Supporting Information: Geometries, Molecular Rayleigh Scattering, Raman and Infrared Frequencies of Polycyclic Aromatic Hydrocarbons and Subunits of Graphite studied by DFT methods

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1 Supporting information

1.1 Geometry optimizations

Table 1: Bond lengths and bond angles of 2H-benzo(cd)pyrene.

Method	Basis set	R(3,8) [Å]	R(3,4) [Å]	A(4,3,8) [degrees]
B3LYP	6-31+G(d,p)	1.4268	1.4268	120.1326
	6-311+G(d,p)	1.4242	1.4242	120.1207
	aug-cc-pVDZ	1.4278	1.4278	120.1294
	aug-cc-pVTZ	1.4207	1.4207	120.1259
ωB97XD	6-31+G(d,p)	1.4242	1.4242	120.0778
	6-311+G(d,p)	1.4219	1.4219	120.0663
	aug-cc-pVDZ	1.4252	1.4252	120.0718
	aug-cc-pVTZ	-	-	-
M06-2X	6-31+G(d,p)	1.425	1.425	120.0352
	6-311+G(d,p)	1.423	1.423	120.0209
	aug-cc-pVDZ	1.4253	1.4253	120.0223
	aug-cc-pVTZ	1.4196	1.4196	120.0358

Table 2: double-layer subunit bond lengths and angles.

Top layer				
	Basis set	R(3,8) [Å]	R(3,4) [Å]	A(4,3,8) [degrees]
B3LYP	6-31+G(d,p)	1.4259	1.4267	120.0404
	6-311+G(d,p)	1.4232	1.4241	120.0269
ωB97XD	6-31+G(d,p)	1.4207	1.4235	119.8446
	6-311+G(d,p)	1.4183	1.4213	119.8296
M06-2X	6-31+G(d,p)	1.4217	1.4242	119.8256
	6-311+G(d,p)	1.4197	1.4223	119.8089
Bottom layer				
	Basis set	R(33,38) [Å]	R(33,34) [Å]	A(34,33,38) [degrees]
B3LYP	6-31+G(d,p)	1.4267	1.4259	120.0411
	6-311+G(d,p)	1.4241	1.4232	120.0269
ωB97XD	6-31+G(d,p)	1.4235	1.4207	119.8449
	6-311+G(d,p)	1.4213	1.4183	119.8298
M06-2X	6-31+G(d,p)	1.4242	1.4217	119.8262
	6-311+G(d,p)	1.4223	1.4197	119.8095

1.2 Raman spectra

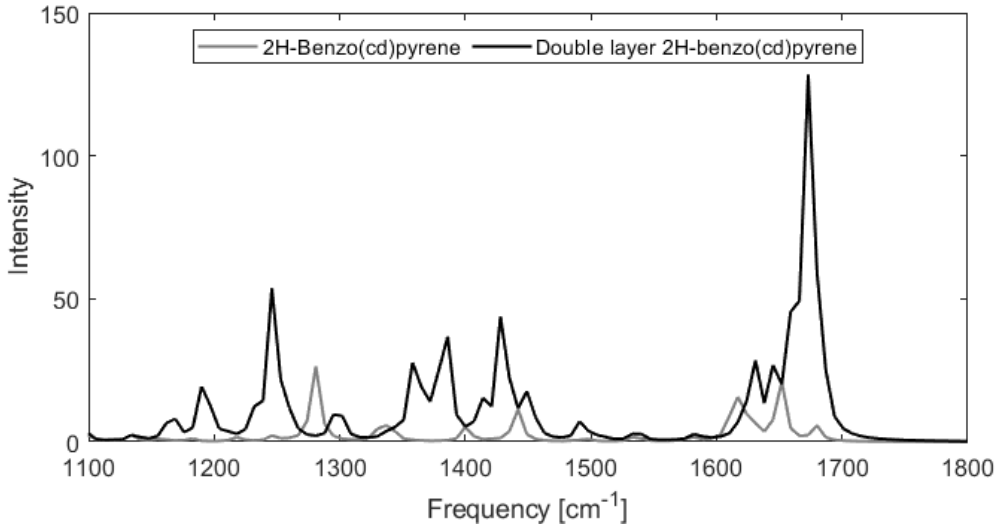

Figure 1: Zoom of Raman spectra obtained from M06-2X/6-311+G(d,p) calculations of a 2H-benzo(cd)pyrene (gray) and the double-layer subunit (black).

