Supporting Information

for

On the reticular construction concept of covalent organic frameworks

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Detailed data of calculated COF parameters

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Table S1: The calculated bond lengths and angles of all studied COFs. Corresponding experimental values found from the literature are shown in brackets.

COF	Building Blocks	C-B	B-O	O-C	∠OBO
COF-1	**I-a**	1.498 (1.600)	1.393 (1.509)		120.3* (120.0)
COF-1M	**I-b**	1.497	1.393		120.3*
COF-2M	**I-c**	1.497	1.392		120.3*
COF-3M	**I-d**	1.496	1.392		120.1*
PPy-COF	**I-e**	1.498	1.393		120.2* (119.0)
COF-5	**II-a**	1.496 (1.530)	1.399 (1.367)	1.443 (1.384)	113.5† (113.9)
COF-10	**II-b**	1.495 (1.553)	1.399 (1.465)	1.443 (1.385)	113.5† (112.0)
COF-8	**II-c**	1.495 (1.548)	1.399 (1.479)	1.443	113.5†
COF-6	**II-d**	1.496	1.399	1.443	113.5†
TP COF	**II-e**	1.496 (1.542)	1.399 (1.396)	1.444 (1.377)	113.5† (118.2)
COF-4M	**III-a**	1.496	1.398	1.449	113.5†
COF-5M	**III-b**	1.496	1.398	1.449	113.6†
COF-6M	**III-c**	1.496	1.399	1.451	113.4†
COF-7M	**III-d**	1.496	1.398	1.449	113.6†
TP COF-1M	**III-e**	1.496	1.398	1.450	113.6†
COF-8M	**IV-a**	1.496	1.398	1.445	113.1†
COF-9M	**IV-b**	1.495	1.398	1.444	113.1†
COF-10M	**IV-c**	1.495	1.391	1.418	112.6†
COF-11M	**IV-d**	1.498	1.399	1.450	113.4†
TP COF-2M	**IV-e**	1.499	1.399	1.447	113.4†

*B_3O_3 connectivity
†C_2B_2O connectivity

It should be noted that the bond lengths of experimentally known COF-1 are much larger compared to our optimized bond lengths as well as that of other synthesized COFs.

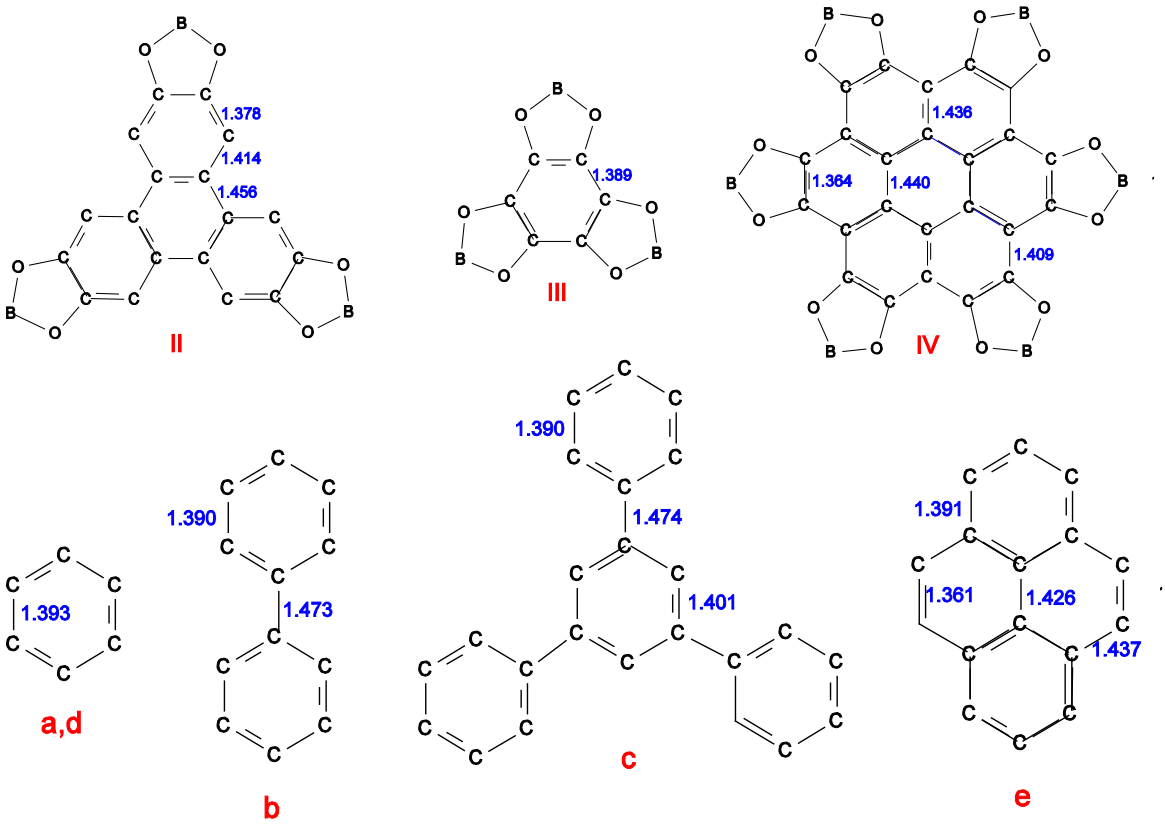

Figure S2: Calculated C-C bond lengths in connectors and linkers. Hydrogen atoms are omitted for clarity.

Table S3: The calculated unit cell parameters a [Å], interlayer distance d [Å] and mass density ρ [g·cm^{-3}] for serrated (S_a: serrated armchair, S_z: serrated zigzag) and inclined (I_a: inclined armchair, I_z: inclined zigzag) stacked COFs.

COF	Building Blocks	a	d				ρ			
			S_a	S_z	I_a	I_z	S_a	S_z	I_a	I_z
COF-1	**I-a**	15.02		3.43		3.43		0.97		0.97
COF-1M	**I-b**	22.41		3.41		3.42		0.69		0.69
COF-2M	**I-c**	14.92		3.40		3.39		0.97		0.97
COF-3M	**I-d**	07.47		3.41		3.42		1.57		1.56
PPy-COF	**I-e**	22.32		3.41		3.41		0.86		0.86
COF-5	**II-a**	30.14	3.42	3.42	3.41	3.40	0.57	0.57	0.58	0.58
COF-10	**II-b**	37.58	3.41	3.41	3.42	3.40	0.46	0.46	0.46	0.46
COF-8	**II-c**	22.51	3.41	3.41	3.42	3.42	0.73	0.73	0.72	0.72
COF-6	**II-d**	15.05	3.42	3.41	3.40	3.40	1.05	1.06	1.06	1.06
TP COF	**II-e**	37.50	3.42	3.41	3.42	3.42	0.52	0.52	0.52	0.52
COF-4M	**III-a**	21.71	3.44	3.44	3.45	3.44	0.74	0.74	0.74	0.74
COF-5M	**III-b**	29.15	3.43	3.42	3.43	3.43	0.56	0.56	0.56	0.56
COF-6M	**III-c**	18.33	3.41	3.41	3.42	3.41	0.84	0.84	0.84	0.84

COF-7M	**III-d**	10.83	3.44	3.43	3.40	3.44	1.31	1.31	1.32	1.31
TP COF-1M	**III-e**	29.05	3.43	3.42	3.43	3.42	0.66	0.67	0.66	0.66
COF-8M	**IV-a**	17.48	3.41	3.41	3.42	3.42	1.42	1.42	1.42	1.42
COF-9M	**IV-b**	21.76	3.41	3.41	3.41	3.42	1.19	1.19	1.19	1.19
COF-10M	**IV-c**	22.54	3.40	3.40	3.40	3.40	1.28	1.28	1.28	1.28
COF-11M	**IV-d**	15.12	3.41	3.41	3.40	3.40	1.71	1.71	1.71	1.71
TP COF-2M	**IV-e**	21.73	3.40	3.40	3.40	3.40	1.37	1.37	1.37	1.37
REF-I	**I**	07.73		3.49		3.45		1.48		1.5
REF-III	**III**	14.45	3.48		3.49		1.06		1.06	

Table S4: The calculated energies [kJ·mol^{-1}] per bond formed between building blocks for serrated (S_a: serrated armchair, S_z: serrated zigzag) and inclined (I_a: inclined armchair, I_z: inclined zigzag) stacked COFs: $E_{c,b}$ is the condensation energy, $E_{s,b}$ is the stacking energy, and $E_{f,b}$ is the COF formation energy ($E_{f,b} = E_{c,b} + E_{s,b}$). The calculated band gaps, Δ [eV], are given as well.

COF	**S_a**			**S_z**			**I_a**			**I_z**		
	$E_{s,b}$	**$E_{f,b}$**	**Δ**	**$E_{s,b}$**	**$E_{f,b}$**	**Δ**	**$E_{s,b}$**	**$E_{f,b}$**	**Δ**	**$E_{s,b}$**	**$E_{f,b}$**	**Δ**
-1				-28.10	-19.04	3.6				-27.86	-18.80	3.6
-1M				-44.26	-34.77	3.0				-43.89	-34.40	3.0
-2M				-59.67	-50.11	3.0				-58.33	-48.77	3.0
-3M				-26.67	-19.04	4.0				-25.91	-18.28	4.0
PPy-				-59.16	-50.58	2.6				-58.65	-50.07	2.6
-5	-30.52	-28.41	2.7	-30.51	-28.40	2.6	-32.75	-30.64	2.6	-32.97	-30.86	2.6
-10	-38.68	-35.51	2.6	-38.69	-35.52	2.5	-38.30	-35.13	2.6	-42.93	-39.76	2.5
-8	-46.15	-43.52	2.7	-46.14	-43.51	2.7	-45.71	-43.08	2.7	-45.73	-43.10	2.7
-6	-29.78	-27.93	3.0	-29.78	-27.93	3.0	-31.17	-29.32	3.0	-30.90	-29.05	3.0
TP	-45.57	-43.26	2.6	-45.62	-43.31	2.6	-45.11	-42.80	2.6	-45.11	-42.80	2.6
-4M	-18.11	-18.44	2.8	-18.13	-18.46	2.8	-17.69	-18.02	2.8	-18.80	-19.13	2.8
-5M	-26.26	-26.19	2.7	-26.30	-26.23	2.6	-25.97	-25.90	2.6	-26.00	-25.93	2.6
-6M	-33.75	-33.61	2.8	-33.81	-33.67	2.8	-34.87	-34.73	2.8	-33.49	-33.35	2.8
-7M	-17.24	-18.94	3.2	-17.26	-18.96	3.1	-23.33	-25.03	3.2	-18.66	-20.36	3.1
TP -1M	-33.27	-33.41	2.6	-33.34	-33.48	2.6	-33.40	-33.54	2.6	-33.53	-33.67	2.6
-8M	-28.97	-36.84	2.1	-28.95	-36.82	2.1	-29.71	-37.58	2.1	-29.83	-37.70	2.1
-9M	-37.32	-45.68	2.0	-37.33	-45.69	2.0	-36.84	-45.20	2.0	-37.06	-45.42	2.0
-10M	-45.12	-54.59	2.1	-45.13	-54.60	2.1	-44.91	-54.38	2.1	-44.95	-54.42	2.1
-11M	-28.31	-32.34	2.4	-28.34	-32.37	2.4	-28.16	-32.19	2.4	-28.30	-32.33	2.4
TP -2M	-45.00	-44.70	2.0	-45.05	-44.75	2.0	-44.95	-44.65	2.0	-44.96	-44.66	2.0

Cartesian coordinates of COF structures

COF-1

Layer I AA, AB, inclined zigzag, and serrated zigzag

C	9.619348	10.595180	0.794835	O	7.077028	12.043170	0.794935
C	9.578448	12.001080	0.795055	B	20.837220	12.738170	0.794775
C	10.816200	12.669210	0.795125	O	13.344850	1.168948	0.794905
C	12.018110	11.975350	0.794975	C	19.541290	11.986090	0.794485
C	12.058630	10.569420	0.794755	C	19.501730	10.580210	0.794805
C	10.821120	9.901537	0.794675	C	18.300440	9.885317	0.794835
B	13.354240	9.816797	0.794755	C	17.062330	10.552590	0.794485
O	14.561420	10.511340	0.794555	C	17.101900	11.958400	0.794135
B	15.762870	9.806707	0.794585	C	18.303200	12.653190	0.794105
O	15.760730	8.414117	0.794805	H	10.802260	0.793766	0.793905
B	14.549710	7.726126	0.794905	H	16.154750	12.522810	0.793925
O	13.344650	8.424098	0.794875	H	20.448893	10.015360	0.795205
C	14.545390	6.227821	0.795005	H	18.317090	8.782715	0.795225
C	15.742780	5.490328	0.795455	H	16.706014	3.565474	0.795925
C	15.743230	4.102874	0.795535	H	16.705240	6.028351	0.795805
C	14.546280	3.364655	0.795125	H	12.385610	3.564683	0.794525
C	13.348490	4.102057	0.794755	H	12.384980	6.026808	0.794405
C	13.348090	5.489797	0.794675	H	12.964940	12.540800	0.795055
B	14.550290	1.866363	0.795105	H	3.348885	0.809891	0.795325
O	0.793766	1.177789	0.795225	H	10.805050	8.798943	0.794505
B	8.279047	12.747040	0.795055	H	8.672658	10.029870	0.794755

Transformation Matrix

a	14.967120	0.000000	0.000000	
b	7.483560	12.961900	0.000000	
c	0.000000	0.000000	3.505888	AA stacking
c	1.204480	0.695407	3.432429	Inclined zigzag stacking

Layer II AB stacking

C	17.10291	14.91582	3.922080	O	14.56059	16.36381	3.922180
C	17.06201	16.32171	3.922300	B	28.32078	17.05881	3.922020
C	18.29976	16.98985	3.922370	O	20.82841	5.489583	3.922150
C	19.50167	16.29599	3.922220	C	27.02485	16.30672	3.921730
C	19.54219	14.89005	3.922000	C	26.98529	14.90084	3.922050
C	18.30468	14.22217	3.921920	C	25.78400	14.20595	3.922080
B	20.83780	14.13743	3.922000	C	24.54589	14.87323	3.921730
O	22.04498	14.83198	3.921800	C	24.58546	16.27904	3.921380
B	23.24643	14.12734	3.921830	C	25.78676	16.97383	3.921350
O	23.24429	12.73475	3.922050	H	18.28582	5.114401	3.921150
B	22.03327	12.04676	3.922150	H	23.63831	16.84344	3.921170
O	20.82821	12.74473	3.922120	H	27.93245	14.33599	3.922450
C	22.02895	10.54846	3.922250	H	25.80065	13.10335	3.922470
C	23.22634	9.810963	3.922700	H	24.18958	7.886109	3.923170
C	23.22679	8.423510	3.922780	H	24.18880	10.34899	3.923050
C	22.02984	7.685290	3.922370	H	19.86917	7.885318	3.921770
C	20.83205	8.422692	3.922000	H	19.86854	10.34744	3.921650
C	20.83165	9.810432	3.921920	H	20.44850	16.86143	3.922300

B	22.03385	6.186998	3.922350	H	10.83245	5.130527	3.922570
O	8.277327	5.498425	3.922470	H	18.28861	13.11958	3.921750
B	15.76261	17.06767	3.922300	H	16.15622	14.35051	3.922000
c	0.00000	0.00000	6.25449	AB stacking			

Layer II serrated zigzag

C	10.82383	11.29059	4.22064	O	8.28151	12.73858	4.220743
C	10.78293	12.69649	4.22086	B	14.55814	0.47168	4.220583
C	4.53712	0.40272	4.22093	O	14.54933	1.86436	4.220713
C	13.22259	12.67076	4.22078	C	20.74577	12.68150	4.220293
C	13.26311	11.26483	4.22056	C	20.70621	11.27562	4.220613
C	12.02560	10.59694	4.22048	C	19.50492	10.58072	4.220643
B	14.55872	10.51220	4.22056	C	18.26681	11.24800	4.220293
O	15.76590	11.20675	4.22036	C	18.30638	12.65381	4.219943
B	16.96735	10.50211	4.22039	C	12.02412	0.38670	4.219913
O	16.96521	9.109524	4.22061	H	12.00674	1.48917	4.219713
B	15.75419	8.421534	4.22071	H	9.87567	0.25632	4.219733
O	14.54913	9.119505	4.22068	H	6.68625	10.71077	4.221013
C	15.74987	6.923228	4.22081	H	19.52157	9.47812	4.221033
C	16.94726	6.185735	4.22126	H	2.94337	4.26088	4.221733
C	16.94771	4.798281	4.22134	H	17.90972	6.72376	4.221613
C	15.75076	4.060062	4.22093	H	13.59009	4.26009	4.220333
C	14.55297	4.797464	4.22056	H	13.58946	6.72222	4.220213
C	14.55257	6.185204	4.22048	H	6.68586	0.27431	4.220863
B	15.75477	2.561770	4.22091	H	4.55336	1.50530	4.221133
O	1.99824	1.873196	4.22103	H	12.00953	9.49435	4.220313
B	1.99996	0.480550	4.22086	H	9.87713	10.72528	4.220563
c	0.00000	0.00000	6.85162	serrated zigzag stacking			

COF-1M

Layer 1 AA, AB, inclined zigzag, and serrated zigzag

C	13.308650	18.473020	0.793916	C	30.716500	18.434470	0.793956
C	13.353690	17.065480	0.793986	C	29.475080	19.099230	0.794056
C	14.555950	16.375820	0.794016	C	28.276480	18.403170	0.794086
C	15.780570	17.061520	0.793986	C	28.257560	16.999700	0.794016
C	15.750000	18.464710	0.793916	C	29.488090	16.324470	0.793886
C	14.544160	19.149250	0.793886	C	30.683890	17.026430	0.793856
C	17.052200	16.327260	0.794016	C	26.985690	16.265890	0.794036
C	17.070910	14.923690	0.793956	C	25.761130	16.951880	0.794016
C	18.269480	14.227490	0.793986	C	24.558700	16.262460	0.794036
C	19.510870	14.892130	0.794086	C	24.513430	14.854960	0.794086
C	19.478510	16.300090	0.794156	C	25.748740	14.178540	0.794116
C	18.282860	17.002340	0.794116	C	26.954810	14.862670	0.794086
B	20.802320	14.134430	0.794116	H	29.494620	15.220760	0.793836
O	22.012470	14.824880	0.794116	H	31.634540	16.467970	0.793766
B	23.211630	14.115310	0.794086	H	18.251610	0.7937660	0.794136
O	23.204290	12.722200	0.794056	H	27.317800	18.950490	0.794186
B	21.990370	12.038150	0.794056	H	25.756300	13.076080	0.794156
O	20.787410	12.741060	0.794086	H	27.907290	14.304970	0.794116
C	21.982510	10.540880	0.794056	H	25.767000	18.055760	0.793956
C	20.781510	9.8055030	0.794186	H	23.613390	16.829830	0.794016

C	20.775990	8.4189450	0.794216	H	24.137390	7.8620570	0.793916
C	21.977800	7.6939080	0.794116	H	24.143150	10.339540	0.793856
C	23.181970	8.4150640	0.793986	H	19.820850	10.346510	0.794286
C	23.180960	9.8012530	0.793956	H	19.818810	7.8691800	0.794286
C	21.977530	6.2254730	0.794116	H	24.142280	3.5794100	0.794116
C	20.775510	5.5006680	0.794086	H	24.137150	6.0568960	0.794136
C	20.780750	4.1141150	0.794056	H	19.818420	6.0505690	0.794086
C	21.981650	3.3785580	0.794056	H	19.819910	3.5732960	0.794036
C	23.180230	4.1179380	0.794116	H	16.702580	19.022280	0.793886
C	23.181600	5.5041230	0.794116	H	3.3468080	0.8438770	0.793806
B	21.989840	1.8812640	0.794016	H	12.408250	16.498420	0.794016
O	0.7937660	1.1976820	0.793986	H	14.561560	15.271920	0.794056
B	12.006670	19.212400	0.793936	H	20.429200	16.858450	0.794236
O	10.807840	18.502380	0.793886	H	18.289510	18.105990	0.794156
B	32.007720	19.192370	0.793956	H	16.112210	14.376520	0.793886
O	20.787130	1.1779250	0.794016	H	18.250840	13.125110	0.793936

Transformation Matrix

a	22.410240	0.000000	0.000000	
b	11.205120	19.407830	0.000000	
c	0.000000	0.000000	3.490500	AA
c	1.199740	0.692670	3.41658	inclined zigzag

Layer II AB stacking

C	24.51377	24.94230	3.830658	C	41.92162	24.90375	3.830698
C	24.55881	23.53476	3.830728	C	40.68020	25.56851	3.830798
C	25.76107	22.84510	3.830758	C	39.48160	24.87245	3.830828
C	26.98569	23.53080	3.830728	C	39.46268	23.46898	3.830758
C	26.95512	24.93399	3.830658	C	40.69321	22.79375	3.830628
C	25.74928	25.61853	3.830628	C	41.88901	23.49571	3.830598
C	28.25732	22.79654	3.830758	C	38.19081	22.73517	3.830778
C	28.27603	21.39297	3.830698	C	36.96625	23.42116	3.830758
C	29.47460	20.69677	3.830728	C	35.76382	22.73174	3.830778
C	30.71599	21.36141	3.830828	C	35.71855	21.32424	3.830828
C	30.68363	22.76937	3.830898	C	36.95386	20.64782	3.830858
C	29.48798	23.47162	3.830858	C	38.15993	21.33195	3.830828
B	32.00744	20.60371	3.830858	H	40.69974	21.69004	3.830578
O	33.21759	21.29416	3.830858	H	42.83966	22.93725	3.830508
B	34.41675	20.58459	3.830828	H	29.45673	7.263045	3.830878
O	34.40941	19.19148	3.830798	H	38.52292	25.41977	3.830928
B	33.19549	18.50743	3.830798	H	36.96142	19.54536	3.830898
O	31.99253	19.21034	3.830828	H	39.11241	20.77425	3.830858
C	33.18763	17.01016	3.830798	H	36.97212	24.52504	3.830698
C	31.98663	16.27478	3.830928	H	34.81851	23.29911	3.830758
C	31.98111	14.88822	3.830958	H	35.34251	14.33134	3.830658
C	33.18292	14.16319	3.830858	H	35.34827	16.80882	3.830598
C	34.38709	14.88434	3.830728	H	31.02597	16.81579	3.831028
C	34.38608	16.27053	3.830698	H	31.02393	14.33846	3.831028
C	33.18265	12.69475	3.830858	H	35.34740	10.04869	3.830858
C	31.98063	11.96995	3.830828	H	35.34227	12.52618	3.830878
C	31.98587	10.58340	3.830798	H	31.02354	12.51985	3.830828
C	33.18677	9.847837	3.830798	H	31.02503	10.04258	3.830778
C	34.38535	10.58722	3.830858	H	27.90770	25.49156	3.830628
C	34.38672	11.97340	3.830858	H	14.55193	7.313156	3.830548
B	33.19496	8.350543	3.830758	H	23.61337	22.96770	3.830758
O	11.99889	7.666961	3.830728	H	25.76668	21.74120	3.830798
B	23.21179	25.68168	3.830678	H	31.63432	23.32773	3.830978

O	22.01296	24.97166	3.830628	H	29.49463	24.57527	3.830898
B	43.21284	25.66165	3.830698	H	27.31733	20.84580	3.830628
O	31.99225	7.647204	3.830758	H	29.45596	19.59439	3.830678
c	0.00000	0.00000	6.073485	AB			

Layer II serrated zigzag

C	14.50839	19.165690	4.207076	C	31.91624	19.127140	4.207116
C	14.55343	17.758150	4.207146	C	19.46970	0.384070	4.207216
C	15.75569	17.068490	4.207176	C	29.47622	19.095840	4.207246
C	16.98031	17.754190	4.207146	C	29.45730	17.692370	4.207176
C	16.94974	19.157380	4.207076	C	30.68783	17.017140	4.207046
C	4.53878	0.434090	4.207046	C	31.88363	17.719100	4.207016
C	18.25194	17.019930	4.207176	C	28.18543	16.958560	4.207196
C	18.27065	15.616360	4.207116	C	26.96087	17.644550	4.207176
C	19.46922	14.920160	4.207146	C	25.75844	16.955130	4.207196
C	20.71061	15.584800	4.207246	C	25.71317	15.547630	4.207246
C	20.67825	16.992760	4.207316	C	26.94848	14.871210	4.207276
C	19.48260	17.695010	4.207276	C	28.15455	15.555340	4.207246
B	22.00206	14.827100	4.207276	H	30.69436	15.913430	4.206996
O	23.21221	15.517550	4.207276	H	10.42404	17.160640	4.206926
B	24.41137	14.807980	4.207246	H	19.45135	1.486436	4.207296
O	24.40403	13.414870	4.207216	H	17.31242	0.235330	4.207346
B	23.19011	12.730820	4.207216	H	26.95604	13.768750	4.207316
O	21.98715	13.433730	4.207246	H	29.10703	14.997640	4.207276
C	23.18225	11.233550	4.207216	H	26.96674	18.748430	4.207116
C	21.98125	10.498170	4.207346	H	24.81313	17.522500	4.207176
C	21.97573	9.111615	4.207376	H	25.33713	8.554728	4.207076
C	23.17754	8.386579	4.207276	H	25.34289	11.032210	4.207016
C	24.38171	9.107734	4.207146	H	21.02059	11.039180	4.207446
C	24.38070	10.493920	4.207116	H	21.01855	8.561851	4.207446
C	23.17727	6.918143	4.207276	H	2.93178	4.272080	4.207276
C	21.97525	6.193338	4.207246	H	25.33689	6.749566	4.207296
C	21.98049	4.806785	4.207216	H	21.01816	6.743239	4.207246
C	23.18139	4.071228	4.207216	H	21.01965	4.265966	4.207196
C	24.37997	4.810608	4.207276	H	6.69720	0.307120	4.207046
C	24.38134	6.196793	4.207276	H	4.54654	1.536547	4.206966
B	23.18958	2.573934	4.207176	H	13.60799	17.191090	4.207176
O	1.99350	1.890352	4.207146	H	15.76130	15.964590	4.207216
B	2.00129	0.497240	4.207096	H	21.62894	17.551120	4.207396
O	12.00758	19.195050	4.207046	H	19.48925	18.798660	4.207316
B	22.00234	0.477210	4.207116	H	17.31195	15.069190	4.207046
O	21.98687	1.870595	4.207176	H	19.45058	13.817780	4.207096
c	0.00000	0.00000	6.82632	serrated zigzag			

COF-2M

Layer I AA, AB, inclined zigzag, and serrated zigzag

C	11.63233	6.210753	0.7964430	C	15.34072	12.66828	0.7999130
C	11.65635	7.613939	0.7969330	B	6.679040	3.364680	0.7965130
C	10.42911	8.294092	0.7959630	O	5.473729	4.063492	0.7958130
C	9.230199	7.598482	0.7947130	B	5.483906	5.456936	0.7949830

C	9.191589	6.190721	0.7944630	O	6.691520	6.151705	0.7942130
C	10.43006	5.520183	0.7952130	B	7.892957	5.445951	0.7944430
C	12.92817	8.352868	0.7981430	O	7.890639	4.052802	0.7953330
C	12.94053	9.753651	0.7989330	H	15.71660	5.673431	0.7978830
C	14.14200	10.47344	0.7995930	H	5.097457	8.180507	0.7954630
C	15.34868	9.762103	0.7995430	H	2.940189	4.434942	0.7955330
C	15.37087	8.361876	0.7987630	H	4.513570	1.667730	0.7984630
C	14.15196	7.672185	0.7981130	H	11.97939	12.11415	0.7994830
C	16.64636	7.629460	0.7979830	H	16.29746	12.11740	0.8004930
C	16.67207	6.226597	0.7973630	H	8.836130	1.671500	0.7994130
C	17.87467	5.537436	0.7961330	H	8.281958	8.161122	0.7939330
C	4.189492	6.208918	0.7954930	H	12.58784	5.657948	0.7971830
C	19.07268	7.616718	0.7960630	H	10.42946	9.397904	0.7962930
C	17.87288	8.311345	0.7973630	H	11.98042	10.30233	0.7988130
C	14.13856	11.94442	0.7997130	H	16.30454	10.31815	0.7999130
C	12.93522	12.66636	0.7993630	H	14.15703	6.566486	0.7973130
C	5.475680	1.129270	0.7987630	H	10.44329	4.417712	0.7948630
C	6.675010	1.867690	0.7983630	H	17.87189	9.415222	0.7978830
C	7.875200	1.130860	0.7992630				

Transformation matrix

a	14.922830	0.000000	0.000000	
b	7.461410	12.923540	0.000000	
c	0.000000	0.000000	3.474490	AA
c	1.221360	0.705152	3.392639	inclined zigzag

Layer II AB stacking

C	19.09374	10.51860	3.913061	C	22.80214	16.97613	3.916531
C	19.11777	11.92179	3.913551	B	14.14046	7.672530	3.913131
C	17.89052	12.60194	3.912581	O	12.93514	8.371342	3.912431
C	16.69161	11.90633	3.911331	B	12.94532	9.764786	3.911601
C	16.65300	10.49857	3.911081	O	14.15294	10.45955	3.910831
C	17.89148	9.828033	3.911831	B	15.35437	9.753801	3.911061
C	20.38959	12.66072	3.914761	O	15.35205	8.360652	3.911951
C	20.40195	14.06150	3.915551	H	23.17801	9.981281	3.914501
C	21.60341	14.78129	3.916211	H	12.55887	12.48836	3.912081
C	22.81009	14.06995	3.916161	H	10.40160	8.742792	3.912151
C	22.83228	12.66973	3.915381	H	11.97499	5.975580	3.915081
C	21.61337	11.98003	3.914731	H	19.44081	16.42200	3.916101
C	24.10777	11.93731	3.914601	H	23.75887	16.42525	3.917111
C	24.13348	10.53445	3.913981	H	16.29754	5.979350	3.916031
C	25.33608	9.845285	3.912751	H	15.74337	12.46897	3.910551
C	11.65091	10.51677	3.912111	H	20.04926	9.965797	3.913801
C	26.53409	11.92457	3.912681	H	17.89087	13.70575	3.912911
C	25.33429	12.61919	3.913981	H	19.44184	14.61018	3.915431
C	21.59998	16.25227	3.916331	H	23.76595	14.62600	3.916531
C	20.39664	16.97421	3.915981	H	21.61844	10.87434	3.913931
C	12.93709	5.437120	3.915381	H	17.90471	8.725562	3.911481
C	14.13643	6.175540	3.914981	H	25.33331	13.72307	3.914501
C	15.33661	5.438710	3.915881				

c	0.00000	0.00000	6.23324	AB

Layer II serrated zigzag

C	12.85369	6.915905	4.192503	C	9.10067	0.449890	4.195973
C	12.87771	8.319091	4.192993	B	7.90040	4.069832	4.192573
C	11.65047	8.999244	4.192023	O	6.69509	4.768644	4.191873

C 10.45156 8.303634 4.190773 B 6.70527 6.162088 4.191043
C 10.41295 6.895873 4.190523 O 7.91288 6.856857 4.190273
C 11.65142 6.225335 4.191273 B 9.11432 6.151103 4.190503
C 14.14953 9.058020 4.194203 O 9.11199 4.757954 4.191393
C 14.16189 10.458800 4.194993 H 16.93796 6.378583 4.193943
C 15.36336 11.178590 4.195653 H 6.31882 8.885658 4.191523
C 16.57004 10.467250 4.195603 H 4.16155 5.140094 4.191593
C 16.59223 9.067027 4.194823 H 5.73493 2.372882 4.194523
C 15.37332 8.377337 4.194173 H 13.20075 12.819300 4.195543
C 17.86772 8.334612 4.194043 H 17.51882 12.822550 4.196553
C 17.89343 6.931749 4.193423 H 10.05749 2.376652 4.195473
C 4.17320 6.242588 4.192193 H 9.50332 8.866274 4.189993
C 5.41085 6.914070 4.191553 H 13.80920 6.363100 4.193243
C 5.37121 8.321870 4.192123 H 11.65082 10.103060 4.192353
C 19.09424 9.016497 4.193423 H 13.20178 11.007480 4.194873
C 15.35992 12.649570 4.195773 H 17.52590 11.023300 4.195973
C 6.69517 0.447970 4.195423 H 15.37839 7.271638 4.193373
C 6.69704 1.834422 4.194823 H 11.66465 5.122864 4.190923
C 7.89637 2.572842 4.194423 H 19.09325 10.120370 4.193943
C 9.09656 1.836012 4.195323
c 0.00000 0.00000 6.79212 serrated zigzag

COF-3M

Layer I AA, AB, inclined zigzag, and serrated zigzag

C 5.821692 5.488254 0.793766
C 5.859315 4.085139 0.793766
C 7.057359 3.353438 0.793766
C 8.253873 4.087584 0.793766
C 8.288739 5.490777 0.793766
C 7.054536 6.159733 0.793766
B 7.057135 1.856436 0.793766
O 5.849398 1.162547 0.793766
B 9.585465 6.238942 0.793766
O 3.319859 5.539076 0.793766
B 4.525276 6.236943 0.793766
O 0.7937660 1.160613 0.793766
H 9.210704 3.538126 0.793766
H 4.903924 3.533164 0.793766
H 3.318080 0.7937660 0.793766

