Electronic supplementary information

Ferrocene-modified polymer-SWCNTs composite film for high-performance flexible thermoelectric generators

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1. SEM measurement

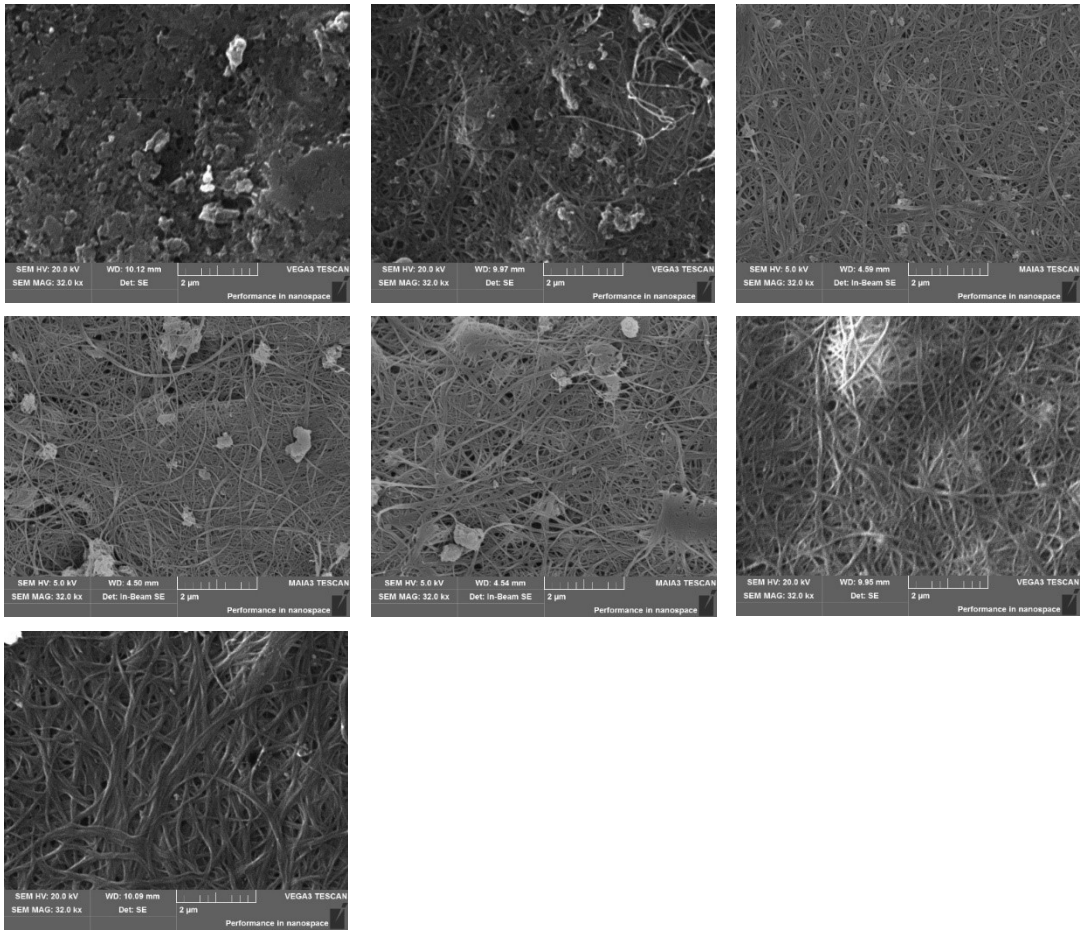


Figure S1. SEM images for the surface morphology of (a-c) **Fc-P2**/SWCNT composite films with various SWCNT mass loadings (f_c): (a) f_c = 30%, (b) f_c = 60%, (c) f_c = 90%; (d-f) **Fc-P3**/SWCNT composite films with various SWCNT mass loadings (f_c): (d) f_c = 30%, (e) f_c = 60%, (f) f_c = 90%; and (g) the pure SWCNT film.

2. XRD measurement

Diffraction peaks located around 26 are present in their XRD patterns, indicating the amorphous nature of the metallopolymer.

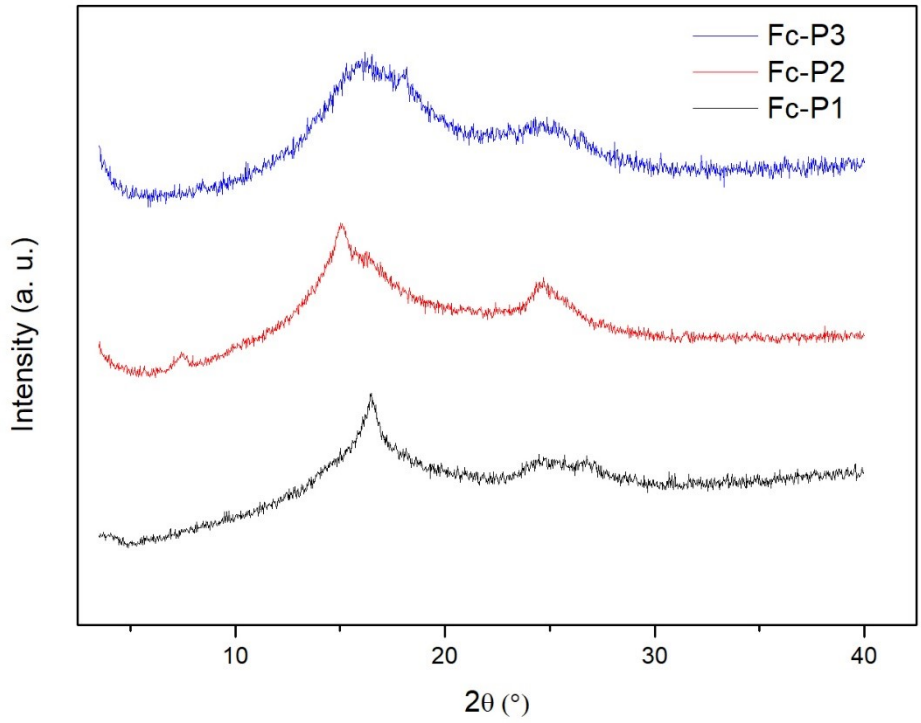


Figure S2. XRD of **Fc-P1**, **Fc-P2**, **Fc-P3**.

3. Thermoelectric parameters of the composites

In testing the thermoelectric performance of the composite films, we ensured the reliability of our experiments by preparing three different films for each data set using the same method.

