000000	1.988703	0.000000
C	0.701143	-6.546236	0.000000
C	-0.701143	-6.546236	0.000000
C	1.420463	-5.358979	0.000000
C	-1.420463	-5.358979	0.000000
C	0.701910	-4.168932	0.000000
C	-0.701910	-4.168932	0.000000
C	1.115691	-2.773148	0.000000
C	-1.115691	-2.773148	0.000000
H	1.229930	-7.493828	0.000000
H	-1.229930	-7.493828	0.000000
H	2.504741	-5.350015	0.000000
H	-2.504741	-5.350015	0.000000
N	0.000000	-1.988703	0.000000
C	6.546236	0.701143	0.000000
C	6.546236	-0.701143	0.000000
C	5.358979	1.420463	0.000000
C	5.358979	-1.420463	0.000000
C	4.168932	0.701910	0.000000
C	4.168932	-0.701910	0.000000
C	2.773148	1.115691	0.000000
C	2.773148	-1.115691	0.000000
H	7.493828	1.229930	0.000000

H	7.493828	-1.229930	0.000000
H	5.350015	2.504741	0.000000
H	5.350015	-2.504741	0.000000
N	1.988703	0.000000	0.000000
C	-6.546236	0.701143	0.000000
C	-6.546236	-0.701143	0.000000
C	-5.358979	1.420463	0.000000
C	-5.358979	-1.420463	0.000000
C	-4.168932	0.701910	0.000000
C	-4.168932	-0.701910	0.000000
C	-2.773148	1.115691	0.000000
C	-2.773148	-1.115691	0.000000
H	-7.493828	1.229930	0.000000
H	-7.493828	-1.229930	0.000000
H	-5.350015	2.504741	0.000000
H	-5.350015	-2.504741	0.000000
N	-1.988703	0.000000	0.000000
N	2.379863	2.379863	0.000000
N	-2.379863	2.379863	0.000000
N	-2.379863	-2.379863	0.000000
N	2.379863	-2.379863	0.000000

4. Atomic coordinates of the SWCNT-MPc-SWCNT molecular junctions

4.1 The SWCNT-MnPc-SWCNT molecular junctions

4.1.1 (3,3) armchair SWCNTs as the electrodes

C	-14.031593	0.724385	1.988705
C	-14.031593	-0.724385	1.988705
C	-14.031593	-2.084847	-0.367052
C	-14.031593	-1.360364	-1.621521
C	-14.031593	1.360364	-1.621521
C	-14.031593	2.084847	-0.367052
C	-12.792100	-1.360364	1.621521
C	-12.792100	-2.084847	0.367052
C	-12.792100	-0.724385	-1.988705
C	-12.792100	0.724385	-1.988705
C	-12.792100	2.084847	0.367052
C	-12.792100	1.360364	1.621521
C	-11.552607	0.724385	1.988705
C	-11.552607	-0.724385	1.988705
C	-11.552607	-2.084847	-0.367052
C	-11.552607	-1.360364	-1.621521

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C	-11.552607	1.360364	-1.621521
C	-11.552607	2.084847	-0.367052
C	-10.313114	-1.360364	1.621521
C	-10.313114	-2.084847	0.367052
C	-10.313114	-0.724385	-1.988705
C	-10.313114	0.724385	-1.988705
C	-10.313114	2.084847	0.367052
C	-10.313114	1.360364	1.621521
C	-9.075675	0.730606	1.988595
C	-9.075675	-0.730606	1.988595
C	-9.080125	-2.086780	-0.368802
C	-9.082599	-1.360479	-1.631757
C	-9.082599	1.360479	-1.631757
C	-9.080125	2.086779	-0.368802
C	-7.827593	-1.354454	1.591001
C	-7.829024	-2.055576	0.356828
C	-7.843566	-0.709098	-1.989645
C	-7.843566	0.709098	-1.989646
C	-7.829023	2.055576	0.356828
C	-7.827593	1.354454	1.591000
C	-6.609200	-2.138991	-0.476361
C	-6.617239	-1.446363	-1.654761
C	-6.617239	1.446364	-1.654761
C	-6.609200	2.138991	-0.476361
H	-5.699445	-2.625990	-0.124591
H	-5.713370	-1.351716	-2.261708
H	-5.713370	1.351716	-2.261708
H	-5.699445	2.625990	-0.124591
C	-2.775229	1.131260	2.268667
C	-2.775215	-1.131280	2.268666
C	-4.164917	0.711512	2.271230
C	-4.164907	-0.711556	2.271231
C	-5.366450	1.439490	2.194787
C	-5.366468	-1.439524	2.194788
C	-6.567033	0.722453	2.032582
C	-6.567031	-0.722452	2.032578
N	-1.960074	-0.000001	2.265993
H	-5.356699	2.532047	2.213285
H	-5.356700	-2.532047	2.213284
C	2.775213	-1.131304	2.268666
C	2.775219	1.131285	2.268667
C	4.164912	-0.711484	2.271231
C	4.164909	0.711506	2.271231
C	5.366468	-1.439523	2.194787

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C	5.366467	1.439521	2.194786
C	6.567031	-0.722451	2.032579
C	6.567034	0.722452	2.032582
N	1.960061	0.000043	2.265992
H	5.356700	-2.532047	2.213284
H	5.356700	2.532047	2.213284
C	1.130669	2.778848	2.190373
C	-1.130669	2.778850	2.190372
C	0.706943	4.180142	2.148558
C	-0.706946	4.180139	2.148559
C	1.436637	5.380317	2.145948
C	-1.436637	5.380330	2.145947
C	0.707761	6.582760	2.149289
C	-0.707759	6.582758	2.149290
N	0.000001	1.957689	2.209893
H	2.528550	5.362959	2.154480
H	-2.528551	5.363051	2.154480
H	-1.240558	7.536436	2.160707
H	1.240558	7.536436	2.160707
C	-1.130669	-2.778849	2.190373
C	1.130667	-2.778851	2.190373
C	-0.706946	-4.180142	2.148559
C	0.706975	-4.180156	2.148558
C	-1.436637	-5.380329	2.145947
C	1.436633	-5.380316	2.145948
C	-0.707757	-6.582758	2.149289
C	0.707790	-6.582746	2.149290
N	-0.000001	-1.957689	2.209892
H	-2.528552	-5.363051	2.154480
H	2.528594	-5.362958	2.154480
H	-1.240559	-7.536436	2.160707
H	1.240558	-7.536434	2.160707
N	2.398349	2.408947	2.222779
N	-2.398351	2.408945	2.222779
N	-2.398351	-2.408949	2.222779
N	2.398364	-2.408886	2.222780
Mn	0.000000	0.000000	2.238538
H	5.699445	-2.625990	-0.124591
H	5.713370	-1.351716	-2.261708
H	5.713370	1.351716	-2.261708
H	5.699445	2.625990	-0.124591
C	6.609200	-2.138990	-0.476361
C	6.617239	-1.446364	-1.654761
C	6.617239	1.446364	-1.654761

C	6.609200	2.138990	-0.476361
C	7.827593	-1.354454	1.591002
C	7.829024	-2.055576	0.356827
C	7.843566	-0.709098	-1.989646
C	7.843566	0.709098	-1.989646
C	7.829023	2.055576	0.356827
C	7.827593	1.354454	1.591000
C	9.075676	0.730607	1.988596
C	9.075675	-0.730606	1.988595
C	9.080125	-2.086779	-0.368802
C	9.082599	-1.360479	-1.631757
C	9.082599	1.360479	-1.631757
C	9.080125	2.086779	-0.368802
C	10.313114	-1.360364	1.621521
C	10.313114	-2.084847	0.367052
C	10.313114	-0.724385	-1.988705
C	10.313114	0.724385	-1.988705
C	10.313114	2.084847	0.367052
C	10.313114	1.360364	1.621521
C	11.552607	0.724385	1.988705
C	11.552607	-0.724385	1.988705
C	11.552607	-2.084847	-0.367052
C	11.552607	-1.360364	-1.621521
C	11.552607	1.360364	-1.621521
C	11.552607	2.084847	-0.367052
C	12.792100	-1.360364	1.621521
C	12.792100	-2.084847	0.367052
C	12.792100	-0.724385	-1.988705
C	12.792100	0.724385	-1.988705
C	12.792100	2.084847	0.367052
C	12.792100	1.360364	1.621521

4.1.2 (4,4) armchair SWCNTs as the electrodes

C	-14.010306	0.718840	2.687080
C	-14.010306	-0.718840	2.687080
C	-14.010306	-2.687080	0.718840
C	-14.010306	-2.687080	-0.718840
C	-14.010306	-0.718840	-2.687080
C	-14.010306	0.718840	-2.687080
C	-14.010306	2.687080	-0.718840
C	-14.010306	2.687080	0.718840
C	-12.769859	-1.391710	2.408430
C	-12.769859	-2.408430	1.391710

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C	-12.769859	-2.408430	-1.391710
C	-12.769859	-1.391710	-2.408430
C	-12.769859	1.391710	-2.408430
C	-12.769859	2.408430	-1.391710
C	-12.769859	2.408430	1.391710
C	-12.769859	1.391710	2.408430
C	-11.529412	0.718840	2.687080
C	-11.529412	-0.718840	2.687080
C	-11.529412	-2.687080	0.718840
C	-11.529412	-2.687080	-0.718840
C	-11.529412	-0.718840	-2.687080
C	-11.529412	0.718840	-2.687080
C	-11.529412	2.687080	-0.718840
C	-11.529412	2.687080	0.718840
C	-10.288965	-1.391710	2.408430
C	-10.288965	-2.408430	1.391710
C	-10.288965	-2.408430	-1.391710
C	-10.288965	-1.391710	-2.408430
C	-10.288965	1.391710	-2.408430
C	-10.288965	2.408430	-1.391710
C	-10.288965	2.408430	1.391710
C	-10.288965	1.391710	2.408430
C	-9.038263	0.729763	2.687723
C	-9.038263	-0.729763	2.687723
C	-9.042925	-2.679756	0.716952
C	-9.045678	-2.684586	-0.730948
C	-9.048667	-0.723878	-2.697473
C	-9.048667	0.723878	-2.697473
C	-9.045678	2.684586	-0.730948
C	-9.042925	2.679756	0.716952
C	-7.806596	-1.410159	2.425848
C	-7.801499	-2.421927	1.385687
C	-7.823167	-2.439325	-1.431412
C	-7.819042	-1.407805	-2.453483
C	-7.819042	1.407805	-2.453483
C	-7.823167	2.439326	-1.431412
C	-7.801499	2.421927	1.385687
C	-7.806596	1.410159	2.425848
C	-6.604366	-2.787912	0.650853
C	-6.616902	-2.788713	-0.731943
C	-6.609922	-0.692212	-2.781951
C	-6.609922	0.692212	-2.781951
C	-6.616902	2.788713	-0.731943
C	-6.604366	2.787912	0.650853