Transformation matrix

a 7.469940 0.000000 0.000000
b 3.734970 6.469160 0.000000
c 0.000000 0.000000 3.488410 AA
c 1.197280 0.691250 3.420000 Inclined zigzag

Layer II AB stacking

C 9.556662 7.644640 4.062411
C 9.594285 6.241525 4.062411
C 10.79233 5.509824 4.062411
C 11.98884 6.243970 4.062411
C 12.02371 7.647163 4.062411
C 10.78951 8.316119 4.062411

B	10.79210	4.012822	4.062411
O	9.584368	3.318933	4.062411
B	13.32044	8.395329	4.062411
O	7.054829	7.695462	4.062411
B	8.260246	8.393329	4.062411
O	4.528736	3.316999	4.062411
H	12.94567	5.694512	4.062411
H	8.638894	5.689550	4.062411
H	7.053050	2.950152	4.062411
c	0.00000	0.00000	6.53729 AB

Layer II serrated zigzag

C	7.018972	6.179504	4.206926
C	7.056595	4.776389	4.206926
C	8.254640	4.044688	4.206926
C	9.451153	4.778834	4.206926
C	9.486019	6.182027	4.206926
C	4.516846	0.381823	4.206926
B	8.254416	2.547686	4.206926
O	7.046678	1.853797	4.206926
B	7.047780	0.461032	4.206926
O	4.517139	6.230326	4.206926
B	1.987586	0.459033	4.206926
O	1.991046	1.851863	4.206926
H	2.938040	4.229376	4.206926
H	6.101204	4.224414	4.206926
H	4.515360	1.485016	4.206926
c	0.00000	0.00000	6.82632 serrated zigzag

PPy-COF

Layer I AA, AB, inclined zigzag, and serrated zigzag

C	11.35865	16.45284	0.793925	C	21.18579	2.159241	0.7941000	C	22.44165	5.668580	0.7939750
C	11.38651	15.04819	0.793975	C	21.21311	3.560100	0.7941000	H	22.13766	8.368893	0.7938500
C	12.58565	14.32387	0.794000	B	31.15145	19.26523	0.7940250	H	17.82290	8.369067	0.7943000
C	13.82106	15.03222	0.793975	O	32.36685	18.58465	0.7939750	C	17.52082	5.666763	0.7942250
C	13.81621	16.45653	0.793925	B	10.05600	17.19214	0.7939250	H	22.13976	1.606842	0.7941250
C	12.58860	17.13289	0.793875	O	31.17973	16.47913	0.7939000	C	22.44209	4.307889	0.7940500
C	15.05371	14.31962	0.794025	B	29.96877	17.16670	0.7939500	C	17.52160	4.305840	0.7941750
C	15.05690	12.89544	0.793975	O	29.95041	18.55973	0.7940000	H	17.82505	1.604832	0.7940250
C	16.28348	12.21823	0.793975	C	28.67703	16.40861	0.7939500	C	15.07907	17.14633	0.7939750
C	17.51485	12.89589	0.794075	C	27.44604	17.08635	0.7940750	H	12.58726	18.23522	0.7938000
C	17.48922	14.30122	0.794150	C	26.21960	16.40935	0.7940750	H	10.43102	14.49862	0.7940500
C	16.29005	15.02674	0.794100	C	26.21594	14.98518	0.7940000	C	12.61698	12.88572	0.7939750
B	18.80745	12.13886	0.794100	C	27.45222	14.27783	0.7939250	H	18.44503	14.85062	0.7942500
O	20.01934	12.82580	0.794100	C	28.65134	15.00327	0.7938750	C	16.25751	16.46517	0.7940750
B	21.21724	12.11402	0.794075	C	24.98299	14.27328	0.7940250	C	13.79484	12.20472	0.7939500
O	21.20629	10.72118	0.794075	C	23.74797	14.98228	0.7940250	H	16.28412	11.11581	0.7939250
B	19.99100	10.03987	0.794075	C	22.54846	14.25844	0.7940250	H	28.37327	12.28811	0.7938500
O	18.79020	10.74570	0.794075	C	22.52000	12.85340	0.7940750	H	26.24156	11.05674	0.7940500
C	19.98093	8.542014	0.794075	C	23.75001	12.17288	0.7941250	H	24.95853	18.20265	0.7941500
C	18.77697	7.816687	0.794200	C	24.97778	12.84901	0.7940500	H	22.82538	16.97153	0.7940500
C	18.74956	6.415403	0.794175	C	27.41899	12.83925	0.7939250	H	23.39572	6.220187	0.7939000
C	19.98089	5.699238	0.794100	H	29.60688	14.45348	0.7937500	H	23.39716	3.757810	0.7940500
C	21.21208	6.415209	0.794000	H	27.44672	18.18865	0.7941750	H	16.56561	6.216244	0.7943000

C	21.18410	7.815895	0.793975	C	24.95805	17.10069	0.7941000	H	16.56737	3.754214	0.7941750
C	19.98162	4.275395	0.794100	H	23.74866	11.07031	0.7941750	H	17.21184	17.01626	0.7941250
C	18.75092	3.558709	0.794100	C	26.24024	12.15864	0.7940250	H	15.08064	18.24831	0.7939250
C	18.77876	2.157579	0.794050	C	23.77973	16.42044	0.7940500	H	13.79363	11.10274	0.7939250
C	19.98266	1.432851	0.794075	H	21.59317	14.80879	0.7939750	H	11.66185	12.33587	0.7940000

Transformation Matrix

a	22.320600	0.000000	0.000000	
b	11.160300	19.330200	0.000000	
c	0.000000	0.000000	3.488000	AA
c	1.21997	0.70435	3.411452	inclined zigzag

Layer II AB stacking

C	22.51895	22.89624	3.762205	C	32.34609	8.602643	3.762380	C	33.60195	12.11198	3.762255
C	22.54681	21.49159	3.762255	C	32.37341	10.00350	3.762380	H	33.29796	14.81229	3.762130
C	23.74595	20.76727	3.762280	B	42.31175	25.70863	3.762305	H	28.98320	14.81247	3.762580
C	24.98136	21.47562	3.762255	O	43.52715	25.02805	3.762255	C	28.68112	12.11016	3.762505
C	24.97651	22.89993	3.762205	B	21.21630	23.63554	3.762205	H	33.30006	8.050244	3.762405
C	23.74890	23.57629	3.762155	O	42.34003	22.92253	3.762180	C	33.60239	10.75129	3.762330
C	26.21401	20.76302	3.762305	B	41.12907	23.61010	3.762230	C	28.68190	10.74924	3.762455
C	26.21720	19.33884	3.762255	O	41.11071	25.00313	3.762280	H	28.98535	8.048234	3.762305
C	27.44378	18.66163	3.762255	C	39.83733	22.85201	3.762230	C	26.23937	23.58973	3.762255
C	28.67515	19.33929	3.762355	C	38.60634	23.52975	3.762355	H	23.74756	24.67862	3.762080
C	28.64952	20.74462	3.762430	C	37.37990	22.85275	3.762355	H	21.59132	20.94202	3.762330
C	27.45035	21.47014	3.762380	C	37.37624	21.42858	3.762280	C	23.77728	19.32912	3.762255
B	29.96775	18.58226	3.762380	C	38.61252	20.72123	3.762205	H	29.60533	21.29402	3.762530
O	31.17964	19.26920	3.762380	C	39.81164	21.44667	3.762155	C	27.41781	22.90857	3.762355
B	32.37754	18.55742	3.762355	C	36.14329	20.71668	3.762305	C	24.95514	18.64812	3.762230
O	32.36659	17.16458	3.762355	C	34.90827	21.42568	3.762305	H	27.44442	17.55921	3.762205
B	31.15130	16.48327	3.762355	C	33.70876	20.70184	3.762305	H	39.53357	18.73151	3.762130
O	29.95050	17.18910	3.762355	C	33.68030	19.29680	3.762355	H	37.40186	17.50014	3.762330
C	31.14123	14.98542	3.762355	C	34.91031	18.61628	3.762405	H	36.11883	24.64605	3.762430
C	29.93727	14.26009	3.762480	C	36.13808	19.29241	3.762330	H	33.98568	23.41493	3.762330
C	29.90986	12.85880	3.762455	C	38.57929	19.28265	3.762205	H	34.55602	12.66359	3.762180
C	31.14119	12.14264	3.762380	H	40.76718	20.89688	3.762030	H	34.55746	10.20121	3.762330
C	32.37238	12.85861	3.762280	H	38.60702	24.63205	3.762455	H	27.72591	12.65965	3.762580
C	32.34440	14.25930	3.762255	C	36.11835	23.54409	3.762380	H	27.72767	10.19762	3.762455
C	31.14192	10.71880	3.762380	H	34.90896	17.51371	3.762455	H	28.37214	23.45966	3.762405
C	29.91122	10.00211	3.762380	C	37.40054	18.60204	3.762305	H	26.24094	24.69171	3.762205
C	29.93906	8.600981	3.762330	C	34.94003	22.86384	3.762330	H	24.95393	17.54614	3.762205
C	31.14296	7.876253	3.762355	H	32.75347	21.25219	3.762255	H	22.82215	18.77927	3.762280
c	0.00000	0.00000	5.93656	AB							

Layer II serrated zigzag

C	12.57862	17.157190	4.203665	C	22.40576	2.863591	4.203840	C	23.66162	6.37293	4.203715
C	12.60648	15.752540	4.203715	C	22.43308	4.264450	4.203840	H	23.35763	9.07324	4.203590
C	13.80562	15.028220	4.203740	B	21.21112	0.639380	4.203765	H	19.04287	9.07341	4.204040
C	15.04103	15.736570	4.203715	O	11.26622	19.289000	4.203715	C	18.74079	6.37111	4.203965
C	15.03618	17.160880	4.203665	B	11.27597	17.896490	4.203665	H	23.35973	2.31119	4.203865
C	13.80857	17.837240	4.203615	O	10.07910	17.183480	4.203640	C	23.66206	5.01223	4.203790
C	16.27368	15.023970	4.203765	B	31.18874	17.871050	4.203690	C	18.74157	5.01019	4.203915
C	16.27687	13.599790	4.203715	O	31.17038	19.264080	4.203740	H	19.04502	2.30918	4.203765
C	17.50345	12.922580	4.203715	C	29.89700	17.112960	4.203690	C	16.29904	17.85068	4.203715
C	18.73482	13.600240	4.203815	C	28.66601	17.790700	4.203815	H	13.80723	18.93957	4.203540
C	18.70919	15.005570	4.203890	C	27.43957	17.113700	4.203815	H	11.65099	15.20297	4.203790
C	17.51002	15.731090	4.203840	C	27.43591	15.689530	4.203740	C	13.83695	13.59007	4.203715
B	20.02742	12.843210	4.203840	C	28.67219	14.982180	4.203665	H	19.66500	15.55497	4.203990
O	21.23931	13.530150	4.203840	C	29.87131	15.707620	4.203615	C	17.47748	17.16952	4.203815
B	22.43721	12.818370	4.203815	C	26.20296	14.977630	4.203765	C	15.01481	12.90907	4.203690
O	22.42626	11.425530	4.203815	C	24.96794	15.686630	4.203765	H	17.50409	11.82016	4.203665

B	21.21097	10.744220	4.203815	C	23.76843	14.962790	4.203765	H	29.59324	12.99246	4.203590	
O	20.01017	11.450050	4.203815	C	23.73997	13.557750	4.203815	H	27.46153	11.76109	4.203790	
C	21.20090	9.246365	4.203815	C	24.96998	12.877230	4.203865	H	26.17850	18.90700	4.203890	
C	19.99694	8.521037	4.203940	C	26.19775	13.553360	4.203790	H	24.04535	17.67588	4.203790	
C	19.96953	7.119753	4.203915	C	28.63896	13.543600	4.203665	H	24.61569	6.92453	4.203640	
C	21.20086	6.403588	4.203840	H	30.82685	15.157830	4.203490	H	24.61713	4.46216	4.203790	
C	22.43205	7.119559	4.203740	H	28.66669	18.893000	4.203915	H	17.78558	6.92059	4.204040	
C	22.40407	8.520245	4.203715	C	26.17802	17.805040	4.203840	H	17.78734	4.45856	4.203915	
C	21.20159	4.979745	4.203840	H	24.96863	11.774660	4.203915	H	18.43181	17.72061	4.203865	
C	19.97089	4.263059	4.203840	C	27.46021	12.862990	4.203765	H	16.30061	18.95266	4.203665	
C	19.99873	2.861929	4.203790	C	24.99970	17.124790	4.203790	H	15.01360	11.80709	4.203665	
C	21.20263	2.137201	4.203815	H	22.81314	15.513140	4.203715	H	12.88182	13.04022	4.203740	

c	0.00000	0.00000	6.81948	serrated zigzag

COF-5

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	39.38465	22.38862	0.8077360	O	20.47563	18.71826	0.8808860	B	35.64685	23.16284	0.8173060	
C	39.41922	20.98273	0.8040060	C	15.45640	10.01228	0.8776360	O	34.40619	22.51739	0.8181660	
C	38.18019	20.31742	0.7978060	C	16.65255	9.272400	0.8877860	C	24.35300	22.27500	0.8515860	
C	36.98136	21.01507	0.7988360	C	16.64961	7.885280	0.8870660	C	24.30941	20.86914	0.8521860	
C	36.94609	22.42116	0.8066160	C	15.45058	7.150020	0.8764060	C	23.10522	20.17951	0.8579360	
C	38.18526	23.08650	0.8090860	C	14.25431	7.889580	0.8657860	C	21.87033	20.85244	0.8632060	
B	40.70932	20.22534	0.8125860	C	14.25719	9.277330	0.8661560	C	21.91408	22.25825	0.8607860	
O	41.96477	20.84153	0.8205360	B	15.45885	5.653904	0.8753560	C	23.11767	22.94780	0.8555060	
C	12.75951	19.73973	0.8336660	O	16.63828	4.902127	0.8771360	H	36.03313	20.45280	0.7953560	
C	14.13734	19.76794	0.8462360	C	16.18376	3.533013	0.8730860	H	38.16029	19.21536	0.7937660	
C	14.82425	18.53141	0.8582860	C	16.92734	2.372618	0.8702360	H	40.33294	22.95052	0.8117860	
C	14.10000	17.30940	0.8571560	C	16.23177	1.141180	0.8641860	H	38.20604	24.18863	0.8138360	
C	12.68582	17.31851	0.8439560	C	14.81144	1.121423	0.8625060	H	13.29518	9.815740	0.8570360	
C	12.04926	18.54070	0.8325360	C	14.08058	2.332607	0.8653360	H	13.29003	7.355373	0.8564160	
C	14.81330	16.03980	0.8681360	C	14.79044	3.514143	0.8701060	H	17.61128	7.346499	0.8952160	
C	16.23385	16.02310	0.8794360	C	29.16997	25.94961	0.8570560	H	17.61656	9.807080	0.8963160	
C	16.97668	17.27594	0.8794860	C	29.89655	24.72903	0.8511660	H	12.98228	14.85730	0.8558360	
C	16.28037	18.51419	0.8695360	C	31.35303	24.74986	0.8490860	H	18.91793	16.28417	0.8931860	
C	16.93177	14.79286	0.8879560	C	32.04632	25.98983	0.8564860	H	16.43995	20.68804	0.8596360	
C	16.19076	13.63059	0.8841660	C	29.21184	23.49104	0.8461360	H	18.03483	14.79542	0.8960660	
C	14.79744	13.64734	0.8730660	C	27.83368	23.51634	0.8477060	H	14.71344	20.70860	0.8467560	
C	14.08506	14.82721	0.8652860	C	27.12170	24.71423	0.8533060	H	12.13732	16.36148	0.8427860	
C	16.99491	19.73474	0.8674060	C	27.75580	25.93760	0.8577160	H	23.10512	24.05012	0.8547660	
C	18.37174	19.67534	0.8727360	C	33.46062	26.01705	0.8532360	H	12.13660	0.7937660	0.8618060	
C	19.05533	18.46110	0.8813860	C	34.12878	24.81158	0.8402860	H	31.52002	22.57643	0.8325560	
C	18.39107	17.25331	0.8862060	C	33.44818	23.59547	0.8326560	H	18.91479	0.8885610	0.8596660	
O	14.30785	12.28935	0.8697560	C	32.07148	23.53168	0.8379660	H	29.78991	22.55151	0.8412660	
B	15.46802	11.50839	0.8787360	O	25.70864	24.42541	0.8541060	H	18.03041	2.372697	0.8713860	
O	16.64678	12.26132	0.8884360	B	25.64560	23.02835	0.8493860	H	12.97787	2.299852	0.8627160	
O	40.77311	18.82814	0.8185360	O	26.90171	22.41331	0.8447660	H	20.96961	22.82688	0.8639060	
O	19.32740	20.75623	0.8671860	O	14.29926	4.871904	0.8716060	H	23.11811	19.07719	0.8582860	
B	20.56945	20.11355	0.8707860	O	35.55002	24.55802	0.8308860	H	25.25342	20.29993	0.8487160	

Transformation Matrix

a	30.137400	0.000000	0.000000	
b	15.068700	26.099740	0.000000	
c	0.000000	0.000000	3.487498	AA
c	1.197700	0.691492	3.405000	inclined zigzag
c	1.387445	0.000000	3.410000	inclined armchair

Layer II AB stacking

C	54.45335	31.08854	4.065051	O	35.54433	27.41818	4.138201	B	50.71555	31.86276	4.074621
C	54.48792	29.68265	4.061321	C	30.52510	18.71220	4.134951	O	49.47488	31.21731	4.075481
C	53.24889	29.01734	4.055121	C	31.72125	17.97232	4.145101	C	39.42170	30.97492	4.108901
C	52.05006	29.71499	4.056151	C	31.71831	16.58520	4.144381	C	39.37811	29.56906	4.109501
C	52.01479	31.12108	4.063931	C	30.51928	15.84994	4.133721	C	38.17392	28.87943	4.115251
C	53.25396	31.78642	4.066401	C	29.32301	16.58950	4.123101	C	36.93903	29.55236	4.120521
B	55.77802	28.92526	4.069901	C	29.32589	17.97725	4.123471	C	36.98278	30.95817	4.118101
O	57.03347	29.54145	4.077851	B	30.52755	14.35382	4.132671	C	38.18637	31.64772	4.112821
C	27.82821	28.43965	4.090981	O	31.70698	13.60205	4.134451	H	51.10183	29.15272	4.052671
C	29.20604	28.46786	4.103551	C	31.25246	12.23293	4.130401	H	53.22898	27.91528	4.051081
C	29.89295	27.23133	4.115601	C	31.99604	11.07254	4.127551	H	55.40164	31.65044	4.069101
C	29.16870	26.00932	4.114471	C	31.30047	9.841098	4.121501	H	53.27474	32.88855	4.071151
C	27.75452	26.01843	4.101271	C	29.88014	9.821341	4.119821	H	28.36388	18.51566	4.114351
C	27.11796	27.24062	4.089851	C	29.14928	11.03253	4.122651	H	28.35873	16.05529	4.113731
C	29.88200	24.73972	4.125451	C	29.85914	12.21406	4.127421	H	32.67998	16.04642	4.152531
C	31.30255	24.72302	4.136751	C	44.23867	34.64953	4.114371	H	32.68526	18.50700	4.153631
C	32.04538	25.97586	4.136801	C	44.96525	33.42895	4.108481	H	28.05098	23.55722	4.113151
C	31.34907	27.21411	4.126851	C	46.42173	33.44978	4.106401	H	33.98663	24.98409	4.150501
C	32.00047	23.49278	4.145271	C	47.11502	34.68975	4.113801	H	31.50865	29.38796	4.116951
C	31.25946	22.33051	4.141481	C	44.28054	32.19096	4.103451	H	33.10353	23.49534	4.153381
C	29.86614	22.34726	4.130381	C	42.90238	32.21626	4.105021	H	29.78214	29.40852	4.104071
C	29.15376	23.52713	4.122601	C	42.19040	33.41415	4.110621	H	27.20602	25.06140	4.100101
C	32.06361	28.43466	4.124721	C	42.82450	34.63752	4.115031	H	38.17382	32.75004	4.112081
C	33.44044	28.37526	4.130051	C	48.52932	34.71697	4.110551	H	27.20530	9.493684	4.119121
C	34.12403	27.16102	4.138701	C	49.19748	33.51150	4.097601	H	46.58872	31.27635	4.089871
C	33.45977	25.95323	4.143521	C	48.51688	32.29539	4.089971	H	33.98349	9.588479	4.116981
O	29.37655	20.98927	4.127071	C	47.14018	32.23160	4.095281	H	44.85861	31.25143	4.098581
B	30.53672	20.20831	4.136051	O	40.77734	33.12533	4.111421	H	33.09911	11.07261	4.128701
O	31.71548	20.96124	4.145751	B	40.71430	31.72827	4.106701	H	28.04657	10.99977	4.120031
O	55.84181	27.52806	4.075851	O	41.97041	31.11323	4.102081	H	36.03831	31.52680	4.121221
O	34.39610	29.45615	4.124501	O	29.36796	13.57182	4.128921	H	38.18681	27.77711	4.115601
B	35.63815	28.81347	4.128101	O	50.61872	33.25794	4.088201	H	40.32212	28.99985	4.106031
c	0.00000	0.00000	6.51463	AB							

Layer II serrated zigzag

C	40.58235	23.08011	4.22612	O	21.67333	19.409750	4.299271	B	36.84455	23.854330	4.23569100
C	40.61692	21.67422	4.22239	C	16.65410	10.703770	4.296021	O	35.60389	23.208880	4.23655100
C	39.37789	21.00891	4.21619	C	17.85025	9.963892	4.306171	C	25.55070	22.966490	4.26997100
C	38.17906	21.70656	4.21722	C	17.84731	8.576772	4.305451	C	25.50711	21.560630	4.27057100
C	38.14380	23.11265	4.22500	C	16.64828	7.841512	4.294791	C	24.30292	20.871000	4.27632100
C	39.38296	23.77799	4.22747	C	15.45201	8.581072	4.284171	C	23.06803	21.543930	4.28159100
B	41.90702	20.91683	4.23097	C	15.45489	9.968822	4.284541	C	23.11178	22.949740	4.27917100
O	13.02507	21.53302	4.23892	B	16.65655	6.345396	4.293741	C	24.31537	23.639290	4.27389100
C	13.95721	20.43122	4.25205	O	17.83598	5.593619	4.295521	H	37.23083	21.144290	4.21374100
C	15.33504	20.45943	4.26462	C	17.38146	4.224505	4.291471	H	39.35799	19.906850	4.21215100
C	16.02195	19.22290	4.27667	C	18.12504	3.064110	4.288621	H	41.53064	23.642010	4.23017100
C	15.29770	18.00089	4.27554	C	17.42947	1.832672	4.282571	H	39.40374	24.880120	4.23222100
C	13.88352	18.01000	4.26234	C	16.00914	1.812915	4.280891	H	14.49288	10.507230	4.27542100
C	13.24696	19.23219	4.25092	C	15.27828	3.024099	4.283721	H	14.48773	8.046865	4.27480100
C	16.01100	16.73129	4.28652	C	15.98814	4.205635	4.288491	H	18.80898	8.037991	4.31360100
C	17.43155	16.71459	4.29782	C	15.29897	0.541360	4.275441	H	18.81426	10.498570	4.31470100
C	18.17438	17.96743	4.29787	C	31.09425	25.420520	4.269551	H	14.17998	15.548790	4.27422100
C	17.47807	19.20568	4.28792	C	32.55073	25.441350	4.267471	H	20.11563	16.975660	4.31157100
C	18.12947	15.48435	4.30634	C	18.17532	0.581580	4.274871	H	17.63765	21.379530	4.27802100
C	17.38846	14.32208	4.30255	C	30.40954	24.182530	4.264521	H	19.23253	15.486910	4.31445100
C	15.99514	14.33883	4.29145	C	29.03138	24.207830	4.266091	H	15.91114	21.400090	4.26514100
C	15.28276	15.51870	4.28367	C	28.31940	25.405720	4.271691	H	13.33502	17.052970	4.26117100
C	18.19261	20.42623	4.28579	C	13.88480	0.529350	4.276101	H	24.30282	24.741610	4.27315100
C	19.56944	20.36683	4.29112	C	19.58962	0.608800	4.271621	H	13.33430	1.485258	4.28019100
C	20.25303	19.15259	4.29977	C	35.32648	25.503070	4.258671	H	32.71772	23.267920	4.25094100

C	19.58877	17.94480	4.30459	C	34.64588	24.286960	4.251041	H	20.11249	1.580053	4.27805100
O	15.50555	12.98084	4.28814	C	33.26918	24.223170	4.256351	H	30.98761	23.243000	4.25965100
B	16.66572	12.19988	4.29712	O	26.90634	25.116900	4.272491	H	19.22811	3.064189	4.28977100
O	17.84448	12.95281	4.30682	B	26.84330	23.719840	4.267771	H	14.17557	2.991344	4.28110100
O	11.83341	19.51963	4.23692	O	28.09941	23.104800	4.263151	H	22.16731	23.518370	4.28229100
O	20.52510	21.44772	4.28557	O	15.49696	5.563396	4.289991	H	24.31581	19.768680	4.27667100
B	21.76715	20.80504	4.28917	O	36.74772	25.249510	4.249271	H	26.45112	20.991420	4.26710100
c	0.00000	0.00000	6.83677	serrated zigzag							

Layer II serrated armchair

C	40.77209	22.38862	4.22813	O	21.86308	18.718260	4.301286	B	37.03430	23.162840	4.23770
C	40.80666	20.98273	4.22440	C	16.84385	10.012280	4.298036	O	35.79363	22.517390	4.23856
C	39.56763	20.31742	4.21820	C	18.04000	9.272400	4.308186	C	25.74045	22.275000	4.27198
C	38.36880	21.01507	4.21923	C	18.03706	7.885280	4.307466	C	25.69686	20.869140	4.27258
C	38.33354	22.42116	4.22701	C	16.83802	7.150020	4.296806	C	24.49267	20.179510	4.27833
C	39.57270	23.08650	4.22948	C	15.64175	7.889580	4.286186	C	23.25778	20.852440	4.28360
B	11.95936	20.22534	4.23298	C	15.64463	9.277330	4.286556	C	23.30153	22.258250	4.28118
O	13.21481	20.84153	4.24093	B	16.84629	5.653904	4.295756	C	24.50512	22.947800	4.27590
C	14.14696	19.73973	4.25406	O	18.02573	4.902127	4.297536	H	37.42057	20.452800	4.21575
C	15.52478	19.76794	4.26663	C	17.57121	3.533013	4.293486	H	39.54773	19.215360	4.21416
C	16.21169	18.53141	4.27868	C	18.31479	2.372618	4.290636	H	41.72038	22.950520	4.23218
C	15.48745	17.30940	4.27755	C	17.61922	1.141180	4.284586	H	39.59349	24.188630	4.23423
C	14.07327	17.31851	4.26435	C	16.19888	1.121423	4.282906	H	14.68262	9.815740	4.27743
C	13.43670	18.54070	4.25293	C	15.46803	2.332607	4.285736	H	14.67747	7.355373	4.27681
C	16.20074	16.03980	4.28853	C	16.17789	3.514143	4.290506	H	18.99873	7.346499	4.31561
C	17.62130	16.02310	4.29983	C	30.55742	25.949610	4.277456	H	19.00401	9.807080	4.31671
C	18.36413	17.27594	4.29988	C	31.28399	24.729030	4.271566	H	14.36972	14.857300	4.27623
C	17.66782	18.51419	4.28993	C	32.74047	24.749860	4.269486	H	20.30538	16.284170	4.31358
C	18.31922	14.79286	4.30835	C	33.43377	25.989830	4.276886	H	17.82740	20.688040	4.28003
C	17.57821	13.63059	4.30456	C	30.59929	23.491040	4.266536	H	19.42228	14.795420	4.31646
C	16.18489	13.64734	4.29346	C	29.22112	23.516340	4.268106	H	16.10089	20.708600	4.26715
C	15.47251	14.82721	4.28568	C	28.50915	24.714230	4.273706	H	13.52477	16.361480	4.26318
C	18.38235	19.73474	4.28780	C	29.14325	25.937600	4.278116	H	24.49257	24.050120	4.27516
C	19.75919	19.67534	4.29313	C	34.84806	26.017050	4.273636	H	13.52404	0.793766	4.28220
C	20.44278	18.46110	4.30178	C	35.51623	24.811580	4.260686	H	32.90746	22.576430	4.25295
C	19.77851	17.25331	4.30660	C	34.83562	23.595470	4.253056	H	20.30223	0.888561	4.28006
O	15.69530	12.28935	4.29015	C	33.45892	23.531680	4.258366	H	31.17735	22.551510	4.26166
B	16.85546	11.50839	4.29913	O	27.09608	24.425410	4.274506	H	19.41786	2.372697	4.29178
O	18.03423	12.26132	4.30883	B	27.03304	23.028350	4.269786	H	14.36531	2.299852	4.28311
O	12.02315	18.82814	4.23893	O	28.28916	22.413310	4.265166	H	22.35706	22.826880	4.28430
O	20.71485	20.75623	4.28758	O	15.68670	4.871904	4.292006	H	24.50556	19.077190	4.27868
B	21.95690	20.11355	4.29118	O	36.93746	24.558020	4.251286	H	26.64087	20.299930	4.26911
c	0.00000	0.00000	6.84080	serrated armchair							

COF-10

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

B	37.50977	27.53210	0.793766	C	19.43546	9.657603	0.793766	C	38.24199	20.51853	0.793766
O	36.34117	26.76319	0.793766	C	19.42151	7.265988	0.793766	C	40.32082	19.33411	0.793766
C	37.50737	29.02741	0.793766	C	20.14871	8.436213	0.793766	C	38.94325	19.28997	0.793766
C	36.30821	29.76566	0.793766	H	21.25162	8.448972	0.793766	H	38.37680	18.34322	0.793766
C	36.30917	31.15210	0.793766	H	20.89360	3.437906	0.793766	H	42.89956	16.15324	0.793766
C	37.51363	31.87336	0.793766	H	20.88455	0.961991	0.793766	H	45.04575	14.91717	0.793766
C	36.80304	23.00954	0.793766	B	13.72391	13.79473	0.793766	O	38.68137	26.76693	0.793766
C	36.81699	25.40116	0.793766	O	13.80313	12.39784	0.793766	C	38.70895	29.76133	0.793766
C	36.08978	24.23090	0.793766	C	12.42878	14.54264	0.793766	C	38.71519	31.14767	0.793766
H	34.98686	24.21814	0.793766	C	11.19060	13.87164	0.793766	C	38.22355	23.00970	0.793766
H	35.34490	29.22924	0.793766	C	9.988718	14.56286	0.793766	C	38.21038	25.40227	0.793766
H	35.35394	31.70512	0.793766	C	9.963801	15.96625	0.793766	C	38.93695	24.23109	0.793766

B	42.51460	18.87242	0.793766	C	17.28637	10.91834	0.793766	H	40.03979	24.21274	0.793766
O	42.43535	20.26927	0.793766	C	15.22095	12.12606	0.793766	H	39.66853	29.21889	0.793766
C	43.80972	18.12450	0.793766	C	15.87178	10.91112	0.793766	H	39.67292	31.69656	0.793766
C	45.04790	18.79551	0.793766	H	15.33533	9.947084	0.793766	O	23.64449	12.39598	0.793766
C	46.24976	18.10426	0.793766	H	11.17634	12.76915	0.793766	C	26.26091	13.86799	0.793766
C	46.27472	16.70086	0.793766	H	9.033188	14.01023	0.793766	C	27.46135	14.56172	0.793766
C	38.95214	21.74880	0.793766	B	23.72578	13.79248	0.793766	C	20.16314	10.91831	0.793766
C	41.01753	20.54105	0.793766	O	22.47722	14.42433	0.793766	C	22.22712	12.12662	0.793766
C	40.36674	21.75599	0.793766	C	25.02214	14.53776	0.793766	C	21.57750	10.91161	0.793766
H	40.90316	22.72006	0.793766	C	25.05735	15.94526	0.793766	H	22.11819	9.950241	0.793766
H	45.06214	19.89797	0.793766	C	26.25503	16.64345	0.793766	H	26.27779	12.76553	0.793766
H	47.20531	18.65692	0.793766	C	27.48411	15.96541	0.793766	H	28.41782	14.01078	0.793766
B	32.51270	18.87463	0.793766	C	19.45278	12.14849	0.793766	O	14.97309	14.42472	0.793766
O	33.76126	18.24278	0.793766	C	21.53118	13.33379	0.793766	C	12.39116	15.95047	0.793766
C	31.21635	18.12935	0.793766	C	20.15363	13.37717	0.793766	C	11.19181	16.64608	0.793766
C	31.18113	16.72185	0.793766	H	19.58600	14.32285	0.793766	C	17.99652	12.14862	0.793766
C	29.98345	16.02367	0.793766	H	24.10795	16.50531	0.793766	C	15.91767	13.33300	0.793766
C	28.75439	16.70174	0.793766	H	26.25166	17.74730	0.793766	C	17.29525	13.37717	0.793766
C	36.78572	20.51866	0.793766	O	32.59399	20.27113	0.793766	H	17.86168	14.32389	0.793766
C	34.70734	19.33333	0.793766	C	29.97759	18.79915	0.793766	H	13.33893	16.51387	0.793766
C	36.08487	19.28997	0.793766	C	28.77713	18.10540	0.793766	H	11.19275	17.74997	0.793766
H	36.65248	18.34426	0.793766	C	36.07534	21.74880	0.793766	O	17.55711	5.900183	0.793766
H	32.13055	16.16183	0.793766	C	34.01139	20.54050	0.793766	C	17.52954	2.905814	0.793766
H	29.98685	14.91981	0.793766	C	34.66100	21.75554	0.793766	C	17.52331	1.519471	0.793766
B	18.72871	5.135015	0.793766	H	34.12031	22.71691	0.793766	C	18.01493	9.657408	0.793766
O	19.89731	5.903926	0.793766	H	29.96070	19.90158	0.793766	C	18.02810	7.264849	0.793766
C	18.73113	3.639735	0.793766	H	27.82068	18.65637	0.793766	C	17.30153	8.436018	0.793766
C	19.93029	2.901485	0.793766	O	41.26539	18.24239	0.793766	H	16.19871	8.454407	0.793766
C	19.92932	1.515012	0.793766	C	43.84734	16.71668	0.793766	H	16.56996	3.448223	0.793766
C	18.72487	0.793784	0.793766	C	45.04671	16.02103	0.793766	H	16.56556	0.970551	0.793766