Table S1 Summary of the thermoelectric parameters of the composites.

films	SWCNT doping ratio (f_c)	σ (S/cm)	S ($\mu V \cdot K^{-1}$)	PF [$\mu W\ m^{-1}\ K^{-2}$]
SWCNT		741.9±11.2	35.5±0.3	93.2±0.4
SWCNT-Fc-P1	15 %	107.5±7.9	69.4±0.4	51.7±3.2
	30 %	218.9±8.6	67.9±0.3	101.1±2.8
	45 %	463.5±12.1	64.0±0.4	189.9±2.7
	60 %	601.6±22.5	61.0±0.2	223.5±7.2

	75 %	604.5±12.8	59.8±0.3	216.2±2.5
	90 %	778.5±18.7	57.5±1.6	331.5±8.3
SWCNT-Fc-P2	15 %	32.6±11.4	69.2±1.3	15.6±5.1
	30 %	184.3±29.3	69.0±0.5	87.8±12.9
	45 %	369.3±18.6	66.6±0.4	163.8±6.4
	60 %	420.1±35.1	61.2±0.3	157.5±11.9
	75 %	597.2±26.4	59.9±0.3	214.3±7.5
	90 %	754.1±32.3	59.1±0.6	263.3±6.1
SWCNT-Fc-P3	15 %	24.1±7.7	73.6±0.4	13.0±4.0
	30 %	112.6±43.8	71.8±0.3	58.0±8.4
	45 %	560.1±36.9	67.0±0.4	251.2±13.5
	60 %	605.3±29.8	63.0±0.3	240.2±9.6
	75 %	637.3±26.7	61.7±0.2	242.3±1.7
	90 %	1051.8±30.1	59.1±0.3	367.4±6.9

Table S2. The thermoelectric performance of different polymers/SWCNT composite films from several related works.

Materials	Electrical conductivity [S cm^{-1}]	Seebeck coefficient [μV K^{-1}]	Power factor [μW m^{-1} K^{-2}]	Ref.
PANI/SWCNT	1390	47.4	407	1
(PEDOT:PSS)/SWCNT	4000	19	140	2
P3HT/SWCNT	1722	34	148	3
MEH-PPV/SWCNT	415	29	33	4
PEDOT-Tos/SWCNT	4731	16	119	5
Fc-P3/SWCNT	1052	59	367	This work

4. DFT Calculations

Computational Details

All density functional theory (DFT) calculations were performed to understand the electrochemical properties for three types of ferrocene-containing cyclopentadithiophene such as **Fc-P1**, **Fc-P2** and **Fc-P3**. The B3LYP-D3[6] method combined with a mixed basis sets of def2-TZVP[7] for Fe atom and 6-31G(d,p)[8] for the other atoms (designed as BS1) were used to fully optimize all the structures in gas phase. Then, vibrational frequency calculations on the fully optimized geometries were carried out at the same level of theory to confirm no imaginary frequency for all local minimum. The effect of 1,4- chlorobenzene solvent was then considered by single-point energy calculation with implicit SMD solvation model.[9] In order to obtain accurate binding energy for molecular dimer, the B3LYP-D3 functional in combination with large basis sets (6-311+G(d,p) & Def2-TZVP (Fe), designed as BS2) were employed in single point calculations with implicit SMD solvation model of chlorobenzene solvent. Moreover, to examine the effect of DFT functional, a few other common and reliable M06L-D3, PBE0-D3, and ωB97X-D methods[10] were also used for the single-point energy calculations in SMD model of chlorobenzene solvent. In addition, non-covalent interaction (NCI) index and topological analysis based on the Quantum Theory of Atoms-In-Molecules (QTAIM) method,[11] HOMO-LUMO orbital and electrostatic potential (ESP) analysis on the basis of the geometry and wavefunction at B3LYP-D3/BS2 level were conducted using Multiwfn.[12] All 3D images of the optimized structures were prepared using GaussView 6.0, and Visual Molecular Dynamics (VMD).[13] All calculations were carried out by Gaussian 16 program.[14]

HOMO-LUMO gap analysis

By analyzing the HOMO and LUMO orbitals energy for **Fc-P1**, **Fc-P2** and **Fc-P3**, the HOMO-LUMO energy gap of **Fc-P3** is the smallest with 2.80 eV, this is ascribed to the large cyclopentadithiophene, which is donor ligand, making the HOMO orbital energy unstable.

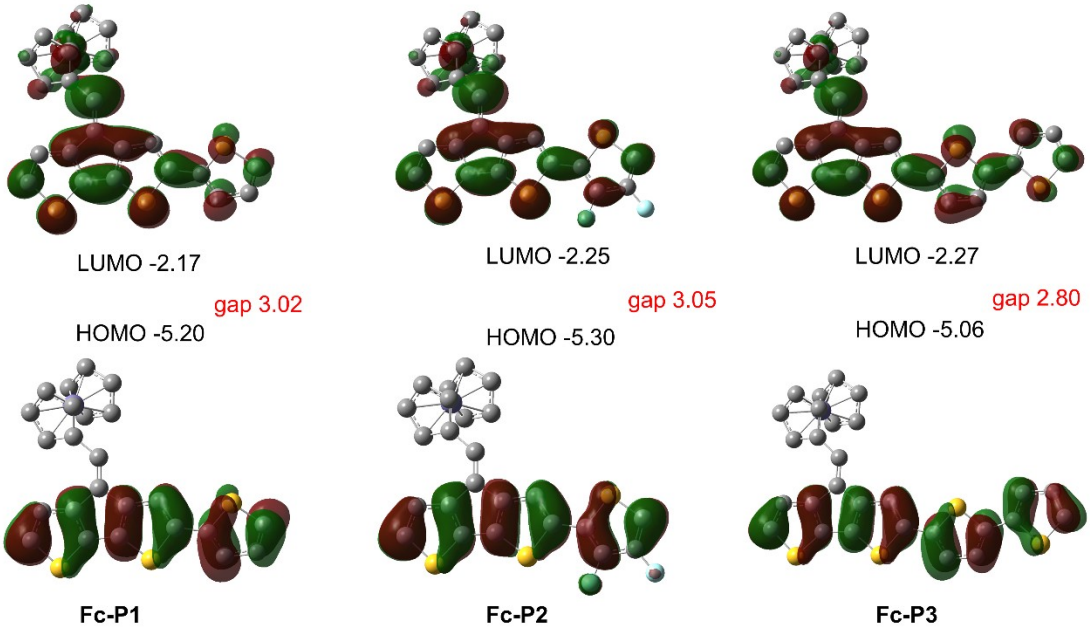


Figure S3. HOMO and LUMO orbital energies and corresponding HOMO-LUMO energy gaps for **Fc-P1**, **Fc-P2** and **Fc-P3**.