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H	-5.641505	-2.890999	1.147726
H	-5.671565	-2.884674	-1.271508
H	-5.656424	-1.220300	-2.852464
H	-5.656424	1.220300	-2.852464
H	-5.671565	2.884674	-1.271508
H	-5.641505	2.890999	1.147726
C	-2.766095	1.132160	2.945523
C	-2.766095	-1.132160	2.945523
C	-4.157872	0.710465	2.970876
C	-4.157872	-0.710465	2.970875
C	-5.354689	1.431208	2.975570
C	-5.354689	-1.431208	2.975570
C	-6.569114	0.725160	2.790456
C	-6.569114	-0.725160	2.790456
N	-1.947810	0.000000	2.920123
H	-5.342280	2.515212	3.102145
H	-5.342280	-2.515212	3.102145
C	2.766095	-1.132160	2.945523
C	2.766095	1.132160	2.945523
C	4.157872	-0.710465	2.970876
C	4.157872	0.710465	2.970875
C	5.354689	-1.431208	2.975570
C	5.354689	1.431208	2.975570
C	6.569114	-0.725160	2.790456
C	6.569114	0.725160	2.790456
N	1.947810	0.000000	2.920123
H	5.342280	-2.515213	3.102145
H	5.342280	2.515213	3.102145
C	1.129114	2.781828	2.882020
C	-1.129114	2.781828	2.882020
C	0.708383	4.178145	2.869488
C	-0.708383	4.178145	2.869489
C	1.437531	5.381045	2.875475
C	-1.437531	5.381045	2.875475
C	0.709143	6.580757	2.877880
C	-0.709143	6.580757	2.877880
N	0.000000	1.962833	2.882351
H	2.529566	5.364484	2.881385
H	-2.529566	5.364484	2.881385
H	-1.240596	7.535173	2.882303
H	1.240596	7.535173	2.882303
C	-1.129114	-2.781828	2.882020
C	1.129114	-2.781828	2.882020
C	-0.708383	-4.178145	2.869488

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C	0.708383	-4.178145	2.869489
C	-1.437531	-5.381045	2.875475
C	1.437531	-5.381045	2.875475
C	-0.709143	-6.580757	2.877880
C	0.709143	-6.580757	2.877880
N	0.000000	-1.962833	2.882351
H	-2.529566	-5.364484	2.881385
H	2.529566	-5.364484	2.881385
H	-1.240596	-7.535173	2.882303
H	1.240596	-7.535173	2.882303
N	2.400697	2.406293	2.911207
N	-2.400697	2.406293	2.911207
N	-2.400697	-2.406293	2.911207
N	2.400697	-2.406293	2.911208
Mn	0.000000	0.000000	2.885174
H	5.641505	-2.890999	1.147726
H	5.671565	-2.884674	-1.271508
H	5.656424	-1.220300	-2.852464
H	5.656424	1.220300	-2.852464
H	5.671565	2.884674	-1.271508
H	5.641505	2.890999	1.147726
C	6.604366	-2.787912	0.650853
C	6.616902	-2.788713	-0.731943
C	6.609922	-0.692212	-2.781951
C	6.609922	0.692212	-2.781951
C	6.616902	2.788713	-0.731943
C	6.604366	2.787912	0.650853
C	7.806596	-1.410159	2.425848
C	7.801499	-2.421927	1.385687
C	7.823167	-2.439326	-1.431412
C	7.819042	-1.407806	-2.453483
C	7.819042	1.407806	-2.453483
C	7.823167	2.439326	-1.431411
C	7.801499	2.421927	1.385687
C	7.806596	1.410160	2.425848
C	9.038263	0.729763	2.687723
C	9.038263	-0.729763	2.687723
C	9.042925	-2.679756	0.716951
C	9.045678	-2.684586	-0.730948
C	9.048667	-0.723878	-2.697473
C	9.048668	0.723878	-2.697473
C	9.045678	2.684586	-0.730948
C	9.042925	2.679756	0.716951
C	10.288965	-1.391710	2.408430

C	10.288965	-2.408430	1.391710
C	10.288965	-2.408430	-1.391710
C	10.288965	-1.391710	-2.408430
C	10.288965	1.391710	-2.408430
C	10.288965	2.408430	-1.391710
C	10.288965	2.408430	1.391710
C	10.288965	1.391710	2.408430
C	11.529412	0.718840	2.687080
C	11.529412	-0.718840	2.687080
C	11.529412	-2.687080	0.718840
C	11.529412	-2.687080	-0.718840
C	11.529412	-0.718840	-2.687080
C	11.529412	0.718840	-2.687080
C	11.529412	2.687080	-0.718840
C	11.529412	2.687080	0.718840
C	12.769859	-1.391710	2.408430
C	12.769859	-2.408430	1.391710
C	12.769859	-2.408430	-1.391710
C	12.769859	-1.391710	-2.408430
C	12.769859	1.391710	-2.408430
C	12.769859	2.408430	-1.391710
C	12.769859	2.408430	1.391710
C	12.769859	1.391710	2.408430

4.1.3 (5,5) armchair SWCNTs as the electrodes

C	-14.0134040	-0.7175070	3.3821310
C	-14.0134040	0.7175070	3.3821310
C	-14.0134040	2.9946940	1.7275320
C	-14.0134040	3.4382620	0.3626190
C	-14.0134040	2.5683390	-2.3143250
C	-14.0134040	1.4072080	-3.1578740
C	-14.0134040	-1.4072080	-3.1578740
C	-14.0134040	-2.5683390	-2.3143250
C	-14.0134040	-3.4382620	0.3626180
C	-14.0134040	-2.9946940	1.7275320
C	-12.7731580	-0.7175070	-3.3821310
C	-12.7731580	0.7175070	-3.3821310
C	-12.7731580	2.9946950	-1.7275320
C	-12.7731580	3.4382630	-0.3626190
C	-12.7731580	2.5683390	2.3143250
C	-12.7731580	1.4072070	3.1578740
C	-12.7731580	-1.4072080	3.1578730
C	-12.7731580	-2.5683390	2.3143250

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C	-12.7731580	-3.4382620	-0.3626180
C	-12.7731580	-2.9946950	-1.7275320
C	-11.5329120	-0.7175070	3.3821310
C	-11.5329120	0.7175070	3.3821310
C	-11.5329120	2.9946940	1.7275320
C	-11.5329120	3.4382620	0.3626190
C	-11.5329120	2.5683390	-2.3143250
C	-11.5329120	1.4072080	-3.1578740
C	-11.5329120	-1.4072080	-3.1578740
C	-11.5329120	-2.5683390	-2.3143250
C	-11.5329120	-3.4382620	0.3626180
C	-11.5329120	-2.9946940	1.7275320
C	-10.2926660	-0.7175070	-3.3821310
C	-10.2926660	0.7175070	-3.3821310
C	-10.2926660	2.9946950	-1.7275320
C	-10.2926660	3.4382630	-0.3626190
C	-10.2926660	2.5683390	2.3143250
C	-10.2926660	1.4072070	3.1578740
C	-10.2926660	-1.4072080	3.1578730
C	-10.2926660	-2.5683390	2.3143250
C	-10.2926660	-3.4382620	-0.3626180
C	-10.2926660	-2.9946950	-1.7275320
C	-9.0450000	-0.7212000	3.3767000
C	-9.0450000	0.7212000	3.3767000
C	-9.0450000	2.9885000	1.7295000
C	-9.0450000	3.4344000	0.3575000
C	-9.0450000	2.5683000	-2.3080000
C	-9.0451000	1.4013000	-3.1559000
C	-9.0451000	-1.4013000	-3.1559000
C	-9.0450000	-2.5683000	-2.3080000
C	-9.0450000	-3.4344000	0.3575000
C	-9.0450000	-2.9885000	1.7295000
C	-7.8109000	-0.7247000	-3.4142000
C	-7.8109000	0.7247000	-3.4142000
C	-7.8106000	3.0230000	-1.7441000
C	-7.8108000	3.4709000	-0.3656000
C	-7.8108000	2.5930000	2.3363000
C	-7.8109000	1.4205000	3.1883000
C	-7.8109000	-1.4205000	3.1883000
C	-7.8108000	-2.5930000	2.3363000
C	-7.8108000	-3.4709000	-0.3656000
C	-7.8106000	-3.0230000	-1.7441000
C	-6.6025000	3.0831000	1.7299000
C	-6.6025000	3.5109000	0.4129000

C	-6.6026000	2.5974000	-2.3978000
C	-6.6025000	1.4777000	-3.2116000
C	-6.6025000	-1.4777000	-3.2116000
C	-6.6026000	-2.5974000	-2.3978000
C	-6.6025000	-3.5109000	0.4129000
C	-6.6025000	-3.0831000	1.7299000
H	-5.6474000	2.9752000	2.2476000
H	-5.6474000	3.7279000	-0.0695000
H	-5.6474000	3.0566000	-2.1349000
H	-5.6474000	1.0857000	-3.5671000
H	-5.6474000	-1.0857000	-3.5671000
H	-5.6474000	-3.0566000	-2.1349000
H	-5.6474000	-3.7279000	-0.0695000
H	-5.6474000	-2.9752000	2.2476000
C	-2.7796000	1.1336000	3.4880000
C	-2.7796000	-1.1336000	3.4880000
C	-4.1805000	0.7168000	3.4880000
C	-4.1805000	-0.7168000	3.4880000
C	-5.3584000	1.4455000	3.4880000
C	-5.3584000	-1.4455000	3.4880000
C	-6.6028000	0.7320000	3.4880000
C	-6.6028000	-0.7320000	3.4880000
N	-1.9605000	0.0000000	3.4880000
H	-5.3372000	2.5382000	3.4880000
H	-5.3372000	-2.5382000	3.4880000
C	2.7796000	-1.1336000	3.4880000
C	2.7796000	1.1336000	3.4880000
C	4.1805000	-0.7168000	3.4880000
C	4.1805000	0.7168000	3.4880000
C	5.3584000	-1.4455000	3.4880000
C	5.3584000	1.4455000	3.4880000
C	6.6028000	-0.7320000	3.4880000
C	6.6028000	0.7320000	3.4880000
N	1.9605000	0.0000000	3.4880000
H	5.3372000	-2.5382000	3.4880000
H	5.3372000	2.5382000	3.4880000
C	1.1311000	2.7777000	3.4880000
C	-1.1311000	2.7777000	3.4880000
C	0.7099000	4.1683000	3.4880000
C	-0.7099000	4.1683000	3.4880000
C	1.4394000	5.3742000	3.4880000
C	-1.4394000	5.3742000	3.4880000
C	0.7104000	6.5707000	3.4880000
C	-0.7104000	6.5707000	3.4880000