Transformation Matrix

a	37.583030	0.000000	0.000000	
b	18.791520	32.547840	0.000000	
c	0.000000	0.000000	3.472000	AA
c	1.203000	0.694552	3.398119	inclined zigzag
c	1.387895	0.00000	3.420000	inclined armchair

Layer II AB stacking

B	56.30128	38.38139	3.970638	C	38.22697	20.50689	3.970638	C	57.03350	31.36782	3.970638
O	55.13269	37.61248	3.970638	C	38.21303	18.11527	3.970638	C	59.11233	30.18340	3.970638
C	56.29889	39.87670	3.970638	C	38.94022	19.28550	3.970638	C	57.73476	30.13926	3.970638
C	55.09972	40.61494	3.970638	H	40.04314	19.29826	3.970638	H	57.16831	29.19251	3.970638
C	55.10069	42.00139	3.970638	H	39.68512	14.28719	3.970638	H	61.69107	27.00253	3.970638
C	56.30515	42.72265	3.970638	H	39.67606	11.81128	3.970638	H	63.83727	25.76646	3.970638
C	55.59455	33.85883	3.970638	B	32.51543	24.64402	3.970638	O	57.47289	37.61622	3.970638
C	55.60851	36.25045	3.970638	O	32.59465	23.24713	3.970638	C	57.50047	40.61062	3.970638
C	54.88129	35.08018	3.970638	C	31.22029	25.39193	3.970638	C	57.50671	41.99696	3.970638
H	53.77837	35.06743	3.970638	C	29.98212	24.72093	3.970638	C	57.01506	33.85899	3.970638
H	54.13641	40.07853	3.970638	C	28.78023	25.41215	3.970638	C	57.00190	36.25156	3.970638
H	54.14545	42.55441	3.970638	C	28.75532	26.81554	3.970638	C	57.72847	35.08038	3.970638
B	61.30611	29.72171	3.970638	C	36.07788	21.76763	3.970638	H	58.83131	35.06203	3.970638
O	61.22686	31.11856	3.970638	C	34.01247	22.97535	3.970638	H	58.46004	40.06818	3.970638
C	62.60124	28.97379	3.970638	C	34.66330	21.76041	3.970638	H	58.46444	42.54585	3.970638
C	63.83941	29.64480	3.970638	H	34.12685	20.79637	3.970638	O	42.43600	23.24527	3.970638
C	65.04128	28.95355	3.970638	H	29.96786	23.61844	3.970638	C	45.05243	24.71728	3.970638
C	65.06624	27.55015	3.970638	H	27.82470	24.85952	3.970638	C	46.25286	25.41101	3.970638
C	57.74366	32.59809	3.970638	B	42.51730	24.64177	3.970638	C	38.95465	21.76760	3.970638
C	59.80904	31.39034	3.970638	O	41.26874	25.27362	3.970638	C	41.01863	22.97591	3.970638
C	59.15826	32.60528	3.970638	C	43.81366	25.38705	3.970638	C	40.36901	21.76090	3.970638
H	59.69468	33.56935	3.970638	C	43.84887	26.79455	3.970638	H	40.90971	20.79953	3.970638
H	63.85366	30.74726	3.970638	C	45.04655	27.49274	3.970638	H	45.06931	23.61482	3.970638

H	65.99683	29.50621	3.970638	C	46.27563	26.81470	3.970638	H	47.20934	24.86007	3.970638
B	51.30421	29.72392	3.970638	C	38.24429	22.99778	3.970638	O	33.76461	25.27401	3.970638
O	52.55278	29.09207	3.970638	C	40.32269	24.18308	3.970638	C	31.18267	26.79976	3.970638
C	50.00787	28.97864	3.970638	C	38.94514	24.22646	3.970638	C	29.98333	27.49537	3.970638
C	49.97264	27.57114	3.970638	H	38.37752	25.17214	3.970638	C	36.78803	22.99791	3.970638
C	48.77496	26.87296	3.970638	H	42.89947	27.35460	3.970638	C	34.70919	24.18229	3.970638
C	47.54591	27.55103	3.970638	H	45.04317	28.59659	3.970638	C	36.08677	24.22646	3.970638
C	55.57724	31.36795	3.970638	O	51.38551	31.12042	3.970638	H	36.65319	25.17318	3.970638
C	53.49886	30.18262	3.970638	C	48.76910	29.64844	3.970638	H	32.13045	27.36316	3.970638
C	54.87638	30.13926	3.970638	C	47.56865	28.95469	3.970638	H	29.98426	28.59926	3.970638
H	55.44400	29.19355	3.970638	C	54.86686	32.59809	3.970638	O	36.34863	16.74947	3.970638
H	50.92207	27.01112	3.970638	C	52.80291	31.38979	3.970638	C	36.32105	13.75510	3.970638
H	48.77837	25.76910	3.970638	C	53.45251	32.60483	3.970638	C	36.31483	12.36876	3.970638
B	37.52023	15.98430	3.970638	H	52.91183	33.56620	3.970638	C	36.80645	20.50669	3.970638
O	38.68883	16.75321	3.970638	H	48.75221	30.75087	3.970638	C	36.81961	18.11414	3.970638
C	37.52264	14.48902	3.970638	H	46.61220	29.50566	3.970638	C	36.09305	19.28531	3.970638
C	38.72181	13.75077	3.970638	O	60.05690	29.09168	3.970638	H	34.99023	19.30369	3.970638
C	38.72083	12.36430	3.970638	C	62.63886	27.56597	3.970638	H	35.36147	14.29751	3.970638
C	37.51639	11.64307	3.970638	C	63.83823	26.87032	3.970638	H	35.35707	11.81984	3.970638
c	0.00000	0.00000	6.35374	AB							

Layer II serrated zigzag

B	38.71277	28.226650	4.206926	C	20.63846	10.35216	4.206926	C	39.44499	21.213080	4.206926
O	37.54417	27.457740	4.206926	C	20.62451	7.96054	4.206926	C	41.52382	20.028660	4.206926
C	38.71037	29.721960	4.206926	C	21.35171	9.13076	4.206926	C	40.14625	19.984520	4.206926
C	37.51121	30.460210	4.206926	H	22.45462	9.14352	4.206926	H	39.57980	19.037770	4.206926
C	37.51217	31.846650	4.206926	H	22.09660	4.13246	4.206926	H	44.10255	16.847790	4.206926
C	19.92511	0.020070	4.206926	H	22.08755	1.65654	4.206926	H	46.24875	15.611720	4.206926
C	38.00604	23.704090	4.206926	B	14.92691	14.48928	4.206926	O	39.88437	27.461480	4.206926
C	38.01999	26.095710	4.206926	O	15.00613	13.09239	4.206926	C	39.91195	30.455880	4.206926
C	37.29278	24.925450	4.206926	C	13.63178	15.23719	4.206926	C	39.91819	31.842220	4.206926
H	36.18986	24.912690	4.206926	C	12.39360	14.56619	4.206926	C	39.42655	23.704250	4.206926
H	36.54790	29.923790	4.206926	C	11.19172	15.25741	4.206926	C	39.41338	26.096820	4.206926
H	36.55694	32.399670	4.206926	C	11.16680	16.66080	4.206926	C	40.13995	24.925640	4.206926
B	43.71759	19.566970	4.206926	C	18.48937	11.61289	4.206926	H	41.24279	24.907290	4.206926
O	43.63835	20.963820	4.206926	C	16.42395	12.82061	4.206926	H	40.87153	29.913440	4.206926
C	45.01272	18.819050	4.206926	C	17.07478	11.60567	4.206926	H	40.87592	32.391110	4.206926
C	46.25090	19.490060	4.206926	H	16.53833	10.64164	4.206926	O	24.84749	13.090530	4.206926
C	47.45276	18.798810	4.206926	H	12.37934	13.46370	4.206926	C	27.46391	14.562540	4.206926
C	47.47772	17.395410	4.206926	H	10.23619	14.70478	4.206926	C	28.66435	15.256270	4.206926
C	40.15514	22.443350	4.206926	B	24.92878	14.48703	4.206926	C	21.36614	11.612860	4.206926
C	42.22053	21.235600	4.206926	O	23.68022	15.11888	4.206926	C	23.43012	12.821170	4.206926
C	41.56974	22.450540	4.206926	C	26.22514	15.23231	4.206926	C	22.78050	11.606160	4.206926
H	42.10616	23.414610	4.206926	C	26.26035	16.63981	4.206926	H	23.32119	10.644790	4.206926
H	46.26514	20.592520	4.206926	C	27.45803	17.33800	4.206926	H	27.48079	13.460080	4.206926
H	48.40831	19.351470	4.206926	C	28.68711	16.65996	4.206926	H	29.62082	14.705330	4.206926
B	33.71570	19.569180	4.206926	C	20.65578	12.84304	4.206926	O	16.17609	15.119270	4.206926
O	34.96426	18.937330	4.206926	C	22.73418	14.02834	4.206926	C	13.59416	16.645020	4.206926
C	32.41935	18.823900	4.206926	C	21.35663	14.07172	4.206926	C	12.39481	17.340630	4.206926
C	32.38413	17.416400	4.206926	H	20.78900	15.01740	4.206926	C	19.19952	12.843170	4.206926
C	31.18645	16.718220	4.206926	H	25.31095	17.19986	4.206926	C	17.12067	14.027550	4.206926
C	29.95739	17.396290	4.206926	H	27.45466	18.44185	4.206926	C	18.49825	14.071720	4.206926
C	37.98872	21.213210	4.206926	O	33.79699	20.96568	4.206926	H	19.06468	15.018440	4.206926
C	35.91034	20.027880	4.206926	C	31.18059	19.49370	4.206926	H	14.54193	17.208420	4.206926
C	37.28787	19.984520	4.206926	C	29.98013	18.79995	4.206926	H	12.39575	18.444520	4.206926
H	37.85548	19.038810	4.206926	C	37.27834	22.44335	4.206926	O	18.76011	6.594735	4.206926
H	33.33355	16.856380	4.206926	C	35.21439	21.23505	4.206926	C	18.73254	3.600366	4.206926
H	31.18985	15.614360	4.206926	C	35.86400	22.45009	4.206926	C	18.72631	2.214023	4.206926
B	19.93171	5.829567	4.206926	H	35.32331	23.41146	4.206926	C	19.21793	10.351960	4.206926
O	21.10031	6.598478	4.206926	H	31.16370	20.59613	4.206926	C	19.23110	7.959401	4.206926
C	19.93413	4.334287	4.206926	H	29.02368	19.35092	4.206926	C	18.50453	9.130570	4.206926
C	21.13329	3.596037	4.206926	O	42.46839	18.93694	4.206926	H	17.40171	9.148959	4.206926
C	21.13232	2.209564	4.206926	C	45.05034	17.41123	4.206926	H	17.77296	4.142775	4.206926

C 19.92787 1.488336 4.206926 C 46.24971 16.71558 4.206926 H 17.76856 1.665103 4.206926
c 0.00000 0.00000 6.82632 serrated zigzag

Layer II serrated armchair

B 38.89766 27.532100 4.20692 C 20.82335 9.657603 4.20692 C 39.62988 20.518530 4.20692
O 37.72906 26.763190 4.20692 C 20.80941 7.265988 4.20692 C 41.70871 19.334110 4.20692
C 38.89526 29.027410 4.20692 C 21.53661 8.436213 4.20692 C 40.33114 19.289970 4.20692
C 37.69610 29.765660 4.20692 H 22.63951 8.448972 4.20692 H 39.76469 18.343220 4.20692
C 37.69706 31.152100 4.20692 H 22.28150 3.437906 4.20692 H 44.28745 16.153240 4.20692
C 38.90152 31.873360 4.20692 H 22.27245 0.961991 4.20692 H 8.850620 14.917170 4.20692
C 38.19093 23.009540 4.20692 B 15.11180 13.794730 4.20692 O 40.06926 26.766930 4.20692
C 38.20488 25.401160 4.20692 O 15.19102 12.397840 4.20692 C 40.09684 29.761330 4.20692
C 37.47767 24.230900 4.20692 C 13.81667 14.542640 4.20692 C 40.10308 31.147670 4.20692
H 36.37475 24.218140 4.20692 C 12.57850 13.871640 4.20692 C 39.61144 23.009700 4.20692
H 36.73279 29.229240 4.20692 C 11.37661 14.562860 4.20692 C 39.59827 25.402270 4.20692
H 36.74183 31.705120 4.20692 C 11.35170 15.966250 4.20692 C 40.32484 24.231090 4.20692
B 43.90249 18.872420 4.20692 C 18.67426 10.918340 4.20692 H 41.42768 24.212740 4.20692
O 43.82324 20.269270 4.20692 C 16.60884 12.126060 4.20692 H 41.05642 29.218890 4.20692
C 45.19762 18.124500 4.20692 C 17.25968 10.911120 4.20692 H 41.06081 31.696560 4.20692
C 46.43579 18.795510 4.20692 H 16.72322 9.947084 4.20692 O 25.03238 12.395980 4.20692
C 47.63766 18.104260 4.20692 H 12.56423 12.769150 4.20692 C 27.64881 13.867990 4.20692
C 10.07958 16.700860 4.20692 H 10.42108 14.010230 4.20692 C 28.84925 14.561720 4.20692
C 40.34003 21.748800 4.20692 B 25.11368 13.792480 4.20692 C 21.55103 10.918310 4.20692
C 42.40542 20.541050 4.20692 O 23.86512 14.424330 4.20692 C 23.61502 12.126620 4.20692
C 41.75463 21.755990 4.20692 C 26.41004 14.537760 4.20692 C 22.96539 10.911610 4.20692
H 42.29106 22.720060 4.20692 C 26.44525 15.945260 4.20692 H 23.50609 9.950241 4.20692
H 46.45004 19.897970 4.20692 C 27.64293 16.643450 4.20692 H 27.66569 12.765530 4.20692
H 11.01017 18.656920 4.20692 C 28.87201 15.965410 4.20692 H 29.80572 14.010780 4.20692
B 33.90059 18.874630 4.20692 C 20.84068 12.148490 4.20692 O 16.36098 14.424720 4.20692
O 35.14915 18.242780 4.20692 C 22.91908 13.333790 4.20692 C 13.77905 15.950470 4.20692
C 32.60424 18.129350 4.20692 C 21.54152 13.377170 4.20692 C 12.57970 16.646080 4.20692
C 32.56902 16.721850 4.20692 H 20.97390 14.322850 4.20692 C 19.38441 12.148620 4.20692
C 31.37135 16.023670 4.20692 H 25.49585 16.505310 4.20692 C 17.30556 13.333000 4.20692
C 30.14229 16.701740 4.20692 H 27.63955 17.747300 4.20692 C 18.68315 13.377170 4.20692
C 38.17361 20.518660 4.20692 O 33.98188 20.271130 4.20692 H 19.24957 14.323890 4.20692
C 36.09523 19.333330 4.20692 C 31.36549 18.799150 4.20692 H 14.72682 16.513870 4.20692
C 37.47276 19.289970 4.20692 C 30.16503 18.105400 4.20692 H 12.58064 17.749970 4.20692
H 38.04037 18.344260 4.20692 C 37.46323 21.748800 4.20692 O 18.94501 5.900183 4.20692
H 33.51844 16.161830 4.20692 C 35.39928 20.540500 4.20692 C 18.91743 2.905814 4.20692
H 31.37475 14.919810 4.20692 C 36.04889 21.755540 4.20692 C 18.91121 1.519471 4.20692
B 20.11661 5.135015 4.20692 H 35.50821 22.716910 4.20692 C 19.40283 9.657408 4.20692
O 21.28521 5.903926 4.20692 H 31.34859 19.901580 4.20692 C 19.41599 7.264849 4.20692
C 20.11903 3.639735 4.20692 H 29.20858 18.656370 4.20692 C 18.68943 8.436018 4.20692
C 21.31819 2.901485 4.20692 O 42.65328 18.242390 4.20692 H 17.58661 8.454407 4.20692
C 21.31721 1.515012 4.20692 C 45.23524 16.716680 4.20692 H 17.95786 3.448223 4.20692
C 20.11277 0.793784 4.20692 C 46.43460 16.021030 4.20692 H 17.95345 0.970551 4.20692
c 0.00000 0.00000 6.82632 serrated armchair

COF-8

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C 25.85511 6.863348 7.860975 C 16.93204 15.12143 7.789575 C 12.00871 9.051265 7.980750
C 4.564046 7.551417 7.906900 C 17.67002 16.28532 7.798175 C 10.76552 9.712545 7.984575
C 27.04152 8.953955 7.932275 C 19.76935 12.61187 7.842400 C 9.568823 9.011315 7.998150
C 25.83477 9.636429 7.915000 C 19.04838 11.38808 7.839901 H 4.968770 0.593880 7.773575
C 24.60197 8.957348 7.872050 C 17.59200 11.40208 7.842575 H 9.290070 0.621960 7.924825
C 24.65039 7.550442 7.845175 C 16.89313 12.63879 7.824075 H 15.82916 15.11616 7.771775
C 5.845753 6.828019 7.928650 C 19.73875 10.15314 7.840800 H 21.73021 13.56432 7.858100
C 5.881123 5.428016 7.906675 C 21.11665 10.18468 7.845775 H 19.16490 9.211218 7.837525

C	7.094083	4.727273	7.928900	C	21.82318	11.38555	7.855025	H	20.88093	15.06828	7.863150
C	8.288683	5.457203	7.971675	C	21.18377	12.60627	7.853175	H	17.43520	9.228512	7.890950
C	8.288533	6.858084	7.988900	C	15.47862	12.65933	7.834900	H	14.95035	13.62760	7.821225
C	7.058663	7.527767	7.969375	C	14.81638	11.45139	7.872100	H	9.268163	3.098184	7.972725
C	7.109643	3.255638	7.901625	C	15.50221	10.23842	7.891925	H	4.953673	3.068884	7.821875
C	5.913613	2.524094	7.844950	C	16.87893	10.18088	7.874175	H	4.931608	4.862563	7.870025
C	5.926420	1.138050	7.817825	O	22.05292	9.084995	7.845775	H	7.043953	8.633483	7.982450
C	7.130610	0.408700	7.844975	B	23.30700	9.705273	7.859050	H	9.253453	4.917077	7.986850
C	8.324480	1.153370	7.901100	O	23.23795	11.10286	7.864675	H	10.79771	5.834665	8.025425
C	8.316553	2.540254	7.928675	O	17.20934	17.65298	7.790775	H	12.93357	7.087914	8.002875
B	18.38553	18.41036	7.823425	O	13.39593	11.19266	7.904350	H	10.74185	10.81479	7.972126
O	19.54858	17.63286	7.843225	B	13.30443	9.797026	7.944225	H	8.609103	9.556862	7.996300
C	19.06316	16.27273	7.827525	O	14.54852	9.156354	7.937501	H	27.99298	9.512935	7.966525
C	19.77834	15.09475	7.841700	C	9.554843	7.608115	8.006650	H	25.84072	10.73869	7.936950
C	19.05345	13.87995	7.831375	C	10.78790	6.938528	8.014576	H	23.70758	6.980115	7.809900
C	17.63319	13.89307	7.810275	C	11.98140	7.643658	8.001800	H	3.348264	5.759680	7.837625

Transformation Matrix

a	22.51323	0.00000	0.00000	
b	11.25662	19.49702	0.00000	
c	0.000000	0.000000	3.476572	AA
c	1.199774	0.69269	3.42000	inclined zigzag
c	1.388105	0.00000	3.42342	inclined armchair

Layer II AB stacking

C	37.11172	13.36236	11.06289	C	28.18865	21.62044	10.99150	C	23.26532	15.55027	11.18267
C	15.82066	14.05043	11.10882	C	28.92663	22.78433	11.00010	C	22.02213	16.21156	11.18649
C	38.29814	15.45296	11.13420	C	31.02596	19.11088	11.04432	C	20.82544	15.51032	11.20007
C	37.09138	16.13544	11.11692	C	30.30499	17.88709	11.04182	H	16.22538	7.092890	10.97549
C	35.85858	15.45636	11.07397	C	28.84861	17.90109	11.04449	H	20.54668	7.120970	11.12675
C	35.90701	14.04945	11.04709	C	28.14974	19.13780	11.02600	H	27.08577	21.61517	10.97369
C	17.10237	13.32703	11.13057	C	30.99537	16.65215	11.04272	H	32.98682	20.06333	11.06002
C	17.13774	11.92703	11.10859	C	32.37326	16.68369	11.04770	H	30.42151	15.71023	11.03944
C	18.35070	11.22628	11.13082	C	33.07980	17.88456	11.05694	H	32.13754	21.56729	11.06507
C	19.54530	11.95621	11.17360	C	32.44038	19.10528	11.05510	H	28.69181	15.72752	11.09287
C	19.54515	13.35709	11.19082	C	26.73523	19.15834	11.03682	H	26.20696	20.12661	11.02315
C	18.31528	14.02678	11.17130	C	26.07299	17.95040	11.07402	H	20.52478	9.597194	11.17464
C	18.36626	9.754647	11.10355	C	26.75882	16.73743	11.09385	H	16.21029	9.567894	11.02380
C	17.17023	9.023104	11.04687	C	28.13554	16.67989	11.07610	H	16.18822	11.36157	11.07195
C	17.18303	7.637060	11.01974	O	33.30953	15.58401	11.04770	H	18.30057	15.13249	11.18437
C	18.38722	6.907710	11.04690	B	34.56361	16.20428	11.06097	H	20.51007	11.41609	11.18877
C	19.58109	7.652380	11.10302	O	34.49456	17.60187	11.06660	H	22.05433	12.33367	11.22734
C	19.57317	9.039264	11.13060	O	28.46595	24.15199	10.99269	H	24.19019	13.58692	11.20480
B	29.64215	24.90937	11.02534	O	24.65255	17.69167	11.10627	H	21.99846	17.31380	11.17405
O	30.80519	24.13187	11.04515	B	24.56104	16.29604	11.14614	H	19.86572	16.05587	11.19822
C	30.31977	22.77174	11.02945	O	25.80513	15.65536	11.13942	H	39.24960	16.01194	11.16845
C	31.03495	21.59376	11.04362	C	20.81146	14.10712	11.20857	H	37.09734	17.23770	11.13887
C	30.31006	20.37896	11.03329	C	22.04451	13.43754	11.21650	H	34.96420	13.47912	11.01182
C	28.88980	20.39208	11.01220	C	23.23801	14.14267	11.20372	H	14.60488	12.25869	11.03955
c	0.00000	0.00000	6.40384	AB							

Layer II serrated zigzag

C	27.07536	7.567857	11.26808	C	18.15228	15.82594	11.19668	C	13.22896	9.755774	11.38786
C	5.784291	8.255926	11.31401	C	18.89026	16.98983	11.20529	C	11.98577	10.41705	11.39168
C	28.26176	9.658463	11.33939	C	20.98960	13.31638	11.24951	C	10.78907	9.715824	11.40526
C	27.05502	10.34094	11.32211	C	20.26863	12.09259	11.24701	H	6.189015	1.298389	11.18069
C	25.82222	9.661857	11.27916	C	18.81224	12.10659	11.24969	H	10.51031	1.326469	11.33193
C	25.87064	8.254951	11.25229	C	18.11337	13.34330	11.23118	H	17.04940	15.82067	11.17888
C	7.065998	7.532528	11.33576	C	20.95900	10.85765	11.24791	H	22.95045	14.26883	11.26521
C	7.101368	6.132525	11.31378	C	22.33689	10.88919	11.25288	H	20.38515	9.915727	11.24463
C	8.314328	5.431782	11.33601	C	23.04342	12.09006	11.26213	H	22.10118	15.77279	11.27026
C	9.508928	6.161712	11.37879	C	22.40401	13.31078	11.26029	H	18.65545	9.933021	11.29806

C	9.508779	7.562593	11.39601	C	16.69886	13.36384	11.24201	H	16.17060	14.33211	11.22834
C	8.278908	8.232276	11.37648	C	16.03662	12.15590	11.27921	H	10.48841	3.802693	11.37984
C	8.329888	3.960147	11.30873	C	16.72245	10.94293	11.29904	H	6.173918	3.773393	11.22898
C	7.133858	3.228603	11.25206	C	18.09917	10.88539	11.28129	H	6.151853	5.567072	11.27713
C	7.146665	1.842559	11.22493	O	23.27316	9.789504	11.25288	H	8.264198	9.337992	11.38956
C	8.350855	1.113209	11.25208	B	24.52724	10.40978	11.26616	H	10.47370	5.621586	11.39396
C	9.544725	1.857879	11.30821	O	24.45819	11.80737	11.27178	H	12.01796	6.539174	11.43254
C	9.536798	3.244763	11.33578	O	18.42958	18.35749	11.19788	H	14.15382	7.792423	11.40999
B	19.60578	19.11487	11.23053	O	14.61618	11.89717	11.31146	H	11.96210	11.51930	11.37924
O	20.76883	18.33737	11.25033	B	14.52468	10.50153	11.35133	H	9.829349	10.26137	11.40341
C	20.28341	16.97724	11.23464	O	15.76877	9.860863	11.34461	H	29.21322	10.21744	11.37364
C	20.99858	15.79926	11.24881	C	10.77509	8.312624	11.41376	H	27.06096	11.44320	11.34406
C	20.27369	14.58446	11.23849	C	12.00815	7.643037	11.42169	H	24.92783	7.684624	11.21701
C	18.85344	14.59758	11.21739	C	13.20164	8.348167	11.40891	H	4.568509	6.464189	11.24473
c	0.00000	0.00000	6.81422	serrated zigzag							

Layer II serrated armchair

C	27.24322	6.863348	11.26808	C	18.32014	15.12143	11.19668	C	13.39682	9.051265	11.38786
C	5.952151	7.551417	11.31401	C	19.05812	16.28532	11.20529	C	12.15363	9.712545	11.39168
C	28.42962	8.953955	11.33939	C	21.15746	12.61187	11.24951	C	10.95693	9.011315	11.40526
C	27.22288	9.636429	11.32211	C	20.43649	11.38808	11.24701	H	6.356875	0.593880	11.18069
C	25.99008	8.957348	11.27916	C	18.98010	11.40208	11.24969	H	10.67817	0.621960	11.33193
C	26.03850	7.550442	11.25229	C	18.28123	12.63879	11.23118	H	17.21726	15.11616	11.17888
C	7.233858	6.828019	11.33576	C	21.12686	10.15314	11.24791	H	23.11831	13.56432	11.26521
C	7.269228	5.428016	11.31378	C	22.50476	10.18468	11.25288	H	20.55301	9.211218	11.24463
C	8.482188	4.727273	11.33601	C	23.21128	11.38555	11.26213	H	22.26904	15.06828	11.27026
C	9.676788	5.457203	11.37879	C	22.57187	12.60627	11.26029	H	18.82331	9.228512	11.29806
C	9.676639	6.858084	11.39601	C	16.86672	12.65933	11.24201	H	16.33846	13.62760	11.22834
C	8.446768	7.527767	11.37648	C	16.20448	11.45139	11.27921	H	10.65627	3.098184	11.37984
C	8.497748	3.255638	11.30873	C	16.89031	10.23842	11.29904	H	6.341778	3.068884	11.22898
C	7.301718	2.524094	11.25206	C	18.26703	10.18088	11.28129	H	6.319713	4.862563	11.27713
C	7.314525	1.138050	11.22493	O	23.44102	9.084995	11.25288	H	8.432058	8.633483	11.38956
C	8.518715	0.408700	11.25208	B	24.69510	9.705273	11.26616	H	10.64156	4.917077	11.39396
C	9.712585	1.153370	11.30821	O	24.62605	11.10286	11.27178	H	12.18582	5.834665	11.43254
C	9.704659	2.540254	11.33578	O	18.59744	17.65298	11.19788	H	14.32168	7.087914	11.40999
B	19.77364	18.41036	11.23053	O	14.78404	11.19266	11.31146	H	12.12996	10.81479	11.37924
O	20.93669	17.63286	11.25033	B	14.69254	9.797026	11.35133	H	9.997209	9.556862	11.40341
C	20.45127	16.27273	11.23464	O	15.93663	9.156354	11.34461	H	29.38108	9.512935	11.37364
C	21.16644	15.09475	11.24881	C	10.94295	7.608115	11.41376	H	27.22882	10.73869	11.34406
C	20.44156	13.87995	11.23849	C	12.17601	6.938528	11.42169	H	25.09569	6.980115	11.21701
C	19.02130	13.89307	11.21739	C	13.36950	7.643658	11.40891	H	4.736369	5.759680	11.24473
c	0.00000	0.00000	6.81422	serrated armchair							

COF-6

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	15.89563	8.845316	0.86161	O	9.288773	5.341016	0.82716
C	14.48142	8.839945	0.84999	B	8.040427	5.971807	0.82076
C	13.76977	7.610588	0.84166	O	8.120573	7.368169	0.81091
C	14.46919	6.381114	0.84331	O	16.79032	5.331043	0.84878
C	15.84657	6.423560	0.85196	B	18.03967	5.960022	0.85468
C	16.54457	7.629647	0.86141	O	17.96170	7.356371	0.86463
C	12.31386	7.612648	0.82996	C	5.521790	3.085190	0.82963
C	11.60519	8.843752	0.81941	C	4.320793	3.811040	0.84141
C	12.33496	10.10368	0.82261	C	4.283533	5.213800	0.84601
C	13.75529	10.10189	0.84169	C	5.512527	5.891126	0.83848
C	14.47044	11.32227	0.85003	C	6.745853	5.221990	0.82658
C	13.74534	12.49412	0.83789	C	6.717893	3.818930	0.82261

C	12.35196	12.49558	0.81744	H	16.43449	9.807772	0.86739
C	11.62342	11.32585	0.80941	H	12.17483	5.437313	0.84011
C	10.19080	8.853007	0.80986	H	9.654883	9.817066	0.80283
C	9.538543	7.639046	0.81301	H	13.90248	5.434823	0.83509
C	10.23402	6.431499	0.82308	H	10.52053	11.31154	0.79376
C	11.61116	6.385260	0.83086	H	15.57334	11.30425	0.86594
O	4.353760	0.823440	0.80971	H	5.508854	6.994033	0.84209
B	5.523970	1.589210	0.82696	H	3.367370	3.256520	0.84836
O	6.693240	0.821640	0.84359	H	7.675120	3.271100	0.81209

Transformation Matrix

a	15.052800	0.000000	0.000000	
b	7.526400	13.036110	0.000000	
c	0.000000	0.000000	3.480887	AA
c	1.198595	0.692009	3.396059	inclined zigzag
c	1.387745	0.000000	3.402900	inclined armchair

Layer II AB stacking

C	23.42203	13.19069	4.13016	O	16.81517	9.686385	4.09571
C	22.00782	13.18531	4.11854	B	15.56683	10.31718	4.08931
C	21.29617	11.95596	4.11021	O	15.64697	11.71354	4.07946
C	21.99559	10.72648	4.11186	O	24.31672	9.676413	4.11733
C	23.37297	10.76893	4.12051	B	25.56607	10.30539	4.12323
C	24.07097	11.97502	4.12996	O	25.48810	11.70174	4.13318
C	19.84026	11.95802	4.09851	C	13.04819	7.430559	4.09818
C	19.13159	13.18912	4.08796	C	11.84719	8.156409	4.10996
C	19.86136	14.44905	4.09116	C	11.80993	9.559170	4.11456
C	21.28169	14.44726	4.11024	C	13.03893	10.23650	4.10703
C	21.99684	15.66764	4.11858	C	14.27225	9.567360	4.09513
C	21.27174	16.83949	4.10644	C	14.24429	8.164299	4.09116
C	19.87836	16.84095	4.08599	H	23.96089	14.15314	4.13594
C	19.14982	15.67122	4.07796	H	19.70123	9.782682	4.10866
C	17.71720	13.19838	4.07841	H	17.18128	14.16244	4.07138
C	17.06494	11.98442	4.08156	H	21.42888	9.780192	4.10364
C	17.76042	10.77687	4.09163	H	18.04693	15.65691	4.06231
C	19.13756	10.73063	4.09941	H	23.09974	15.64962	4.13449
O	11.88016	5.168809	4.07826	H	13.03525	11.33940	4.11064
B	13.05037	5.934579	4.09551	H	10.89377	7.601890	4.11691
O	14.21964	5.167009	4.11214	H	15.20152	7.616469	4.08064

c	0.00000	0.00000	6.537105	AB

Layer II serrated zigzag

C	17.094220	9.537325	4.27655	O	10.487370	6.033025	4.24210
C	15.680010	9.531954	4.26493	B	9.239022	6.663816	4.23570
C	14.968360	8.302597	4.25660	O	9.319168	8.060178	4.22585
C	15.667780	7.073123	4.25825	O	17.988920	6.023052	4.26372
C	17.045160	7.115569	4.26690	B	4.185460	6.652031	4.26962
C	17.743170	8.321655	4.27635	O	19.160290	8.048380	4.27957
C	13.512450	8.304657	4.24490	C	6.720385	3.777199	4.24457
C	12.803790	9.535761	4.23435	C	5.519388	4.503049	4.25635
C	13.533560	10.795690	4.23755	C	5.482128	5.905809	4.26095
C	14.953890	10.793900	4.25663	C	6.711122	6.583135	4.25342
C	15.669030	12.014280	4.26497	C	7.944448	5.913999	4.24152
C	7.417540	0.150020	4.25283	C	7.916488	4.510939	4.23755
C	6.024160	0.151480	4.23238	H	17.633090	10.499780	4.28233
C	12.822010	12.017860	4.22435	H	13.373430	6.129322	4.25505
C	11.389390	9.545016	4.22480	H	10.853480	10.509080	4.21777