Single layer:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.244592	2.706640	-0.000007
2	6	0	-0.000002	2.017341	-0.000007
3	6	0	-0.000001	0.602626	-0.000003
4	6	0	1.232160	-0.108343	-0.000005
5	6	0	2.458281	0.599868	-0.000008
6	6	0	2.426804	2.027988	-0.000007
7	1	0	1.237145	3.791263	-0.000005
8	6	0	-1.232158	-0.108342	0.000004
9	6	0	1.230297	-1.538553	-0.000003
10	1	0	3.367887	2.566844	-0.000006
11	6	0	-0.000001	-2.223611	0.000002
12	6	0	-1.230299	-1.538558	0.000007
13	1	0	0.000004	-3.308637	0.000002
14	6	0	3.668568	-0.122003	-0.000010
15	1	0	4.606253	0.422103	-0.000011
16	6	0	3.663814	-1.510726	-0.000011
17	1	0	4.603471	-2.049994	-0.000013
18	6	0	2.468365	-2.215723	-0.000008
19	1	0	2.472979	-3.299879	-0.000009
20	6	0	-2.468366	-2.215721	0.000016
21	1	0	-2.472991	-3.299876	0.000018
22	6	0	-3.663819	-1.510718	0.000021
23	1	0	-4.603472	-2.049994	0.000029
24	6	0	-3.668572	-0.122003	0.000017
25	1	0	-4.606251	0.422114	0.000018
26	6	0	-2.458276	0.599872	0.000008
27	6	0	-2.426803	2.027983	-0.000003
28	6	0	-1.244585	2.706640	-0.000004
29	1	0	-3.367882	2.566845	-0.000003
30	1	0	-1.237144	3.791263	-0.000011

Double layer:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.406079	2.971957	1.669141
2	6	0	-0.482553	1.863904	1.750102
3	6	0	0.052221	0.554119	1.660585
4	6	0	1.453090	0.360097	1.509613
5	6	0	2.313586	1.479454	1.424210
6	6	0	1.746200	2.789408	1.499583
7	1	0	-0.008574	3.973100	1.725588

8	6	0	-0.817995	-0.567452	1.675740
9	6	0	1.988268	-0.965919	1.428335
10	1	0	2.411175	3.643736	1.425523
11	6	0	1.108868	-2.066663	1.462430
12	6	0	-0.278203	-1.889205	1.556602
13	1	0	1.516052	-3.071228	1.425902
14	6	0	3.694575	1.271369	1.242237
15	1	0	4.350725	2.131994	1.167604
16	6	0	4.215138	-0.013277	1.180977
17	1	0	5.282528	-0.154774	1.054149
18	6	0	3.381123	-1.122311	1.265201
19	1	0	3.793405	-2.123956	1.218254
20	6	0	-1.184232	-2.970999	1.459394
21	1	0	-0.786138	-3.973076	1.334640
22	6	0	-2.553029	-2.771707	1.563370
23	1	0	-3.224851	-3.620541	1.503630
24	6	0	-3.072543	-1.492706	1.717789
25	1	0	-4.143207	-1.341441	1.799326
26	6	0	-2.217928	-0.372860	1.781450
27	6	0	-2.724820	0.955142	1.914525
28	6	0	-1.883721	2.030338	1.902321
29	1	0	-3.795918	1.092698	2.013103
30	1	0	-2.279431	3.037549	1.983438
31	6	0	1.883588	2.033280	-1.900022