From Figure S4 it can be seen that the positive and negative ESP maps of **Fc-P1**, **Fc-P2** and **Fc-P3**. The large positive ESP was shown in the center of molecules, whereas the negative ESP was located on the edge. Therefore, from a pure electrostatic point of view, **Fc-P1** to **Fc-P3** molecules may be more prone to as the polymer donor.

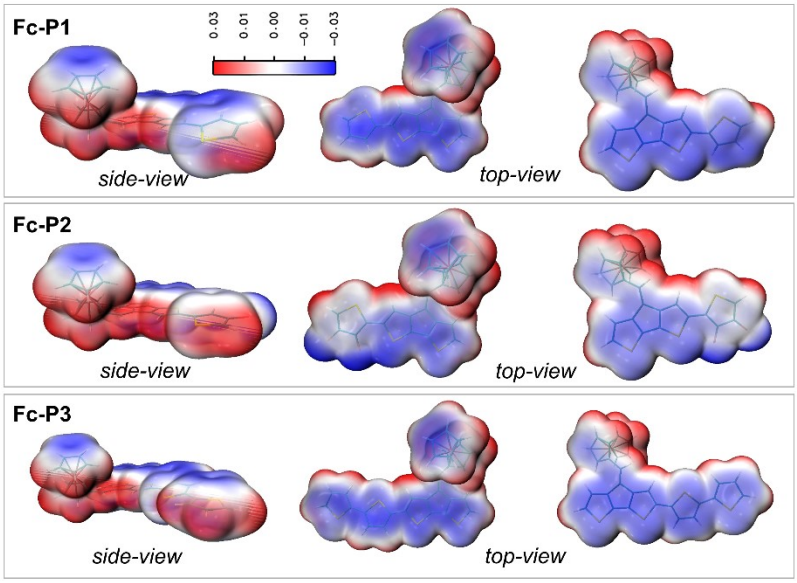
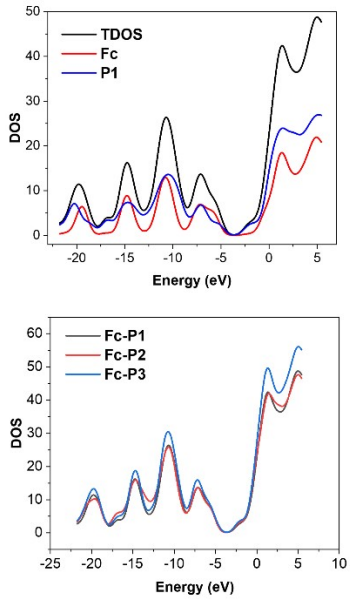
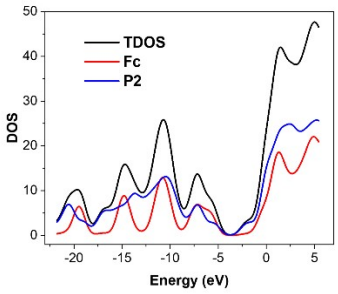
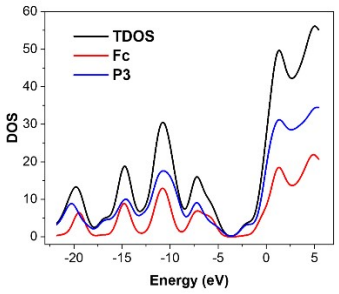


Figure S4. Isosurface maps of the electrostatic potential (ESP) for **Fc-P1**, **Fc-P2** and **Fc-P3** fragments. Red and blue colors correspond to positive and negative parts of ESP, respectively.







	HOMO (eV)	LUMO (eV)	HOMO-LUMO gap
Fc-P1	-5.20	-2.17	-3.02
Fc-P2	-5.30	-2.25	3.05
Fc-P3	-5.06	-2.27	2.80
SWCNT	-4.82	-2.62	

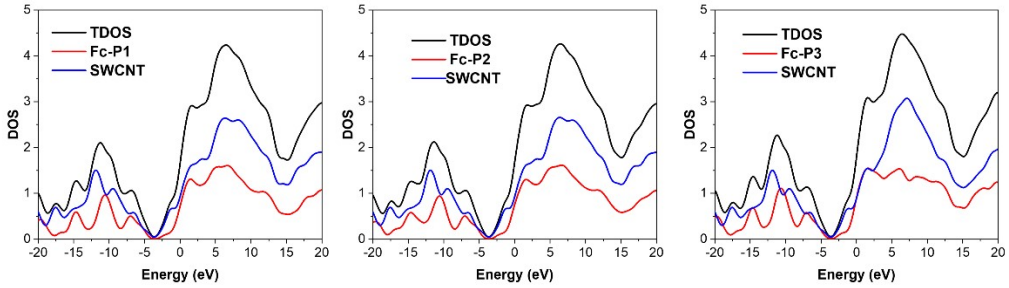


Figure S5. Density-of-state (DOS) map (curve) and HOMO and LUMO energies of the polymer and SWCNT fragments, as well as their complexes.

Table S3. Redox potentials and frontier orbital energy levels of the polymers.

Compound	*E*1/2 ox *vs.* Fc^+/Fc (V)	*E*1/2 red *vs.* Fc^+/Fc (V)	HOMO[a] (eV)	LUMO[a] (eV)	Energy gap[a]
Fc-P1	0.95	-0.86	-5.27	-3.46	1.81
Fc-P2	1.08	-0.83	-5.40	-3.49	1.91
Fc-P3	0.82	-0.85	-5.14	-3.47	1.67

[a]Measured by cyclic voltammetry in dilute dichloromethane solution.