C	10.737140	8.331055	4.22795	H	15.101080	6.126832	4.25003	
C	11.432620	7.123508	4.23802	H	11.719120	12.003550	4.20870	
C	12.809760	7.077269	4.24580	H	16.771930	11.996260	4.28088	
O	5.552355	1.515449	4.22465	H	6.707449	7.686042	4.25703	
B	6.722565	2.281219	4.24190	H	4.565965	3.948529	4.26330	
O	7.891835	1.513649	4.25853	H	8.873714	3.963109	4.22703	
c	0.00000	0.00000	6.82988	serrated zigzag				

Layer II serrated armchair

C	17.283370	8.845316	4.27996	O	10.676520	5.341016	4.24551	
C	15.869160	8.839945	4.26834	B	9.428172	5.971807	4.23911	
C	15.157510	7.610588	4.26001	O	9.508318	7.368169	4.22926	
C	15.856930	6.381114	4.26166	O	3.125270	5.331043	4.26713	
C	17.234310	6.423560	4.27031	B	4.374610	5.960022	4.27303	
C	17.932320	7.629647	4.27976	O	4.296640	7.356371	4.28298	
C	13.701600	7.612648	4.24831	C	6.909535	3.085190	4.24798	
C	12.992940	8.843752	4.23776	C	5.708538	3.811040	4.25976	
C	13.722700	10.103680	4.24096	C	5.671278	5.213800	4.26436	
C	15.143030	10.101890	4.26004	C	6.900272	5.891126	4.25683	
C	15.858180	11.322270	4.26838	C	8.133598	5.221990	4.24493	
C	15.133090	12.494120	4.25624	C	8.105639	3.818930	4.24096	
C	13.739710	12.495580	4.23579	H	17.822240	9.807772	4.28574	
C	13.011160	11.325850	4.22776	H	13.562580	5.437313	4.25846	
C	11.578540	8.853007	4.22821	H	11.042630	9.817066	4.22118	
C	10.926290	7.639046	4.23136	H	15.290230	5.434823	4.25344	
C	11.621770	6.431499	4.24143	H	11.908270	11.311540	4.21211	
C	12.998910	6.385260	4.24921	H	16.961090	11.304250	4.28429	
O	5.741505	0.823440	4.22806	H	6.896599	6.994033	4.26044	
B	6.911715	1.589210	4.24531	H	4.755115	3.256520	4.26671	
O	8.080985	0.821640	4.26194	H	9.062865	3.271100	4.23044	
c	0.00000	0.00000	6.83669	serrated armchair				

TP COF

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	34.39868	29.87646	0.8851000	C	24.37890	16.82335	1.032600	B	11.84997	13.94665	0.9876250
C	36.83124	31.28005	0.9077250	C	25.61187	16.11050	1.034250	C	16.85226	0.9500470	0.8756500
C	36.80484	29.87837	0.9170500	C	25.60210	14.68645	1.042625	C	18.08207	1.668191	0.8882250
C	35.60217	29.15006	0.9062250	C	24.37281	14.01387	1.039150	C	18.05348	3.069575	0.8809500
H	33.44363	29.32625	0.8758000	C	23.14563	14.69843	1.027075	C	16.84923	3.794051	0.8623500
C	36.31152	23.12550	0.9099250	H	24.36958	12.91163	1.040475	C	15.64649	3.067074	0.8480500
C	37.02438	24.34742	0.9158250	H	22.22370	16.65756	1.022275	C	15.62094	1.665626	0.8540750
C	38.45328	21.86251	0.9374750	C	28.04238	14.66603	1.033025	H	19.00718	3.622121	0.8918250
C	36.29857	25.51970	0.9156250	C	26.86112	13.99045	1.046875	H	14.69127	3.617120	0.8324500
C	34.89022	23.12622	0.9052000	H	26.85656	12.88845	1.058825	C	19.31136	0.9209210	0.9099000
C	34.16021	21.86543	0.9001500	H	28.99457	14.11092	1.033850	H	20.26561	1.472396	0.9195500
C	34.87082	20.63552	0.8890250	H	37.76038	29.32940	0.9335250	H	20.24120	10.10662	0.9359750
C	36.32595	20.63432	0.8965750	H	38.99637	22.82239	0.9526250	H	19.37732	8.607212	0.8973250
C	37.03899	21.86257	0.9123750	H	38.12735	24.33161	0.9198250	H	14.32416	8.609713	0.8674250
C	34.17387	19.40526	0.8849000	H	36.45034	18.45755	0.8907000	H	13.46097	10.10351	0.9084250
C	37.02020	19.40224	0.9024250	H	34.74218	18.45969	0.8769500	H	17.71272	14.48212	0.9219500
C	32.79719	19.44526	0.8987000	H	33.07544	24.33291	0.9043250	H	15.98495	14.48153	0.9239750
C	32.74545	21.86793	0.9114750	H	32.20335	22.82837	0.9240000	C	41.87809	18.21613	1.031250
C	34.17826	24.34885	0.9069750	C	14.39298	0.9160510	0.8412250	C	43.10454	18.90112	1.055425
C	32.09827	20.65075	0.9128750	H	13.43777	1.465609	0.8237000	C	44.33380	18.22957	1.074325
C	34.90507	25.52051	0.9113000	C	17.57832	12.30619	0.9074750	C	44.34391	16.80553	1.069575

O	30.68187	20.37381	0.9355250	C	18.27864	13.53516	0.9240000	C	43.11116	16.09209	1.056575
O	31.85747	18.35059	0.9119000	C	19.65576	13.49148	0.9479500	C	41.90845	16.81111	1.037300
O	36.77170	26.88481	0.9179000	C	20.35256	12.28453	0.9534500	H	43.09948	20.00329	1.053900
O	34.43290	26.88552	0.9100750	C	19.70287	11.06943	0.9320000	H	40.95639	16.25577	1.021600
B	30.60740	18.97701	0.9375750	O	20.60011	14.58300	0.9765000	C	39.09807	20.64413	0.9491000
B	35.60246	27.65364	0.9126750	O	21.76957	12.55647	0.9865500	C	38.39683	19.43987	0.9309250
C	38.05931	32.03014	0.9193000	C	16.12204	12.30593	0.9025000	O	40.51356	20.36410	0.9872000
H	39.01498	31.48159	0.9364750	C	15.41295	11.07515	0.8962750	O	39.33394	18.34341	0.9565000
C	24.41733	18.26152	1.027250	C	16.14113	9.814229	0.8848000	B	40.58493	18.96701	0.9929000
C	34.37049	31.27794	0.8740250	C	17.56149	9.813969	0.8926750	C	45.59208	18.92632	1.090825
C	35.60035	31.99605	0.8855750	C	18.28873	11.07605	0.9091000	C	45.57991	16.09949	1.068700
C	33.14102	32.02530	0.8509750	C	15.42718	8.593088	0.8720250	C	43.15001	14.65392	1.056175
C	26.84758	16.81718	1.020575	C	16.15344	7.421854	0.8680250	H	42.19825	14.09806	1.053025
C	28.08053	16.10404	1.014725	C	17.54702	7.421431	0.8769250	C	46.81231	16.81342	1.072000
C	29.28315	16.82283	0.9879500	C	18.27422	8.592146	0.8890250	C	46.77369	18.25139	1.089550
C	29.31319	18.22769	0.9686000	O	15.67979	6.058103	0.8582000	H	47.72544	18.80706	1.098950
C	28.08663	18.91288	0.9813000	O	18.01930	6.056999	0.8738000	H	45.58649	20.02830	1.101200
C	26.85737	18.24126	1.006300	C	13.99864	11.06667	0.9098500	C	45.59021	14.67545	1.055400
H	30.23537	16.26740	0.9804000	C	13.34772	12.28106	0.9324750	C	44.33161	13.97873	1.055775
H	28.09240	20.01511	0.9679500	C	14.04313	13.48859	0.9356250	H	44.33682	12.87656	1.052275
C	25.59852	18.93723	1.014650	C	15.42030	13.53392	0.9186500	C	9.326377	14.00396	1.035200
H	25.60300	20.03930	1.008300	O	11.93065	12.55056	0.9637250	C	10.55260	14.69006	1.027125
H	23.46556	18.81709	1.031025	O	13.09771	14.57885	0.9686750	C	10.52161	16.09469	1.050875
H	32.18653	31.47438	0.8413000	B	21.84881	13.95298	0.9997500	H	9.331083	12.90176	1.019800
C	23.17641	16.10342	1.029025	B	16.84910	5.290247	0.8633000	H	11.47402	16.64954	1.048075

Transformation Matrix

a	**3**7.493430	0.000000	0.000000	
b	18.746710	32.470250	0.000000	
c	0.000000	0.000000	3.472000	AA
c	1.203185	0.69466	3.42000	inclined zigzag
c	1.386345	0.000000	3.425000	inclined armchair

Layer II AB stacking

C	53.14540	40.69988	4.086278	C	43.12562	27.64677	4.233778	B	30.59669	24.77007	4.188803
C	55.57796	42.10347	4.108903	C	44.35859	26.93392	4.235428	C	35.59898	11.77347	4.076828
C	55.55156	40.70179	4.118228	C	44.34882	25.50987	4.243803	C	36.82878	12.49161	4.089403
C	54.34888	39.97348	4.107403	C	43.11953	24.83729	4.240328	C	36.80019	13.89300	4.082128
H	52.19035	40.14967	4.076978	C	41.89235	25.52185	4.228253	C	35.59595	14.61747	4.063528
C	55.05824	33.94892	4.111103	H	43.11629	23.73505	4.241653	C	34.39320	13.89050	4.049228
C	55.77110	35.17084	4.117003	H	40.97041	27.48098	4.223453	C	34.36766	12.48905	4.055253
C	57.20000	32.68593	4.138653	C	46.78909	25.48945	4.234203	H	37.75389	14.44554	4.093003
C	55.04528	36.34312	4.116803	C	45.60783	24.81387	4.248053	H	33.43798	14.44054	4.033628
C	53.63694	33.94964	4.106378	H	45.60328	23.71187	4.260003	C	38.05807	11.74434	4.111078
C	52.90693	32.68885	4.101328	H	47.74129	24.93434	4.235028	H	39.01233	12.29582	4.120728
C	53.61753	31.45894	4.090203	H	56.50710	40.15282	4.134703	H	38.98792	20.93004	4.137153
C	55.07267	31.45774	4.097753	H	57.74308	33.64581	4.153803	H	38.12403	19.43063	4.098503
C	55.78571	32.68599	4.113553	H	56.87407	35.15503	4.121003	H	33.07088	19.43313	4.068603
C	52.92059	30.22868	4.086078	H	55.19706	29.28097	4.091878	H	32.20769	20.92693	4.109603
C	55.76691	30.22566	4.103603	H	53.48890	29.28311	4.078128	H	36.45943	25.30554	4.123128
C	51.54391	30.26868	4.099878	H	51.82215	35.15633	4.105503	H	34.73167	25.30495	4.125153
C	51.49216	32.69135	4.112653	H	50.95007	33.65179	4.125178	C	60.62481	29.03955	4.232428
C	52.92498	35.17227	4.108153	C	33.13969	11.73947	4.042403	C	61.85126	29.72454	4.256603
C	50.84499	31.47417	4.114053	H	32.18449	12.28903	4.024878	C	63.08052	29.05299	4.275503
C	53.65179	36.34393	4.112478	C	36.32504	23.12961	4.108653	C	63.09063	27.62895	4.270753
O	49.42859	31.19723	4.136703	C	37.02536	24.35858	4.125178	C	61.85788	26.91551	4.257753
O	50.60419	29.17401	4.113078	C	38.40247	24.31490	4.149128	C	60.65517	27.63453	4.238478
O	55.51842	37.70823	4.119078	C	39.09927	23.10795	4.154628	H	61.84620	30.82671	4.255078
O	53.17962	37.70894	4.111253	C	38.44958	21.89285	4.133178	H	59.70311	27.07919	4.222778
B	49.35412	29.80043	4.138753	O	39.34682	25.40642	4.177678	C	57.84478	31.46755	4.150278
B	54.34917	38.47706	4.113853	O	40.51628	23.37989	4.187728	C	57.14355	30.26329	4.132103
C	56.80603	42.85356	4.120478	C	34.86876	23.12935	4.103678	O	59.26028	31.18752	4.188378

H	57.76170	42.30501	4.137653	C	34.15966	21.89857	4.097453	O	58.08065	29.16683	4.157678
C	43.16405	29.08494	4.228428	C	34.88785	20.63765	4.085978	B	59.33165	29.79043	4.194078
C	53.11721	42.10136	4.075203	C	36.30820	20.63739	4.093853	C	64.33879	29.74974	4.292003
C	54.34706	42.81947	4.086753	C	37.03545	21.89947	4.110278	C	64.32663	26.92291	4.269878
C	51.88774	42.84872	4.052153	C	34.17390	19.41651	4.073203	C	61.89672	25.47734	4.257353
C	45.59430	27.64060	4.221753	C	34.90015	18.24528	4.069203	H	60.94497	24.92148	4.254203
C	46.82725	26.92746	4.215903	C	36.29374	18.24485	4.078103	C	65.55902	27.63684	4.273178
C	48.02987	27.64625	4.189128	C	37.02094	19.41557	4.090203	C	65.52040	29.07481	4.290728
C	48.05991	29.05111	4.169778	O	34.42651	16.88153	4.059378	H	66.47215	29.63048	4.300128
C	46.83334	29.73630	4.182478	O	36.76601	16.88042	4.074978	H	64.33321	30.85172	4.302378
C	45.60409	29.06468	4.207478	C	32.74535	21.89009	4.111028	C	64.33693	25.49887	4.256578
H	48.98209	27.09082	4.181578	C	32.09444	23.10448	4.133653	C	63.07833	24.80215	4.256953
H	46.83912	30.83853	4.169128	C	32.78984	24.31201	4.136803	H	63.08353	23.69998	4.253453
C	44.34524	29.76065	4.215828	C	34.16702	24.35734	4.119828	C	28.07309	24.82738	4.236378
H	44.34972	30.86272	4.209478	O	30.67736	23.37398	4.164903	C	29.29932	25.51348	4.228303
H	42.21228	29.64051	4.232203	O	31.84443	25.40227	4.169853	C	29.26833	26.91811	4.252053
H	50.93325	42.29780	4.042478	B	40.59553	24.77640	4.200928	H	28.07780	23.72518	4.220978
C	41.92313	26.92684	4.230203	B	35.59582	16.11367	4.064478	H	30.22074	27.47296	4.249253
c	0.00000	0.00000	6.402355	AB							

Layer II serrated zigzag

C	35.60187	30.57112	4.297788	C	25.58208	17.51801	4.445288	B	13.05315	14.64131	4.400313
C	38.03443	31.97471	4.320413	C	26.81505	16.80516	4.446938	C	18.05544	1.64470	4.288338
C	38.00803	30.57303	4.329738	C	26.80528	15.38111	4.455313	C	19.28525	2.36285	4.300913
C	36.80536	29.84472	4.318913	C	25.57599	14.70853	4.451838	C	19.25666	3.76423	4.293638
H	34.64682	30.02091	4.288488	C	24.34881	15.39309	4.439763	C	18.05241	4.48871	4.275038
C	37.51471	23.82016	4.322613	H	25.57276	13.60629	4.453163	C	16.84967	3.76173	4.260738
C	38.22757	25.04208	4.328513	H	23.42688	17.35222	4.434963	C	16.82413	2.36028	4.266763
C	39.65647	22.55717	4.350163	C	29.24556	15.36069	4.445713	H	20.21036	4.31678	4.304513
C	37.50175	26.21436	4.328313	C	28.06430	14.68511	4.459563	H	15.89445	4.31178	4.245138
C	36.09341	23.82088	4.317888	H	28.05974	13.58311	4.471513	C	20.51454	1.61558	4.322588
C	35.36340	22.56009	4.312838	H	30.19775	14.80558	4.446538	H	21.46879	2.16705	4.332238
C	36.07401	21.33018	4.301713	H	38.96357	30.02406	4.346213	H	21.44438	10.80128	4.348663
C	37.52914	21.32898	4.309263	H	40.19955	23.51705	4.365313	H	20.58050	9.30187	4.310013
C	38.24218	22.55723	4.325063	H	39.33054	25.02627	4.332513	H	15.52734	9.30437	4.280113
C	35.37706	20.09992	4.297588	H	37.65353	19.15221	4.303388	H	14.66416	10.79817	4.321113
C	38.22338	20.09690	4.315113	H	35.94537	19.15435	4.289638	H	18.91590	15.17678	4.334638
C	34.00038	20.13992	4.311388	H	34.27863	25.02757	4.317013	H	17.18814	15.17619	4.336663
C	33.94864	22.56259	4.324163	H	33.40654	23.52303	4.336688	C	43.08128	18.91079	4.443938
C	35.38145	25.04351	4.319663	C	15.59616	1.61071	4.253913	C	44.30773	19.59578	4.468113
C	33.30146	21.34541	4.325563	H	14.64095	2.16026	4.236388	C	45.53699	18.92423	4.487013
C	36.10826	26.21517	4.323988	C	18.78150	13.00085	4.320163	C	45.54710	17.50019	4.482263
O	31.88505	21.06847	4.348213	C	19.48182	14.22982	4.336688	C	44.31435	16.78675	4.469263
O	33.06065	19.04525	4.324588	C	20.85894	14.18614	4.360638	C	43.11164	17.50577	4.449988
O	37.97489	27.57947	4.330588	C	21.55574	12.97919	4.366138	H	44.30267	20.69795	4.466588
O	35.63609	27.58018	4.322763	C	20.90605	11.76409	4.344688	H	42.15958	16.95043	4.434288
B	31.81059	19.67167	4.350263	O	21.80329	15.27766	4.389188	C	40.30125	21.33879	4.361788
B	36.80564	28.34830	4.325363	O	22.97275	13.25113	4.399238	C	39.60002	20.13453	4.343613
C	20.51579	0.25455	4.331988	C	17.32522	13.00059	4.315188	O	41.71675	21.05876	4.399888
H	40.21817	32.17625	4.349163	C	16.61613	11.76981	4.308963	O	40.53712	19.03807	4.369188
C	25.62051	18.95618	4.439938	C	17.34431	10.50889	4.297488	B	41.78812	19.66167	4.405588
C	35.57368	31.97260	4.286713	C	18.76467	10.50863	4.305363	C	46.79527	19.62098	4.503513
C	18.05683	0.22046	4.298263	C	19.49191	11.77071	4.321788	C	46.78310	16.79415	4.481388
C	15.59750	0.24971	4.263663	C	16.63037	9.28774	4.284713	C	44.35320	15.34858	4.468863
C	28.05076	17.51184	4.433263	C	17.35662	8.11651	4.280713	H	43.40144	14.79272	4.465713
C	29.28371	16.79870	4.427413	C	18.75020	8.11609	4.289613	C	10.52207	17.50808	4.484688
C	30.48633	17.51749	4.400638	C	19.47740	9.28680	4.301713	C	47.97688	18.94605	4.502238
C	30.51637	18.92235	4.381288	O	16.88297	6.75276	4.270888	H	11.43520	19.50172	4.511638
C	29.28981	19.60754	4.393988	O	19.22248	6.75165	4.286488	H	46.78968	20.72296	4.513888
C	28.06055	18.93592	4.418988	C	15.20183	11.76133	4.322538	C	9.29997	15.37011	4.468088
H	31.43855	16.96206	4.393088	C	14.55091	12.97572	4.345163	C	45.53480	14.67339	4.468463
H	29.29558	20.70977	4.380638	C	15.24632	14.18325	4.348313	H	8.04657	13.57122	4.464963

C	26.80170	19.63189	4.427338	C	16.62348	14.22858	4.331338	C	10.52956	14.69862	4.447888
H	26.80618	20.73396	4.420988	O	13.13383	13.24522	4.376413	C	11.75578	15.38472	4.439813
H	24.66875	19.51175	4.443713	O	14.30089	15.27351	4.381363	C	11.72480	16.78935	4.463563
H	33.38972	32.16904	4.253988	B	23.05199	14.64764	4.412438	H	10.53427	13.59642	4.432488
C	24.37959	16.79808	4.441713	B	18.05228	5.98490	4.275988	H	12.67721	17.34420	4.460763
c	0.00000	0.00000	6.82538	serrated zigzag							

Layer II serrated armchair

C	35.78503	29.876460	4.301190	C	25.76525	16.823350	4.448690	B	13.23631	13.946650	4.403715
C	38.21759	31.280050	4.323815	C	26.99821	16.110500	4.450340	C	18.23861	0.950047	4.291740
C	38.19118	29.878370	4.333140	C	26.98845	14.686450	4.458715	C	19.46841	1.668191	4.304315
C	36.98851	29.150060	4.322315	C	25.75916	14.013870	4.455240	C	19.43983	3.069575	4.297040
H	34.82998	29.326250	4.291890	C	24.53197	14.698430	4.443165	C	18.23557	3.794051	4.278440
C	37.69786	23.125500	4.326015	H	25.75592	12.911630	4.456565	C	17.03284	3.067074	4.264140
C	38.41072	24.347420	4.331915	H	23.61004	16.657560	4.438365	C	17.00729	1.665626	4.270165
C	39.83963	21.862510	4.353565	C	29.42872	14.666030	4.449115	H	20.39352	3.622121	4.307915
C	37.68491	25.519700	4.331715	C	28.24747	13.990450	4.462965	H	16.07762	3.617120	4.248540
C	36.27657	23.126220	4.321290	H	28.24290	12.888450	4.474915	C	20.69770	0.920921	4.325990
C	35.54655	21.865430	4.316240	H	30.38091	14.110920	4.449940	H	21.65195	1.472396	4.335640
C	36.25716	20.635520	4.305115	H	39.14672	29.329400	4.349615	H	21.62754	10.106620	4.352065
C	37.71230	20.634320	4.312665	H	40.38271	22.822390	4.368715	H	20.76366	8.607212	4.313415
C	38.42533	21.862570	4.328465	H	39.51369	24.331610	4.335915	H	15.71050	8.609713	4.283515
C	35.56021	19.405260	4.300990	H	37.83669	18.457550	4.306790	H	14.84731	10.103510	4.324515
C	38.40654	19.402240	4.318515	H	36.12852	18.459690	4.293040	H	19.09907	14.482120	4.338040
C	34.18354	19.445260	4.314790	H	34.46178	24.332910	4.320415	H	17.37130	14.481530	4.340065
C	34.13179	21.867930	4.327565	H	33.58969	22.828370	4.340090	C	43.26443	18.216130	4.447340
C	35.56461	24.348850	4.323065	C	15.77932	0.916051	4.257315	C	44.49089	18.901120	4.471515
C	33.48462	20.650750	4.328965	H	14.82411	1.465609	4.239790	C	45.72015	18.229570	4.490415
C	36.29142	25.520510	4.327390	C	18.96466	12.306190	4.323565	C	45.73026	16.805530	4.485665
O	32.06821	20.373810	4.351615	C	19.66499	13.535160	4.340090	C	44.49751	16.092090	4.472665
O	33.24382	18.350590	4.327990	C	21.04210	13.491480	4.364040	C	43.29480	16.811110	4.453390
O	38.15805	26.884810	4.333990	C	21.73890	12.284530	4.369540	H	44.48582	20.003290	4.469990
O	35.81924	26.885520	4.326165	C	21.08921	11.069430	4.348090	H	42.34274	16.255770	4.437690
B	31.99375	18.977010	4.353665	O	21.98645	14.583000	4.392590	C	40.48441	20.644130	4.365190
B	36.98880	27.653640	4.328765	O	23.15591	12.556470	4.402640	C	39.78318	19.439870	4.347015
C	39.44566	32.030140	4.335390	C	17.50838	12.305930	4.318590	O	41.89991	20.364100	4.403290
H	40.40133	31.481590	4.352565	C	16.79930	11.075150	4.312365	O	40.72028	18.343410	4.372590
C	25.80367	18.261520	4.443340	C	17.52748	9.814229	4.300890	B	41.97128	18.967010	4.408990
C	35.75684	31.277940	4.290115	C	18.94783	9.813969	4.308765	C	46.97842	18.926320	4.506915
C	36.98669	31.996050	4.301665	C	19.67508	11.076050	4.325190	C	9.47283	16.099490	4.484790
C	34.52737	32.025300	4.267065	C	16.81353	8.593088	4.288115	C	44.53635	14.653920	4.472265
C	28.23392	16.817180	4.436665	C	17.53979	7.421854	4.284115	H	43.58459	14.098060	4.469115
C	29.46688	16.104040	4.430815	C	18.93336	7.421431	4.293015	C	10.70522	16.813420	4.488090
C	30.66949	16.822830	4.404040	C	19.66056	8.592146	4.305115	C	10.66660	18.251390	4.505640
C	30.69954	18.227690	4.384690	O	17.06614	6.058103	4.274290	H	11.61836	18.807060	4.515040
C	29.47297	18.912880	4.397390	O	19.40565	6.056999	4.289890	H	46.97284	20.028300	4.517290
C	28.24372	18.241260	4.422390	C	15.38498	11.066670	4.325940	C	9.48312	14.675450	4.471490
H	31.62172	16.267400	4.396490	C	14.73407	12.281060	4.348565	C	8.22453	13.978730	4.471865
H	29.47874	20.015110	4.384040	C	15.42947	13.488590	4.351715	H	8.22973	12.876560	4.468365
C	26.98487	18.937230	4.430740	C	16.80664	13.533920	4.334740	C	10.71272	14.003960	4.451290
H	26.98935	20.039300	4.424390	O	13.31699	12.550560	4.379815	C	11.93894	14.690060	4.443215
H	24.85191	18.817090	4.447115	O	14.48405	14.578850	4.384765	C	11.90796	16.094690	4.466965
H	33.57288	31.474380	4.257390	B	23.23516	13.952980	4.415840	H	10.71743	12.901760	4.435890
C	24.56276	16.103420	4.445115	B	18.23545	5.290247	4.279390	H	12.86036	16.649540	4.464165
c	0.00000	0.00000	6.83218	serrated armchair							

COF-4M

Layer I AA, AB, inclined zigzag & armchair, serrated zigzag & armchair

C	16.65795	14.57413	0.8662960	O	11.20571	9.554735	0.8149160
C	16.69869	15.98028	0.8642160	O	8.386591	14.42251	0.9112960
C	15.46072	16.64832	0.8602260	B	28.85009	13.79134	0.9119460
C	14.25893	15.95477	0.8594960	B	12.92274	13.79939	0.8610660
C	14.21803	14.54852	0.8606960	B	10.03714	8.786865	0.8151160
C	15.45619	13.88052	0.8633260	C	26.31219	16.63906	0.9244460
H	15.44348	17.75057	0.8584760	C	25.07378	15.97165	0.9219960
H	13.31323	16.52131	0.8566460	C	25.11413	14.56548	0.9248460
H	15.47330	12.77820	0.8640760	C	26.31559	13.87148	0.9253160
H	17.60369	14.00774	0.8695460	C	27.55387	14.53887	0.9241960
C	11.23588	6.552347	0.7979460	C	27.51373	15.94491	0.9261160
C	10.03838	7.290568	0.8001260	H	24.16820	13.99940	0.9243960
C	8.840971	6.552197	0.7960960	H	26.29782	12.76925	0.9250460
C	8.840961	5.164634	0.7951960	H	28.45984	16.51109	0.9265760
C	10.03848	4.426489	0.7995760	H	26.33001	17.74158	0.9237460
C	11.23590	5.164728	0.7984960	C	9.340211	0.795383	0.8400960
H	7.877671	7.088386	0.7953460	C	19.49931	18.39517	0.8532960
H	7.877801	4.628389	0.7937660	C	20.19245	17.19146	0.8764660
H	12.19921	4.628671	0.8001960	C	21.58226	17.18971	0.8876260
H	12.19940	7.088141	0.7988760	C	22.27837	18.39192	0.8747960
C	10.72633	13.33004	0.8750660	C	10.72945	0.793766	0.8504260
C	9.336611	13.32796	0.8885460	O	19.24258	16.09653	0.8840160
C	8.643501	12.12411	0.8777660	O	22.52935	16.09253	0.9102460
C	9.340001	10.92161	0.8529160	O	11.20607	2.162620	0.8326760
C	10.72909	10.92367	0.8395160	O	8.867001	2.165328	0.8159160
C	11.42252	12.12811	0.8508760	O	23.70144	18.11697	0.8890960
O	7.219531	12.39550	0.8935960	O	18.07539	18.12346	0.8460460
O	8.866661	9.551425	0.8371960	B	17.99500	16.72763	0.8650460
O	12.84555	12.40333	0.8417960	B	10.03749	2.930173	0.8134960
O	11.67349	14.42733	0.8815960	B	23.77861	16.72083	0.9089960

Transformation Matrix

a	21.711180	0.000000	0.000000	
b	10.855590	18.802430	0.000000	
c	0.000000	0.000000	3.505078	AA
c	1.19747	0.691360	3.437101	inclined zigzag
c	1.38958	0.00000	3.45078	inclined armchair

Layer II AB stacking

C	27.51354	20.84161	4.048914	O	22.06130	15.82221	3.997534
C	27.55428	22.24776	4.046834	O	19.24218	20.68999	4.093914
C	26.31631	22.91580	4.042844	B	39.70568	20.05882	4.094564
C	25.11452	22.22225	4.042114	B	23.77833	20.06687	4.043684
C	25.07362	20.81600	4.043314	B	20.89273	15.05434	3.997734
C	26.31178	20.14800	4.045944	C	37.16778	22.90654	4.107064
H	26.29907	24.01805	4.041094	C	35.92937	22.23913	4.104614
H	24.16882	22.78879	4.039264	C	35.96972	20.83296	4.107464
H	26.32889	19.04568	4.046694	C	37.17118	20.13896	4.107934
H	28.45928	20.27522	4.052164	C	38.40946	20.80635	4.106814
C	22.09147	12.81983	3.980564	C	38.36932	22.21239	4.108734
C	20.89397	13.55805	3.982744	H	35.02379	20.26688	4.107014
C	19.69656	12.81968	3.978714	H	37.15341	19.03673	4.107664
C	19.69655	11.43211	3.977814	H	39.31543	22.77857	4.109194

C	20.89407	10.69397	3.982194	H	37.18560	24.00906	4.106364
C	22.09149	11.43221	3.981114	C	20.19580	7.062861	4.022714
H	18.73326	13.35586	3.977964	C	30.35490	24.66265	4.035914
H	18.73339	10.89587	3.976384	C	31.04804	23.45894	4.059084
H	23.05480	10.89615	3.982814	C	32.43785	23.45719	4.070244
H	23.05499	13.35562	3.981494	C	33.13396	24.65940	4.057414
C	21.58192	19.59752	4.057684	C	21.58504	7.061244	4.033044
C	20.19220	19.59544	4.071164	O	30.09817	22.36401	4.066634
C	19.49909	18.39159	4.060384	O	33.38494	22.36001	4.092864
C	20.19559	17.18909	4.035534	O	22.06166	8.430098	4.015294
C	21.58468	17.19115	4.022134	O	19.72259	8.432806	3.998534
C	22.27811	18.39559	4.033494	O	34.55703	24.38445	4.071714
O	18.07512	18.66298	4.076214	O	28.93098	24.39094	4.028664
O	19.72225	15.81890	4.019814	B	28.85059	22.99511	4.047664
O	23.70114	18.67081	4.024414	B	20.89308	9.197651	3.996114
O	22.52908	20.69481	4.064214	B	34.63420	22.98831	4.091614
c	0.00000	0.00000	6.36524	AB			