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N	0.0000000	1.9630000	3.4880000
H	2.5314000	5.3613000	3.4880000
H	-2.5314000	5.3613000	3.4880000
H	1.2406000	7.5259000	3.4880000
H	-1.2406000	7.5259000	3.4880000
C	-1.1311000	-2.7777000	3.4880000
C	1.1311000	-2.7777000	3.4880000
C	-0.7099000	-4.1683000	3.4880000
C	0.7099000	-4.1683000	3.4880000
C	-1.4394000	-5.3742000	3.4880000
C	1.4394000	-5.3742000	3.4880000
C	-0.7104000	-6.5707000	3.4880000
C	0.7104000	-6.5707000	3.4880000
N	0.0000000	-1.9630000	3.4880000
H	-2.5314000	-5.3613000	3.4880000
H	2.5314000	-5.3613000	3.4880000
H	-1.2406000	-7.5259000	3.4880000
H	1.2406000	-7.5259000	3.4880000
N	2.4068000	2.4015000	3.4880000
N	-2.4068000	2.4015000	3.4880000
N	-2.4068000	-2.4015000	3.4880000
N	2.4068000	-2.4015000	3.4880000
Mn	0.0000000	0.0000000	3.4880000
H	5.6474000	2.9752000	2.2476000
H	5.6474000	3.7279000	-0.0695000
H	5.6474000	3.0566000	-2.1349000
H	5.6474000	1.0857000	-3.5671000
H	5.6474000	-1.0857000	-3.5671000
H	5.6474000	-3.0566000	-2.1349000
H	5.6474000	-3.7279000	-0.0695000
H	5.6474000	-2.9752000	2.2476000
C	6.6025000	3.0831000	1.7299000
C	6.6025000	3.5109000	0.4129000
C	6.6026000	2.5974000	-2.3978000
C	6.6025000	1.4777000	-3.2116000
C	6.6025000	-1.4777000	-3.2116000
C	6.6026000	-2.5974000	-2.3978000
C	6.6025000	-3.5109000	0.4129000
C	6.6025000	-3.0831000	1.7299000
C	7.8109000	-0.7247000	-3.4142000
C	7.8109000	0.7247000	-3.4142000
C	7.8106000	3.0230000	-1.7441000
C	7.8108000	3.4709000	-0.3656000
C	7.8108000	2.5930000	2.3363000

C	7.8109000	1.4205000	3.1883000
C	7.8109000	-1.4205000	3.1883000
C	7.8108000	-2.5930000	2.3363000
C	7.8108000	-3.4709000	-0.3656000
C	7.8106000	-3.0230000	-1.7441000
C	9.0450000	-0.7212000	3.3767000
C	9.0450000	0.7212000	3.3767000
C	9.0450000	2.9885000	1.7295000
C	9.0450000	3.4344000	0.3575000
C	9.0450000	2.5683000	-2.3080000
C	9.0451000	1.4013000	-3.1559000
C	9.0451000	-1.4013000	-3.1559000
C	9.0450000	-2.5683000	-2.3080000
C	9.0450000	-3.4344000	0.3575000
C	9.0450000	-2.9885000	1.7295000
C	10.2926660	-0.7175070	-3.3821310
C	10.2926660	0.7175070	-3.3821310
C	10.2926660	2.9946950	-1.7275320
C	10.2926660	3.4382630	-0.3626190
C	10.2926660	2.5683390	2.3143250
C	10.2926660	1.4072070	3.1578740
C	10.2926660	-1.4072080	3.1578730
C	10.2926660	-2.5683390	2.3143250
C	10.2926660	-3.4382620	-0.3626180
C	10.2926660	-2.9946950	-1.7275320
C	11.5329120	-0.7175070	3.3821310
C	11.5329120	0.7175070	3.3821310
C	11.5329120	2.9946940	1.7275320
C	11.5329120	3.4382620	0.3626190
C	11.5329120	2.5683390	-2.3143250
C	11.5329120	1.4072080	-3.1578740
C	11.5329120	-1.4072080	-3.1578740
C	11.5329120	-2.5683390	-2.3143250
C	11.5329120	-3.4382620	0.3626180
C	11.5329120	-2.9946940	1.7275320
C	12.7731580	-0.7175070	-3.3821310
C	12.7731580	0.7175070	-3.3821310
C	12.7731580	2.9946950	-1.7275320
C	12.7731580	3.4382630	-0.3626190
C	12.7731580	2.5683390	2.3143250
C	12.7731580	1.4072070	3.1578740
C	12.7731580	-1.4072080	3.1578730
C	12.7731580	-2.5683390	2.3143250
C	12.7731580	-3.4382620	-0.3626180

C	12.7731580	-2.9946950	-1.7275320

4.1.4 (4,4) armchair SWCNTs as the electrodes and one CO molecule adsorbed at the Mn atom

C	-14.010306	0.718840	2.687080
C	-14.010306	-0.718840	2.687080
C	-14.010306	-2.687080	0.718840
C	-14.010306	-2.687080	-0.718840
C	-14.010306	-0.718840	-2.687080
C	-14.010306	0.718840	-2.687080
C	-14.010306	2.687080	-0.718840
C	-14.010306	2.687080	0.718840
C	-12.769859	-1.391710	2.408430
C	-12.769859	-2.408430	1.391710
C	-12.769859	-2.408430	-1.391710
C	-12.769859	-1.391710	-2.408430
C	-12.769859	1.391710	-2.408430
C	-12.769859	2.408430	-1.391710
C	-12.769859	2.408430	1.391710
C	-12.769859	1.391710	2.408430
C	-11.529412	0.718840	2.687080
C	-11.529412	-0.718840	2.687080
C	-11.529412	-2.687080	0.718840
C	-11.529412	-2.687080	-0.718840
C	-11.529412	-0.718840	-2.687080
C	-11.529412	0.718840	-2.687080
C	-11.529412	2.687080	-0.718840
C	-11.529412	2.687080	0.718840
C	-10.288965	-1.391710	2.408430
C	-10.288965	-2.408430	1.391710
C	-10.288965	-2.408430	-1.391710
C	-10.288965	-1.391710	-2.408430
C	-10.288965	1.391710	-2.408430
C	-10.288965	2.408430	-1.391710
C	-10.288965	2.408430	1.391710
C	-10.288965	1.391710	2.408430
C	-9.043756	0.731310	2.717548
C	-9.043713	-0.731309	2.717554
C	-9.036518	-2.662772	0.725206
C	-9.039559	-2.673237	-0.723354
C	-9.047003	-0.724287	-2.697723
C	-9.047004	0.724290	-2.697723
C	-9.039561	2.673249	-0.723361

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C	-9.036534	2.662796	0.725194
C	-7.809986	-1.405504	2.473310
C	-7.801074	-2.391880	1.406290
C	-7.814508	-2.427490	-1.417929
C	-7.816808	-1.407062	-2.457595
C	-7.816805	1.407074	-2.457613
C	-7.814514	2.427479	-1.417929
C	-7.801102	2.391913	1.406286
C	-7.810053	1.405552	2.473302
C	-6.593682	-2.708340	0.678766
C	-6.603102	-2.730074	-0.705617
C	-6.612722	-0.692768	-2.799155
C	-6.612719	0.692768	-2.799159
C	-6.603093	2.730058	-0.705610
C	-6.593690	2.708312	0.678761
H	-5.629045	-2.728046	1.184869
H	-5.648232	-2.784272	-1.233337
H	-5.659860	-1.219767	-2.883848
H	-5.659852	1.219757	-2.883851
H	-5.648229	2.784253	-1.233336
H	-5.629052	2.727978	1.184869
C	-2.782420	1.126279	3.399454
C	-2.782260	-1.125597	3.398647
C	-4.185055	0.710114	3.314181
C	-4.184945	-0.709595	3.314065
C	-5.377954	1.430764	3.170456
C	-5.377757	-1.430426	3.170264
C	-6.578632	0.726051	2.894511
C	-6.578552	-0.725908	2.894464
N	-1.967012	0.000417	3.445603
H	-5.373279	2.519386	3.262121
H	-5.372853	-2.519029	3.261969
C	2.782590	-1.125604	3.403376
C	2.782696	1.126261	3.404197
C	4.184972	-0.709562	3.315112
C	4.185086	0.710090	3.315232
C	5.377606	-1.430409	3.169909
C	5.377798	1.430767	3.170105
C	6.578343	-0.725881	2.893931
C	6.578407	0.726058	2.893987
N	1.967269	0.000409	3.455474
H	5.372806	-2.518975	3.261934
H	5.373181	2.519358	3.262119
C	1.125786	2.760497	3.300199

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C	-1.125309	2.760483	3.299603
C	0.707324	4.150285	3.120579
C	-0.706872	4.150275	3.120486
C	1.437476	5.336883	2.939297
C	-1.437222	5.336776	2.939157
C	0.708159	6.523810	2.758895
C	-0.708006	6.523771	2.758892
N	0.000278	1.946343	3.392885
H	2.529330	5.321489	2.939142
H	-2.529052	5.321280	2.939024
H	-1.240342	7.466713	2.615454
H	1.240432	7.466774	2.615348
C	-1.125311	-2.759853	3.293770
C	1.125820	-2.759849	3.294329
C	-0.706875	-4.150272	3.119235
C	0.707350	-4.150278	3.119317
C	-1.437165	-5.337039	2.939727
C	1.437494	-5.337153	2.939856
C	-0.707944	-6.524118	2.759721
C	0.708178	-6.524175	2.759721
N	0.000342	-1.945412	3.381322
H	-2.529002	-5.321505	2.939143
H	2.529333	-5.321652	2.939263
H	-1.240299	-7.466966	2.615608
H	1.240463	-7.467030	2.615503
N	2.401442	2.395433	3.332248
N	-2.400958	2.395551	3.330705
N	-2.400841	-2.394812	3.328630
N	2.401404	-2.394702	3.330124
Mn	0.000000	0.000000	3.642260
C	-0.026562	-0.027539	5.394187
O	-0.055781	-0.057044	6.572496
H	5.629054	-2.728114	1.184842
H	5.648239	-2.784276	-1.233373
H	5.659865	-1.219766	-2.883893
H	5.659862	1.219771	-2.883888
H	5.648240	2.784273	-1.233370
H	5.629065	2.728093	1.184847
C	6.593688	-2.708396	0.678730
C	6.603099	-2.730093	-0.705641
C	6.612722	-0.692751	-2.799187
C	6.612727	0.692768	-2.799177
C	6.603098	2.730094	-0.705634
C	6.593701	2.708393	0.678732