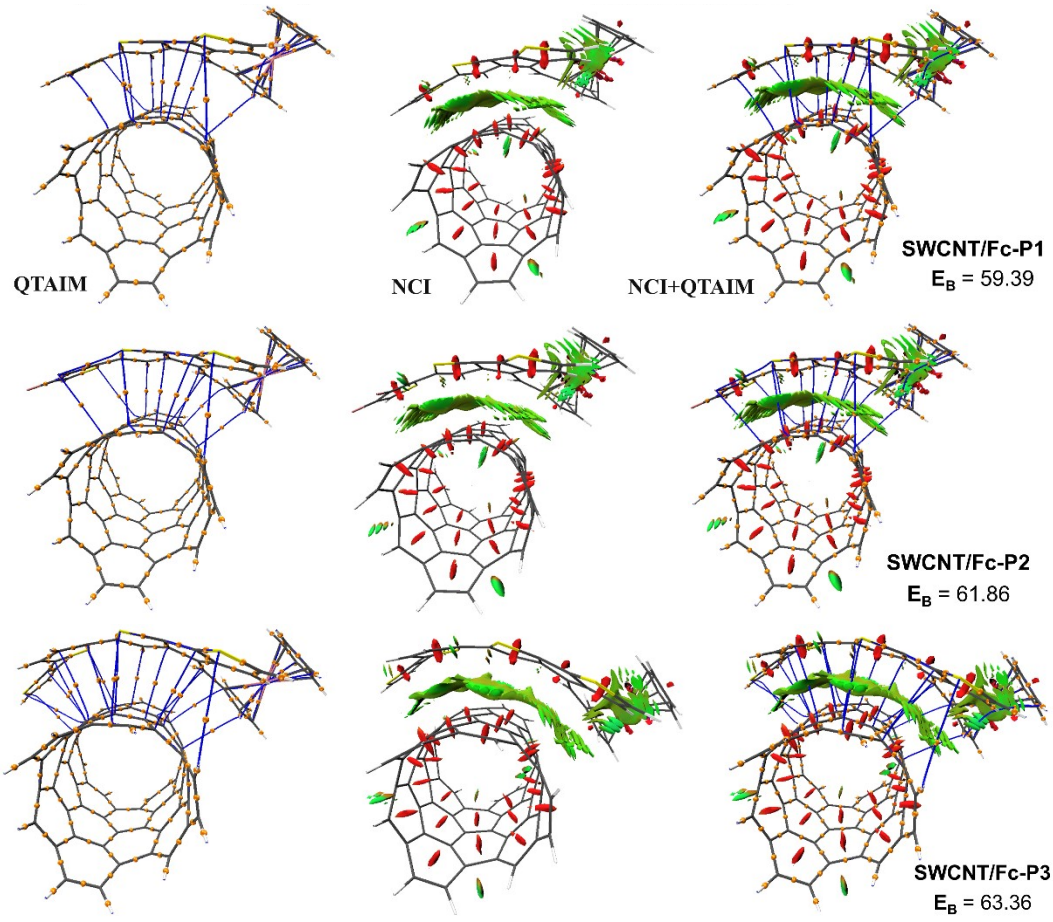


Figure S6. (Medium) Non-covalent interactions (NCIs) plot (red: strong repulsion; green: weak attraction; blue: strong attraction), (left) topological analysis based on the Quantum Theory of Atoms-In-Molecules (QTAIM) method; bond-critical points (BCPs) in a color sphere form based on their electron density (highest (red) and lowest (blue)); their corresponding bond paths in magenta lines, as well as (right) the NCIs combined with topological analysis of the molecule dimers (structures shown by VDW representation).

Table S4. Calculated binding energies (kJ/mol) of polymer fragments (**Fc-P1** to **Fc-P3**) and SWCNT using various DFT methods

E_B	B3LYP-D3	M06L-D3	PBE-D3	ωB97X-D
Fc-P1	59.39	65.82	57.87	75.03
Fc-P2	61.86	67.40	60.17	78.01
Fc-P3	63.36	71.51	61.00	77.91

From Figure S6 and Table S2, it can be seen that the binding energies between polymer fragments and SWCNT can quantitatively explain the interaction. The interaction between **Fc-P3** and SWCNT is stronger than others, the binding energy is 63.36 kJ/mol using B3LYP-D3 method. The ordering of binding energy: **Fc-P1** < **Fc-P2** < **Fc-P3**. The calculated results are quantitively consistent with experimental data.

Table S5. Cartesian coordinates

Fc-P1.xyz

Fe	-3.675783	-1.068857	0.064319
C	-0.989541	0.015955	-0.975923
C	-0.071751	0.924865	-0.565158
C	1.351939	0.601708	-0.343743
C	2.013422	1.738802	0.110951
C	1.069396	2.821253	0.170889
C	-0.186515	2.361314	-0.237941
S	1.079474	4.517606	0.495638
C	-0.614008	4.625896	0.057228
C	-1.141336	3.417021	-0.315451
C	2.189746	-0.537028	-0.401225
C	3.488044	-0.268516	-0.008580
S	3.681118	1.437185	0.448718
C	4.620517	-1.166363	0.049977
S	4.639590	-2.655716	-0.885006
C	6.206575	-3.084812	-0.269250
C	6.689693	-2.131788	0.584305
C	5.791147	-1.042961	0.768761
C	-3.365179	-1.431120	2.076842
H	-0.609446	-0.964517	-1.259061
H	-2.165360	3.306243	-0.645765
H	1.871171	-1.529060	-0.701498
H	6.671626	-4.011684	-0.574844
H	7.652228	-2.206858	1.076845
H	5.986835	-0.204295	1.427167
C	-4.699308	-1.787318	1.713700
H	-5.604426	-1.347494	2.108835
C	-4.624912	-0.370682	-1.642576
C	-4.660146	0.621698	-0.616155
C	-3.318789	0.933464	-0.252953
C	-2.433139	0.141745	-1.064702
C	-2.470390	-2.217443	1.291739
C	-3.249919	-3.057860	0.440626
C	-4.628286	-2.792594	0.702732
H	-5.469928	-3.247053	0.198788
C	-3.262314	-0.680198	-1.909389
H	-2.897510	-1.410788	-2.618285
H	-5.483837	-0.834079	-2.107382
H	-5.550963	1.032495	-0.161767
H	-3.011717	1.597056	0.540984
H	-1.391338	-2.146998	1.303255
H	-3.080596	-0.672146	2.792052
H	-2.864954	-3.748986	-0.296255
H	-1.113995	5.583032	0.106799