Layer II serrated zigzag

C	17.85542	15.265490	4.306816	O	12.40318	10.246100	4.255436
C	17.89616	16.671640	4.304736	O	9.58406	15.113870	4.351816
C	16.65819	17.339680	4.300746	B	30.04756	14.482700	4.352466
C	15.45640	16.646130	4.300016	B	14.12021	14.490750	4.301586
C	15.41550	15.239880	4.301216	B	11.23461	9.478226	4.255636
C	16.65366	14.571880	4.303846	C	27.50966	17.330420	4.364966
H	16.64095	18.441930	4.298996	C	26.27125	16.663010	4.362516
H	14.51070	17.212670	4.297166	C	26.31160	15.256840	4.365366
H	16.67077	13.469560	4.304596	C	27.51306	14.562840	4.365836
H	18.80116	14.699100	4.310066	C	28.75134	15.230230	4.364716
C	12.43335	7.243707	4.238466	C	28.71120	16.636270	4.366636
C	11.23585	7.981928	4.240646	H	25.36567	14.690760	4.364916
C	10.03844	7.243557	4.236616	H	27.49529	13.460610	4.365566
C	10.03843	5.855994	4.235716	H	29.65731	17.202450	4.367096
C	11.23595	5.117849	4.240096	H	27.52748	18.432940	4.364266
C	12.43337	5.856088	4.239016	C	10.53768	1.486743	4.280616
H	9.07514	7.779746	4.235866	C	9.84119	0.284100	4.293816
H	9.07527	5.319749	4.234286	C	21.38992	17.882820	4.316986
H	13.39668	5.320031	4.240716	C	22.77973	17.881070	4.328146
H	13.39687	7.779501	4.239396	C	12.62025	0.280850	4.315316
C	11.92380	14.021400	4.315586	C	11.92692	1.485126	4.290946
C	10.53408	14.019320	4.329066	O	20.44005	16.787890	4.324536
C	9.84097	12.815470	4.318286	O	23.72682	16.783890	4.350766
C	10.53747	11.612970	4.293436	O	12.40354	2.853980	4.273196
C	11.92656	11.615030	4.280036	O	10.06447	2.856688	4.256436
C	12.61999	12.819470	4.291396	O	14.04332	0.005900	4.329616
O	8.41700	13.086860	4.334116	O	8.41727	0.012390	4.286566
O	10.06413	10.242780	4.277716	B	19.19247	17.418990	4.305566
O	14.04302	13.094690	4.282316	B	11.23496	3.621533	4.254016
O	12.87096	15.118690	4.322116	B	24.97608	17.412190	4.349516
c	0.00000	0.00000	6.88104	serrated zigzag			

Layer II serrated armchair

C	18.047530	14.574130	4.310236	O	12.595290	9.554735	4.258856
C	18.088270	15.980280	4.308156	O	9.776171	14.422510	4.355236
C	16.850300	16.648320	4.304166	B	8.528490	13.791340	4.355886
C	15.648510	15.954770	4.303436	B	14.312320	13.799390	4.305006

C	15.607610	14.548520	4.304636	B	11.426720	8.786865	4.259056
C	16.845770	13.880520	4.307266	C	27.701770	16.639060	4.368386
H	16.833060	17.750570	4.302416	C	26.463360	15.971650	4.365936
H	14.702810	16.521310	4.300586	C	26.503710	14.565480	4.368786
H	16.862880	12.778200	4.308016	C	27.705170	13.871480	4.369256
H	18.993270	14.007740	4.313486	C	28.943450	14.538870	4.368136
C	12.625460	6.552347	4.241886	C	28.903310	15.944910	4.370056
C	11.427960	7.290568	4.244066	H	25.557780	13.999400	4.368336
C	10.230550	6.552197	4.240036	H	27.687400	12.769250	4.368986
C	10.230540	5.164634	4.239136	H	29.849420	16.511090	4.370516
C	11.428060	4.426489	4.243516	H	27.719590	17.741580	4.367686
C	12.625480	5.164728	4.242436	C	10.729790	0.795383	4.284036
H	9.267251	7.088386	4.239286	C	20.888890	18.395170	4.297236
H	9.267381	4.628389	4.237706	C	21.582030	17.191460	4.320406
H	13.588790	4.628671	4.244136	C	22.971840	17.189710	4.331566
H	13.588980	7.088141	4.242816	C	23.667950	18.391920	4.318736
C	12.115910	13.330040	4.319006	C	12.119030	0.793766	4.294366
C	10.726190	13.327960	4.332486	O	20.632160	16.096530	4.327956
C	10.033080	12.124110	4.321706	O	23.918930	16.092530	4.354186
C	10.729580	10.921610	4.296856	O	12.595650	2.162620	4.276616
C	12.118670	10.923670	4.283456	O	10.256580	2.165328	4.259856
C	12.812100	12.128110	4.294816	O	25.091020	18.116970	4.333036
O	8.609111	12.395500	4.337536	O	19.464970	18.123460	4.289986
O	10.256240	9.551425	4.281136	B	19.384580	16.727630	4.308986
O	14.235130	12.403330	4.285736	B	11.427070	2.930173	4.257436
O	13.063070	14.427330	4.325536	B	25.168190	16.720830	4.352936
c	0.00000	0.00000	6.88788	serrated armchair			

COF-5M

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	13.01181	22.34097	0.9135870	C	27.58970	2.790600	0.8839620	C	22.23723	10.86297	1.022137
C	15.41276	23.73070	0.9347870	C	27.58465	1.403850	0.8886370	H	25.59842	12.79208	1.050612
C	15.41148	22.34430	0.9440870	H	30.95196	3.323317	0.9137120	H	23.41300	9.062314	1.004562
C	14.21256	21.60599	0.9334870	H	26.62894	3.330941	0.8722620	C	10.05809	12.90808	0.8579870
H	41.20082	21.80104	0.9047870	O	31.64852	8.606116	0.8449620	C	8.858518	12.21246	0.8419870
C	14.96698	15.57696	0.9486620	O	30.49775	10.64400	0.8876870	C	7.630246	12.89205	0.8480120
C	15.64707	16.78833	0.9593370	B	31.73979	10.00195	0.8538870	C	36.80516	14.29538	0.8685620
C	14.93871	17.98314	0.9511120	O	26.02376	8.666956	0.9843370	C	8.856944	14.98615	0.8834870
C	13.57766	15.56085	0.9302120	B	25.96297	10.06458	0.9972620	H	11.00543	12.34449	0.8538120
C	12.86939	16.75619	0.9236620	O	27.21853	10.67924	0.9731370	C	35.50769	12.15967	0.8380370
C	13.54972	17.96746	0.9337370	O	17.07419	16.53399	0.9789870	H	37.99348	16.08834	0.9006370
O	15.39925	19.35711	0.9559620	O	15.92897	14.49269	0.9607870	C	34.28146	12.84275	0.8498120
O	13.05913	19.33217	0.9269120	O	12.64145	14.45389	0.9142620	C	33.08038	12.15033	0.8502120
B	14.22106	20.11042	0.9397870	O	11.44886	16.46757	0.9046370	C	33.03878	10.74288	0.8382120
C	42.15765	23.72782	0.9043120	B	17.16970	15.13879	0.9795870	C	34.27464	10.06875	0.8206120
C	14.20938	24.45350	0.9143370	B	11.38620	15.07040	0.8991620	C	6.328531	10.75647	0.8206620
H	16.37365	21.80646	0.9598370	C	18.47296	14.40545	0.9982620	H	32.13431	12.71617	0.8616120
C	28.15192	9.571300	0.9397620	C	10.09526	14.31548	0.8796370	H	34.28576	8.966738	0.8086620
C	29.54024	9.556532	0.9030870	C	18.52074	12.99846	0.9926370	H	23.46207	14.04228	1.061062
C	27.44410	8.375884	0.9472370	C	19.72498	12.31243	1.006762	H	21.27807	10.31708	1.013437
C	28.12549	7.164942	0.9204370	C	20.94826	13.00050	1.027462	H	21.86387	14.96439	1.051237
C	29.51459	7.150704	0.8873120	C	20.91346	14.40361	1.035062	H	19.73294	11.20832	1.000262
C	30.22199	8.346423	0.8773870	C	19.70584	15.08559	1.020637	H	16.36911	24.28176	0.9433620
O	27.63679	5.798896	0.9228870	H	17.57731	12.42820	0.9751370	H	1.794930	0.846800	0.9256120
O	29.97603	5.776882	0.8704870	C	22.22023	12.26659	1.034562	H	26.62709	0.855000	0.8810370

B	28.79922	5.021281	0.8938120	H	19.71152	16.18803	1.025862	H	41.20013	24.27656	0.8885120
C	28.78563	0.677480	0.9047870	C	23.45246	12.93888	1.048287	H	35.84981	14.84786	0.8738370
C	0.839300	1.399460	0.9128370	C	24.64747	12.23470	1.042037	H	8.859699	11.10883	0.8255620
C	29.98927	2.786030	0.9059120	C	24.67650	10.82685	1.023087	H	34.28357	13.94647	0.8612370
C	28.79080	3.525527	0.8927620	C	23.43431	10.16420	1.017012	H	7.281887	10.20058	0.8091370

Transformation Matrix

a	29.150180	0.000000	0.000000	
b	14.575090	25.244790	0.000000	
c	0.000000	0.000000	3.504000	AA
c	1.19993	0.69278	3.433682	inclined zigzag
c	1.38905	0.00000	3.43368	inclined armchair

Layer II AB stacking

C	27.58690	30.75590	4.091712	C	42.16479	11.20553	4.062087	C	36.81232	19.27790	4.200262
C	29.98785	32.14563	4.112912	C	42.15974	9.818782	4.066762	H	40.17351	21.20701	4.228737
C	29.98657	30.75923	4.122212	H	45.52705	11.73825	4.091837	H	37.98809	17.47725	4.182687
C	28.78765	30.02092	4.111612	H	41.20403	11.74587	4.050387	C	24.63318	21.32301	4.036112
H	55.77591	30.21597	4.082912	O	46.22361	17.02105	4.023087	C	23.43361	20.62739	4.020112
C	29.54207	23.99189	4.126787	O	45.07284	19.05893	4.065812	C	22.20534	21.30698	4.026137
C	30.22216	25.20326	4.137462	B	46.31488	18.41688	4.032012	C	51.38025	22.71031	4.046687
C	29.51380	26.39807	4.129237	O	40.59885	17.08189	4.162462	C	23.43203	23.40108	4.061612
C	28.15275	23.97578	4.108337	B	40.53806	18.47951	4.175387	H	25.58052	20.75942	4.031937
C	27.44448	25.17112	4.101787	O	41.79362	19.09417	4.151262	C	50.08278	20.57460	4.016162
C	28.12481	26.38239	4.111862	O	31.64928	24.94892	4.157112	H	52.56857	24.50327	4.078762
O	29.97434	27.77204	4.134087	O	30.50406	22.90762	4.138912	C	48.85655	21.25768	4.027937
O	27.63422	27.74710	4.105037	O	27.21654	22.86882	4.092387	C	47.65547	20.56526	4.028337
B	28.79615	28.52535	4.117912	O	26.02395	24.88250	4.082762	C	47.61387	19.15781	4.016337
C	56.73274	32.14275	4.082437	B	31.74479	23.55372	4.157712	C	48.84973	18.48368	3.998737
C	28.78447	32.86843	4.092462	B	25.96129	23.48533	4.077287	C	20.90362	19.17140	3.998787
H	30.94874	30.22139	4.137962	C	33.04805	22.82038	4.176387	H	46.70940	21.13110	4.039737
C	42.72701	17.98623	4.117887	C	24.67035	22.73041	4.057762	H	48.86085	17.38167	3.986787
C	44.11533	17.97146	4.081212	C	33.09583	21.41339	4.170762	H	38.03716	22.45721	4.239187
C	42.01919	16.79082	4.125362	C	34.30007	20.72736	4.184887	H	35.85316	18.73201	4.191562
C	42.70058	15.57987	4.098562	C	35.52335	21.41543	4.205587	H	36.43896	23.37932	4.229362
C	44.08968	15.56564	4.065437	C	35.48855	22.81854	4.213187	H	34.30803	19.62325	4.178387
C	44.79708	16.76136	4.055512	C	34.28093	23.50052	4.198762	H	30.94420	32.69669	4.121487
O	42.21188	14.21383	4.101012	H	32.15240	20.84313	4.153262	H	16.37002	9.261732	4.103737
O	44.55112	14.19181	4.048612	C	36.79532	20.68152	4.212687	H	41.20218	9.269932	4.059162
B	43.37431	13.43621	4.071937	H	34.28661	24.60296	4.203987	H	55.77522	32.69149	4.066637
C	43.36072	9.092412	4.082912	C	38.02755	21.35381	4.226412	H	50.42490	23.26279	4.051962
C	15.41439	9.814392	4.090962	C	39.22256	20.64963	4.220162	H	23.43479	19.52376	4.003687
C	44.56436	11.20096	4.084037	C	39.25159	19.24178	4.201212	H	48.85866	22.36140	4.039362
C	43.36589	11.94046	4.070887	C	38.00940	18.57913	4.195137	H	21.85698	18.61551	3.987262

c	0.00000	0.00000	6.35625	AB

Layer II serrated zigzag

C	14.21174	23.033750	4.337007	C	28.78963	3.483380	4.307382	C	23.43716	11.555750	4.445557
C	16.61269	24.423480	4.358207	C	28.78458	2.096630	4.312057	H	26.79835	13.484860	4.474032
C	16.61141	23.037080	4.367507	H	3.00171	4.016097	4.337132	H	24.61293	9.755095	4.427982
C	15.41249	22.298770	4.356907	H	27.82887	4.023721	4.295682	C	11.25802	13.600860	4.281407
H	13.25057	22.493820	4.328207	O	32.84845	9.298897	4.268382	C	10.05845	12.905240	4.265407
C	16.16691	16.269740	4.372082	O	31.69768	11.336780	4.311107	C	8.83017	13.584830	4.271432
C	16.84700	17.481110	4.382757	B	32.93972	10.694730	4.277307	C	8.85491	14.988160	4.291982
C	16.13864	18.675920	4.374532	O	27.22369	9.359735	4.407757	C	10.05687	15.678930	4.306907
C	14.77759	16.253630	4.353632	B	27.16290	10.757360	4.420682	H	12.20536	13.037270	4.277232
C	14.06932	17.448970	4.347082	O	28.41846	11.372020	4.396557	C	7.55744	12.852450	4.261457
C	14.74965	18.660240	4.357157	O	18.27412	17.226770	4.402407	H	10.04323	16.781120	4.324057
O	16.59918	20.049890	4.379382	O	17.12890	15.185470	4.384207	C	35.48139	13.535530	4.273232
O	14.25906	20.024950	4.350332	O	13.84138	15.146670	4.337682	C	34.28031	12.843110	4.273632
B	15.42099	20.803200	4.363207	O	12.64879	17.160350	4.328057	C	34.23871	11.435660	4.261632

C	14.20740	24.420600	4.327732	B	18.36963	15.831570	4.403007	C	6.32439	10.761530	4.244032
C	15.40931	25.146280	4.337757	B	12.58613	15.763180	4.322582	C	7.52846	11.449250	4.244082
H	17.57358	22.499240	4.383257	C	19.67289	15.098230	4.421682	H	33.33424	13.408950	4.285032
C	29.35185	10.264080	4.363182	C	11.29519	15.008260	4.303057	H	6.33550	9.659517	4.232082
C	30.74017	10.249310	4.326507	C	19.72067	13.691240	4.416057	H	24.66200	14.735060	4.484482
C	28.64403	9.068665	4.370657	C	20.92491	13.005210	4.430182	H	22.47800	11.009860	4.436857
C	29.32542	7.857722	4.343857	C	22.14819	13.693280	4.450882	H	23.06380	15.657170	4.474657
C	30.71452	7.843484	4.310732	C	22.11339	15.096390	4.458482	H	20.93287	11.901100	4.423682
C	31.42192	9.039204	4.300807	C	20.90577	15.778370	4.444057	H	17.56904	24.974540	4.366782
O	28.83672	6.491676	4.346307	H	18.77724	13.120980	4.398557	H	2.99486	1.539580	4.349032
O	31.17596	6.469662	4.293907	C	23.42016	12.959370	4.457982	H	27.82702	1.547780	4.304457
B	29.99915	5.714061	4.317232	H	20.91145	16.880810	4.449282	H	42.40006	24.969340	4.311932
C	0.83538	1.370260	4.328207	C	24.65239	13.631660	4.471707	H	37.04974	15.540640	4.297257
C	2.03923	2.092240	4.336257	C	25.84740	12.927480	4.465457	H	10.05963	11.801610	4.248982
C	2.03902	3.478810	4.329332	C	25.87643	11.519630	4.446507	H	35.48350	14.639250	4.284657
C	29.99073	4.218307	4.316182	C	24.63424	10.856980	4.440432	H	8.48181	10.893360	4.232557
c	0.00000	0.00000	6.84684	serrated zigzag							

Layer II serrated armchair

C	14.400860	22.340970	4.340427	C	28.978750	2.790600	4.310802	C	23.626280	10.862970	4.448977
C	16.801810	23.730700	4.361627	C	28.973700	1.403850	4.315477	H	26.987470	12.792080	4.477452
C	16.800530	22.344300	4.370927	H	3.190830	3.323317	4.340552	H	24.802050	9.062314	4.431402
C	15.601610	21.605990	4.360327	H	28.017990	3.330941	4.299102	C	11.447140	12.908080	4.284827
H	13.439690	21.801040	4.331627	O	33.037570	8.606116	4.271802	C	10.247570	12.212460	4.268827
C	16.356030	15.576960	4.375502	O	31.886800	10.644000	4.314527	C	9.019297	12.892050	4.274852
C	17.036120	16.788330	4.386177	B	33.128840	10.001950	4.280727	C	9.044030	14.295380	4.295402
C	16.327760	17.983140	4.377952	O	27.412810	8.666956	4.411177	C	10.245990	14.986150	4.310327
C	14.966710	15.560850	4.357052	B	27.352020	10.064580	4.424102	H	12.394480	12.344490	4.280652
C	14.258440	16.756190	4.350502	O	28.607580	10.679240	4.399977	C	7.746560	12.159670	4.264877
C	14.938770	17.967460	4.360577	O	18.463240	16.533990	4.405827	H	10.232350	16.088340	4.327477
O	16.788300	19.357110	4.382802	O	17.318020	14.492690	4.387627	C	35.670510	12.842750	4.276652
O	14.448180	19.332170	4.353752	O	14.030500	14.453890	4.341102	C	34.469430	12.150330	4.277052
B	15.610110	20.110420	4.366627	O	12.837910	16.467570	4.331477	C	34.427830	10.742880	4.265052
C	14.396520	23.727820	4.331152	B	18.558750	15.138790	4.406427	C	6.513510	10.068750	4.247452
C	15.598430	24.453500	4.341177	B	12.775250	15.070400	4.326002	C	7.717581	10.756470	4.247502
H	17.762700	21.806460	4.386677	C	19.862010	14.405450	4.425102	H	33.523360	12.716170	4.288452
C	29.540970	9.571300	4.366602	C	11.484310	14.315480	4.306477	H	6.524620	8.966738	4.235502
C	30.929290	9.556532	4.329927	C	19.909790	12.998460	4.419477	H	24.851120	14.042280	4.487902
C	28.833150	8.375884	4.374077	C	21.114030	12.312430	4.433602	H	22.667120	10.317080	4.440277
C	29.514540	7.164942	4.347277	C	22.337310	13.000500	4.454302	H	23.252920	14.964390	4.478077
C	30.903640	7.150704	4.314152	C	22.302510	14.403610	4.461902	H	21.121990	11.208320	4.427102
C	31.611040	8.346423	4.304227	C	21.094890	15.085590	4.447477	H	17.758160	24.281760	4.370202
O	29.025840	5.798896	4.349727	H	18.966360	12.428200	4.401977	H	3.183980	0.846800	4.352452
O	31.365080	5.776882	4.297327	C	23.609280	12.266590	4.461402	H	28.016140	0.855000	4.307877
B	30.188270	5.021281	4.320652	H	21.100570	16.188030	4.452702	H	42.589180	24.276560	4.315352
C	1.024500	0.677480	4.331627	C	24.841510	12.938880	4.475127	H	37.238860	14.847860	4.300677
C	2.228350	1.399460	4.339677	C	26.036520	12.234700	4.468877	H	10.248750	11.108830	4.252402
C	2.228140	2.786030	4.332752	C	26.065550	10.826850	4.449927	H	35.672620	13.946470	4.288077
C	30.179850	3.525527	4.319602	C	24.823360	10.164200	4.443852	H	8.670937	10.200580	4.235977
c	0.00000	0.00000	6.85368	serrated armchair							

COF-6M

Layer I AA, AB, inclined zigzag & armchair, serrated zigzag & armchair

C	2.069789	2.222231	0.9642750	B	24.51850	15.19163	0.9585000
C	4.503057	3.615478	0.9920000	O	18.81151	13.76917	0.9918500
C	4.516872	2.213752	1.004500	B	18.72369	15.16558	1.007625
C	3.290919	1.533999	0.9900750	O	19.97116	15.79992	1.001375

C	19.12395	1.488225	0.9549250	H	5.462789	4.164466	1.002400
C	2.094722	3.623877	0.9524000	H	5.465576	5.986796	0.9831000
C	3.301635	4.337306	0.9658750	H	19.48176	5.994481	0.9224500
C	5.791527	1.472347	1.023550	H	19.47330	4.180899	0.9322500
C	20.92758	14.70809	0.9810750	H	3.287207	0.428162	0.9989750
C	22.31848	14.71442	0.9700000	C	5.816369	0.068796	1.027350
C	20.23823	13.50168	0.9754750	C	16.18345	15.24957	1.026825
C	20.93885	12.30068	0.9595250	C	8.260023	0.034787	1.023850
C	22.32830	12.30689	0.9511500	C	8.221853	1.443006	1.029450
C	23.01829	13.51413	0.9560750	C	7.024327	2.143892	1.029575
O	20.47047	10.92726	0.9532000	H	14.02684	15.39445	1.026575
O	22.80925	10.93757	0.9409500	H	16.16085	14.14730	1.025400
B	21.64331	10.16396	0.9437500	H	9.170374	2.004966	1.030050
C	21.63993	5.811987	0.9546500	H	7.033475	3.247776	1.030375
C	4.508557	6.536959	0.9669000	C	17.89443	2.165613	0.9377000
C	22.84239	7.924728	0.9602750	C	16.69275	1.471379	0.9388750
C	21.64565	8.667626	0.9422000	C	16.64719	0.063382	0.9549250
C	20.44625	7.929031	0.9281750	C	27.05415	15.27235	0.9677500
C	20.44070	6.541469	0.9334750	C	0.757990	0.084705	0.9681500
H	5.472964	8.459459	0.9717250	H	17.89104	3.269416	0.9252500
H	19.48475	8.468255	0.9127250	H	15.74778	2.039150	0.9272750
O	24.44228	13.79426	0.9496500	H	8.736521	14.17002	0.9806750
O	23.26568	15.81503	0.9714500	H	10.87745	15.40432	0.9807750

Transformation Matrix

a	18.333510	0.000000	0.000000	
b	9.166750	15.877270	0.000000	
c	0.000000	0.000000	3.446880	AA
c	1.22371	0.70651	3.41316	inclined zigzag
c	1.390080	0.000000	3.423420	inclined armchair

Layer II AB stacking

C	11.23654	7.514659	4.145750	B	33.68525	20.48406	4.139975
C	13.66981	8.907907	4.173475	O	27.97826	19.06160	4.173325
C	13.68363	7.506181	4.185975	B	27.89045	20.45801	4.189100
C	12.45767	6.826427	4.171550	O	29.13792	21.09235	4.182850
C	28.29070	6.780653	4.136400	H	14.62954	9.456894	4.183875
C	11.26148	8.916306	4.133875	H	14.63233	11.27922	4.164575
C	12.46839	9.629734	4.147350	H	28.64851	11.28691	4.103925
C	14.95828	6.764775	4.205025	H	28.64006	9.473328	4.113725
C	30.09433	20.00052	4.162550	H	12.45396	5.720591	4.180450
C	31.48523	20.00685	4.151475	C	14.98312	5.361225	4.208825
C	29.40498	18.79411	4.156950	C	25.35020	20.54200	4.208300
C	30.10561	17.59311	4.141000	C	17.42678	5.327216	4.205325
C	31.49506	17.59932	4.132625	C	17.38861	6.735435	4.210925
C	32.18504	18.80656	4.137550	C	16.19108	7.436320	4.211050
O	29.63723	16.21969	4.134675	H	23.19360	20.68688	4.208050
O	31.97601	16.23000	4.122425	H	25.32761	19.43973	4.206875
B	30.81007	15.45639	4.125225	H	18.33713	7.297395	4.211525
C	30.80669	11.10442	4.136125	H	16.20023	8.540205	4.211850
C	13.67531	11.82939	4.148375	C	27.06118	7.458041	4.119175
C	32.00914	13.21716	4.141750	C	25.85950	6.763807	4.120350
C	30.81240	13.96005	4.123675	C	25.81395	5.355811	4.136400
C	29.61301	13.22146	4.109650	C	36.22091	20.56478	4.149225
C	29.60746	11.83390	4.114950	C	9.924745	5.377133	4.149625
H	14.63972	13.75189	4.153200	H	27.05780	8.561845	4.106725
H	28.65150	13.76068	4.094200	H	24.91454	7.331578	4.108750

O 33.60904 19.08669 4.131125 H 17.90327 19.46245 4.162150
O 32.43243 21.10746 4.152925 H 20.04420 20.69675 4.162250
c 0.00000 0.00000 6.36295 AB

Layer II serrated zigzag

C 3.293499 2.928741 4.374015 B 16.575460 0.020870 4.368240
C 5.726767 4.321988 4.401740 O 20.035220 14.475680 4.401590
C 5.740582 2.920262 4.414240 B 19.947400 15.872090 4.417365
C 4.514629 2.240509 4.399815 O 12.028120 0.629160 4.411115
C 2.014150 2.194735 4.364665 H 6.686499 4.870976 4.412140
C 3.318432 4.330387 4.362140 H 6.689286 6.693306 4.392840
C 4.525345 5.043816 4.375615 H 20.705470 6.700991 4.332190
C 7.015237 2.178857 4.433290 H 20.697010 4.887409 4.341990
C 22.151290 15.414600 4.390815 H 4.510917 1.134672 4.408715
C 23.542190 15.420930 4.379740 C 7.040079 0.775306 4.437090
C 21.461940 14.208190 4.385215 C 8.240410 0.078810 4.436565
C 22.162560 13.007190 4.369265 C 9.483733 0.741297 4.433590
C 23.552010 13.013400 4.360890 C 9.445563 2.149516 4.439190
C 24.242000 14.220640 4.365815 C 8.248036 2.850402 4.439315
O 21.694180 11.633770 4.362940 H 6.083800 0.223690 4.436315
O 24.032960 11.644080 4.350690 H 17.384560 14.853810 4.435140
B 22.867020 10.870470 4.353490 H 10.394080 2.711476 4.439790
C 4.530130 6.518497 4.364390 H 8.257185 3.954286 4.440115
C 5.732267 7.243469 4.376640 C 19.118140 2.872123 4.347440
C 5.732590 8.631238 4.370015 C 17.916460 2.177889 4.348615
C 22.869360 9.374136 4.351940 C 17.870900 0.769892 4.364665
C 21.669960 8.635541 4.337915 C 0.777600 0.101590 4.377490
C 21.664410 7.247979 4.343215 C 1.981700 0.791215 4.377890
H 6.696674 9.165969 4.381465 H 19.114750 3.975926 4.334990
H 20.708460 9.174765 4.322465 H 16.971490 2.745660 4.337015
O 25.665990 14.500770 4.359390 H 9.960231 14.876530 4.390415
O 15.322640 0.644270 4.381190 H 2.934410 0.233560 4.390515
c 0.00000 0.00000 6.81948 serrated zigzag

Layer II serrated armchair

C 3.459869 2.222231 4.377435 B 25.908580 15.191630 4.371660
C 5.893137 3.615478 4.405160 O 20.201590 13.769170 4.405010
C 5.906952 2.213752 4.417660 B 20.113770 15.165580 4.420785
C 4.680999 1.533999 4.403235 O 21.361240 15.799920 4.414535
C 2.180520 1.488225 4.368085 H 6.852869 4.164466 4.415560
C 3.484802 3.623877 4.365560 H 6.855656 5.986796 4.396260
C 4.691715 4.337306 4.379035 H 20.871840 5.994481 4.335610
C 7.181607 1.472347 4.436710 H 2.529870 4.180899 4.345410
C 22.317660 14.708090 4.394235 H 4.677287 0.428162 4.412135
C 23.708560 14.714420 4.383160 C 7.206449 0.068796 4.440510
C 21.628310 13.501680 4.388635 C 17.573530 15.249570 4.439985
C 22.328930 12.300680 4.372685 C 9.650103 0.034787 4.437010
C 23.718380 12.306890 4.364310 C 9.611933 1.443006 4.442610
C 24.408370 13.514130 4.369235 C 8.414407 2.143892 4.442735
O 21.860550 10.927260 4.366360 H 15.416920 15.394450 4.439735
O 24.199330 10.937570 4.354110 H 17.550930 14.147300 4.438560
B 23.033390 10.163960 4.356910 H 10.560450 2.004966 4.443210
C 4.696500 5.811987 4.367810 H 8.423555 3.247776 4.443535
C 5.898637 6.536959 4.380060 C 19.284510 2.165613 4.350860
C 5.898960 7.924728 4.373435 C 18.082830 1.471379 4.352035
C 23.035730 8.667626 4.355360 C 18.037270 0.063382 4.368085

C 21.836330 7.929031 4.341335 C 10.110720 15.272350 4.380910
C 21.830780 6.541469 4.346635 C 2.148070 0.084705 4.381310
H 6.863044 8.459459 4.384885 H 19.281120 3.269416 4.338410
H 20.874830 8.468255 4.325885 H 17.137860 2.039150 4.340435
O 25.832360 13.794260 4.362810 H 10.126600 14.170020 4.393835
O 24.655760 15.815030 4.384610 H 12.267530 15.404320 4.393935
c 0.00000 0.00000 6.82632 serrated armchair

COF-7M

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C 2.089298 3.482910 0.8291060 C 9.432521 4.695974 0.8271560
C 3.321002 4.155495 0.8423260 C 8.043071 4.695796 0.8329760
C 4.552149 3.481775 0.8406360 O 9.906851 8.471457 0.8017060
C 4.518664 2.078683 0.8270560 O 11.54991 5.626999 0.8141760
C 3.319577 1.349452 0.8149560 O 7.095810 3.599552 0.8441360
C 2.121119 2.079809 0.8155560 O 5.925208 5.625911 0.8349760
H 5.473324 1.526728 0.8256260 O 10.38063 3.600256 0.8340060
H 1.165733 1.529205 0.8037860 O 7.566726 8.470697 0.8124060
C 7.348151 5.898857 0.8271560 B 8.736531 9.236634 0.8072560
C 8.042571 7.102210 0.8149560 B 5.847724 4.229781 0.8428760
C 9.432001 7.102548 0.8085560 B 11.62851 4.231011 0.8263060
C 10.12681 5.899374 0.8149560 H 3.321609 5.258204 0.8550860

Transformation Matrix

a 10.834740 0.000000 0.000000
b 5.417370 9.383160 0.000000
c 0.000000 0.000000 3.495390 AA
c 1.198785 0.692119 3.443941 inclined zigzag
c 1.389345 0.000000 3.402900 inclined armchair

Layer II AB stacking

C 7.506668 6.610630 4.132246 C 14.84989 7.823694 4.130296
C 8.738372 7.283215 4.145466 C 13.46044 7.823516 4.136116
C 9.969519 6.609495 4.143776 O 15.32422 11.59918 4.104846
C 9.936033 5.206403 4.130196 O 16.96728 8.754719 4.117316
C 8.736947 4.477172 4.118096 O 12.51318 6.727272 4.147276
C 7.538489 5.207529 4.118696 O 11.34258 8.753632 4.138116
H 10.89069 4.654448 4.128766 O 15.79800 6.727976 4.137146
H 6.583103 4.656925 4.106926 O 12.98410 11.59842 4.115546
C 12.76552 9.026577 4.130296 B 14.15390 12.36435 4.110396
C 13.45994 10.22993 4.118096 B 11.26509 7.357501 4.146016
C 14.84937 10.23027 4.111696 B 17.04588 7.358731 4.129446
C 15.54418 9.027094 4.118096 H 8.738979 8.385923 4.158226
c 0.00000 0.00000 6.60628 AB

Layer II serrated zigzag

C 3.288083 4.175029 4.26278 C 10.631310 5.388093 4.26083
C 4.519787 4.847614 4.27600 C 9.241856 5.387915 4.26665
C 5.750934 4.173894 4.27431 O 11.105640 9.163575 4.23538
C 5.717449 2.770802 4.26073 O 12.748690 6.319118 4.24785
C 4.518362 2.041571 4.24863 O 8.294595 4.291671 4.27781
C 3.319904 2.771928 4.24923 O 7.123993 6.318030 4.26865
H 6.672109 2.218847 4.25930 O 11.579410 4.292375 4.26768

H	2.364518	2.221324	4.23746	O	8.765512	9.162816	4.24608	
C	8.546936	6.590976	4.26083	B	4.517946	0.545593	4.24093	
C	9.241356	7.794329	4.24863	B	7.046509	4.921900	4.27655	
C	10.630790	7.794667	4.24223	B	12.827290	4.923130	4.25998	
C	11.325590	6.591493	4.24863	H	4.520394	5.950323	4.28876	
c	0.00000	0.00000	6.86736	serrated zigzag				