C	7.809938	-1.405482	2.473177
C	7.801081	-2.391921	1.406248
C	7.814513	-2.427499	-1.417946
C	7.816809	-1.407070	-2.457610
C	7.816809	1.407081	-2.457619
C	7.814517	2.427497	-1.417941
C	7.801115	2.391975	1.406250
C	7.810014	1.405554	2.473176
C	9.043701	0.731329	2.717543
C	9.043673	-0.731323	2.717542
C	9.036529	-2.662808	0.725190
C	9.039565	-2.673253	-0.723366
C	9.047006	-0.724289	-2.697735
C	9.047005	0.724291	-2.697733
C	9.039574	2.673266	-0.723374
C	9.036543	2.662836	0.725177
C	10.288965	-1.391710	2.408430
C	10.288965	-2.408430	1.391710
C	10.288965	-2.408430	-1.391710
C	10.288965	-1.391710	-2.408430
C	10.288965	1.391710	-2.408430
C	10.288965	2.408430	-1.391710
C	10.288965	2.408430	1.391710
C	10.288965	1.391710	2.408430
C	11.529412	0.718840	2.687080
C	11.529412	-0.718840	2.687080
C	11.529412	-2.687080	0.718840
C	11.529412	-2.687080	-0.718840
C	11.529412	-0.718840	-2.687080
C	11.529412	0.718840	-2.687080
C	11.529412	2.687080	-0.718840
C	11.529412	2.687080	0.718840
C	12.769859	-1.391710	2.408430
C	12.769859	-2.408430	1.391710
C	12.769859	-2.408430	-1.391710
C	12.769859	-1.391710	-2.408430
C	12.769859	1.391710	-2.408430
C	12.769859	2.408430	-1.391710
C	12.769859	2.408430	1.391710
C	12.769859	1.391710	2.408430

4.2 The SWCNT-FePc-SWCNT molecular junctions

4.2.1 (3,3) armchair SWCNTs as the electrodes

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C	-14.015214	0.724385	1.988705
C	-14.015214	-0.724385	1.988705
C	-14.015214	-2.084847	-0.367052
C	-14.015214	-1.360364	-1.621521
C	-14.015214	1.360364	-1.621521
C	-14.015214	2.084847	-0.367052
C	-12.775721	-1.360364	1.621521
C	-12.775721	-2.084847	0.367052
C	-12.775721	-0.724385	-1.988705
C	-12.775721	0.724385	-1.988705
C	-12.775721	2.084847	0.367052
C	-12.775721	1.360364	1.621521
C	-11.536228	0.724385	1.988705
C	-11.536228	-0.724385	1.988705
C	-11.536228	-2.084847	-0.367052
C	-11.536228	-1.360364	-1.621521
C	-11.536228	1.360364	-1.621521
C	-11.536228	2.084847	-0.367052
C	-10.296735	-1.360364	1.621521
C	-10.296735	-2.084847	0.367052
C	-10.296735	-0.724385	-1.988705
C	-10.296735	0.724385	-1.988705
C	-10.296735	2.084847	0.367052
C	-10.296735	1.360364	1.621521
C	-9.060068	0.730462	1.991514
C	-9.060075	-0.730464	1.991513
C	-9.062382	-2.084936	-0.368316
C	-9.065578	-1.362133	-1.634452
C	-9.065577	1.362136	-1.634460
C	-9.062379	2.084931	-0.368318
C	-7.812354	-1.354672	1.596505
C	-7.812556	-2.050135	0.357980
C	-7.830583	-0.710630	-1.998051
C	-7.830581	0.710628	-1.998048
C	-7.812553	2.050146	0.357986
C	-7.812344	1.354665	1.596497
C	-6.589417	-2.116433	-0.468112
C	-6.598674	-1.428956	-1.649769
C	-6.598677	1.428962	-1.649779
C	-6.589418	2.116441	-0.468116
H	-5.663319	-2.551850	-0.091707
H	-5.682395	-1.297592	-2.230610
H	-5.682394	1.297597	-2.230610

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H	-5.663317	2.551846	-0.091706
C	-6.551344	0.721956	2.034857
C	-6.551329	-0.721975	2.034876
C	-5.349757	1.439299	2.197776
C	-5.349804	-1.439337	2.197795
C	-4.149896	0.710441	2.255671
C	-4.149885	-0.710464	2.255680
C	-2.755738	1.125418	2.238024
C	-2.755749	-1.125426	2.238027
H	-5.339565	2.531470	2.234281
H	-5.339607	-2.531493	2.234305
N	-1.934770	-0.000013	2.220781
C	6.551329	0.721974	2.034877
C	6.551344	-0.721955	2.034857
C	5.349804	1.439337	2.197796
C	5.349758	-1.439299	2.197777
C	4.149886	0.710464	2.255681
C	4.149892	-0.710438	2.255671
C	2.755748	1.125426	2.238028
C	2.755737	-1.125419	2.238023
H	5.339607	2.531492	2.234306
H	5.339566	-2.531469	2.234282
N	1.934772	0.000014	2.220780
C	0.707904	6.571750	2.168558
C	-0.707899	6.571752	2.168558
C	1.436976	5.369588	2.165308
C	-1.436972	5.369593	2.165308
C	0.706353	4.170915	2.157342
C	-0.706355	4.170911	2.157341
C	1.120317	2.766298	2.171593
C	-1.120329	2.766295	2.171591
H	1.240055	7.525729	2.173969
H	-1.240042	7.525728	2.173967
H	2.529442	5.352351	2.172569
H	-2.529442	5.352364	2.172567
N	0.000001	1.941999	2.172910
C	0.707898	-6.571753	2.168557
C	-0.707905	-6.571750	2.168559
C	1.436973	-5.369593	2.165306
C	-1.436976	-5.369588	2.165309
C	0.706356	-4.170912	2.157339
C	-0.706353	-4.170915	2.157341
C	1.120330	-2.766295	2.171589
C	-1.120317	-2.766298	2.171594

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H	1.240041	-7.525729	2.173967
H	-1.240056	-7.525728	2.173969
H	2.529441	-5.352365	2.172566
H	-2.529442	-5.352350	2.172570
N	-0.000001	-1.941999	2.172910
N	2.393959	2.403703	2.202176
N	2.393962	-2.403682	2.202172
N	-2.393958	-2.403703	2.202176
N	-2.393961	2.403681	2.202174
Fe	0.000000	0.000000	2.183864
H	5.663319	-2.551838	-0.091712
H	5.682398	-1.297592	-2.230620
H	5.682397	1.297593	-2.230610
H	5.663320	2.551849	-0.091709
C	6.589421	-2.116441	-0.468117
C	6.598682	-1.428956	-1.649784
C	6.598677	1.428954	-1.649770
C	6.589417	2.116433	-0.468110
C	7.812345	-1.354664	1.596498
C	7.812553	-2.050144	0.357986
C	7.830581	-0.710629	-1.998048
C	7.830583	0.710631	-1.998053
C	7.812557	2.050135	0.357979
C	7.812354	1.354671	1.596506
C	9.060075	0.730464	1.991514
C	9.060067	-0.730462	1.991515
C	9.062382	-2.084931	-0.368317
C	9.065579	-1.362136	-1.634459
C	9.065580	1.362134	-1.634452
C	9.062381	2.084937	-0.368316
C	10.296735	-1.360364	1.621521
C	10.296735	-2.084847	0.367052
C	10.296735	-0.724385	-1.988705
C	10.296735	0.724385	-1.988705
C	10.296735	2.084847	0.367052
C	10.296735	1.360364	1.621521
C	11.536228	0.724385	1.988705
C	11.536228	-0.724385	1.988705
C	11.536228	-2.084847	-0.367052
C	11.536228	-1.360364	-1.621521
C	11.536228	1.360364	-1.621521
C	11.536228	2.084847	-0.367052
C	12.775721	-1.360364	1.621521
C	12.775721	-2.084847	0.367052

C	12.775721	-0.724385	-1.988705
C	12.775721	0.724385	-1.988705
C	12.775721	2.084847	0.367052
C	12.775721	1.360364	1.621521

4.2.2 (4,4) armchair SWCNTs as the electrodes

C	-13.997506	0.718840	2.687080
C	-13.997506	-0.718840	2.687080
C	-13.997506	-2.687080	0.718840
C	-13.997506	-2.687080	-0.718840
C	-13.997506	-0.718840	-2.687080
C	-13.997506	0.718840	-2.687080
C	-13.997506	2.687080	-0.718840
C	-13.997506	2.687080	0.718840
C	-12.757059	-1.391710	2.408430
C	-12.757059	-2.408430	1.391710
C	-12.757059	-2.408430	-1.391710
C	-12.757059	-1.391710	-2.408430
C	-12.757059	1.391710	-2.408430
C	-12.757059	2.408430	-1.391710
C	-12.757059	2.408430	1.391710
C	-12.757059	1.391710	2.408430
C	-11.516612	0.718840	2.687080
C	-11.516612	-0.718840	2.687080
C	-11.516612	-2.687080	0.718840
C	-11.516612	-2.687080	-0.718840
C	-11.516612	-0.718840	-2.687080
C	-11.516612	0.718840	-2.687080
C	-11.516612	2.687080	-0.718840
C	-11.516612	2.687080	0.718840
C	-10.276165	-1.391710	2.408430
C	-10.276165	-2.408430	1.391710
C	-10.276165	-2.408430	-1.391710
C	-10.276165	-1.391710	-2.408430
C	-10.276165	1.391710	-2.408430
C	-10.276165	2.408430	-1.391710
C	-10.276165	2.408430	1.391710
C	-10.276165	1.391710	2.408430
C	-9.028319	0.730369	2.698834
C	-9.028332	-0.730336	2.698820
C	-9.028202	-2.673763	0.720081
C	-9.031437	-2.679034	-0.728174
C	-9.034546	-0.723938	-2.695821