Fc-P2.xyz

C	-1.467240	0.027095	-0.986578
C	-0.577728	0.968597	-0.587081
C	0.862993	0.702822	-0.402013
C	1.489699	1.862504	0.047697
C	0.503982	2.904209	0.138801
C	-0.741953	2.396204	-0.243845
S	0.452471	4.596016	0.482264
C	-1.253987	4.637682	0.087054
C	-1.741161	3.411962	-0.285517
C	1.748477	-0.392048	-0.505948
C	3.047567	-0.067972	-0.151079
S	3.175085	1.635995	0.341532
C	4.205232	-0.928199	-0.157944
S	4.118533	-2.603032	-0.701326
C	5.812182	-2.877108	-0.395337
C	6.396783	-1.748014	0.088560
C	5.496754	-0.654164	0.222390
F	7.688095	-1.630567	0.421454
F	5.903826	0.539430	0.686589
H	-1.054769	-0.934769	-1.287782
H	-2.767661	3.262679	-0.591828
H	1.464408	-1.387090	-0.830726
H	6.271276	-3.834639	-0.587120
Fe	-4.094787	-1.172775	0.086351
C	-2.831694	-2.299674	1.275983
C	-3.734710	-1.550947	2.087937
H	-3.459757	-0.792978	2.807955
C	-5.096603	-0.487936	-1.595793
C	-5.151030	0.489319	-0.555766
C	-3.816152	0.845167	-0.209755
C	-2.915898	0.097026	-1.046360
C	-3.601405	-3.152658	0.428448
C	-4.981907	-2.932751	0.719618
C	-5.063997	-1.943042	1.744945
H	-5.974279	-1.535884	2.162517
C	-3.728294	-0.744355	-1.888265
H	-3.348994	-1.451798	-2.612835
H	-5.945667	-0.976480	-2.052903

H	-6.048661	0.861207	-0.081706
H	-3.520342	1.509203	0.588077
H	-3.209933	-3.822644	-0.324362
H	-1.755143	-2.197462	1.269429
H	-5.818887	-3.405987	0.225336
H	-1.791301	5.573031	0.158024

Fc-P3.xyz

Fe	-4.383182	-2.076498	0.088078
C	-2.272186	-0.092632	-0.953098
C	-1.789524	1.117684	-0.579731
C	-0.361396	1.377706	-0.308924
C	-0.205517	2.703913	0.086566
C	-1.492352	3.341861	0.058012
C	-2.458415	2.414121	-0.346068
S	-2.145994	4.925829	0.275740
C	-3.731579	4.352033	-0.202062
C	-3.740137	3.016119	-0.508429
C	0.848943	0.648332	-0.279357
C	1.929659	1.415359	0.121773
S	1.434067	3.085373	0.476691
C	3.311452	1.026180	0.259159
S	3.910140	-0.446891	-0.492952
C	5.525359	-0.195489	0.154109
C	5.572453	0.981666	0.871433
C	4.334600	1.665815	0.931404
C	-4.044129	-2.208334	2.124590
H	-1.535227	-0.864994	-1.168249
H	-4.628967	2.503590	-0.850888
H	0.946154	-0.403471	-0.524350
H	6.472185	1.327049	1.367920
H	4.186992	2.589585	1.479052
C	-5.123923	-3.063997	1.749881
H	-6.144388	-2.989438	2.099020
C	-5.456699	-1.867273	-1.674234
C	-5.908099	-0.920540	-0.704914
C	-4.801915	-0.105114	-0.331178
C	-3.649742	-0.532897	-1.079317
C	-2.884088	-2.622598	1.404890
C	-3.246032	-3.732229	0.582636
C	-4.630982	-4.005740	0.797147
H	-5.212745	-4.768689	0.298868
C	-4.069091	-1.644591	-1.894751
H	-3.425742	-2.210302	-2.554625
H	-6.055449	-2.642940	-2.130717
H	-6.905822	-0.861990	-0.292755
H	-4.802144	0.658747	0.431447
H	-1.915392	-2.143061	1.438194
H	-4.102210	-1.369620	2.804100
H	-2.595069	-4.252307	-0.106285
C	6.580687	-1.151482	-0.099418
C	6.480810	-2.463167	-0.514230
S	8.269510	-0.707044	0.101721
C	7.739722	-3.110859	-0.660096
H	5.528028	-2.950312	-0.687498
C	8.796395	-2.297043	-0.356672
H	7.853046	-4.143267	-0.969716
H	9.851685	-2.531231	-0.374442
H	-4.561398	5.044508	-0.223051

SWCNT-FcP1.xyz

C	0.622916	0.326145	-4.216649
C	-0.257893	1.143868	-3.415046
C	0.404945	1.163395	0.823024
C	-1.509841	1.548261	-3.884298
C	-2.555584	1.793578	-2.958289
C	0.012341	1.193136	-2.010264
C	-0.856811	1.926382	-1.164556
C	-0.549663	2.040914	0.238077
C	-1.463374	2.693569	1.102494
C	-0.040117	2.144213	3.011824
C	-4.229444	0.564407	-4.415803
C	-3.857357	1.196120	-3.172532
C	-4.559536	0.785658	-2.011226
C	-2.187084	2.148392	-1.615594
C	-3.192623	2.253470	-0.601123
C	-2.843438	2.710036	0.713037
C	-3.820567	2.738650	1.739039
C	-1.117991	2.858390	2.481918
C	-2.120416	3.447909	3.337638
C	-4.838874	-0.655364	-4.419901
C	-5.038939	-1.348413	-3.168418
C	-5.095559	-0.544535	-1.984878
C	-5.206031	-1.182980	-0.723274
C	-4.353408	1.467609	-0.766290
C	-5.000081	1.002930	0.424151
C	-4.875300	1.750485	1.644815
C	-5.395251	1.168141	2.827780
C	-3.435493	3.352133	2.987564
C	-2.683406	-4.756261	-2.917497
C	-4.801557	-2.720011	-3.055903
C	-4.408155	-3.262841	-1.807393