Layer II serrated armchair

C	3.478643	3.482910	4.26620	C	10.821870	4.695974	4.26425	
C	4.710347	4.155495	4.27942	C	9.432416	4.695796	4.27007	
C	5.941494	3.481775	4.27773	O	11.296200	8.471457	4.23880	
C	5.908009	2.078683	4.26415	O	12.939250	5.626999	4.25127	
C	4.708922	1.349452	4.25205	O	8.485155	3.599552	4.28123	
C	3.510464	2.079809	4.25265	O	7.314553	5.625911	4.27207	
H	6.862669	1.526728	4.26272	O	11.769970	3.600256	4.27110	
H	2.555078	1.529205	4.24088	O	8.956071	8.470697	4.24950	
C	8.737496	5.898857	4.26425	B	10.125880	9.236634	4.24435	
C	9.431916	7.102210	4.25205	B	7.237069	4.229781	4.27997	
C	10.821350	7.102548	4.24565	B	13.017850	4.231011	4.26340	
C	11.516160	5.899374	4.25205	H	4.710954	5.258204	4.29218	
c	0.00000	0.00000	6.87420	serrated armchair				

TP COF-1M

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	41.93071	22.44135	0.9456780	C	29.81555	2.941544	0.9388030	C	24.50818	10.96620	1.062253
C	15.31735	23.84314	0.9692280	C	28.61193	3.666409	0.9219280	C	23.27786	10.28848	1.054703
C	15.29007	22.44251	0.9782280	C	27.40732	2.943154	0.9112030	C	22.05271	10.96706	1.057953
C	14.08640	21.71777	0.9667030	C	27.37994	1.542002	0.9168030	C	23.25423	14.53541	1.105878
H	40.97625	21.88984	0.9363030	H	30.76978	3.493206	0.9481530	H	25.44198	12.91995	1.090878
C	14.84988	15.69144	0.9781780	H	26.45344	3.495369	0.8969780	H	23.27742	9.186367	1.040328
C	15.52798	16.90401	0.9862280	C	2.022967	0.793766	0.9708530	C	20.79098	10.27623	1.043678
C	14.81742	18.09719	0.9812280	H	2.977441	1.344597	0.9803780	H	24.20850	15.08624	1.125428
C	13.46063	15.67280	0.9653030	O	31.47836	8.738125	0.8700030	H	22.07697	16.31894	1.110603
C	12.75065	16.86703	0.9621030	O	30.33164	10.77838	0.9177030	H	20.79141	9.174468	1.038578
C	13.42875	18.07931	0.9697780	B	31.57160	10.13326	0.8815030	H	18.65771	10.40866	1.022203
O	15.27568	19.47153	0.9842780	O	25.85447	8.808589	1.021228	C	9.952588	13.02103	0.8913030
O	12.93524	19.44270	0.9651780	B	25.79604	10.20572	1.035003	C	8.752552	12.29745	0.8716030
B	14.09600	20.22198	0.9731280	O	27.05160	10.81994	1.008928	C	7.516801	13.00546	0.8795530
C	16.54692	24.58981	0.9810280	O	16.95549	16.65313	1.001678	C	36.56987	14.42960	0.9020530
H	17.50093	24.03838	0.9986280	O	15.81476	14.60929	0.9879030	C	8.748195	15.10579	0.9199530
C	41.90369	23.84248	0.9354780	O	12.52497	14.56424	0.9505280	H	10.90689	12.46984	0.8863780
C	43.13467	24.55867	0.9472530	O	11.33105	16.57718	0.9465530	C	8.718841	10.85926	0.8442280
C	40.67483	24.59019	0.9128780	B	17.05346	15.25841	1.003378	C	35.33230	12.29438	0.8677530
H	39.72037	24.03938	0.9025780	B	11.26967	15.18058	0.9388280	C	35.30775	15.12076	0.9061530
H	16.24449	21.89103	0.9948280	C	18.35656	14.52386	1.023653	H	37.79769	16.20793	0.9384780
C	26.15078	0.794345	0.9041030	C	9.978078	14.42570	0.9171530	C	34.09654	13.00241	0.8798280
H	25.19615	1.344748	0.8867780	C	18.38367	13.11909	1.020153	C	32.89714	12.27868	0.8793780
C	27.98384	9.710557	0.9723030	C	19.58266	12.39556	1.038228	C	32.87125	10.87385	0.8659280
C	29.37176	9.693224	0.9327780	C	20.81815	13.10377	1.060628	C	34.10009	10.19311	0.8474030
C	27.27371	8.516394	0.9804280	C	20.81289	14.52804	1.069503	C	6.278407	10.87041	0.8480030
C	27.95286	7.304898	0.9506780	C	19.58573	15.20523	1.050303	C	34.12928	14.44057	0.8957780
C	29.34174	7.288068	0.9140030	H	17.42910	12.56838	1.001678	H	31.94200	12.82916	0.8929530
C	30.05164	8.482030	0.9040530	C	19.61335	10.95752	1.034203	H	34.09911	9.090973	0.8358030
O	27.46063	5.940952	0.9541280	C	22.05026	12.39115	1.070653	C	7.539982	10.17945	0.8329030
O	29.80042	5.913657	0.8952280	C	22.07599	15.21701	1.097228	H	9.672662	10.30770	0.8328530
B	28.62153	5.162302	0.9218530	H	19.58529	16.30750	1.056078	H	7.538297	9.077640	0.8129530

C	28.61072	0.825489	0.9373280	C	23.28708	13.09705	1.088128	H	35.30721	16.22285	0.9187030	
C	29.84224	1.540845	0.9485530	C	24.48596	12.37125	1.082478	H	33.17422	14.99055	0.9004530	

Transformation Matrix

a	29.048470	0.000000	0.000000	
b	14.524230	25.156700	0.000000	
c	0.000000	0.000000	3.488000	AA
c	1.21743	0.70288	3.42821	inclined zigzag
c	1.38884	0.00000	3.431975	inclined armchair

Layer II AB stacking

C	56.45494	30.82692	4.043016	C	44.33978	11.32712	4.036141	C	39.03242	19.35177	4.159591	
C	29.84159	32.22871	4.066566	C	43.13617	12.05198	4.019266	C	37.80209	18.67405	4.152041	
C	29.81430	30.82808	4.075566	C	41.93156	11.32873	4.008541	C	36.57694	19.35263	4.155291	
C	28.61063	30.10334	4.064041	C	41.90417	9.927573	4.014141	C	37.77847	22.92098	4.203216	
H	55.50048	30.27541	4.033641	H	45.29401	11.87878	4.045491	H	39.96622	21.30552	4.188216	
C	29.37411	24.07701	4.075516	H	40.97768	11.88094	3.994316	H	37.80165	17.57194	4.137666	
C	30.05222	25.28958	4.083566	C	16.54720	9.179338	4.068191	C	35.31522	18.66180	4.141016	
C	29.34166	26.48276	4.078566	H	17.50168	9.730168	4.077716	H	38.73273	23.47181	4.222766	
C	27.98487	24.05837	4.062641	O	46.00259	17.12370	3.967341	H	36.60120	24.70451	4.207941	
C	27.27489	25.25260	4.059441	O	44.85587	19.16395	4.015041	H	35.31564	17.56004	4.135916	
C	27.95298	26.46488	4.067116	B	46.09583	18.51883	3.978841	H	33.18195	18.79423	4.119541	
O	29.79992	27.85710	4.081616	O	40.37870	17.19416	4.118566	C	24.47682	21.40660	3.988641	
O	27.45947	27.82827	4.062516	B	40.32027	18.59129	4.132341	C	23.27679	20.68302	3.968941	
B	28.62024	28.60755	4.070466	O	41.57584	19.20551	4.106266	C	22.04103	21.39103	3.976891	
C	31.07116	32.97538	4.078366	O	31.47972	25.03870	4.099016	C	51.09410	22.81517	3.999391	
H	32.02517	32.42395	4.095966	O	30.33899	22.99486	4.085241	C	23.27243	23.49136	4.017291	
C	56.42793	32.22805	4.032816	O	27.04921	22.94981	4.047866	H	25.43113	20.85541	3.983716	
C	57.65891	32.94424	4.044591	O	25.85529	24.96275	4.043891	C	23.24308	19.24483	3.941566	
C	55.19907	32.97576	4.010216	B	31.57769	23.64398	4.100716	C	49.85653	20.67995	3.965091	
H	54.24461	32.42495	3.999916	B	25.79390	23.56615	4.036166	C	49.83199	23.50633	4.003491	
H	30.76872	30.27660	4.092166	C	32.88079	22.90943	4.120991	H	52.32193	24.59350	4.035816	
C	40.67501	9.179916	4.001441	C	24.50231	22.81127	4.014491	C	48.62077	21.38798	3.977166	
H	39.72038	9.730320	3.984116	C	32.90791	21.50466	4.117491	C	47.42138	20.66425	3.976716	
C	42.50808	18.09613	4.069641	C	34.10690	20.78113	4.135566	C	47.39548	19.25942	3.963266	
C	43.89600	18.07880	4.030116	C	35.34238	21.48934	4.157966	C	48.62432	18.57868	3.944741	
C	41.79794	16.90197	4.077766	C	35.33712	22.91361	4.166841	C	20.80264	19.25598	3.945341	
C	42.47710	15.69047	4.048016	C	34.10996	23.59080	4.147641	C	48.65351	22.82614	3.993116	
C	43.86597	15.67364	4.011341	H	31.95333	20.95395	4.099016	H	46.46623	21.21473	3.990291	
C	44.57587	16.86760	4.001391	C	34.13758	19.34309	4.131541	H	48.62334	17.47654	3.933141	
O	41.98486	14.32652	4.051466	C	36.57449	20.77672	4.167991	C	22.06422	18.56502	3.930241	
O	44.32465	14.29923	3.992566	C	36.60023	23.60258	4.194566	H	24.19690	18.69327	3.930191	
B	43.14577	13.54787	4.019191	H	34.10953	24.69307	4.153416	H	22.06253	17.46321	3.910291	
C	43.13496	9.211061	4.034666	C	37.81132	21.48262	4.185466	H	49.83144	24.60842	4.016041	
C	44.36647	9.926416	4.045891	C	39.01019	20.75682	4.179816	H	47.69846	23.37612	3.997791	
c	0.00000	0.00000	6.194675	AB								

Layer II serrated zigzag

C	14.099670	23.144230	4.365678	C	31.032980	3.644424	4.358803	C	25.725610	11.669080	4.482253	
C	16.534780	24.546020	4.389228	C	29.829360	4.369289	4.341928	C	24.495290	10.991360	4.474703	
C	16.507500	23.145390	4.398228	C	28.624750	3.646034	4.331203	C	23.270140	11.669940	4.477953	
C	15.303830	22.420650	4.386703	C	28.597370	2.244882	4.336803	C	24.471660	15.238290	4.525878	
H	13.145210	22.592720	4.356303	H	2.938740	4.196086	4.368153	H	26.659410	13.622830	4.510878	
C	16.067310	16.394320	4.398178	H	27.670870	4.198249	4.316978	H	24.494850	9.889247	4.460328	
C	16.745410	17.606890	4.406228	C	3.240397	1.496646	4.390853	C	22.008410	10.979110	4.463678	
C	16.034850	18.800070	4.401228	H	4.194871	2.047477	4.400378	H	25.425930	15.789120	4.545428	
C	14.678060	16.375680	4.385303	O	32.695790	9.441005	4.290003	H	23.294400	17.021820	4.530603	
C	13.968080	17.569910	4.382103	O	31.549070	11.481260	4.337703	H	22.008840	9.877348	4.458578	
C	14.646180	18.782190	4.389778	B	32.789030	10.836140	4.301503	H	19.875140	11.111540	4.442203	
O	16.493110	20.174410	4.404278	O	27.071900	9.511469	4.441228	C	11.170020	13.723910	4.311303	
O	14.152670	20.145580	4.385178	B	27.013470	10.908600	4.455003	C	9.969982	13.000330	4.291603	
B	15.313430	20.924860	4.393128	O	28.269030	11.522820	4.428928	C	8.734231	13.708340	4.299553	

C 3.240120 0.135990 4.401028 O 18.172920 17.356010 4.421678 C 8.738830 15.132480 4.322053
H 18.718360 24.741260 4.418628 O 17.032190 15.312170 4.407903 C 9.965625 15.808670 4.339953
C 43.121120 24.545360 4.355478 O 13.742400 15.267120 4.370528 H 12.124320 13.172720 4.306378
C 0.779400 0.104850 4.367253 O 12.548480 17.280060 4.366553 C 9.936271 11.562140 4.264228
C 27.368030 0.136370 4.332878 B 18.270890 15.961290 4.423378 C 36.549730 12.997260 4.287753
H 40.937800 24.742260 4.322578 B 12.487100 15.883460 4.358828 C 36.525180 15.823640 4.326153
H 17.461920 22.593910 4.414828 C 19.573990 15.226740 4.443653 H 9.966650 16.910810 4.358478
C 27.368210 1.497225 4.324103 C 11.195510 15.128580 4.337153 C 35.313970 13.705290 4.299828
H 26.413580 2.047628 4.306778 C 19.601100 13.821970 4.440153 C 34.114570 12.981560 4.299378
C 29.201270 10.413440 4.392303 C 20.800090 13.098440 4.458228 C 34.088680 11.576730 4.285928
C 30.589190 10.396100 4.352778 C 22.035580 13.806650 4.480628 C 35.317520 10.895990 4.267403
C 28.491140 9.219274 4.400428 C 22.030320 15.230920 4.489503 C 7.495837 11.573290 4.268003
C 29.170290 8.007778 4.370678 C 20.803160 15.908110 4.470303 C 35.346710 15.143450 4.315778
C 30.559170 7.990948 4.334003 H 18.646530 13.271260 4.421678 H 33.159430 13.532040 4.312953
C 31.269070 9.184910 4.324053 C 20.830780 11.660400 4.454203 H 6.268070 9.793853 4.255803
O 28.678060 6.643832 4.374128 C 23.267690 13.094030 4.490653 C 8.757412 10.882330 4.252903
O 31.017850 6.616537 4.315228 C 23.293420 15.919890 4.517228 H 10.890090 11.010580 4.252853
B 29.838960 5.865182 4.341853 H 20.802720 17.010380 4.476078 H 8.755727 9.780519 4.232953
C 29.828150 1.528369 4.357328 C 24.504510 13.799930 4.508128 H 36.524640 16.925730 4.338703
C 2.011200 2.243725 4.368553 C 25.703390 13.074130 4.502478 H 34.391650 15.693430 4.320453
c 0.00000 0.00000 6.84000 serrated zigzag

Layer II serrated armchair

C 14.271080 22.441350 4.372518 C 2.155920 2.941544 4.365643 C 25.897020 10.966200 4.489093
C 16.706190 23.843140 4.396068 C 30.000770 3.666409 4.348768 C 24.666700 10.288480 4.481543
C 16.678910 22.442510 4.405068 C 28.796160 2.943154 4.338043 C 23.441550 10.967060 4.484793
C 15.475240 21.717770 4.393543 C 28.768780 1.542002 4.343643 C 24.643070 14.535410 4.532718
H 13.316620 21.889840 4.363143 H 3.110150 3.493206 4.374993 H 26.830820 12.919950 4.517718
C 16.238720 15.691440 4.405018 H 27.842280 3.495369 4.323818 H 24.666260 9.186367 4.467168
C 16.916820 16.904010 4.413068 C 3.411807 0.793766 4.397693 C 22.179820 10.276230 4.470518
C 16.206260 18.097190 4.408068 H 4.366281 1.344597 4.407218 H 25.597340 15.086240 4.552268
C 14.849470 15.672800 4.392143 O 32.867200 8.738125 4.296843 H 23.465810 16.318940 4.537443
C 14.139490 16.867030 4.388943 O 31.720480 10.778380 4.344543 H 22.180250 9.174468 4.465418
C 14.817590 18.079310 4.396618 B 32.960440 10.133260 4.308343 H 20.046550 10.408660 4.449043
O 16.664520 19.471530 4.411118 O 27.243310 8.808589 4.448068 C 11.341430 13.021030 4.318143
O 14.324080 19.442700 4.392018 B 27.184880 10.205720 4.461843 C 10.141390 12.297450 4.298443
B 15.484840 20.221980 4.399968 O 28.440440 10.819940 4.435768 C 8.905641 13.005460 4.306393
C 17.935760 24.589810 4.407868 O 18.344330 16.653130 4.428518 C 8.910240 14.429600 4.328893
H 18.889770 24.038380 4.425468 O 17.203600 14.609290 4.414743 C 10.137030 15.105790 4.346793
C 14.244060 23.842480 4.362318 O 13.913810 14.564240 4.377368 H 12.295730 12.469840 4.313218
C 15.475040 24.558670 4.374093 O 12.719890 16.577180 4.373393 C 10.107680 10.859260 4.271068
C 42.063670 24.590190 4.339718 B 18.442300 15.258410 4.430218 C 7.672670 12.294380 4.294593
H 41.109210 24.039380 4.329418 B 12.658510 15.180580 4.365668 C 36.696590 15.120760 4.332993
H 17.633330 21.891030 4.421668 C 19.745400 14.523860 4.450493 H 10.138060 16.207930 4.365318
C 27.539620 0.794345 4.330943 C 11.366920 14.425700 4.343993 C 35.485380 13.002410 4.306668
H 26.584990 1.344748 4.313618 C 19.772510 13.119090 4.446993 C 34.285980 12.278680 4.306218
C 29.372680 9.710557 4.399143 C 20.971500 12.395560 4.465068 C 34.260090 10.873850 4.292768
C 30.760600 9.693224 4.359618 C 22.206990 13.103770 4.487468 C 6.440460 10.193110 4.274243
C 28.662550 8.516394 4.407268 C 22.201730 14.528040 4.496343 C 7.667247 10.870410 4.274843
C 29.341700 7.304898 4.377518 C 20.974570 15.205230 4.477143 C 35.518120 14.440570 4.322618
C 30.730580 7.288068 4.340843 H 18.817940 12.568380 4.428518 H 33.330840 12.829160 4.319793
C 31.440480 8.482030 4.330893 C 21.002190 10.957520 4.461043 H 6.439480 9.090973 4.262643
O 28.849470 5.940952 4.380968 C 23.439100 12.391150 4.497493 C 8.928822 10.179450 4.259743
O 31.189260 5.913657 4.322068 C 23.464830 15.217010 4.524068 H 11.061500 10.307700 4.259693
B 30.010370 5.162302 4.348693 H 20.974130 16.307500 4.482918 H 8.927137 9.077640 4.239793
C 0.951090 0.825489 4.364168 C 24.675920 13.097050 4.514968 H 36.696050 16.222850 4.345543
C 2.182610 1.540845 4.375393 C 25.874800 12.371250 4.509318 H 34.563060 14.990550 4.327293
c 0.00000 0.00000 6.85368 serrated armchair

COF-8M

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	14.87100	13.10092	12.53652	C	9.994664	10.25464	12.48675	B	4.657629	8.066248	12.49980
C	15.60762	14.29931	12.54615	C	10.05393	11.66229	12.50093	B	13.39624	2.998720	12.47470
C	16.99475	14.29966	12.54198	C	6.314614	9.571654	12.48913	H	17.53230	10.94041	12.51272
C	17.73172	13.10140	12.52777	O	9.075429	8.150852	12.46467	H	8.793394	0.127528	12.54862
C	16.99497	11.90296	12.52248	O	11.09507	9.318142	12.47698	C	19.28621	5.530660	12.52065
C	15.60790	11.90277	12.52615	C	11.24319	12.41787	12.51398	C	19.97979	6.731958	12.51320
H	6.332169	0.126983	12.55585	C	22.54893	11.66186	12.49982	C	3.909664	6.770794	12.50930
H	15.07095	10.94000	12.51947	C	21.35955	12.41766	12.50475	C	4.579064	5.533536	12.51765
C	25.03966	14.53985	12.50580	C	21.35980	13.78255	12.50263	C	3.885240	4.332313	12.52560
C	16.30157	0.840782	12.50650	C	22.54915	14.53802	12.49840	C	2.479138	4.293537	12.52580
C	17.55042	1.493011	12.51538	C	22.60887	10.25408	12.49687	H	19.41463	7.678579	12.50865
C	1.255848	0.810617	12.52420	O	19.99767	11.93435	12.51305	H	5.681329	5.517084	12.51720
C	10.05366	14.53797	12.52137	O	19.99862	14.26709	12.50978	H	4.450455	3.385723	12.53092
C	15.05264	1.493086	12.49675	C	13.87068	0.810799	12.49273	H	18.18408	5.547112	12.52210
O	17.81232	2.914312	12.51670	B	1.731129	2.998160	12.52627	C	11.24289	4.333766	12.44150
O	2.355929	1.747764	12.53140	B	10.47093	8.067413	12.46348	C	10.54974	5.535216	12.43835
C	11.24303	13.78254	12.52532	B	19.22758	13.10107	12.51723	C	11.21933	6.772308	12.45425
C	23.79268	13.81988	12.50110	O	12.60461	14.26672	12.53745	C	12.62550	6.732987	12.46800
C	23.79267	12.37991	12.49920	O	12.60503	11.93408	12.51793	C	13.31859	5.531432	12.47097
C	7.563324	11.65993	12.49578	O	21.50914	9.316689	12.50257	C	12.64889	4.294324	12.46085
C	8.810241	12.38004	12.50228	O	6.052922	8.150474	12.48980	H	9.447520	5.519505	12.42425
C	8.810172	13.81989	12.51038	O	14.79147	2.914312	12.48668	H	13.19118	7.679184	12.47850
C	7.563577	10.22387	12.48703	O	12.77095	1.748475	12.47910	H	14.42101	5.547339	12.48378
C	8.812889	9.571866	12.47962	B	13.37519	13.10052	12.53230	H	10.67745	3.387569	12.42988

Transformation Matrix

a	17.476440	0.000000	0.000000	
b	8.738220	15.135040	0.000000	
c	0.000000	0.000000	3.472735	AA stacking
c	1.384650	0.000000	3.416581	inclined zigzag
c	1.219300	0.703963	3.419316	inclined armchair

Layer II AB stacking

C	23.60922	18.14593	15.82520	C	18.73288	15.29965	15.77542	B	13.39585	13.11126	15.78848
C	24.34584	19.34432	15.83483	C	18.79215	16.70730	15.78961	B	22.13446	8.043734	15.76338
C	25.73297	19.34467	15.83066	C	15.05283	14.61667	15.77781	H	26.27052	15.98542	15.80140
C	26.46994	18.14641	15.81645	O	17.81365	13.19587	15.75335	H	17.53161	5.172542	15.83730
C	25.73319	16.94797	15.81116	O	19.83329	14.36316	15.76566	C	28.02443	10.57567	15.80933
C	24.34612	16.94778	15.81483	C	19.98141	17.46288	15.80266	C	28.71801	11.77697	15.80188
H	15.07039	5.171997	15.84453	C	31.28715	16.70687	15.78850	C	12.64788	11.81581	15.79798
H	23.80917	15.98501	15.80815	C	30.09777	17.46267	15.79343	C	13.31728	10.57855	15.80632
C	33.77788	19.58486	15.79448	C	30.09802	18.82756	15.79131	C	12.62346	9.377327	15.81428
C	25.03979	5.885796	15.79518	C	31.28737	19.58303	15.78708	C	11.21736	9.338551	15.81448
C	26.28864	6.538025	15.80406	C	31.34709	15.29909	15.78555	H	28.15285	12.72359	15.79733
C	9.994068	5.855631	15.81288	O	28.73589	16.97936	15.80173	H	14.41955	10.56210	15.80588
C	18.79188	19.58298	15.81005	O	28.73684	19.31210	15.79846	H	13.18867	8.430737	15.81960
C	23.79086	6.538100	15.78543	C	22.60890	5.855813	15.78141	H	26.92230	10.59213	15.81078
O	26.55054	7.959326	15.80538	B	10.46935	8.043174	15.81495	C	19.98111	9.378780	15.73018
O	11.09415	6.792778	15.82008	B	19.20915	13.11243	15.75216	C	19.28796	10.58023	15.72703
C	19.98125	18.82755	15.81400	B	27.96580	18.14608	15.80591	C	19.95755	11.81732	15.74293
C	32.53090	18.86489	15.78977	O	21.34283	19.31173	15.82613	C	21.36372	11.77800	15.75668
C	32.53089	17.42492	15.78788	O	21.34325	16.97909	15.80661	C	22.05681	10.57645	15.75965
C	16.30154	16.70494	15.78446	O	30.24736	14.36170	15.79125	C	21.38711	9.339338	15.74953
C	17.54846	17.42505	15.79096	O	14.79114	13.19549	15.77848	H	18.18574	10.56452	15.71292
C	17.54839	18.86490	15.79906	O	23.52969	7.959326	15.77536	H	21.92940	12.72420	15.76718
C	16.30180	15.26888	15.77571	O	21.50917	6.793489	15.76778	H	23.15923	10.59235	15.77246
C	17.55111	14.61688	15.76830	B	22.11341	18.14553	15.82098	H	19.41567	8.432583	15.71856

c	0.00000	0.00000	13.15470	AB

Layer II serrated zigzag

C	16.09030	13.80488	15.94626	C	11.21396	10.95860	15.89649	B	5.876929	8.770211	15.90954
C	16.82692	15.00327	15.95589	C	11.27323	12.36625	15.91067	B	14.61554	3.702683	15.88444
C	18.21405	15.00362	15.95172	C	7.533914	10.27562	15.89887	H	18.75160	11.64437	15.92246
C	18.95102	13.80536	15.93751	O	10.29473	8.854815	15.87441	H	10.01269	0.831491	15.95836
C	18.21427	12.60692	15.93222	O	12.31437	10.02211	15.88672	C	20.50551	6.234623	15.93039
C	16.82720	12.60673	15.93589	C	12.46249	13.12183	15.92372	C	21.19909	7.435921	15.92294
H	7.551469	0.830946	15.96559	C	23.76823	12.36582	15.90956	C	5.128964	7.474757	15.91904
H	16.29025	11.64396	15.92921	C	22.57885	13.12162	15.91449	C	5.798364	6.237499	15.92739
C	26.25896	15.24381	15.91554	C	22.57910	14.48651	15.91237	C	5.104540	5.036276	15.93534
C	17.52087	1.544745	15.91624	C	23.76845	15.24198	15.90814	C	3.698438	4.997500	15.93554
C	18.76972	2.196974	15.92512	C	23.82817	10.95804	15.90661	H	20.63393	8.382542	15.91839
C	2.475148	1.514580	15.93394	O	21.21697	12.63831	15.92279	H	6.900629	6.221047	15.92694
C	11.27296	15.24193	15.93111	O	21.21792	14.97105	15.91952	H	5.669755	4.089686	15.94066
C	16.27194	2.197049	15.90649	C	15.08998	1.514762	15.90247	H	19.40338	6.251075	15.93184
O	19.03162	3.618275	15.92644	B	2.950429	3.702123	15.93601	C	12.46219	5.037729	15.85124
O	3.575229	2.451727	15.94114	B	11.69023	8.771377	15.87322	C	11.76904	6.239179	15.84809
C	12.46233	14.48650	15.93506	B	20.44688	13.80503	15.92697	C	12.43863	7.476271	15.86399
C	25.01198	14.52384	15.91084	O	13.82391	14.97068	15.94719	C	13.84480	7.436950	15.87774
C	25.01197	13.08387	15.90894	O	13.82433	12.63804	15.92767	C	14.53789	6.235395	15.88071
C	8.782624	12.36389	15.90552	O	22.72844	10.02065	15.91231	C	13.86819	4.998287	15.87059
C	10.02954	13.08400	15.91202	O	7.272222	8.854437	15.89954	H	10.66682	6.223468	15.83399
C	10.02947	14.52385	15.92012	O	16.01077	3.618275	15.89642	H	14.41048	8.383147	15.88824
C	8.782877	10.92783	15.89677	O	13.99025	2.452438	15.88884	H	15.64031	6.251302	15.89352
C	10.03219	10.27583	15.88936	B	14.59449	13.80448	15.94204	H	11.89675	4.091532	15.83962
c	0.00000	0.00000	6.81948	serrated zigzag							

Layer II serrated armchair

C	16.25565	13.10092	15.94626	C	11.37931	10.25464	15.89649	B	6.042279	8.066248	15.90954
C	16.99227	14.29931	15.95589	C	11.43858	11.66229	15.91067	B	14.78089	2.998720	15.88444
C	18.37940	14.29966	15.95172	C	7.699264	9.571654	15.89887	H	18.91695	10.94041	15.92246
C	19.11637	13.10140	15.93751	O	10.46008	8.150852	15.87441	H	10.17804	0.127528	15.95836
C	18.37962	11.90296	15.93222	O	12.47972	9.318142	15.88672	C	20.67086	5.530660	15.93039
C	16.99255	11.90277	15.93589	C	12.62784	12.41787	15.92372	C	21.36444	6.731958	15.92294
H	7.716819	0.126983	15.96559	C	23.93358	11.66186	15.90956	C	5.294314	6.770794	15.91904
H	16.45560	10.94000	15.92921	C	22.74420	12.41766	15.91449	C	5.963714	5.533536	15.92739
C	26.42431	14.53985	15.91554	C	22.74445	13.78255	15.91237	C	5.269890	4.332313	15.93534
C	17.68622	0.840782	15.91624	C	23.93380	14.53802	15.90814	C	3.863788	4.293537	15.93554
C	18.93507	1.493011	15.92512	C	23.99352	10.25408	15.90661	H	20.79928	7.678579	15.91839
C	2.640498	0.810617	15.93394	O	21.38232	11.93435	15.92279	H	7.065979	5.517084	15.92694
C	11.43831	14.53797	15.93111	O	21.38327	14.26709	15.91952	H	5.835105	3.385723	15.94066
C	16.43729	1.493086	15.90649	C	15.25533	0.810799	15.90247	H	19.56873	5.547112	15.93184
O	19.19697	2.914312	15.92644	B	3.115779	2.998160	15.93601	C	12.62754	4.333766	15.85124
O	3.740579	1.747764	15.94114	B	11.85558	8.067413	15.87322	C	11.93439	5.535216	15.84809
C	12.62768	13.78254	15.93506	B	20.61223	13.10107	15.92697	C	12.60398	6.772308	15.86399
C	25.17733	13.81988	15.91084	O	13.98926	14.26672	15.94719	C	14.01015	6.732987	15.87774
C	25.17732	12.37991	15.90894	O	13.98968	11.93408	15.92767	C	14.70324	5.531432	15.88071
C	8.947974	11.65993	15.90552	O	22.89379	9.316689	15.91231	C	14.03354	4.294324	15.87059
C	10.19489	12.38004	15.91202	O	7.437572	8.150474	15.89954	H	10.83217	5.519505	15.83399
C	10.19482	13.81989	15.92012	O	16.17612	2.914312	15.89642	H	14.57583	7.679184	15.88824
C	8.948227	10.22387	15.89677	O	14.15560	1.748475	15.88884	H	15.80566	5.547339	15.89352
C	10.19754	9.571866	15.88936	B	14.75984	13.10052	15.94204	H	12.06210	3.387569	15.83962
c	0.00000	0.00000	6.81948	serrated armchair							

COF-9M

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	14.59178	3.372689	0.8041910	C	11.20542	13.01756	0.9207410	H	22.76201	6.737653	0.9634910
C	13.89448	4.570645	0.8000910	C	11.26492	14.42487	0.9335410	H	4.741983	4.584498	1.050616
C	14.57390	5.799003	0.8085410	C	7.526185	12.33444	0.9405160	H	3.509206	2.435057	1.030366
C	15.97742	5.776763	0.8152160	O	10.28352	10.91457	0.8990910	H	21.52552	4.591133	0.9420910
C	16.67005	4.576300	0.8188910	O	12.30498	12.08092	0.9052410	C	12.43730	7.096361	0.8189410
C	15.99938	3.338292	0.8165410	C	12.45361	15.18074	0.9523410	C	11.74939	8.299501	0.8403160
H	12.79071	4.568421	0.7937660	C	28.04780	14.42404	0.9369160	C	12.42443	9.535039	0.8623910
H	16.52786	6.733695	0.8211410	C	26.85874	15.17908	0.9367160	C	13.83190	9.496081	0.8580660
H	17.77229	4.590982	0.8270910	C	26.85885	16.54380	0.9158660	C	14.52433	8.295693	0.8370410
H	14.03087	2.423710	0.8002660	C	28.04751	17.29885	0.8990160	C	13.84081	7.069730	0.8189160
C	16.07924	15.86807	1.017216	C	28.10753	13.01686	0.9479160	H	10.64704	8.289003	0.8411660
C	16.81173	17.07067	1.014266	O	25.49746	14.69534	0.9585160	H	14.39634	10.44282	0.8734910
C	18.19785	17.07721	1.019991	O	25.49861	17.02901	0.9232410	H	15.62817	8.292979	0.8365410
C	18.92305	15.87533	1.030216	C	28.10630	18.70596	0.8757660	H	11.88279	6.142143	0.8037910
C	18.20316	14.67029	1.041591	B	22.55716	2.047775	0.9600160	C	24.77636	8.307850	0.9863910
C	16.81724	14.66902	1.034516	B	11.67911	10.83068	0.8893910	C	25.47579	9.504525	0.9763160
H	16.26928	18.03031	1.003291	B	24.72792	15.86281	0.9517160	C	26.88352	9.536773	0.9833910
H	16.28000	13.70649	1.040341	O	13.81292	17.03118	0.9851660	C	5.788726	8.297616	1.004091
C	30.53716	17.30121	0.9112910	O	13.81525	14.69754	0.9736160	C	5.093962	7.098472	1.015991
C	30.53635	18.73719	0.8999910	O	27.00774	12.08085	0.9642660	C	25.45391	7.078588	1.005641
C	20.90273	0.541890	0.9192160	O	7.265470	10.91354	0.9530160	H	24.91649	10.45439	0.9597660
C	11.20333	18.70792	0.9433910	O	18.14427	1.962037	0.8520410	H	6.891042	8.280691	1.010316
C	11.26375	17.30048	0.9436160	O	16.12396	0.793766	0.8513410	H	5.642541	6.140729	1.031316
C	18.40620	0.541360	0.8760160	B	14.58440	15.86510	0.9939160	H	23.67278	8.312147	0.9775910
O	21.16193	1.962659	0.9276160	B	27.63308	10.83017	0.9673660	C	21.11555	17.07632	0.9937410
O	1.420584	0.797856	0.9689660	B	16.74851	2.044647	0.8373160	C	22.50151	17.06893	0.9722910
C	12.45272	16.54561	0.9598660	H	18.75806	13.71599	1.052166	C	23.23318	15.86591	0.9759910
C	29.29102	16.58125	0.9105410	H	18.74669	18.03484	1.012941	C	22.49501	14.66727	1.004991
C	29.29134	15.14210	0.9249160	C	22.62760	4.580050	0.9666410	C	21.10926	14.66940	1.026141
C	8.774544	14.42274	0.9261410	C	23.31602	5.783171	0.9787660	C	20.39008	15.87488	1.019666
C	10.02105	15.14259	0.9282160	C	24.71927	5.808954	1.006491	H	23.04468	18.02798	0.9507410
C	10.02046	16.58204	0.9277410	C	3.638383	4.582425	1.027216	H	23.03190	13.70448	1.009716
C	8.774642	12.98680	0.9277660	C	2.945480	3.382245	1.015341	H	20.55391	13.71558	1.046541
C	10.02321	12.33531	0.9173660	C	23.30188	3.343890	0.9819910	H	20.56711	18.03412	0.9883660