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C	-9.034536	0.723937	-2.695823
C	-9.031411	2.679017	-0.728151
C	-9.028194	2.673756	0.720072
C	-7.794056	-1.406606	2.440385
C	-7.788632	-2.411136	1.393693
C	-7.807038	-2.436186	-1.426736
C	-7.803951	-1.407652	-2.452783
C	-7.803961	1.407666	-2.452774
C	-7.807030	2.436188	-1.426729
C	-7.788581	2.411142	1.393709
C	-7.794076	1.406643	2.440384
C	-6.588563	-2.764961	0.662017
C	-6.600433	-2.776679	-0.721048
C	-6.596492	-0.692176	-2.786355
C	-6.596487	0.692172	-2.786358
C	-6.600425	2.776695	-0.721037
C	-6.588523	2.764966	0.661984
H	-5.625745	2.842109	1.163360
H	-5.650828	2.871091	-1.252396
H	-5.644984	1.221454	-2.865215
H	-5.644989	-1.221447	-2.865211
H	-5.650851	-2.871067	-1.252408
H	-5.625810	-2.842088	1.163353
C	-6.556862	0.725885	2.825488
C	-6.556818	-0.725871	2.825487
C	-5.344698	1.432200	3.032745
C	-5.344761	-1.432262	3.032739
C	-4.148315	0.709711	3.060828
C	-4.148254	-0.709671	3.060825
C	-2.751457	1.124070	3.033397
C	-2.751469	-1.124122	3.033404
H	-5.329615	2.518304	3.147752
H	-5.329690	-2.518296	3.147758
N	-1.929686	-0.000005	3.010789
C	6.556965	0.725785	2.825518
C	6.556953	-0.725860	2.825558
C	5.344770	1.432227	3.032752
C	5.344714	-1.432260	3.032699
C	4.148322	0.709592	3.060782
C	4.148233	-0.709699	3.060779
C	2.751458	1.124166	3.033410
C	2.751533	-1.124132	3.033400
H	5.329726	2.518216	3.147769
H	5.329518	-2.518475	3.147721

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N	1.929601	-0.000275	3.010820
C	0.708929	6.560607	2.860884
C	-0.708836	6.560650	2.860884
C	1.437960	5.361091	2.860676
C	-1.437814	5.361128	2.860688
C	0.707547	4.160208	2.865481
C	-0.707301	4.160245	2.865463
C	1.121251	2.761449	2.913217
C	-1.121203	2.761436	2.913202
H	1.240291	7.515243	2.867218
H	-1.240121	7.515192	2.867220
H	2.530142	5.343207	2.866982
H	-2.530048	5.343234	2.867012
N	0.000031	1.937203	2.928943
C	0.708820	-6.560663	2.860891
C	-0.708921	-6.560688	2.860892
C	1.437879	-5.361174	2.860680
C	-1.437945	-5.361139	2.860679
C	0.707444	-4.160194	2.865467
C	-0.707445	-4.160311	2.865467
C	1.121282	-2.761465	2.913213
C	-1.121219	-2.761469	2.913191
H	1.240177	-7.515253	2.867226
H	-1.240237	-7.515219	2.867210
H	2.530058	-5.343310	2.866986
H	-2.530182	-5.343254	2.866996
N	-0.000020	-1.937241	2.928929
N	2.395917	2.400255	2.969090
N	2.395851	-2.400171	2.969101
N	-2.395876	-2.400184	2.969109
N	-2.395863	2.400138	2.969093
Fe	0.000000	0.000000	2.962070
H	5.625815	2.842014	1.163391
H	5.651002	2.871107	-1.252300
H	5.644924	1.221469	-2.865228
H	5.644813	-1.221559	-2.865237
H	5.650989	-2.871153	-1.252386
H	5.625815	-2.842130	1.163322
C	6.588615	-2.764964	0.661951
C	6.600400	-2.776766	-0.721028
C	6.596514	-0.692259	-2.786287
C	6.596443	0.692357	-2.786272
C	6.600356	2.776736	-0.720945
C	6.588609	2.764915	0.661996

C	7.794125	-1.406760	2.440450
C	7.788720	-2.411116	1.393633
C	7.806922	-2.436211	-1.426701
C	7.803981	-1.407712	-2.452765
C	7.803903	1.407718	-2.452625
C	7.806837	2.436129	-1.426640
C	7.788632	2.411056	1.393744
C	7.794099	1.406578	2.440459
C	9.028227	0.730353	2.698892
C	9.028325	-0.730360	2.698833
C	9.028184	-2.673684	0.720175
C	9.031317	-2.679057	-0.728134
C	9.034651	-0.723944	-2.695838
C	9.034513	0.723944	-2.695804
C	9.031168	2.679056	-0.728163
C	9.028132	2.673736	0.720192
C	10.276165	-1.391710	2.408430
C	10.276165	-2.408430	1.391710
C	10.276165	-2.408430	-1.391710
C	10.276165	-1.391710	-2.408430
C	10.276165	1.391710	-2.408430
C	10.276165	2.408430	-1.391710
C	10.276165	2.408430	1.391710
C	10.276165	1.391710	2.408430
C	11.516612	0.718840	2.687080
C	11.516612	-0.718840	2.687080
C	11.516612	-2.687080	0.718840
C	11.516612	-2.687080	-0.718840
C	11.516612	-0.718840	-2.687080
C	11.516612	0.718840	-2.687080
C	11.516612	2.687080	-0.718840
C	11.516612	2.687080	0.718840
C	12.757059	-1.391710	2.408430
C	12.757059	-2.408430	1.391710
C	12.757059	-2.408430	-1.391710
C	12.757059	-1.391710	-2.408430
C	12.757059	1.391710	-2.408430
C	12.757059	2.408430	-1.391710
C	12.757059	2.408430	1.391710
C	12.757059	1.391710	2.408430

4.2.3 (4,4) armchair SWCNTs as the electrodes and one CO molecule adsorbed at the Fe atom

C	-13.9975060	0.7188400	2.6870800
C	-13.9975060	-0.7188400	2.6870800
C	-13.9975060	-2.6870800	0.7188400
C	-13.9975060	-2.6870800	-0.7188400
C	-13.9975060	-0.7188400	-2.6870800
C	-13.9975060	0.7188400	-2.6870800
C	-13.9975060	2.6870800	-0.7188400
C	-13.9975060	2.6870800	0.7188400
C	-12.7570590	-1.3917100	2.4084300
C	-12.7570590	-2.4084300	1.3917100
C	-12.7570590	-2.4084300	-1.3917100
C	-12.7570590	-1.3917100	-2.4084300
C	-12.7570590	1.3917100	-2.4084300
C	-12.7570590	2.4084300	-1.3917100
C	-12.7570590	2.4084300	1.3917100
C	-12.7570590	1.3917100	2.4084300
C	-11.5166120	0.7188400	2.6870800
C	-11.5166120	-0.7188400	2.6870800
C	-11.5166120	-2.6870800	0.7188400
C	-11.5166120	-2.6870800	-0.7188400
C	-11.5166120	-0.7188400	-2.6870800
C	-11.5166120	0.7188400	-2.6870800
C	-11.5166120	2.6870800	-0.7188400
C	-11.5166120	2.6870800	0.7188400
C	-10.2761650	-1.3917100	2.4084300
C	-10.2761650	-2.4084300	1.3917100
C	-10.2761650	-2.4084300	-1.3917100
C	-10.2761650	-1.3917100	-2.4084300
C	-10.2761650	1.3917100	-2.4084300
C	-10.2761650	2.4084300	-1.3917100
C	-10.2761650	2.4084300	1.3917100
C	-10.2761650	1.3917100	2.4084300
C	-9.0281036	0.7323450	2.7142019
C	-9.0281669	-0.7317159	2.7143311
C	-9.0232569	-2.6646511	0.7237160
C	-9.0268592	-2.6747538	-0.7253778
C	-9.0343853	-0.7244613	-2.7003478
C	-9.0343015	0.7247766	-2.7000283
C	-9.0269134	2.6751823	-0.7253009
C	-9.0236068	2.6652674	0.7237447
C	-7.7955807	-1.4066800	2.4661219
C	-7.7861773	-2.3981189	1.4026525
C	-7.8035926	-2.4300531	-1.4229813
C	-7.8048286	-1.4079049	-2.4626729

C	-7.8046185	1.4081580	-2.4620508
C	-7.8033668	2.4303530	-1.4222798
C	-7.7867799	2.3994584	1.4032368
C	-7.7960424	1.4086339	2.4669940
C	-6.5819447	-2.7200200	0.6719552
C	-6.5934948	-2.7374964	-0.7129393
C	-6.6009094	-0.6929049	-2.8031457
C	-6.6008475	0.6933073	-2.8027543
C	-6.5934688	2.7382674	-0.7118017
C	-6.5823310	2.7210920	0.6731886
H	-5.6156703	2.7503798	1.1752868
H	-5.6401059	2.7950589	-1.2420762
H	-5.6478163	1.2209853	-2.8853681
H	-5.6476960	-1.2201087	-2.8858264
H	-5.6404064	-2.7942803	-1.2438904
H	-5.6147357	-2.7494356	1.1730875
C	-6.5639492	0.7278903	2.8834061
C	-6.5635663	-0.7247570	2.8816752
C	-5.3658542	1.4338646	3.1674785
C	-5.3635633	-1.4288600	3.1608480
C	-4.1752980	0.7125143	3.3315296
C	-4.1743315	-0.7054429	3.3252626
C	-2.7737043	1.1258415	3.4381878
C	-2.7726185	-1.1185451	3.4234141
H	-5.3627519	2.5231809	3.2481929
H	-5.3574674	-2.5183389	3.2399596
N	-1.9539062	0.0039787	3.4735051
C	6.5669413	0.7277368	2.8913498
C	6.5667671	-0.7254673	2.8895865
C	5.3701878	1.4332096	3.1818237
C	5.3686634	-1.4300797	3.1755242
C	4.1812306	0.7109728	3.3560213
C	4.1808279	-0.7065911	3.3500772
C	2.7797616	1.1232908	3.4700139
C	2.7793940	-1.1190716	3.4556765
H	5.3669192	2.5227559	3.2625488
H	5.3639090	-2.5197384	3.2545617
N	1.9591214	0.0021646	3.5187267
C	0.7129284	6.4965452	2.7418826
C	-0.7046330	6.4957882	2.7406875
C	1.4436649	5.3180611	2.9666947
C	-1.4342035	5.3167590	2.9642851
C	0.7124145	4.1384520	3.1909347
C	-0.7011402	4.1382997	3.1883242