C	-4.764675	-2.533650	-0.622184
C	-4.257071	-2.948931	0.650739
C	-5.327904	-0.382701	0.470138
C	-5.339181	-1.017086	1.738441
C	-5.523449	-0.219768	2.913458
C	-5.441495	-0.900563	4.184611
C	-1.328682	-4.770125	-3.073403
C	-0.498770	-4.121298	-2.085268
C	-3.281645	-4.170552	-1.742057
C	-2.466596	-4.079917	-0.586311
C	-3.029961	-3.646260	0.659542
C	-2.192088	-3.479235	1.809071
C	-4.694963	-2.293578	1.848643
C	-4.135793	-2.652152	3.100663
C	-4.733003	-2.062244	4.274423
C	0.584560	-3.324164	-2.464515
C	0.981939	-2.248902	-1.633114
C	-1.047347	-3.983161	-0.769892
C	-0.307764	-3.278172	0.214152
C	-0.820967	-3.183924	1.559470
C	-0.131190	-2.397948	2.517870
C	-2.776277	-3.150023	3.079599
C	-1.896507	-2.835193	4.146206
C	1.296462	-0.706708	-3.629843
C	1.195277	-0.937419	-2.209643
C	0.810625	0.166919	-1.411320
C	0.653590	-2.330792	-0.237377
C	0.886728	-1.204711	0.616774
C	0.670324	-1.312812	2.029389
C	0.825139	-0.175174	2.860647
C	-0.614967	-2.357655	3.865093
C	0.074477	-1.474996	4.780022
C	0.849748	0.070120	0.017409
C	0.552985	1.107390	2.250162
C	0.742452	-0.394385	4.285080
H	-0.085317	-1.583588	5.849183
H	1.128061	0.363744	4.959566
H	0.109156	2.174409	4.085618
H	-1.836710	3.808297	4.322531
H	-4.203268	3.640415	3.699172
H	-5.797446	-0.400998	5.081326
H	-4.527815	-2.492278	5.250027
H	-5.379307	1.729751	3.755822
H	-2.297692	-2.645501	5.136174
H	1.831165	-1.422246	-4.247079
H	0.613460	0.433533	-5.297779
H	-1.746471	1.348917	-4.924101
H	-3.924975	1.016244	-5.354999
H	-5.019132	-1.178905	-5.354671
H	-4.606404	-3.272960	-3.968643
H	-3.321350	-5.091127	-3.729759
H	-0.884194	-5.108708	-4.005182
H	0.873325	-3.330417	-3.510283
Fe	6.198503	-1.924665	-0.646156
C	4.078098	0.446173	-1.071087
C	3.890531	1.300978	-0.034894
C	3.193874	2.593854	-0.193144
C	3.004673	3.170777	1.061104
C	3.598635	2.309796	2.046448
C	4.127643	1.178003	1.416242
S	3.802464	2.266798	3.760230
C	4.628582	0.724319	3.639440
C	4.732192	0.283243	2.346148
C	2.431755	3.220498	-1.207363
C	1.651186	4.255265	-0.727234
S	1.907571	4.503649	1.010598
C	0.608136	4.978970	-1.417372
S	0.560045	5.051968	-3.171270
C	-0.972401	5.867994	-3.147424
C	-1.409521	6.082649	-1.868837
C	-0.516421	5.575794	-0.884021
C	7.443290	-1.788339	1.007730
H	3.854755	0.846984	-2.058156
H	5.215693	-0.643922	2.076257
H	2.363434	2.875866	-2.231905
H	-1.454264	6.139204	-4.076317
H	-2.348789	6.569706	-1.634335
H	-0.717349	5.594323	0.180574
C	7.867611	-2.852939	0.157196
H	7.915096	-3.899492	0.424123
C	5.011859	-3.044310	-1.932229
C	4.578006	-3.226834	-0.584832
C	4.213863	-1.958444	-0.057845
C	4.409570	-0.967223	-1.083684
C	7.483959	-0.576169	0.255268
C	7.938042	-0.891279	-1.060528
C	8.176977	-2.297740	-1.120492
H	8.497056	-2.851474	-1.992337
C	4.905529	-1.661397	-2.240800
H	5.178044	-1.189663	-3.175347
H	5.388998	-3.815794	-2.589015
H	4.552902	-4.163852	-0.046452

H	3.805253	-1.771903	0.922045
H	7.171342	0.398056	0.604727
H	7.126021	-1.889897	2.036053
H	8.042496	-0.193199	-1.879366
H	4.985325	0.241619	4.538358

SWCNT-FcP2.xyz

C	-2.289739	3.291101	3.229589
C	-1.245876	2.720376	2.412451
C	-2.197568	1.844119	-1.681716
C	-0.148260	2.072202	2.983998
C	0.510523	1.043746	2.265300
C	-1.554803	2.498988	1.032830
C	-0.595391	1.863713	0.206595
C	-0.868201	1.694036	-1.198114
C	0.051349	0.978454	-2.005286
C	-1.447881	1.207503	-3.917758
C	0.729228	-0.386867	4.347914
C	0.830020	-0.206068	2.919208
C	0.745143	-1.373872	2.120181
C	0.388821	1.050425	0.834798
C	0.900748	-0.043504	0.070826
C	0.884574	0.008694	-1.360783
C	1.334414	-1.099730	-2.118061
C	-0.188671	0.874656	-3.412779
C	0.744947	0.075817	-4.172841
C	0.101321	-1.482044	4.862797
C	-0.529000	-2.421657	3.962137
C	-0.016752	-2.479405	2.626070
C	-0.651585	-3.323466	1.679152
C	0.985143	-1.297414	0.709245
C	0.819474	-2.457749	-0.114667
C	1.170582	-2.402052	-1.506144
C	0.838907	-3.518340	-2.311876
C	1.453183	-0.906783	-3.542436
C	-4.663867	-2.300707	4.285182
C	-1.793441	-2.947813	4.233406
C	-2.636761	-3.333344	3.160576
C	-2.012987	-3.672871	1.911788
C	-2.819361	-3.911460	0.752443
C	-0.107804	-3.433916	0.347229
C	-0.795465	-4.200067	-0.628789
C	-0.215053	-4.352206	-1.928867
C	-0.995045	-5.067244	-2.911942
C	-5.422568	-1.176073	4.146822
C	-5.510738	-0.537922	2.854168
C	-4.017260	-2.896998	3.141181
C	-4.567051	-2.601670	1.868651
C	-4.076243	-3.271493	0.699632
C	-4.577223	-2.918327	-0.594478
C	-2.212344	-4.355628	-0.468905
C	-2.999294	-4.517756	-1.636245
C	-2.351906	-5.110184	-2.781857
C	-5.445232	0.851228	2.728316
C	-4.929719	1.421837	1.537630
C	-5.266611	-1.360322	1.707650
C	-5.260170	-0.764285	0.420899
C	-5.078161	-1.593230	-0.744958
C	-4.972485	-0.988286	-2.023401
C	-4.164426	-3.665187	-1.750075
C	-4.557621	-3.178692	-3.021659
C	-3.591641	3.127324	2.857586
C	-3.923133	2.459620	1.621664
C	-2.925271	2.444745	0.615672
C	-4.996126	0.633234	0.338393
C	-4.348001	1.091723	-0.853538
C	-4.497271	0.363894	-2.080421
C	-3.791691	0.771528	-3.240607
C	-4.855266	-1.823537	-3.180484
C	-4.662292	-1.159592	-4.448768
C	-3.227350	1.934112	-0.690143
C	-2.522305	1.432897	-3.019842
C	-4.109472	0.086639	-4.470685
H	-4.800059	-1.718433	-5.370221
H	-3.807387	0.523964	-5.417520
H	-1.654596	0.964280	-4.954663
H	0.751799	0.150256	-5.256800
H	2.033660	-1.614139	-4.126775
H	-0.517257	-5.412917	-3.824433
H	-2.957728	-5.497839	-3.595231
H	1.148444	-3.541976	-3.351427
H	-4.319578	-3.749016	-3.913277
H	-4.386211	3.404432	3.543623
H	-2.041590	3.696027	4.206597
H	-0.023182	2.140624	4.059205
H	1.065329	0.407865	5.006632
H	-0.074890	-1.566343	5.931564
H	-2.222434	-2.747468	5.209516
H	-4.458675	-2.691641	5.277089
H	-5.818585	-0.667055	5.021127
H	-5.474015	1.440770	3.638528
Fe	6.365047	-1.730446	-0.670602