Transformation Matrix

a	21.763390	0.000000	0.000000	
b	10.881700	18.847640	0.000000	
c	0.000000	0.000000	3.472735	AA
c	1.38742	0.000000	3.415897	inclined zigzag
c	1.21549	0.70176	3.41316	inclined armchair

Layer II AB stacking

C	25.47347	9.655238	4.144956	C	22.08711	19.30011	4.261506	H	33.64371	13.02020	4.304256
C	24.77617	10.85319	4.140856	C	22.14661	20.70742	4.274306	H	15.62368	10.86705	4.391381
C	25.45560	12.08155	4.149306	C	18.40788	18.61699	4.281281	H	14.39090	8.717607	4.371131
C	26.85912	12.05931	4.155981	O	21.16521	17.19712	4.239856	H	32.40722	10.87368	4.282856
C	27.55174	10.85885	4.159656	O	23.18668	18.36347	4.246006	C	23.31899	13.37891	4.159706
C	26.88107	9.620841	4.157306	C	23.33530	21.46329	4.293106	C	22.63108	14.58205	4.181081
H	23.67241	10.85097	4.134531	C	38.92950	20.70659	4.277681	C	23.30613	15.81759	4.203156
H	27.40956	13.01624	4.161906	C	37.74043	21.46163	4.277481	C	24.71359	15.77863	4.198831
H	28.65398	10.87353	4.167856	C	37.74055	22.82635	4.256631	C	25.40602	14.57824	4.177806
H	24.91257	8.706260	4.141031	C	38.92921	23.58140	4.239781	C	24.72250	13.35228	4.159681
C	26.96094	22.15062	4.357981	C	38.98923	19.29941	4.288681	H	21.52874	14.57155	4.181931
C	27.69342	23.35322	4.355031	O	36.37915	20.97789	4.299281	H	25.27803	16.72537	4.214256
C	29.07954	23.35976	4.360756	O	36.38030	23.31156	4.264006	H	26.50986	14.57553	4.177306
C	29.80474	22.15788	4.370981	C	38.98800	24.98851	4.216531	H	22.76448	12.42469	4.144556
C	29.08485	20.95284	4.382356	B	33.43885	8.330324	4.300781	C	35.65805	14.59040	4.327156

C	27.69893	20.95157	4.375281	B	22.56080	17.11323	4.230156	C	36.35748	15.78708	4.317081
H	27.15097	24.31286	4.344056	B	35.60962	22.14536	4.292481	C	37.76522	15.81932	4.324156
H	27.16170	19.98904	4.381106	O	24.69461	23.31373	4.325931	C	16.67042	14.58017	4.344856
C	41.41885	23.58376	4.252056	O	24.69695	20.98009	4.314381	C	15.97566	13.38102	4.356756
C	41.41805	25.01974	4.240756	O	37.88943	18.36340	4.305031	C	36.33560	13.36114	4.346406
C	31.78443	6.824440	4.259981	O	18.14717	17.19609	4.293781	H	35.79819	16.73694	4.300531
C	22.08503	24.99047	4.284156	O	29.02596	8.244586	4.192806	H	17.77274	14.56324	4.351081
C	22.14544	23.58303	4.284381	O	27.00566	7.076315	4.192106	H	16.52423	12.42328	4.372081
C	29.28790	6.823909	4.216781	B	25.46609	22.14765	4.334681	H	34.55447	14.59470	4.318356
O	32.04362	8.245209	4.268381	B	38.51477	17.11272	4.308131	C	31.99724	23.35887	4.334506
O	12.30228	7.080405	4.309731	B	27.63021	8.327196	4.178081	C	33.38321	23.35148	4.313056
C	23.33442	22.82816	4.300631	H	29.63976	19.99854	4.392931	C	34.11488	22.14846	4.316756
C	40.17271	22.86380	4.251306	H	29.62839	24.31739	4.353706	C	33.37671	20.94982	4.345756
C	40.17303	21.42465	4.265681	C	33.50929	10.86260	4.307406	C	31.99096	20.95195	4.366906
C	19.65624	20.70529	4.266906	C	34.19772	12.06572	4.319531	C	31.27177	22.15743	4.360431
C	20.90274	21.42514	4.268981	C	35.60097	12.09150	4.347256	H	33.92638	24.31053	4.291506
C	20.90215	22.86459	4.268506	C	14.52008	10.86497	4.367981	H	33.91360	19.98703	4.350481
C	19.65634	19.26935	4.268531	C	13.82718	9.664795	4.356106	H	31.43560	19.99813	4.387306
C	20.90490	18.61786	4.258131	C	34.18357	9.626439	4.322756	H	31.44880	24.31667	4.329131
c	0.00000	0.00000	6.68153	AB							

Layer II serrated zigzag

C	15.97920	3.372689	4.210511	C	12.59284	13.017560	4.327061	H	24.14943	6.737653	4.369811
C	15.28190	4.570645	4.206411	C	12.65234	14.424870	4.339861	H	6.12940	4.584498	4.456936
C	15.96132	5.799003	4.214861	C	8.91360	12.334440	4.346836	H	4.89662	2.435057	4.436686
C	17.36484	5.776763	4.221536	O	11.67094	10.914570	4.305411	H	22.91294	4.591133	4.348411
C	18.05747	4.576300	4.225211	O	13.69240	12.080920	4.311561	C	13.82472	7.096361	4.225261
C	17.38680	3.338292	4.222861	C	13.84103	15.180740	4.358661	C	13.13681	8.299501	4.246636
H	14.17813	4.568421	4.200086	C	29.43522	14.424040	4.343236	C	13.81185	9.535039	4.268711
H	17.91528	6.733695	4.227461	C	28.24616	15.179080	4.343036	C	15.21932	9.496081	4.264386
H	19.15971	4.590982	4.233411	C	28.24627	16.543800	4.322186	C	15.91175	8.295693	4.243361
H	15.41829	2.423710	4.206586	C	29.43493	17.298850	4.305336	C	15.22823	7.069730	4.225236
C	17.46666	15.868070	4.423536	C	7.73156	13.016860	4.354236	H	12.03446	8.289003	4.247486
C	18.19915	17.070670	4.420586	O	26.88488	14.695340	4.364836	H	15.78376	10.442820	4.279811
C	19.58527	17.077210	4.426311	O	26.88603	17.029010	4.329561	H	17.01559	8.292979	4.242861
C	20.31047	15.875330	4.436536	C	29.49372	18.705960	4.282086	H	13.27021	6.142143	4.210111
C	19.59058	14.670290	4.447911	B	2.18119	2.047775	4.366336	C	26.16378	8.307850	4.392711
C	18.20466	14.669020	4.440836	B	13.06653	10.830680	4.295711	C	26.86321	9.504525	4.382636
H	17.65670	18.030310	4.409611	B	26.11534	15.862810	4.358036	C	6.50755	9.536773	4.389711
H	17.66742	13.706490	4.446661	O	15.20034	17.031180	4.391486	C	7.17614	8.297616	4.410411
C	10.16119	17.301210	4.317611	O	15.20267	14.697540	4.379936	C	6.48138	7.098472	4.422311
C	31.92377	18.737190	4.306311	O	28.39516	12.080850	4.370586	C	5.07794	7.078588	4.411961
C	0.52676	0.541890	4.325536	O	8.65289	10.913540	4.359336	H	26.30391	10.454390	4.366086
C	12.59075	18.707920	4.349711	O	19.53169	1.962037	4.258361	H	8.27846	8.280691	4.416636
C	12.65117	17.300480	4.349936	O	17.51138	0.793766	4.257661	H	7.02996	6.140729	4.437636
C	19.79362	0.541360	4.282336	B	15.97182	15.865100	4.400236	H	25.06020	8.312147	4.383911
O	22.54935	1.962659	4.333936	B	7.25711	10.830170	4.373686	C	22.50297	17.076320	4.400061
O	2.80800	0.797856	4.375286	B	18.13593	2.044647	4.243636	C	23.88893	17.068930	4.378611
C	13.84014	16.545610	4.366186	H	20.14548	13.715990	4.458486	C	24.62060	15.865910	4.382311
C	30.67844	16.581250	4.316861	H	20.13411	18.034840	4.419261	C	23.88243	14.667270	4.411311
C	8.91537	15.142100	4.331236	C	24.01502	4.580050	4.372961	C	22.49668	14.669400	4.432461
C	10.16196	14.422740	4.332461	C	24.70344	5.783171	4.385086	C	21.77750	15.874880	4.425986
C	11.40847	15.142590	4.334536	C	4.34330	5.808954	4.412811	H	24.43210	18.027980	4.357061
C	11.40788	16.582040	4.334061	C	5.02580	4.582425	4.433536	H	24.41932	13.704480	4.416036
C	10.16206	12.986800	4.334086	C	4.33290	3.382245	4.421661	H	21.94133	13.715580	4.452861
C	11.41063	12.335310	4.323686	C	2.92591	3.343890	4.388311	H	21.95453	18.034120	4.394686
c	0.00000	0.00000	6.81264	serrated zigzag							

Layer II serrated armchair

C	15.807270	4.074449	4.210511	C	12.420910	13.719320	4.327061	H	23.977500	7.439413	4.369811
C	15.109970	5.272405	4.206411	C	12.480410	15.126630	4.339861	H	5.957473	5.286258	4.456936

C	15.789390	6.500763	4.214861	C	8.741675	13.036200	4.346836	H	4.724696	3.136817	4.436686
C	17.192910	6.478523	4.221536	O	11.499010	11.616330	4.305411	H	22.741010	5.292893	4.348411
C	17.885540	5.278060	4.225211	O	13.520470	12.782680	4.311561	C	13.652790	7.798121	4.225261
C	17.214870	4.040052	4.222861	C	13.669100	15.882500	4.358661	C	12.964880	9.001262	4.246636
H	14.006200	5.270181	4.200086	C	29.263290	15.125800	4.343236	C	13.639920	10.236800	4.268711
H	17.743350	7.435455	4.227461	C	28.074230	15.880840	4.343036	C	15.047390	10.197840	4.264386
H	18.987780	5.292742	4.233411	C	28.074340	17.245560	4.322186	C	15.739820	8.997454	4.243361
H	15.246360	3.125470	4.206586	C	29.263000	18.000610	4.305336	C	15.056300	7.771490	4.225236
C	17.294730	16.569830	4.423536	C	29.323020	13.718620	4.354236	H	11.862530	8.990764	4.247486
C	18.027220	17.772430	4.420586	O	26.712950	15.397100	4.364836	H	15.611830	11.144580	4.279811
C	19.413340	17.778970	4.426311	O	26.714100	17.730770	4.329561	H	16.843660	8.994740	4.242861
C	20.138540	16.577090	4.436536	C	18.440090	0.560080	4.282086	H	13.098280	6.843903	4.210111
C	19.418650	15.372050	4.447911	B	2.009260	2.749535	4.366336	C	25.991850	9.009610	4.392711
C	18.032730	15.370780	4.440836	B	12.894600	11.532440	4.295711	C	26.691280	10.206290	4.382636
H	17.484770	18.732070	4.409611	B	25.943410	16.564570	4.358036	C	6.335620	10.238530	4.389711
H	17.495490	14.408250	4.446661	O	15.028410	17.732940	4.391486	C	7.004216	8.999376	4.410411
C	31.752650	18.002970	4.317611	O	15.030740	15.399300	4.379936	C	6.309452	7.800232	4.422311
C	20.870140	0.591310	4.306311	O	28.223230	12.782610	4.370586	C	4.906010	7.780348	4.411961
C	22.118220	1.243650	4.325536	O	8.480960	11.615300	4.359336	H	26.131980	11.156150	4.366086
C	1.537120	0.562040	4.349711	O	19.359760	2.663797	4.258361	H	8.106532	8.982451	4.416636
C	12.479240	18.002240	4.349936	O	17.339450	1.495526	4.257661	H	6.858031	6.842489	4.437636
C	19.621690	1.243120	4.282336	B	15.799890	16.566860	4.400236	H	24.888270	9.013907	4.383911
O	22.377420	2.664419	4.333936	B	7.085180	11.531930	4.373686	C	22.331040	17.778080	4.400061
O	2.636074	1.499616	4.375286	B	17.964000	2.746407	4.243636	C	23.717000	17.770690	4.378611
C	13.668210	17.247370	4.366186	H	19.973550	14.417750	4.458486	C	24.448670	16.567670	4.382311
C	30.506510	17.283010	4.316861	H	19.962180	18.736600	4.419261	C	23.710500	15.369030	4.411311
C	30.506830	15.843860	4.331236	C	23.843090	5.281810	4.372961	C	22.324750	15.371160	4.432461
C	9.990034	15.124500	4.332461	C	24.531510	6.484931	4.385086	C	21.605570	16.576640	4.425986
C	11.236540	15.844350	4.334536	C	4.171370	6.510714	4.412811	H	24.260170	18.729740	4.357061
C	11.235950	17.283800	4.334061	C	4.853873	5.284185	4.433536	H	24.247390	14.406240	4.416036
C	9.990132	13.688560	4.334086	C	4.160970	4.084005	4.421661	H	21.769400	14.417340	4.452861
C	11.238700	13.037070	4.323686	C	2.753980	4.045650	4.388311	H	21.782600	18.735880	4.394686
c	0.00000	0.00000	6.81264	serrated armchair							

COF-10M

Layer I AA, AB, inclined zigzag & armchair, and serrated zigzag & armchair

C	16.57332	12.16294	0.814356	C	20.62796	19.13068	0.902936	C	25.32753	18.59247	0.914636
C	17.77586	11.44018	0.814516	C	19.21583	19.08032	0.900016	C	24.09156	17.91935	0.918856
C	18.97789	12.16352	0.828336	C	18.46343	17.88479	0.892766	C	24.12646	16.51218	0.932736
C	18.97659	13.54880	0.844436	C	17.09066	17.88596	0.890156	C	25.32587	15.81852	0.942006
C	17.77513	14.28179	0.847666	O	7.671621	7.067490	0.936066	C	15.28373	7.113374	0.803886
C	16.57405	13.54829	0.830836	B	6.515409	7.841362	0.948236	C	14.05487	7.790636	0.807086
C	17.77726	9.968939	0.806816	O	5.356762	7.070887	0.939356	C	12.85693	7.094708	0.823616
C	16.57504	9.250811	0.798486	O	25.28426	5.565122	0.892136	C	12.82444	5.687621	0.836786
C	16.55731	7.850500	0.800456	O	14.00620	18.05991	0.898636	C	14.06156	5.016470	0.828516
C	17.78079	7.168805	0.808686	B	12.75822	18.67559	0.900236	C	15.26056	5.710602	0.812536
C	19.00276	7.853272	0.816356	C	11.46452	17.92673	0.907886	H	21.48687	0.175720	0.896186
C	18.98126	9.253584	0.815506	C	32.77322	18.59870	0.905736	H	30.61651	18.45701	0.913516
C	20.27827	7.119095	0.830066	C	31.57336	17.90601	0.915616	H	10.23199	14.72098	0.941416
C	21.50558	7.798915	0.841436	C	31.54857	16.50340	0.928956	H	12.37858	15.95767	0.923116
C	22.70539	7.105876	0.856886	C	10.23131	15.82520	0.931016	H	8.669429	13.81456	0.959056
C	22.74164	5.698829	0.861806	C	11.43031	16.51954	0.920556	H	26.89355	13.80858	0.967386
C	21.50576	5.025237	0.849186	O	1.575940	0.539410	0.897136	H	29.04920	17.55431	0.922016
C	20.30502	5.716323	0.833916	O	16.61842	16.54940	0.874986	H	27.48455	18.45185	0.919466
B	24.03574	4.950769	0.878316	B	17.77531	15.77627	0.867836	H	14.06743	0.169370	0.903936
O	24.12467	3.561997	0.879736	O	18.93337	16.54752	0.879716	H	23.17825	15.95051	0.936736
C	2.972248	3.299269	0.893536	O	21.54908	18.05305	0.909036	H	25.32609	14.71442	0.953266
C	3.631523	2.049202	0.896586	B	22.79765	18.66766	0.910306	H	26.89911	12.00369	0.978186

C	5.067356	2.047992	0.901166	O	11.43621	0.531490	0.904156	H	26.89981	9.524688	0.970436
C	5.788824	3.293977	0.906416	O	11.43922	3.551238	0.869056	H	8.677974	9.532068	0.965736
C	5.072328	4.537913	0.910486	B	11.53050	4.939757	0.860686	H	8.669823	12.01055	0.973466
C	3.660156	4.487441	0.901066	O	10.28333	5.556746	0.876836	H	23.65301	7.668761	0.865466
C	5.825573	5.733271	0.922416	C	30.27453	15.76684	0.940656	H	21.50498	8.902993	0.838316
C	7.198402	5.731416	0.920416	C	30.25672	14.36666	0.956036	H	19.34894	5.164138	0.824916
C	7.948356	4.534379	0.907216	C	29.05454	13.64834	0.965806	H	21.49355	3.923150	0.851736
C	7.228782	3.292298	0.905656	C	27.85025	14.36334	0.960666	H	17.78187	6.062794	0.812036
C	7.947905	2.044985	0.901736	C	27.82890	15.76352	0.945156	H	15.61671	9.803075	0.793766
C	9.383546	2.043364	0.897316	C	29.05074	16.44824	0.935286	H	19.93805	9.808386	0.824316
C	10.04565	3.291537	0.888756	C	29.05698	12.17717	0.974036	H	19.93378	11.61083	0.827966
C	9.360223	4.481037	0.893756	C	27.85581	11.45246	0.975886	H	19.93720	14.08908	0.856206
C	7.226426	0.799057	0.901336	C	27.85928	10.06717	0.971306	H	15.61331	14.08849	0.831566
C	5.786580	0.800659	0.900016	C	6.516085	9.335764	0.964886	H	15.61756	11.61013	0.802706
C	16.34050	19.08315	0.895956	C	7.716351	10.07074	0.968686	H	14.05293	8.894695	0.798816
C	14.92855	19.13630	0.895916	C	7.714987	11.45613	0.973236	H	11.90755	7.654508	0.828006
C	2.969599	0.800444	0.895316	C	26.55372	16.49787	0.937136	H	14.07635	3.914481	0.837066
C	10.04314	0.793766	0.900286	C	26.52789	17.90045	0.923286	H	16.21818	5.161092	0.808836

Transformation Matrix

a	22.545500	0.000000	0.000000	
b	11.272750	19.524970	0.000000	
c	0.000000	0.000000	3.415248	AA
c	1.20129	0.693564	3.399478	iclined zigzag
c	1.408306	0.00000	3.39914	iclined armchair

Layer II AB stacking

C	27.84607	18.67126	4.182771	C	31.90071	25.63901	4.271351	C	36.60028	25.10080	4.283051
C	29.04861	17.94851	4.182931	C	30.48858	25.58865	4.268431	C	35.36431	24.42768	4.287271
C	30.25064	18.67184	4.196751	C	29.73618	24.39312	4.261181	C	35.39921	23.02051	4.301151
C	30.24934	20.05713	4.212851	C	28.36341	24.39429	4.258571	C	36.59862	22.32685	4.310421
C	29.04788	20.79012	4.216081	O	18.94437	13.57582	4.304481	C	26.55648	13.62170	4.172301
C	27.84680	20.05662	4.199251	B	17.78816	14.34969	4.316651	C	25.32762	14.29896	4.175501
C	29.05001	16.47726	4.175231	O	16.62951	13.57921	4.307771	C	24.12968	13.60303	4.192031
C	27.84779	15.75914	4.166901	O	36.55701	12.07345	4.260551	C	24.09719	12.19595	4.205201
C	27.83006	14.35883	4.168871	O	25.27895	24.56824	4.267051	C	25.33431	11.52480	4.196931
C	29.05354	13.67713	4.177101	B	24.03097	25.18392	4.268651	C	26.53331	12.21893	4.180951
C	30.27551	14.36160	4.184771	C	22.73727	24.43505	4.276301	H	32.75962	6.684045	4.264601
C	30.25401	15.76191	4.183921	C	44.04597	25.10703	4.274151	H	41.88926	24.96534	4.281931
C	31.55102	13.62742	4.198481	C	42.84611	24.41434	4.284031	H	21.50474	21.22931	4.309831
C	32.77833	14.30724	4.209851	C	42.82132	23.01173	4.297371	H	23.65133	22.46600	4.291531
C	33.97814	13.61420	4.225301	C	21.50406	22.33352	4.299431	H	19.94218	20.32289	4.327471
C	34.01439	12.20715	4.230221	C	22.70306	23.02787	4.288971	H	38.16630	20.31691	4.335801
C	32.77851	11.53356	4.217601	O	12.84869	7.047735	4.265551	H	40.32195	24.06264	4.290431
C	31.57777	12.22465	4.202331	O	27.89117	23.05773	4.243401	H	38.75730	24.96018	4.287881
B	35.30849	11.45909	4.246731	B	29.04806	22.28460	4.236251	H	25.34018	6.677695	4.272351
O	35.39742	10.07032	4.248151	O	30.20612	23.05585	4.248131	H	34.45100	22.45884	4.305151
C	14.24500	9.807594	4.261951	O	32.82183	24.56137	4.277451	H	36.59884	21.22275	4.321681
C	14.90427	8.557528	4.265001	B	34.07040	25.17599	4.278721	H	38.17186	18.51201	4.346601
C	16.34011	8.556317	4.269581	O	22.70896	7.039815	4.272571	H	38.17256	16.03301	4.338851
C	17.06157	9.802302	4.274831	O	22.71197	10.05956	4.237471	H	19.95072	16.04039	4.334151
C	16.34508	11.04624	4.278901	B	22.80325	11.44808	4.229101	H	19.94257	18.51888	4.341881
C	14.93291	10.99577	4.269481	O	21.55608	12.06507	4.245251	H	34.92576	14.17709	4.233881
C	17.09832	12.24160	4.290831	C	41.54728	22.27517	4.309071	H	32.77773	15.41132	4.206731
C	18.47115	12.23974	4.288831	C	41.52947	20.87498	4.324451	H	30.62169	11.67246	4.193331
C	19.22111	11.04270	4.275631	C	40.32729	20.15667	4.334221	H	32.76630	10.43147	4.220151
C	18.50153	9.800623	4.274071	C	39.12300	20.87167	4.329081	H	29.05462	12.57112	4.180451
C	19.22066	8.553310	4.270151	C	39.10165	22.27184	4.313571	H	26.88946	16.31140	4.162181
C	20.65630	8.551689	4.265731	C	40.32349	22.95657	4.303701	H	31.21080	16.31671	4.192731
C	21.31840	9.799862	4.257171	C	40.32973	18.68550	4.342451	H	31.20653	18.11916	4.196381
C	20.63297	10.98936	4.262171	C	39.12856	17.96078	4.344301	H	31.20995	20.59740	4.224621
C	18.49918	7.307382	4.269751	C	39.13203	16.57549	4.339721	H	26.88606	20.59682	4.199981

C	17.05933	7.308984	4.268431	C	17.78884	15.84409	4.333301	H	26.89031	18.11846	4.171121
C	27.61325	25.59148	4.264371	C	18.98910	16.57907	4.337101	H	25.32568	15.40302	4.167231
C	26.20130	25.64462	4.264331	C	18.98774	17.96445	4.341651	H	23.18030	14.16283	4.196421
C	14.24235	7.308769	4.263731	C	37.82647	23.00620	4.305551	H	25.34910	10.42281	4.205481
C	21.31589	7.302091	4.268701	C	37.80064	24.40878	4.291701	H	27.49093	11.66942	4.177251
c	0.00000	0.00000	6.73683	AB							

Layer II serrated zigzag

C	17.77461	12.85650	4.21071	C	10.55650	0.299270	4.299296	C	26.52882	19.28603	4.310996
C	18.97715	12.13374	4.210876	C	9.144370	0.248910	4.296376	C	25.29285	18.61291	4.315216
C	20.17918	12.85708	4.224696	C	19.66472	18.57835	4.289126	C	25.32775	17.20574	4.329096
C	20.17788	14.24236	4.240796	C	18.29195	18.57952	4.286516	C	26.52716	16.51208	4.338366
C	18.97642	14.97535	4.244026	O	8.872910	7.761054	4.332426	C	16.48502	7.806938	4.200246
C	17.77534	14.24185	4.227196	B	7.716699	8.534926	4.344596	C	15.25616	8.484200	4.203446
C	18.97855	10.66250	4.203176	O	6.558052	7.764451	4.335716	C	14.05822	7.788272	4.219976
C	17.77633	9.944375	4.194846	O	3.940050	6.258686	4.288496	C	14.02573	6.381185	4.233146
C	17.75860	8.544065	4.196816	O	15.20749	18.75347	4.294996	C	15.26285	5.710034	4.224876
C	18.98208	7.862369	4.205046	B	13.95951	19.36915	4.296596	C	16.46185	6.404166	4.208896
C	20.20405	8.546836	4.212716	C	12.66581	18.62029	4.304246	H	22.68816	0.869284	4.292546
C	20.18255	9.947148	4.211866	C	11.42901	19.29226	4.302096	H	31.81780	19.15057	4.309876
C	21.47956	7.812659	4.226426	C	32.77465	18.59957	4.311976	H	11.43328	15.41454	4.337776
C	22.70687	8.492479	4.237796	C	10.20436	17.19696	4.325316	H	13.57987	16.65123	4.319476
C	23.90668	7.799440	4.253246	C	11.43260	16.51876	4.327376	H	9.870719	14.50812	4.355416
C	23.94293	6.392393	4.258166	C	12.63160	17.21310	4.316916	H	28.09484	14.50214	4.363746
C	22.70705	5.718801	4.245546	O	2.777230	1.232974	4.293496	H	30.25049	18.24787	4.318376
C	21.50631	6.409887	4.230276	O	17.81971	17.24296	4.271346	H	28.68584	19.14541	4.315826
B	25.23703	5.644333	4.274676	B	18.97660	16.46983	4.264196	H	15.26872	0.862934	4.300296
O	2.780460	4.255561	4.276096	O	20.13466	17.24108	4.276076	H	24.37954	16.64407	4.333096
C	4.173538	3.992833	4.289896	O	22.75037	18.74661	4.305396	H	26.52738	15.40798	4.349626
C	4.832813	2.742766	4.292946	B	23.99894	19.36122	4.306666	H	28.10040	12.69725	4.374546
C	6.268646	2.741556	4.297526	O	12.63750	1.225054	4.300516	H	28.10110	10.21825	4.366796
C	6.990114	3.987541	4.302776	O	12.64051	4.244802	4.265416	H	9.879264	10.22563	4.362096
C	6.273618	5.231477	4.306846	B	12.73179	5.633321	4.257046	H	9.871113	12.70411	4.369826
C	4.861446	5.181005	4.297426	O	11.48462	6.250310	4.273196	H	24.85430	8.362325	4.261826
C	7.026863	6.426835	4.318776	C	31.47582	16.46040	4.337016	H	22.70627	9.596558	4.234676
C	8.399692	6.424980	4.316776	C	8.912510	15.06022	4.352396	H	20.55023	5.857702	4.221276
C	9.149646	5.227943	4.303576	C	30.25583	14.34190	4.362166	H	22.69484	4.616714	4.248096
C	8.430072	3.985862	4.302016	C	29.05154	15.05690	4.357026	H	18.98316	6.756358	4.208396
C	9.149195	2.738549	4.298096	C	29.03019	16.45708	4.341516	H	16.81800	10.49664	4.190126
C	10.58484	2.736928	4.293676	C	30.25203	17.14180	4.331646	H	21.13934	10.50195	4.220676
C	11.24694	3.985101	4.285116	C	7.712770	12.87073	4.370396	H	21.13507	12.30439	4.224326
C	10.56151	5.174601	4.290116	C	29.05710	12.14602	4.372246	H	21.13849	14.78264	4.252566
C	8.427716	1.492621	4.297696	C	6.515070	10.76073	4.367666	H	16.81460	14.78205	4.227926
C	6.987870	1.494223	4.296376	C	7.717375	10.02933	4.361246	H	16.81885	12.30369	4.199066
C	6.269040	0.251740	4.292316	C	8.917641	10.76430	4.365046	H	15.25422	9.588260	4.195176
C	4.857090	0.304890	4.292276	C	8.916277	12.14969	4.369596	H	13.10884	8.348072	4.224366
C	4.170889	1.494008	4.291676	C	27.75501	17.19143	4.333496	H	15.27764	4.608045	4.233426
C	11.24443	1.487330	4.296646	C	27.72918	18.59401	4.319646	H	17.41947	5.854656	4.205196
c	0.00000	0.00000	6.79272	serrated zigzag							

Layer II serrated armchair

C	17.98163	12.16294	4.210716	C	22.03627	19.13068	4.299296	C	26.73584	18.59247	4.310996
C	19.18417	11.44018	4.210876	C	20.62414	19.08032	4.296376	C	25.49987	17.91935	4.315216
C	20.38620	12.16352	4.224696	C	19.87174	17.88479	4.289126	C	25.53477	16.51218	4.329096
C	20.38490	13.54880	4.240796	C	18.49897	17.88596	4.286516	C	26.73418	15.81852	4.338366
C	19.18344	14.28179	4.244026	O	9.079926	7.067490	4.332426	C	16.69204	7.113374	4.200246
C	17.98236	13.54829	4.227196	B	7.923715	7.841362	4.344596	C	15.46318	7.790636	4.203446
C	19.18557	9.968939	4.203176	O	6.765068	7.070887	4.335716	C	14.26524	7.094708	4.219976
C	17.98335	9.250811	4.194846	O	4.147070	5.565122	4.288496	C	14.23275	5.687621	4.233146
C	17.96562	7.850500	4.196816	O	15.41451	18.05991	4.294996	C	15.46987	5.016470	4.224876
C	19.18910	7.168805	4.205046	B	14.16653	18.67559	4.296596	C	16.66887	5.710602	4.208896