C	1.1272634	2.7505141	3.3829088
C	-1.1174987	2.7508285	3.3731877
H	1.2437272	7.4323728	2.5521534
H	-1.2358373	7.4311710	2.5497698
H	2.5355992	5.3014245	2.9566687
H	-2.5260752	5.2986768	2.9552277
N	0.0049771	1.9335752	3.4669980
C	0.7125986	-6.4980144	2.7487446
C	-0.7046908	-6.4973068	2.7482767
C	1.4431985	-5.3161079	2.9541763
C	-1.4344296	-5.3148823	2.9528176
C	0.7120025	-4.1337500	3.1618270
C	-0.7017071	-4.1332631	3.1594766
C	1.1275816	-2.7460535	3.3493867
C	-1.1179085	-2.7452894	3.3397733
H	1.2434517	-7.4376602	2.5787601
H	-1.2360696	-7.4364603	2.5779327
H	2.5350204	-5.2994541	2.9452921
H	-2.5262615	-5.2974882	2.9456743
N	0.0051816	-1.9292430	3.4318226
N	2.4047969	2.3938162	3.4131380
N	2.4048454	-2.3887650	3.3838942
N	-2.3954060	-2.3880195	3.3628824
N	-2.3956768	2.3958427	3.3927158
Fe	0.0000000	0.0000000	3.7063117
C	-0.1164583	-0.0588539	5.4095173
O	-0.2582027	-0.1261965	6.5731790
H	5.6162284	2.7485846	1.1799925
H	5.6384012	2.7944888	-1.2380979
H	5.6470875	1.2207325	-2.8831687
H	5.6471651	-1.2203813	-2.8837769
H	5.6387209	-2.7942356	-1.2398705
H	5.6156934	-2.7477273	1.1780320
C	6.5820887	-2.7194905	0.6750368
C	6.5927300	-2.7386892	-0.7102357
C	6.6003864	-0.6931481	-2.8013078
C	6.6002942	0.6932353	-2.8009722
C	6.5926553	2.7387838	-0.7090005
C	6.5822919	2.7202154	0.6761818
C	7.7970718	-1.4071209	2.4684959
C	7.7869559	-2.3978105	1.4043139
C	7.8026064	-2.4313744	-1.4215602
C	7.8039757	-1.4081267	-2.4605801
C	7.8038339	1.4082473	-2.4599534

C	7.8023055	2.4311836	-1.4207288
C	7.7874112	2.3987309	1.4050028
C	7.7972738	1.4086517	2.4696100
C	9.0292539	0.7321500	2.7149471
C	9.0292480	-0.7316302	2.7149938
C	9.0234599	-2.6645674	0.7241352
C	9.0266965	-2.6749418	-0.7249054
C	9.0337196	-0.7245588	-2.6985109
C	9.0335753	0.7246846	-2.6983435
C	9.0267356	2.6750588	-0.7248059
C	9.0236250	2.6650108	0.7242928
C	10.2761650	-1.3917100	2.4084300
C	10.2761650	-2.4084300	1.3917100
C	10.2761650	-2.4084300	-1.3917100
C	10.2761650	-1.3917100	-2.4084300
C	10.2761650	1.3917100	-2.4084300
C	10.2761650	2.4084300	-1.3917100
C	10.2761650	2.4084300	1.3917100
C	10.2761650	1.3917100	2.4084300
C	11.5166120	0.7188400	2.6870800
C	11.5166120	-0.7188400	2.6870800
C	11.5166120	-2.6870800	0.7188400
C	11.5166120	-2.6870800	-0.7188400
C	11.5166120	-0.7188400	-2.6870800
C	11.5166120	0.7188400	-2.6870800
C	11.5166120	2.6870800	-0.7188400
C	11.5166120	2.6870800	0.7188400
C	12.7570590	-1.3917100	2.4084300
C	12.7570590	-2.4084300	1.3917100
C	12.7570590	-2.4084300	-1.3917100
C	12.7570590	-1.3917100	-2.4084300
C	12.7570590	1.3917100	-2.4084300
C	12.7570590	2.4084300	-1.3917100
C	12.7570590	2.4084300	1.3917100
C	12.7570590	1.3917100	2.4084300

4.3 The SWCNT-CoPc-SWCNT molecular junction with (4,4) SWCNTs as the electrodes

C	-13.985806	0.718840	2.687080
C	-13.985806	-0.718840	2.687080
C	-13.985806	-2.687080	0.718840
C	-13.985806	-2.687080	-0.718840
C	-13.985806	-0.718840	-2.687080

C	-13.985806	0.718840	-2.687080
C	-13.985806	2.687080	-0.718840
C	-13.985806	2.687080	0.718840
C	-12.745359	-1.391710	2.408430
C	-12.745359	-2.408430	1.391710
C	-12.745359	-2.408430	-1.391710
C	-12.745359	-1.391710	-2.408430
C	-12.745359	1.391710	-2.408430
C	-12.745359	2.408430	-1.391710
C	-12.745359	2.408430	1.391710
C	-12.745359	1.391710	2.408430
C	-11.504912	0.718840	2.687080
C	-11.504912	-0.718840	2.687080
C	-11.504912	-2.687080	0.718840
C	-11.504912	-2.687080	-0.718840
C	-11.504912	-0.718840	-2.687080
C	-11.504912	0.718840	-2.687080
C	-11.504912	2.687080	-0.718840
C	-11.504912	2.687080	0.718840
C	-10.264465	-1.391710	2.408430
C	-10.264465	-2.408430	1.391710
C	-10.264465	-2.408430	-1.391710
C	-10.264465	-1.391710	-2.408430
C	-10.264465	1.391710	-2.408430
C	-10.264465	2.408430	-1.391710
C	-10.264465	2.408430	1.391710
C	-10.264465	1.391710	2.408430
C	-9.015447	0.730387	2.698653
C	-9.015442	-0.730376	2.698653
C	-9.016487	-2.673939	0.721095
C	-9.019597	-2.679636	-0.726987
C	-9.022736	-0.724731	-2.697132
C	-9.022738	0.724709	-2.697131
C	-9.019619	2.679634	-0.726991
C	-9.016487	2.673932	0.721083
C	-7.782944	-1.408619	2.445559
C	-7.777814	-2.410782	1.394178
C	-7.796134	-2.437456	-1.426297
C	-7.792700	-1.408779	-2.454060
C	-7.792699	1.408766	-2.454071
C	-7.796146	2.437457	-1.426289
C	-7.777807	2.410777	1.394187
C	-7.782969	1.408624	2.445555
C	-6.579828	-2.768441	0.661043

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C	-6.591349	-2.781583	-0.722562
C	-6.585286	-0.692368	-2.786488
C	-6.585291	0.692364	-2.786483
C	-6.591351	2.781572	-0.722548
C	-6.579832	2.768436	0.661031
H	-5.613983	2.844947	1.159160
H	-5.642647	2.883785	-1.253751
H	-5.633940	1.222173	-2.864253
H	-5.633940	-1.222185	-2.864236
H	-5.642647	-2.883793	-1.253729
H	-5.614000	-2.844961	1.159163
C	-6.548142	0.725529	2.833512
C	-6.548112	-0.725537	2.833517
C	-5.335977	1.431581	3.038080
C	-5.335976	-1.431591	3.038079
C	-4.140415	0.708451	3.070280
C	-4.140405	-0.708408	3.070277
C	-2.741115	1.119637	3.031750
C	-2.741102	-1.119552	3.031751
H	-5.324280	2.518264	3.142771
H	-5.324281	-2.518245	3.142771
N	-1.918095	-0.000017	2.995689
C	6.548375	0.725677	2.833428
C	6.548226	-0.725792	2.833502
C	5.335823	1.431596	3.038051
C	5.336172	-1.431586	3.038041
C	4.140477	0.708440	3.070278
C	4.140324	-0.708350	3.070267
C	2.741031	1.119703	3.031741
C	2.740923	-1.119653	3.031735
H	5.324222	2.518241	3.142727
H	5.324258	-2.518358	3.142772
N	1.917879	-0.000045	2.995685
C	0.707992	6.552647	2.862851
C	-0.708075	6.552667	2.862851
C	1.437006	5.351980	2.862148
C	-1.437006	5.351892	2.862152
C	0.706066	4.152604	2.862849
C	-0.706020	4.152692	2.862835
C	1.116328	2.749873	2.903827
C	-1.116313	2.749978	2.903822
H	1.240060	7.507367	2.867957
H	-1.240103	7.507332	2.867956
H	2.529107	5.335260	2.868814

H	-2.529203	5.335276	2.868820
N	-0.000058	1.923534	2.909623
C	0.707980	-6.552670	2.862848
C	-0.708036	-6.552731	2.862858
C	1.437009	-5.351948	2.862139
C	-1.437061	-5.351917	2.862152
C	0.705960	-4.152613	2.862839
C	-0.705931	-4.152723	2.862829
C	1.116203	-2.749973	2.903802
C	-1.116369	-2.750004	2.903823
H	1.240105	-7.507398	2.867953
H	-1.240082	-7.507410	2.867958
H	2.529072	-5.335199	2.868795
H	-2.529240	-5.335347	2.868819
N	-0.000132	-1.923520	2.909619
N	2.390447	2.395759	2.965439
N	2.390488	-2.395878	2.965410
N	-2.390469	-2.395642	2.965452
N	-2.390520	2.395638	2.965451
Co	0.000000	0.000000	2.924635
H	5.614232	2.844978	1.158906
H	5.642741	2.883875	-1.253799
H	5.633802	1.222230	-2.864225
H	5.633822	-1.222265	-2.864146
H	5.642527	-2.883897	-1.253830
H	5.614139	-2.845002	1.159013
C	6.579484	-2.768447	0.661141
C	6.591414	-2.781629	-0.722152
C	6.585498	-0.692608	-2.786390
C	6.585438	0.692515	-2.786422
C	6.591323	2.781669	-0.722291
C	6.579440	2.768455	0.661206
C	7.782682	-1.408675	2.445454
C	7.777725	-2.410776	1.394130
C	7.795990	-2.437516	-1.426392
C	7.792665	-1.408621	-2.454126
C	7.792927	1.408553	-2.454127
C	7.795982	2.437458	-1.426446
C	7.777548	2.410730	1.394127
C	7.782800	1.408766	2.445348
C	9.015179	0.730139	2.698771
C	9.015251	-0.730183	2.698767
C	9.016578	-2.673862	0.721316
C	9.019741	-2.679654	-0.727179