C	4.115509	0.524497	-1.083806
C	3.888369	1.365961	-0.044805
C	3.117970	2.617846	-0.192590
C	2.910353	3.182652	1.065327
C	3.559036	2.352401	2.042307
C	4.143735	1.253226	1.403861
S	3.778501	2.315878	3.754263
C	4.686747	0.821963	3.621087
C	4.804115	0.390233	2.325813
C	2.303000	3.195162	-1.191644
C	1.462970	4.176906	-0.694603
S	1.721720	4.431266	1.042436
C	0.366515	4.812317	-1.383244
S	0.183583	4.707677	-3.130037
C	-1.398898	5.429852	-3.090303
C	-1.749397	5.741808	-1.812195
C	-0.758463	5.398119	-0.852393
C	7.610652	-1.534182	0.977069
H	3.862536	0.912540	-2.068908
H	5.334942	-0.508454	2.048823
H	2.243222	2.845778	-2.215175
H	-1.965685	5.596459	-3.993177
C	8.084205	-2.573373	0.121180
H	8.186960	-3.616765	0.384860
C	5.234849	-2.908434	-1.955028
C	4.815200	-3.116436	-0.606797
C	4.386157	-1.870230	-0.075920
C	4.526055	-0.868043	-1.100054
C	7.584653	-0.319615	0.227803
C	8.046637	-0.607607	-1.091396
C	8.357261	-1.999747	-1.156627
H	8.700343	-2.534060	-2.031826
C	5.054574	-1.532335	-2.260218
H	5.298562	-1.044816	-3.194525
H	5.650620	-3.657447	-2.614517
H	4.840959	-4.054637	-0.070547
H	3.969850	-1.707695	0.905138
H	7.224809	0.636366	0.582183
H	7.305340	-1.654522	2.007000
H	8.110457	0.096969	-1.908842
H	5.075753	0.356377	4.515685
F	-0.956329	5.591384	0.462357
F	-2.905955	6.308642	-1.446880

SWCNT-FcP3.xyz

C	-5.009403	0.139924	-3.767409
C	-4.891293	-1.086334	-3.010089
C	-4.617538	-0.748347	1.262167
C	-4.430657	-2.263974	-3.602228
C	-3.764628	-3.234170	-2.811509
C	-4.877348	-0.966050	-1.583133
C	-4.683934	-2.128690	-0.794164
C	-4.728318	-2.027169	0.644022
C	-4.439315	-3.168573	1.434519
C	-4.636667	-1.814738	3.457988
C	-2.039443	-3.642686	-4.627018
C	-2.520789	-3.811273	-3.277170
C	-1.553569	-4.110954	-2.285300
C	-4.031693	-3.240975	-1.400043
C	-3.269500	-4.088667	-0.533113
C	-3.602099	-4.180693	0.858881
C	-2.802040	-4.959861	1.731629
C	-4.546603	-3.073212	2.859327
C	-4.161546	-4.237107	3.622919
C	-0.737746	-3.312440	-4.864582
C	0.139303	-3.053169	-3.746750
C	-0.209107	-3.658523	-2.496822
C	0.571276	-3.365893	-1.348730
C	-1.967476	-4.437693	-0.951540
C	-0.989768	-4.663103	0.070770
C	-1.404932	-5.095647	1.376234
C	-0.421493	-5.145255	2.396480
C	-3.283622	-5.128968	3.081359
C	1.145773	0.961113	-3.547544
C	1.028438	-1.975427	-3.762982
C	1.396465	-1.359040	-2.541904
C	1.308344	-2.148095	-1.345397
C	1.509519	-1.530763	-0.068047
C	0.268453	-4.016466	-0.096995
C	0.983689	-3.651152	1.072506
C	0.717834	-4.344158	2.296995
C	1.410368	-3.874207	3.476435
C	0.230373	1.973792	-3.507957
C	-0.620752	2.115767	-2.350198
C	1.317722	0.081943	-2.417236
C	0.904155	0.577628	-1.156770
C	1.189905	-0.162196	0.036707
C	0.721145	0.308048	1.303066
C	1.537201	-2.328165	1.122673
C	1.657825	-1.706430	2.391005
C	1.832333	-2.578744	3.528241
C	-1.977060	2.428214	-2.469377