C	20.41107	7.853272	4.212716	C	12.87283	17.92673	4.304246	H	0.349680	0.175720	4.292546
C	20.38957	9.253584	4.211866	C	11.63603	18.59870	4.302096	H	32.02481	18.45701	4.309876
C	21.68658	7.119095	4.226426	C	10.43617	17.90601	4.311976	H	11.64030	14.72098	4.337776
C	22.91389	7.798915	4.237796	C	10.41137	16.50340	4.325316	H	13.78689	15.95767	4.319476
C	24.11370	7.105876	4.253246	C	11.63962	15.82520	4.327376	H	10.07773	13.81456	4.355416
C	24.14995	5.698829	4.258166	C	12.83862	16.51954	4.316916	H	28.30186	13.80858	4.363746
C	22.91407	5.025237	4.245546	O	2.984246	0.539410	4.293496	H	30.45751	17.55431	4.318376
C	21.71333	5.716323	4.230276	O	18.02673	16.54940	4.271346	H	28.89286	18.45185	4.315826
B	2.898550	4.950769	4.274676	B	19.18362	15.77627	4.264196	H	15.47574	0.169370	4.300296
O	2.987480	3.561997	4.276096	O	20.34168	16.54752	4.276076	H	24.58656	15.95051	4.333096
C	4.380554	3.299269	4.289896	O	22.95739	18.05305	4.305396	H	26.73440	14.71442	4.349626
C	5.039829	2.049202	4.292946	B	24.20596	18.66766	4.306666	H	28.30742	12.00369	4.374546
C	6.475662	2.047992	4.297526	O	12.84452	0.531490	4.300516	H	5.762620	9.524688	4.366796
C	7.197130	3.293977	4.302776	O	12.84753	3.551238	4.265416	H	10.08628	9.532068	4.362096
C	6.480634	4.537913	4.306846	B	12.93881	4.939757	4.257046	H	10.07813	12.01055	4.369826
C	5.068462	4.487441	4.297426	O	11.69164	5.556746	4.273196	H	25.06132	7.668761	4.261826
C	7.233879	5.733271	4.318776	C	9.137340	15.76684	4.337016	H	22.91329	8.902993	4.234676
C	8.606708	5.731416	4.316776	C	9.119530	14.36666	4.352396	H	20.75725	5.164138	4.221276
C	9.356662	4.534379	4.303576	C	7.917350	13.64834	4.362166	H	22.90186	3.923150	4.248096
C	8.637088	3.292298	4.302016	C	29.25856	14.36334	4.357026	H	19.19018	6.062794	4.208396
C	9.356211	2.044985	4.298096	C	29.23721	15.76352	4.341516	H	17.02501	9.803075	4.190126
C	10.79185	2.043364	4.293676	C	30.45905	16.44824	4.331646	H	21.34636	9.808386	4.220676
C	11.45396	3.291537	4.285116	C	7.919790	12.17717	4.370396	H	21.34209	11.61083	4.224326
C	10.76853	4.481037	4.290116	C	6.718620	11.45246	4.372246	H	21.34551	14.08908	4.252566
C	8.634732	0.799057	4.297696	C	6.722090	10.06717	4.367666	H	17.02162	14.08849	4.227926
C	7.194886	0.800659	4.296376	C	7.924391	9.335764	4.361246	H	17.02587	11.61013	4.199066
C	17.74881	19.08315	4.292316	C	9.124657	10.07074	4.365046	H	15.46124	8.894695	4.195176
C	16.33685	19.13630	4.292276	C	9.123293	11.45613	4.369596	H	13.31586	7.654508	4.224366
C	4.377905	0.800444	4.291676	C	27.96203	16.49787	4.333496	H	15.48466	3.914481	4.233426
C	11.45145	0.793766	4.296646	C	27.93620	17.90045	4.319646	H	17.62649	5.161092	4.205196
c	0.00000	0.00000	6.79272	serrated armchair							

COF-11M

Layer I AA, AB, inclined zigzag & armchair, serrated zigzag & armchair

C	6.029330	8.768199	7.743065	C	17.15021	6.996589	7.808554
C	7.277517	9.427519	7.752586	C	16.46681	8.179989	7.816382
C	7.252033	10.83956	7.750654	O	8.650606	7.269379	7.767845
C	21.17628	11.55042	7.740655	O	17.41270	9.284769	7.825348
C	19.95718	10.86990	7.732084	B	18.64921	8.651609	7.822211
C	19.95041	9.473769	7.733063	O	18.57954	7.264169	7.812064
B	8.567448	8.666579	7.765151	O	2.290272	2.200259	7.780051
O	9.823492	9.282629	7.775844	B	3.526822	2.833349	7.776802
C	10.76074	8.178919	7.784836	O	3.457262	4.220809	7.784103
C	12.17156	8.240099	7.796441	O	12.44407	10.80364	7.812343
C	12.89116	6.993119	7.797756	B	13.60999	11.55898	7.825169
C	12.16734	5.742769	7.793236	O	14.77729	10.80555	7.828099
C	10.72626	5.742849	7.786936	O	8.650353	4.216689	7.789758
C	10.07482	6.997209	7.780148	B	8.566852	2.819509	7.798276
C	14.33581	6.993719	7.804075	C	7.276627	2.059149	7.805703
C	15.05524	8.241649	7.813150	C	6.028722	2.719139	7.802707
C	14.29536	9.433119	7.816544	C	4.827250	2.014289	7.811697
C	12.92917	9.432439	7.807315	C	4.833230	0.618220	7.824137
C	15.05847	5.742629	7.800000	C	13.61305	13.03318	7.827328
C	14.33569	4.491589	7.796688	C	7.250310	0.647160	7.818232
C	12.89101	4.492319	7.796258	O	9.822869	2.203239	7.801608
C	12.17126	3.245409	7.798302	O	12.44368	0.681820	7.808698

C	10.76039	3.306769	7.796534	B	21.17066	13.02252	7.809775
C	10.07465	4.488579	7.789561	O	14.77694	0.679700	7.803260
C	12.92882	2.052999	7.801846	H	5.996126	3.823479	7.793185
C	14.29506	2.052179	7.798633	H	3.882250	0.057630	7.831465
C	15.05502	3.243589	7.794485	H	8.200110	0.082340	7.821305
C	16.46660	3.305119	7.789248	H	8.202126	11.40385	7.757337
C	17.15010	4.488489	7.791566	H	19.00654	11.43107	7.724606
C	16.49860	5.742569	7.799910	H	5.996109	7.663829	7.743672

Transformation Matrix

a	15.122130	0.000000	0.000000	
b	7.561060	13.096150	0.000000	
c	0.000000	0.000000	3.465420	AA
c	1.22487	0.70718	3.40974	inclined zigzag
c	1.407205	0.000000	3.407183	inclined armchair

Layer II AB stacking

C	13.59039	13.13358	11.12486	C	24.71128	11.36197	11.19035
C	14.83858	13.79290	11.13438	C	24.02788	12.54537	11.19818
C	14.81310	15.20494	11.13245	O	16.21167	11.63476	11.14964
C	28.73735	15.91580	11.12245	O	24.97377	13.65015	11.20714
C	27.51825	15.23528	11.11388	B	26.21028	13.01699	11.20401
C	27.51148	13.83915	11.11486	O	26.14061	11.62955	11.19386
B	16.12851	13.03196	11.14695	O	9.851337	6.565642	11.16185
O	17.38456	13.64801	11.15764	B	11.08789	7.198732	11.15860
C	18.32181	12.54430	11.16663	O	11.01833	8.586192	11.16590
C	19.73263	12.60548	11.17824	O	20.00513	15.16902	11.19414
C	20.45222	11.35850	11.17955	B	21.17105	15.92436	11.20696
C	19.72840	10.10815	11.17503	O	22.33836	15.17093	11.20989
C	18.28732	10.10823	11.16873	O	16.21142	8.582072	11.17155
C	17.63589	11.36259	11.16194	B	16.12792	7.184892	11.18007
C	21.89688	11.35910	11.18587	C	14.83769	6.424532	11.18750
C	22.61630	12.60703	11.19494	C	13.58979	7.084522	11.18450
C	21.85642	13.79850	11.19834	C	12.38832	6.379672	11.19349
C	20.49023	13.79782	11.18911	C	12.39429	4.983603	11.20593
C	22.61954	10.10801	11.18180	C	21.17412	17.39856	11.20912
C	21.89676	8.856972	11.17848	C	14.81137	5.012543	11.20003
C	20.45208	8.857702	11.17805	O	17.38393	6.568622	11.18340
C	19.73232	7.610792	11.18010	O	20.00475	5.047203	11.19049
C	18.32146	7.672152	11.17833	B	28.73173	17.38790	11.19157
C	17.63572	8.853962	11.17136	O	22.33801	5.045083	11.18505
C	20.48989	6.418382	11.18364	H	13.55719	8.188862	11.17498
C	21.85612	6.417562	11.18043	H	11.44332	4.423013	11.21326
C	22.61609	7.608972	11.17628	H	15.76118	4.447723	11.20310
C	24.02767	7.670502	11.17104	H	15.76319	15.76923	11.13913
C	24.71117	8.853872	11.17336	H	26.56761	15.79645	11.10640
C	24.05967	10.10795	11.18171	H	13.55717	12.02921	11.12547
c	0.00000	0.00000	6.76359	AB			

Layer II serrated zigzag

C	7.254205	9.475381	11.1493	C	18.37508	7.703771	11.2148
C	8.502392	10.13470	11.1589	C	17.69168	8.887171	11.2227
C	8.476908	11.54674	11.1569	O	9.875481	7.976561	11.1741
C	22.40115	12.25760	11.1469	O	18.63758	9.991951	11.2316
C	21.18205	11.57708	11.1384	B	19.87408	9.358791	11.2285
C	21.17529	10.18095	11.1393	O	19.80441	7.971351	11.2183
B	9.792322	9.373761	11.1714	O	3.515147	2.907441	11.1863

O	11.04837	9.989811	11.1821	B	4.751697	3.540531	11.1831
C	11.98561	8.886101	11.1911	O	4.682137	4.927991	11.1904
C	13.39643	8.947281	11.2027	O	13.66895	11.51082	11.2186
C	14.11604	7.700301	11.2040	B	14.83487	12.26616	11.2314
C	13.39222	6.449951	11.1995	O	16.00216	11.51273	11.2344
C	11.95114	6.450031	11.1932	O	9.875229	4.923871	11.1960
C	11.29969	7.704391	11.1864	B	9.791727	3.526691	11.2046
C	15.56068	7.700901	11.2103	C	8.501502	2.766331	11.2120
C	16.28012	8.948831	11.2194	C	7.253597	3.426321	11.2090
C	15.52024	10.14030	11.2228	C	6.052125	2.721471	11.2180
C	14.15405	10.13962	11.2136	C	6.058105	1.325402	11.2304
C	16.28334	6.449811	11.2063	C	14.83792	13.74036	11.2336
C	15.56056	5.198771	11.2030	C	8.475185	1.354342	11.2245
C	14.11588	5.199501	11.2025	O	11.04774	2.910421	11.2079
C	13.39614	3.952591	11.2046	O	13.66855	1.389002	11.2150
C	11.98527	4.013951	11.2028	B	22.39553	13.72970	11.2160
C	11.29952	5.195761	11.1958	O	16.00182	1.386882	11.2095
C	14.15369	2.760181	11.2081	H	7.221001	4.530661	11.1995
C	15.51994	2.759361	11.2049	H	5.107125	0.764812	11.2377
C	16.27990	3.950771	11.2008	H	9.424986	0.789522	11.2276
C	17.69147	4.012301	11.1955	H	9.427000	12.11103	11.1636
C	18.37498	5.195671	11.1978	H	20.23141	12.13825	11.1309
C	17.72347	6.449751	11.2062	H	7.220984	8.371011	11.1499
c	0.00000	0.00000	6.81264	serrated zigzag			

Layer II serrated armchair

C	7.436535	8.768199	11.14939	C	18.55742	6.996589	11.21487
C	8.684722	9.427519	11.15891	C	17.87402	8.179989	11.22270
C	8.659238	10.83956	11.15697	O	10.05781	7.269379	11.17417
C	22.58348	11.55042	11.14697	O	18.81991	9.284769	11.23167
C	21.36439	10.86990	11.13840	B	20.05642	8.651609	11.22853
C	21.35762	9.473769	11.13938	O	19.98675	7.264169	11.21838
B	9.974652	8.666579	11.17147	O	3.697477	2.200259	11.18637
O	11.23070	9.282629	11.18216	B	4.934027	2.833349	11.18312
C	12.16794	8.178919	11.19116	O	4.864467	4.220809	11.19042
C	13.57876	8.240099	11.20276	O	13.85127	10.80364	11.21866
C	14.29836	6.993119	11.20408	B	15.01719	11.55898	11.23149
C	13.57454	5.742769	11.19956	O	16.18450	10.80555	11.23442
C	12.13346	5.742849	11.19326	O	10.05756	4.216689	11.19608
C	11.48202	6.997209	11.18647	B	9.974056	2.819509	11.20460
C	15.74301	6.993719	11.21039	C	8.683832	2.059149	11.21202
C	16.46244	8.241649	11.21947	C	7.435927	2.719139	11.20903
C	15.70256	9.433119	11.22286	C	6.234455	2.014289	11.21802
C	14.33637	9.432439	11.21363	C	6.240435	0.618220	11.23046
C	16.46568	5.742629	11.20632	C	15.02026	13.03318	11.23365
C	15.74289	4.491589	11.20301	C	8.657515	0.647160	11.22455
C	14.29821	4.492319	11.20258	O	11.23007	2.203239	11.20793
C	13.57846	3.245409	11.20462	O	13.85088	0.681820	11.21502
C	12.16759	3.306769	11.20285	B	22.57787	13.02252	11.21609
C	11.48185	4.488579	11.19588	O	16.18414	0.679700	11.20958
C	14.33602	2.052999	11.20817	H	7.403331	3.823479	11.19950
C	15.70226	2.052179	11.20495	H	5.289455	0.057630	11.23779
C	16.46222	3.243589	11.20081	H	9.607315	0.082340	11.22762
C	17.87381	3.305119	11.19557	H	9.609330	11.40385	11.16366
C	18.55731	4.488489	11.19789	H	20.41375	11.43107	11.13093
C	17.90581	5.742569	11.20623	H	7.403314	7.663829	11.14999

c 0.00000 0.00000 6.81264 serrated armchair

TP COF-2M

Layer I AA, AB, inclined zigzag & armchair, serrated zigzag & armchair

C	11.53373	17.29940	7.897015	C	6.948308	5.495443	7.790462	C	15.51659	5.074529	7.910435
C	10.81540	16.08678	7.889568	C	6.963305	6.861492	7.807947	C	14.79675	6.309104	7.922283
C	9.386423	16.12945	7.891382	C	5.650118	3.343056	7.768093	C	15.52279	7.539138	7.913510
C	30.43892	17.38967	7.900753	C	4.452850	2.681089	7.770287	C	16.92713	7.509400	7.893935
C	31.20175	18.57367	7.907957	O	19.92867	5.149659	7.851935	C	13.36539	6.316542	7.942979
C	10.86680	18.52356	7.906059	B	19.15823	6.316537	7.864342	C	12.65723	7.558408	7.954891
C	28.99692	17.39786	7.902335	O	19.94037	7.478925	7.860467	C	13.41708	8.783940	7.945538
C	28.27953	16.23948	7.894841	O	21.52952	10.09981	7.846352	C	14.77946	8.775408	7.925808
C	28.93109	14.95246	7.884808	B	22.17415	11.34171	7.846267	C	14.75644	3.845973	7.919866
C	8.631410	14.91323	7.883423	C	21.44998	12.65246	7.848131	C	13.39303	3.851842	7.939608
C	9.294085	13.64705	7.873590	C	22.15148	13.87463	7.849526	C	12.64163	5.083708	7.951964
C	8.522690	12.47073	7.864807	C	21.49758	15.11753	7.853895	C	11.23282	5.120296	7.972434
C	28.83890	12.48731	7.865308	C	20.06886	15.15289	7.856809	C	10.55090	6.336157	7.983824
C	28.20938	13.74730	7.875818	C	19.33805	13.92472	7.854147	C	11.24899	7.542093	7.975286
C	11.45896	14.79528	7.880022	C	20.04195	12.70941	7.849787	H	27.10604	13.79462	7.876607
C	10.73877	13.63745	7.872524	C	19.37718	16.40523	7.862851	H	9.048549	11.49908	7.856876
B	28.03353	11.22390	7.854322	C	20.11559	17.62964	7.865990	H	23.25629	13.85647	7.847719
O	6.884225	9.950203	7.842186	C	21.55708	17.56425	7.862517	H	19.46911	11.76453	7.848138
C	5.755644	9.046624	7.834604	C	22.21482	16.37033	7.856641	H	17.47370	8.468995	7.887759
C	5.783925	7.635924	7.820360	C	17.94759	16.43221	7.866268	H	17.46608	4.140168	7.882244
C	4.526696	6.938115	7.817264	C	17.23538	15.17725	7.863058	H	12.63820	17.29018	7.895675
C	25.01942	7.688411	7.828087	C	17.89570	13.98475	7.857155	H	19.83174	0.738500	7.915137
C	25.05096	9.130285	7.837695	C	17.29024	17.67784	7.872745	H	16.18677	17.71970	7.875516
C	26.31880	9.760226	7.841638	C	7.153850	0.050300	7.875762	H	9.099760	0.989080	7.875019
C	23.75442	6.989074	7.829306	C	8.547570	0.032790	7.872471	H	10.65328	4.180081	7.979670
C	22.51656	7.729205	7.839743	O	23.56869	11.22691	7.844745	H	10.68723	8.492787	7.984669
C	22.61078	9.138580	7.843066	O	26.63275	11.17893	7.854360	H	23.31998	16.35819	7.854279
C	23.80739	9.800035	7.842160	O	21.36941	2.531600	7.825842	H	22.13660	18.50505	7.864892
C	23.73321	5.544355	7.820461	B	21.96362	1.276360	7.811249	H	17.31745	13.04286	7.854983
C	22.47369	4.850706	7.826912	O	1.626130	1.303490	7.794398	H	16.13047	15.18767	7.865653
C	21.29406	5.624925	7.841077	O	4.694230	1.246050	7.748926	H	15.32964	9.733315	7.919179
C	21.30888	6.990464	7.845919	B	6.080430	1.151040	7.734575	H	12.87823	9.748173	7.954705
C	4.505702	5.492987	7.802299	O	6.737047	2.375562	7.745324	H	15.29094	2.878303	7.911016
C	3.240720	4.793623	7.804294	O	8.320065	5.004504	7.780248	H	12.84489	2.892184	7.946462
C	3.208953	3.352280	7.790728	B	9.082167	6.167326	7.793336	H	12.56318	14.74916	7.878684
C	1.939740	2.726316	7.799774	O	8.335097	7.338007	7.810074	H	11.27392	12.67013	7.865308
C	22.50238	3.440037	7.818167	C	17.65861	6.306237	7.882397	H	28.46698	18.36703	7.909660
C	5.743215	4.753431	7.786190	C	16.92294	5.102267	7.890790	H	27.17570	16.28299	7.896270

Transformation Matrix

a	21.727490	0.000000	0.000000	
b	10.863740	18.816550	0.000000	
c	0.000000	0.000000	3.468760	AA
c	1.40699	0.00000	3.400518	inclined zigzag
c	1.22029	0.70453	3.404958	inclined armchair

Layer II serrated zigzag

C	12.75401	18.00393	11.29992	C	8.168593	6.199975	11.19336	C	16.73688	5.779061	11.31334
C	12.03569	16.79131	11.29247	C	8.183590	7.566024	11.21085	C	16.01703	7.013636	11.32518
C	10.60671	16.83398	11.29428	C	6.870403	4.047588	11.17099	C	16.74307	8.243670	11.31641
C	31.65920	18.09420	11.30365	C	5.673135	3.385621	11.17319	C	18.14742	8.213932	11.29683
C	32.42204	19.27820	11.31086	O	21.14896	5.854191	11.25484	C	14.58568	7.021074	11.34588
C	12.08709	19.22809	11.30896	B	20.37852	7.021069	11.26724	C	13.87752	8.262939	11.35779
C	30.21721	18.10239	11.30523	O	21.16066	8.183457	11.26337	C	14.63737	9.488472	11.34844

C	29.49981	16.94401	11.29774	O	22.74981	10.80434	11.24925	C	15.99975	9.479939	11.32871
C	30.15137	15.65699	11.28771	B	23.39444	12.04624	11.24917	C	15.97673	4.550505	11.32277
C	9.851695	15.61776	11.28632	C	22.67027	13.35699	11.25103	C	14.61332	4.556374	11.34251
C	10.51437	14.35158	11.27649	C	23.37177	14.57916	11.25243	C	13.86192	5.788239	11.35486
C	9.742975	13.17526	11.26771	C	22.71786	15.82206	11.25679	C	12.45310	5.824828	11.37533
C	30.05919	13.19184	11.26821	C	21.28914	15.85742	11.25971	C	11.77119	7.040689	11.38672
C	29.42966	14.45183	11.27872	C	20.55834	14.62925	11.25705	C	12.46928	8.246625	11.37819
C	12.67924	15.49981	11.28292	C	21.26224	13.41394	11.25269	H	28.32632	14.49915	11.27951
C	11.95905	14.34198	11.27542	C	20.59747	17.10976	11.26575	H	10.26883	12.20361	11.25978
B	29.25381	11.92843	11.25722	C	21.33587	18.33417	11.26889	H	24.47658	14.56100	11.25062
O	8.104510	10.65473	11.24509	C	22.77736	18.26878	11.26542	H	20.68940	12.46906	11.25104
C	6.975929	9.751156	11.23750	C	23.43511	17.07486	11.25954	H	18.69398	9.173527	11.29066
C	7.004210	8.340456	11.22326	C	19.16788	17.13674	11.26917	H	18.68637	4.844700	11.28514
C	5.746981	7.642647	11.22016	C	18.45567	15.88178	11.26596	H	13.85849	17.99471	11.29858
C	26.23971	8.392943	11.23099	C	19.11599	14.68928	11.26005	H	21.05202	1.443032	11.31804
C	26.27125	9.834817	11.24059	C	18.51052	18.38237	11.27565	H	17.40705	18.42423	11.27842
C	27.53909	10.46476	11.24454	C	8.374135	0.7548319	11.27866	H	10.32005	1.693612	11.27792
C	24.97470	7.693606	11.23221	C	9.767856	0.7373219	11.27537	H	11.87357	4.884613	11.38257
C	23.73685	8.433737	11.24264	O	24.78897	11.93144	11.24765	H	11.90752	9.197319	11.38757
C	23.83107	9.843112	11.24597	O	27.85303	11.88346	11.25726	H	24.54027	17.06272	11.25718
C	25.02768	10.50457	11.24506	O	22.58969	3.236132	11.22874	H	23.35689	19.20958	11.26779
C	24.95350	6.248887	11.22336	B	23.18390	1.980892	11.21415	H	18.53773	13.74739	11.25788
C	23.69398	5.555238	11.22981	O	2.846415	2.008022	11.19730	H	17.35076	15.89220	11.26855
C	22.51435	6.329457	11.24398	O	5.914515	1.950582	11.15183	H	16.54992	10.43785	11.32208
C	22.52917	7.694996	11.24882	B	7.300715	1.855572	11.13748	H	14.09852	10.45270	11.35760
C	5.725987	6.197519	11.20520	O	7.957332	3.080094	11.14822	H	16.51122	3.582835	11.31392
C	4.461005	5.498155	11.20719	O	9.540350	5.709036	11.18315	H	14.06518	3.596716	11.34936
C	4.429238	4.056812	11.19363	B	10.30245	6.871858	11.19624	H	13.78347	15.45369	11.28158
C	3.160025	3.430848	11.20267	O	9.555383	8.042539	11.21297	H	12.49421	13.37466	11.26821
C	23.72267	4.144569	11.22107	C	18.87889	7.010769	11.28530	H	29.68727	19.07156	11.31256
C	6.963500	5.457963	11.18909	C	18.14322	5.806799	11.29369	H	28.39598	16.98752	11.29917
c	0.00000	0.00000	6.80580	serrated zigzag							

Layer II serrated armchair

C	12.94072	17.29940	11.29992	C	8.355298	5.495443	11.19336	C	16.92358	5.074529	11.31334
C	12.22239	16.08678	11.29247	C	8.370295	6.861492	11.21085	C	16.20374	6.309104	11.32518
C	10.79341	16.12945	11.29428	C	7.057108	3.343056	11.17099	C	16.92978	7.539138	11.31641
C	31.84591	17.38967	11.30365	C	5.859840	2.681089	11.17319	C	18.33412	7.509400	11.29683
C	32.60874	18.57367	11.31086	O	21.33566	5.149659	11.25484	C	14.77238	6.316542	11.34588
C	12.27379	18.52356	11.30896	B	20.56522	6.316537	11.26724	C	14.06422	7.558408	11.35779
C	30.40391	17.39786	11.30523	O	21.34736	7.478925	11.26337	C	14.82407	8.783940	11.34844
C	29.68652	16.23948	11.29774	O	22.93651	10.09981	11.24925	C	16.18645	8.775408	11.32871
C	30.33808	14.95246	11.28771	B	23.58114	11.34171	11.24917	C	16.16343	3.845973	11.32277
C	10.03840	14.91323	11.28632	C	22.85697	12.65246	11.25103	C	14.80002	3.851842	11.34251
C	10.70107	13.64705	11.27649	C	23.55847	13.87463	11.25243	C	14.04862	5.083708	11.35486
C	9.929680	12.47073	11.26771	C	22.90457	15.11753	11.25679	C	12.63981	5.120296	11.37533
C	30.24589	12.48731	11.26821	C	21.47585	15.15289	11.25971	C	11.95789	6.336157	11.38672
C	29.61637	13.74730	11.27872	C	20.74504	13.92472	11.25705	C	12.65598	7.542093	11.37819
C	12.86595	14.79528	11.28292	C	21.44894	12.70941	11.25269	H	28.51303	13.79462	11.27951
C	12.14576	13.63745	11.27542	C	20.78417	16.40523	11.26575	H	10.45554	11.49908	11.25978
B	29.44052	11.22390	11.25722	C	21.52258	17.62964	11.26889	H	24.66328	13.85647	11.25062
O	8.291215	9.950203	11.24509	C	22.96407	17.56425	11.26542	H	20.87610	11.76453	11.25104
C	7.162634	9.046624	11.23750	C	23.62181	16.37033	11.25954	H	18.88069	8.468995	11.29066
C	7.190915	7.635924	11.22326	C	19.35458	16.43221	11.26917	H	18.87307	4.140168	11.28514
C	5.933686	6.938115	11.22016	C	18.64237	15.17725	11.26596	H	14.04519	17.29018	11.29858
C	26.42641	7.688411	11.23099	C	19.30269	13.98475	11.26005	H	21.23873	0.738500	11.31804
C	26.45795	9.130285	11.24059	C	18.69723	17.67784	11.27565	H	17.59376	17.71970	11.27842
C	27.72579	9.760226	11.24454	C	8.560841	0.050300	11.27866	H	10.50675	0.989080	11.27792
C	25.16141	6.989074	11.23221	C	9.954560	0.032790	11.27537	H	12.06027	4.180081	11.38257
C	23.92355	7.729205	11.24264	O	24.97568	11.22691	11.24765	H	12.09422	8.492787	11.38757
C	24.01777	9.138580	11.24597	O	28.03974	11.17893	11.25726	H	24.72697	16.35819	11.25718
C	25.21438	9.800035	11.24506	O	22.77640	2.531600	11.22874	H	23.54359	18.50505	11.26779

C	25.14020	5.544355	11.22336	B	23.37061	1.276360	11.21415	H	18.72444	13.04286	11.25788
C	23.88068	4.850706	11.22981	O	3.033120	1.303490	11.19730	H	17.53746	15.18767	11.26855
C	22.70105	5.624925	11.24398	O	6.101220	1.246050	11.15183	H	16.73663	9.733315	11.32208
C	22.71587	6.990464	11.24882	B	7.487420	1.151040	11.13748	H	14.28522	9.748173	11.35760
C	5.912692	5.492987	11.20520	O	8.144037	2.375562	11.14822	H	16.69793	2.878303	11.31392
C	4.647710	4.793623	11.20719	O	9.727055	5.004504	11.18315	H	14.25188	2.892184	11.34936
C	4.615943	3.352280	11.19363	B	10.48916	6.167326	11.19624	H	13.97017	14.74916	11.28158
C	3.346730	2.726316	11.20267	O	9.742087	7.338007	11.21297	H	12.68091	12.67013	11.26821
C	23.90937	3.440037	11.22107	C	19.06560	6.306237	11.28530	H	29.87397	18.36703	11.31256
C	7.150205	4.753431	11.18909	C	18.32993	5.102267	11.29369	H	28.58269	16.28299	11.29917
c	0.00000	0.00000	6.80580	serrated armchair							

REF-I

Layer I AA, AB, inclined zigzag, and serrated zigzag

O	8.53482300	5.11449700	0.79376800
B	5.86856000	0.79392900	0.79376800
B	7.07711000	2.88729900	0.79376800
O	5.86856000	3.57514900	0.79376800
B	4.66000000	2.88729900	0.79376800
O	4.66869000	1.49697900	0.79376800
B	9.73479300	5.81749700	0.79376800
B	3.21081700	3.72373700	0.79376800
O	2.00231700	3.03588700	0.79376800
O	3.20228700	5.11449700	0.79376800
B	8.52630300	3.72373700	0.79376800
O	7.06842000	1.49697900	0.79376800

Transformation Matrix

a	7.732466	0.000000	0.000000	
b	3.866233	6.696508	0.000000	
c	0.000000	0.000000	3.592001	AA
c	1.208490	0.697722	3.446160	inclined zigzag

Layer II AB stacking

O	12.40106	7.346668	4.158838
B	9.734793	3.026100	4.158838
B	10.94334	5.119470	4.158838
O	9.734793	5.807320	4.158838
B	8.526233	5.119470	4.158838
O	8.534924	3.729150	4.158838
B	13.60103	8.049667	4.158838
B	7.077050	5.955908	4.158838
O	5.868550	5.268058	4.158838
O	7.068520	7.346668	4.158838
B	12.39254	5.955908	4.158838
O	10.93465	3.729150	4.158838
c	0.00000	0.00000	6.73014	AB

Layer II serrated zigzag

O	9.743313	5.812217	4.285588
B	7.077050	1.491659	4.285588
B	8.285600	3.585029	4.285588
O	7.077050	4.272869	4.285588
B	5.868490	3.585029	4.285588
O	5.877180	2.194699	4.285588

B 10.94328 6.515227 4.285588
B 4.419297 4.421457 4.285588
O 3.210807 3.733607 4.285588
O 4.410777 5.812217 4.285588
B 9.734793 4.421457 4.285588
O 8.276910 2.194699 4.285588
c 0.000000 0.000000 6.98364 serrated zigzag

REF-II

Layer I AA, AB, inclined armchair, and serrated armchair

O 15.328768 8.0298630 0.793768 B 15.243038 6.6372530 0.793768
O 16.974848 10.881153 0.793768 O 16.491958 6.0148430 0.793768
C 11.608732 2.9338220 0.793768 C 16.749358 8.3077030 0.793768
C 10.221312 2.9345120 0.793768 C 17.443178 7.1061530 0.793768
C 9.5268420 4.1387820 0.793768 C 4.3841160 7.1063330 0.793768
C 10.220672 5.3405120 0.793768 C 17.444578 9.5118230 0.793768
C 11.611122 5.3399020 0.793768 C 5.0784360 8.3079230 0.793768
C 12.304472 4.1378520 0.793768 C 18.832338 9.5120830 0.793768
B 10.913192 0.7940220 0.793768 O 5.3337660 6.0145530 0.793768
O 9.7503720 1.5653020 0.793768 O 6.4986960 8.0284530 0.793768
O 8.1061320 4.4158220 0.793768 B 6.5831160 6.6357230 0.793768
B 8.0199620 5.8084320 0.793768 O 19.301238 10.881833 0.793768
O 9.2685720 6.4313320 0.793768 B 18.137838 11.652123 0.793768
O 12.563232 6.4312020 0.793768 O 12.077002 1.5636820 0.793768
B 13.809412 5.8101220 0.793768 O 13.725892 4.4157220 0.793768
Transformation Matrix
a 14.449272 0.000000 0.000000
b 7.224636 12.513431 0.000000
c 0.000000 0.000000 3.528001 AA
c 1.389180 0.000000 3.487678 inclined armchair

Layer II AB stacking

O 22.55340 12.20101 4.103020 B 22.46767 10.80840 4.103020
O 24.19948 15.05230 4.103020 O 23.71659 10.18599 4.103020
C 18.83337 7.104967 4.103020 C 23.97399 12.47885 4.103020
C 17.44595 7.105658 4.103020 C 24.66781 11.27730 4.103020
C 16.75148 8.309927 4.103020 C 11.60875 11.27748 4.103020
C 17.44531 9.511658 4.103020 C 24.66921 13.68297 4.103020
C 18.83576 9.511047 4.103020 C 12.30307 12.47907 4.103020
C 19.52911 8.308998 4.103020 C 26.05697 13.68323 4.103020
B 18.13783 4.965168 4.103020 O 12.55840 10.18570 4.103020
O 16.97501 5.736447 4.103020 O 13.72333 12.19960 4.103020
O 15.33077 8.586967 4.103020 B 13.80775 10.80687 4.103020
B 15.24460 9.979578 4.103020 O 26.52587 15.05298 4.103020
O 16.49321 10.60248 4.103020 B 25.36247 15.82327 4.103020
O 19.78787 10.60235 4.103020 O 19.30164 5.734828 4.103020
B 21.03405 9.981268 4.103020 O 20.95053 8.586867 4.103020
c 0.00000 0.00000 6.618505 AB

Layer II serrated armchair

O 16.717948 8.0298630 4.271908 B 16.632218 6.6372530 4.271908
O 18.364028 10.881153 4.271908 O 17.881138 6.0148430 4.271908

C	12.997912	2.9338220	4.271908	C	18.138538	8.3077030	4.271908
C	11.610492	2.9345120	4.271908	C	4.3830860	7.1061530	4.271908
C	10.916022	4.1387820	4.271908	C	5.7732960	7.1063330	4.271908
C	11.609842	5.3405120	4.271908	C	18.833758	9.5118230	4.271908
C	13.000302	5.3399020	4.271908	C	6.4676160	8.3079230	4.271908
C	13.693652	4.1378520	4.271908	C	5.7722460	9.5120830	4.271908
B	12.302372	0.7940220	4.271908	O	6.7229460	6.0145530	4.271908
O	11.139552	1.5653020	4.271908	O	7.8878760	8.0284530	4.271908
O	9.4953020	4.4158220	4.271908	B	7.9722960	6.6357230	4.271908
B	9.4091420	5.8084320	4.271908	O	20.690418	10.881833	4.271908
O	10.657752	6.4313320	4.271908	B	19.527018	11.652123	4.271908
O	13.952402	6.4312020	4.271908	O	13.466182	1.5636820	4.271908
B	15.198592	5.8101220	4.271908	O	15.115072	4.4157220	4.271908
c	0.00000	0.00000	6.95628	serrated armchair			