C	9.022459	-0.724438	-2.697168
C	9.022487	0.724472	-2.697160
C	9.019703	2.679614	-0.727337
C	9.016537	2.673860	0.721316
C	10.264465	-1.391710	2.408430
C	10.264465	-2.408430	1.391710
C	10.264465	-2.408430	-1.391710
C	10.264465	-1.391710	-2.408430
C	10.264465	1.391710	-2.408430
C	10.264465	2.408430	-1.391710
C	10.264465	2.408430	1.391710
C	10.264465	1.391710	2.408430
C	11.504912	0.718840	2.687080
C	11.504912	-0.718840	2.687080
C	11.504912	-2.687080	0.718840
C	11.504912	-2.687080	-0.718840
C	11.504912	-0.718840	-2.687080
C	11.504912	0.718840	-2.687080
C	11.504912	2.687080	-0.718840
C	11.504912	2.687080	0.718840
C	12.745359	-1.391710	2.408430
C	12.745359	-2.408430	1.391710
C	12.745359	-2.408430	-1.391710
C	12.745359	-1.391710	-2.408430
C	12.745359	1.391710	-2.408430
C	12.745359	2.408430	-1.391710
C	12.745359	2.408430	1.391710
C	12.745359	1.391710	2.408430

4.4 The SWCNT-NiPc-SWCNT molecular junction with (4,4) SWCNTs as the electrodes

C	-13.977706	0.718840	2.687080
C	-13.977706	-0.718840	2.687080
C	-13.977706	-2.687080	0.718840
C	-13.977706	-2.687080	-0.718840
C	-13.977706	-0.718840	-2.687080
C	-13.977706	0.718840	-2.687080
C	-13.977706	2.687080	-0.718840
C	-13.977706	2.687080	0.718840
C	-12.737259	-1.391710	2.408430
C	-12.737259	-2.408430	1.391710
C	-12.737259	-2.408430	-1.391710
C	-12.737259	-1.391710	-2.408430

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C	-12.737259	1.391710	-2.408430
C	-12.737259	2.408430	-1.391710
C	-12.737259	2.408430	1.391710
C	-12.737259	1.391710	2.408430
C	-11.496812	0.718840	2.687080
C	-11.496812	-0.718840	2.687080
C	-11.496812	-2.687080	0.718840
C	-11.496812	-2.687080	-0.718840
C	-11.496812	-0.718840	-2.687080
C	-11.496812	0.718840	-2.687080
C	-11.496812	2.687080	-0.718840
C	-11.496812	2.687080	0.718840
C	-10.256365	-1.391710	2.408430
C	-10.256365	-2.408430	1.391710
C	-10.256365	-2.408430	-1.391710
C	-10.256365	-1.391710	-2.408430
C	-10.256365	1.391710	-2.408430
C	-10.256365	2.408430	-1.391710
C	-10.256365	2.408430	1.391710
C	-10.256365	1.391710	2.408430
C	-9.009242	0.732179	2.713190
C	-9.009275	-0.732175	2.713199
C	-9.004991	-2.666928	0.722904
C	-9.008162	-2.677676	-0.725886
C	-9.013875	-0.724162	-2.697554
C	-9.013892	0.724166	-2.697567
C	-9.008133	2.677656	-0.725870
C	-9.004996	2.666917	0.722867
C	-7.779293	-1.408228	2.462988
C	-7.768256	-2.400830	1.400887
C	-7.784780	-2.433976	-1.422842
C	-7.784736	-1.409215	-2.459779
C	-7.784752	1.409214	-2.459797
C	-7.784735	2.433974	-1.422858
C	-7.768285	2.400798	1.400890
C	-7.779257	1.408206	2.462971
C	-6.565023	-2.727086	0.670931
C	-6.575151	-2.746226	-0.713773
C	-6.578345	-0.693090	-2.786406
C	-6.578354	0.693112	-2.786418
C	-6.575172	2.746200	-0.713788
C	-6.564960	2.727052	0.670950
H	-5.598032	2.761013	1.170984
H	-5.620970	2.803725	-1.243028

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H	-5.621957	1.216747	-2.853892
H	-5.621948	-1.216719	-2.853867
H	-5.620987	-2.803717	-1.243047
H	-5.598007	-2.761041	1.170998
C	-6.547081	0.725685	2.869090
C	-6.547045	-0.725799	2.869090
C	-5.343758	1.432467	3.123143
C	-5.343826	-1.432511	3.123129
C	-4.150444	0.706962	3.223688
C	-4.150458	-0.707013	3.223695
C	-2.748834	1.119276	3.251968
C	-2.748795	-1.119445	3.251957
H	-5.337403	2.520173	3.216137
H	-5.337502	-2.520285	3.216144
N	-1.925579	-0.000057	3.261919
C	6.546909	0.725766	2.869119
C	6.546910	-0.725786	2.869153
C	5.343653	1.432504	3.123254
C	5.343593	-1.432205	3.123259
C	4.150456	0.707105	3.223817
C	4.150306	-0.707145	3.223767
C	2.748552	1.119354	3.251928
C	2.748710	-1.119194	3.251921
H	5.337238	2.520251	3.216214
H	5.337259	-2.520330	3.216167
N	1.925713	-0.000091	3.261895
C	0.708889	6.524984	2.816908
C	-0.709139	6.524939	2.816919
C	1.439545	5.330438	2.924967
C	-1.439751	5.330513	2.924957
C	0.705409	4.136302	3.032633
C	-0.705508	4.136486	3.032658
C	1.118291	2.741173	3.145389
C	-1.118498	2.741100	3.145443
H	1.239244	7.475562	2.728461
H	-1.239366	7.475511	2.728492
H	2.531550	5.314731	2.922114
H	-2.531692	5.314718	2.922110
N	0.000019	1.919304	3.194699
C	0.709008	-6.524942	2.816888
C	-0.709015	-6.525027	2.816894
C	1.439598	-5.330433	2.924918
C	-1.439699	-5.330518	2.924917
C	0.705456	-4.136289	3.032622

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C	-0.705492	-4.136483	3.032610
C	1.118351	-2.741146	3.145364
C	-1.118384	-2.741052	3.145397
H	1.239358	-7.475586	2.728468
H	-1.239299	-7.475557	2.728486
H	2.531706	-5.314688	2.922079
H	-2.531684	-5.314794	2.922061
N	0.000123	-1.919384	3.194673
N	2.394531	2.392143	3.185997
N	2.394577	-2.392146	3.185956
N	-2.394725	-2.392387	3.186002
N	-2.394697	2.392402	3.186026
Ni	0.000000	0.000000	3.237770
H	5.597652	2.760843	1.171185
H	5.620995	2.803558	-1.243106
H	5.621893	1.216866	-2.854246
H	5.621843	-1.216688	-2.854036
H	5.620726	-2.803546	-1.243156
H	5.597856	-2.760838	1.171042
C	6.564669	-2.727129	0.670761
C	6.575306	-2.746081	-0.713890
C	6.578246	-0.693017	-2.786448
C	6.578499	0.693110	-2.786497
C	6.574869	2.746137	-0.713909
C	6.565006	2.727120	0.670876
C	7.779193	-1.408145	2.463150
C	7.768461	-2.400819	1.400993
C	7.784562	-2.434063	-1.423043
C	7.784739	-1.409200	-2.459759
C	7.784365	1.409193	-2.459953
C	7.785048	2.434055	-1.422996
C	7.768107	2.400941	1.400975
C	7.779394	1.408136	2.463206
C	9.009199	0.732071	2.713268
C	9.009533	-0.732127	2.713246
C	9.004879	-2.666941	0.722909
C	9.008435	-2.677613	-0.725828
C	9.013595	-0.724200	-2.697711
C	9.013922	0.724209	-2.697587
C	9.007913	2.677665	-0.725833
C	9.005287	2.667056	0.722998
C	10.256365	-1.391710	2.408430
C	10.256365	-2.408430	1.391710
C	10.256365	-2.408430	-1.391710

C	10.256365	-1.391710	-2.408430
C	10.256365	1.391710	-2.408430
C	10.256365	2.408430	-1.391710
C	10.256365	2.408430	1.391710
C	10.256365	1.391710	2.408430
C	11.496812	0.718840	2.687080
C	11.496812	-0.718840	2.687080
C	11.496812	-2.687080	0.718840
C	11.496812	-2.687080	-0.718840
C	11.496812	-0.718840	-2.687080
C	11.496812	0.718840	-2.687080
C	11.496812	2.687080	-0.718840
C	11.496812	2.687080	0.718840
C	12.737259	-1.391710	2.408430
C	12.737259	-2.408430	1.391710
C	12.737259	-2.408430	-1.391710
C	12.737259	-1.391710	-2.408430
C	12.737259	1.391710	-2.408430
C	12.737259	2.408430	-1.391710
C	12.737259	2.408430	1.391710
C	12.737259	1.391710	2.408430

4.5 The SWCNT-CuPc-SWCNT molecular junction with (4,4) SWCNTs as the electrodes

C	-14.014206	0.718840	2.687080
C	-14.014206	-0.718840	2.687080
C	-14.014206	-2.687080	0.718840
C	-14.014206	-2.687080	-0.718840
C	-14.014206	-0.718840	-2.687080
C	-14.014206	0.718840	-2.687080
C	-14.014206	2.687080	-0.718840
C	-14.014206	2.687080	0.718840
C	-12.773759	-1.391710	2.408430
C	-12.773759	-2.408430	1.391710
C	-12.773759	-2.408430	-1.391710
C	-12.773759	-1.391710	-2.408430
C	-12.773759	1.391710	-2.408430
C	-12.773759	2.408430	-1.391710
C	-12.773759	2.408430	1.391710
C	-12.773759	1.391710	2.408430
C	-11.533312	0.718840	2.687080
C	-11.533312	-0.718840	2.687080
C	-11.533312	-2.687080	0.718840