C	-2.882199	1.998893	-1.466850
C	-0.133487	1.563104	-1.122622
C	-0.952639	1.615683	0.032758
C	-0.441503	1.127170	1.288084
C	-1.288742	1.096238	2.422915
C	1.106286	-0.373702	2.506736
C	0.492534	0.034898	3.716715
C	-4.595097	1.311315	-3.206011
C	-4.111848	1.338055	-1.845882
C	-4.553287	0.298871	-0.989234
C	-2.355448	1.747710	-0.154582
C	-3.190847	1.168327	0.853275
C	-2.701498	1.014478	2.192460
C	-3.495648	0.363944	3.169277
C	-0.752047	0.668623	3.679417
C	-1.677933	0.571639	4.782976
C	-4.244941	0.341002	0.410434
C	-4.403258	-0.653438	2.679731
C	-3.004975	0.385325	4.526516
H	-1.293891	0.480020	5.795162
H	-3.680969	0.144943	5.341544
H	-4.551613	-1.764725	4.538378
H	-4.438414	-4.303021	4.671428
H	-2.862772	-5.913520	3.702829
H	1.437703	-4.499866	4.364277
H	2.206001	-2.165257	4.459917
H	-0.683399	-5.526924	3.377654
H	0.807669	-0.408293	4.655006
H	-4.530323	2.212951	-3.807460
H	-5.268912	0.093518	-4.821442
H	-4.302803	-2.268386	-4.679565
H	-2.744326	-3.676413	-5.452173
H	-0.403291	-3.077853	-5.871334
H	1.145914	-1.433565	-4.695523
H	1.674660	0.747822	-4.471454
H	0.024721	2.564719	-4.396278
H	-2.351786	2.702677	-3.449280
Fe	6.557343	-0.169053	-1.713212
C	4.008350	1.547536	-0.790348
C	3.864250	1.774542	0.539162
C	2.923657	2.781883	1.071034
C	2.855772	2.660744	2.458157
C	3.769806	1.630225	2.864856
C	4.378062	1.076216	1.732249
S	4.276041	0.863317	4.326620
C	5.338838	-0.198060	3.420537
C	5.291352	0.036639	2.071195
C	1.884509	3.576050	0.537244
C	1.010172	4.041352	1.505391
S	1.530496	3.543304	3.129123
C	-0.311405	4.581546	1.298493
S	-0.823464	5.087093	-0.303753
C	-2.507236	5.150972	0.185064
C	-2.625551	4.859730	1.528844
C	-1.397784	4.538582	2.153780
C	8.041183	-0.489380	-0.298539
H	3.539400	2.278613	-1.446587
H	5.881010	-0.515508	1.354409
H	1.694759	3.705955	-0.521047
H	-3.581584	4.828701	2.038734
H	-1.322589	4.196325	3.178830
C	8.483226	-0.922461	-1.584574
H	8.763463	-1.931245	-1.853974
C	5.374428	-0.844221	-3.281740
C	5.231916	-1.710064	-2.156083
C	4.750075	-0.943038	-1.061411
C	4.577945	0.417250	-1.501213
C	7.727375	0.900494	-0.382105
C	7.979816	1.327941	-1.720152
C	8.448843	0.202012	-2.462543
H	8.695643	0.192908	-3.515245
C	4.970288	0.458322	-2.883722
H	4.978769	1.348697	-3.497915
H	5.756387	-1.122838	-4.253976
H	5.471322	-2.763843	-2.130257
H	4.499771	-1.321007	-0.083374
H	7.317377	1.507115	0.413473
H	7.942199	-1.113687	0.578324
H	7.806053	2.320328	-2.112171
C	-3.548196	5.335370	-0.801441
C	-3.452616	5.831568	-2.084874
S	-5.173240	4.740270	-0.501035
C	-4.670763	5.750015	-2.817248
H	-2.533377	6.244268	-2.484612
C	-5.690404	5.190657	-2.095107
H	-4.786296	6.103789	-3.835332
H	-6.715287	5.025933	-2.397201
H	5.933909	-0.929605	3.948848

SWCNT.xyz

C	-4.146232	3.003129	1.133917
C	-3.095079	2.443854	1.951862

C	0.954343	3.071185	0.669757
C	-3.347234	1.386561	2.828242
C	-2.308061	0.474636	3.140813
C	-1.747811	2.722292	1.554570
C	-0.680262	2.129252	2.275096
C	0.680348	2.451758	1.923098
C	1.747909	1.785480	2.576485
C	3.347343	2.938364	1.135208
C	-3.887106	-1.501603	2.943886
C	-2.559645	-0.949249	3.070616
C	-1.484814	-1.755581	2.620189
C	-0.954244	0.934377	3.000954
C	0.130979	0.012314	3.147578
C	1.485012	0.483244	3.116537
C	2.559852	-0.437871	3.183797
C	3.095177	2.157092	2.264595
C	4.146326	1.390857	2.892866
C	-4.146179	-2.483542	2.034022
C	-3.095100	-2.912274	1.140628
C	-1.747793	-2.707387	1.580285
C	-0.680298	-3.035006	0.706413
C	-0.130739	-1.342017	2.847458
C	0.954422	-2.115687	2.324735
C	2.308266	-1.758092	2.645693
C	3.347382	-2.452401	1.976790
C	3.887308	0.116360	3.302377
C	-3.887306	-1.798502	-2.772221
C	-3.347336	-3.142697	-0.213171
C	-2.308233	-2.957359	-1.159275
C	-0.954387	-3.066214	-0.691310
C	0.130775	-2.732287	-1.563259
C	0.680344	-2.891580	1.161681
C	1.747823	-3.124292	0.257882
C	3.095139	-3.039912	0.735554
C	4.146228	-3.200979	-0.242211
C	-4.146337	-0.519569	-3.167666
C	-3.095190	0.468430	-3.092266
C	-2.559849	-2.184531	-2.357284
C	-1.484997	-1.391415	-2.830545
C	-0.130933	-1.795054	-2.585977
C	0.954280	-0.955526	-2.994485
C	1.484831	-2.940819	-1.139896
C	2.559666	-2.538556	-1.971294
C	3.887132	-2.918388	-1.550707
C	-3.347369	1.756097	-2.614925
C	-2.308210	2.482745	-1.981408
C	-1.747910	-0.014860	-3.134669
C	-0.680355	0.905648	-2.981329
C	0.680268	0.439643	-3.084831
C	1.747800	1.338655	-2.834438
C	2.308110	-1.412340	-2.845361
C	3.347295	-0.485932	-3.111936
C	-3.887233	3.300181	-0.171393
C	-2.559788	3.133867	-0.713160
C	-1.484929	3.147127	0.210321
C	-0.954389	2.131775	-2.309634
C	0.130811	2.719884	-1.584509
C	1.484850	2.457507	-1.976805
C	2.559685	2.976541	-1.212818
C	3.095092	0.882771	-3.000175
C	4.146184	1.810118	-2.650900
C	-0.130883	3.137117	-0.261547
C	2.308150	3.170553	0.199563
C	3.887120	2.802173	-1.752088
H	5.164110	1.609435	-2.973122
H	4.704780	3.398610	-1.358955
H	4.381462	3.069268	0.834656
H	5.164246	1.770273	2.880166
H	4.705007	-0.522345	3.622184
H	5.164154	-3.379767	0.092648
H	4.704764	-2.876063	-2.263827
H	4.381535	-2.257842	2.240490
H	4.381409	-0.811675	-3.074990
H	-4.704946	3.563112	-0.835519
H	-5.164148	3.023467	1.513011
H	-4.381345	1.098532	2.984803
H	-4.704747	-1.057936	3.503773
H	-5.164098	-2.822069	1.862225
H	-4.381487	-3.134544	-0.540776
H	-4.705020	-2.505112	-2.667839
H	-5.164265	-0.201457	-3.374803
H	-4.381505	2.035746	-2.443949

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