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C	-11.533312	-2.687080	-0.718840
C	-11.533312	-0.718840	-2.687080
C	-11.533312	0.718840	-2.687080
C	-11.533312	2.687080	-0.718840
C	-11.533312	2.687080	0.718840
C	-10.292865	-1.391710	2.408430
C	-10.292865	-2.408430	1.391710
C	-10.292865	-2.408430	-1.391710
C	-10.292865	-1.391710	-2.408430
C	-10.292865	1.391710	-2.408430
C	-10.292865	2.408430	-1.391710
C	-10.292865	2.408430	1.391710
C	-10.292865	1.391710	2.408430
C	-9.045716	0.731330	2.707855
C	-9.045644	-0.731355	2.707866
C	-9.042182	-2.667236	0.720617
C	-9.044454	-2.677281	-0.728016
C	-9.050806	-0.724089	-2.697288
C	-9.050822	0.724136	-2.697304
C	-9.044460	2.677345	-0.728014
C	-9.042184	2.667188	0.720563
C	-7.817057	-1.411071	2.460038
C	-7.805547	-2.407037	1.399623
C	-7.821581	-2.435121	-1.426872
C	-7.821593	-1.409469	-2.462820
C	-7.821584	1.409429	-2.462819
C	-7.821605	2.435166	-1.426863
C	-7.805541	2.407065	1.399571
C	-7.817089	1.411054	2.460023
C	-6.603050	-2.736389	0.667129
C	-6.613937	-2.753598	-0.717796
C	-6.618943	-0.693126	-2.803426
C	-6.618922	0.693142	-2.803413
C	-6.613950	2.753554	-0.717764
C	-6.603044	2.736453	0.667208
H	-5.636076	2.783944	1.167516
H	-5.662159	2.824262	-1.249520
H	-5.666210	1.220802	-2.891237
H	-5.666212	-1.220750	-2.891218
H	-5.662091	-2.824256	-1.249520
H	-5.636073	-2.783927	1.167522
C	-6.587276	0.725701	2.860094
C	-6.587250	-0.725718	2.860099
C	-5.382722	1.431713	3.106696

C	-5.382752	-1.431754	3.106720
C	-4.188869	0.710519	3.201815
C	-4.188856	-0.710587	3.201854
C	-2.783339	1.127823	3.229936
C	-2.783403	-1.127799	3.229972
H	-5.378398	2.519455	3.203771
H	-5.378452	-2.519430	3.203828
N	-1.985998	-0.000008	3.243412
C	6.586971	0.725562	2.860032
C	6.587091	-0.725733	2.860040
C	5.382472	1.431858	3.106500
C	5.382705	-1.431860	3.106586
C	4.188723	0.710507	3.202005
C	4.188848	-0.710457	3.202041
C	2.783393	1.127702	3.230123
C	2.783314	-1.127663	3.230130
H	5.378387	2.519496	3.203846
H	5.378488	-2.519552	3.203938
N	1.985727	0.000016	3.243504
C	0.708343	6.577897	2.846287
C	-0.708258	6.577767	2.846266
C	1.437372	5.380378	2.940082
C	-1.437487	5.380086	2.940065
C	0.708565	4.182494	3.032580
C	-0.708710	4.182346	3.032621
C	1.125996	2.779892	3.132307
C	-1.126031	2.779954	3.132318
H	1.239898	7.529338	2.772774
H	-1.240053	7.529360	2.772782
H	2.529007	5.365032	2.943053
H	-2.529298	5.364996	2.943035
N	-0.000293	1.981280	3.178523
C	0.708229	-6.577944	2.846271
C	-0.708220	-6.577848	2.846308
C	1.437419	-5.380317	2.940092
C	-1.437648	-5.380119	2.940098
C	0.708439	-4.182443	3.032648
C	-0.708579	-4.182406	3.032618
C	1.125824	-2.780053	3.132343
C	-1.126046	-2.779957	3.132290
H	1.239879	-7.529402	2.772799
H	-1.240077	-7.529437	2.772772
H	2.528988	-5.365086	2.943096
H	-2.529262	-5.365073	2.943066

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N	-0.000261	-1.981298	3.178543
N	2.403438	2.403111	3.169301
N	2.403433	-2.403251	3.169298
N	-2.403289	-2.403229	3.169220
N	-2.403305	2.403117	3.169188
Cu	0.000000	0.000000	3.203139
H	5.636356	2.783761	1.167281
H	5.662085	2.824367	-1.249874
H	5.666377	1.220769	-2.891575
H	5.666457	-1.220682	-2.891434
H	5.662162	-2.824575	-1.249756
H	5.636143	-2.783968	1.167565
C	6.603191	-2.736290	0.667234
C	6.613938	-2.753512	-0.717733
C	6.618772	-0.693149	-2.803390
C	6.618627	0.693016	-2.803501
C	6.613939	2.753522	-0.717853
C	6.603074	2.736090	0.667261
C	7.816918	-1.411154	2.460151
C	7.805580	-2.407175	1.399514
C	7.821575	-2.435358	-1.427057
C	7.821512	-1.409462	-2.463017
C	7.821688	1.409594	-2.463080
C	7.821659	2.435364	-1.426976
C	7.805309	2.407045	1.399572
C	7.817250	1.411097	2.460184
C	9.045654	0.731564	2.707795
C	9.045653	-0.731420	2.707909
C	9.042075	-2.667180	0.720483
C	9.044413	-2.677418	-0.727823
C	9.050977	-0.724313	-2.697253
C	9.051024	0.724297	-2.697234
C	9.044489	2.677230	-0.727976
C	9.041900	2.667338	0.720394
C	10.292865	-1.391710	2.408430
C	10.292865	-2.408430	1.391710
C	10.292865	-2.408430	-1.391710
C	10.292865	-1.391710	-2.408430
C	10.292865	1.391710	-2.408430
C	10.292865	2.408430	-1.391710
C	10.292865	2.408430	1.391710
C	10.292865	1.391710	2.408430
C	11.533312	0.718840	2.687080
C	11.533312	-0.718840	2.687080

C	11.533312	-2.687080	0.718840
C	11.533312	-2.687080	-0.718840
C	11.533312	-0.718840	-2.687080
C	11.533312	0.718840	-2.687080
C	11.533312	2.687080	-0.718840
C	11.533312	2.687080	0.718840
C	12.773759	-1.391710	2.408430
C	12.773759	-2.408430	1.391710
C	12.773759	-2.408430	-1.391710
C	12.773759	-1.391710	-2.408430
C	12.773759	1.391710	-2.408430
C	12.773759	2.408430	-1.391710
C	12.773759	2.408430	1.391710
C	12.773759	1.391710	2.408430

4.6 The SWCNT-ZnPc-SWCNT molecular junction with (4,4) SWCNTs as the electrodes

C	-14.039006	0.718840	2.687080
C	-14.039006	-0.718840	2.687080
C	-14.039006	-2.687080	0.718840
C	-14.039006	-2.687080	-0.718840
C	-14.039006	-0.718840	-2.687080
C	-14.039006	0.718840	-2.687080
C	-14.039006	2.687080	-0.718840
C	-14.039006	2.687080	0.718840
C	-12.798559	-1.391710	2.408430
C	-12.798559	-2.408430	1.391710
C	-12.798559	-2.408430	-1.391710
C	-12.798559	-1.391710	-2.408430
C	-12.798559	1.391710	-2.408430
C	-12.798559	2.408430	-1.391710
C	-12.798559	2.408430	1.391710
C	-12.798559	1.391710	2.408430
C	-11.558112	0.718840	2.687080
C	-11.558112	-0.718840	2.687080
C	-11.558112	-2.687080	0.718840
C	-11.558112	-2.687080	-0.718840
C	-11.558112	-0.718840	-2.687080
C	-11.558112	0.718840	-2.687080
C	-11.558112	2.687080	-0.718840
C	-11.558112	2.687080	0.718840
C	-10.317665	-1.391710	2.408430
C	-10.317665	-2.408430	1.391710

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C	-10.317665	-2.408430	-1.391710
C	-10.317665	-1.391710	-2.408430
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C	-9.072571	-0.731669	2.718538
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C	-9.067618	-2.673498	-0.725174
C	-9.075432	-0.724569	-2.701725
C	-9.075416	0.724548	-2.701729
C	-9.067631	2.673497	-0.725201
C	-9.064342	2.661288	0.723246
C	-7.840812	-1.406747	2.472925
C	-7.827811	-2.391108	1.402915
C	-7.844716	-2.430752	-1.424313
C	-7.845807	-1.408142	-2.464527
C	-7.845858	1.408207	-2.464474
C	-7.844743	2.430788	-1.424279
C	-7.827841	2.391167	1.402955
C	-7.840854	1.406785	2.472885
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C	-6.640466	-0.693387	-2.801765
C	-6.640471	0.693397	-2.801724
C	-6.633188	2.727562	-0.712493
C	-6.621034	2.701412	0.672740
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H	-5.686107	1.221086	-2.875543
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H	-5.680125	-2.778201	-1.244460
H	-5.652581	-2.708611	1.172162
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C	-6.612898	-0.725354	2.896167
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C	-4.224570	-0.712671	3.348554
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C	-2.817565	-1.131737	3.454872
H	-5.413978	2.520353	3.267727
H	-5.413859	-2.520350	3.267775

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N	-2.030145	0.000049	3.521159
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C	1.132175	2.790226	3.381727
C	-1.132048	2.790162	3.381731
H	1.240062	7.499830	2.669234
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C	0.709930	-4.185255	3.208227
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C	1.132149	-2.790111	3.381687
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H	5.680141	2.778252	-1.244378
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H	5.686170	-1.221118	-2.875597
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H	5.652506	-2.708501	1.172206
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C	6.640431	0.693383	-2.801751
C	6.633168	2.727476	-0.712551
C	6.621014	2.701293	0.672727
C	7.840850	-1.406790	2.472952
C	7.827751	-2.391124	1.402919
C	7.844729	-2.430825	-1.424332
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C	7.845865	1.408202	-2.464499
C	7.844638	2.430812	-1.424309
C	7.827791	2.391160	1.402976
C	7.840854	1.406839	2.472959
C	9.072569	0.731706	2.718522
C	9.072553	-0.731680	2.718551
C	9.064367	-2.661313	0.723202
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C	9.075419	-0.724552	-2.701751
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C	11.558112	0.718840	-2.687080
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C	12.798559	-2.408430	1.391710
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C	12.798559	1.391710	2.408430