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Calculation of Vibrationally Resolved Absorption Spectra of Acenes and Pyrene

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1 Ground state structures

1.1 Napthalene

18

C	-1.2367440	-1.3940257	0.0000000
C	-2.4178490	-0.7044030	0.0000000
C	-2.4178490	0.7044030	0.0000000
C	-1.2367440	1.3940257	0.0000000
C	0.0000000	0.7112416	0.0000000
C	0.0000000	-0.7112416	0.0000000
C	1.2367440	-1.3940257	0.0000000
C	2.4178490	-0.7044030	0.0000000
C	2.4178490	0.7044030	0.0000000
C	1.2367440	1.3940257	0.0000000
H	-1.2336450	-2.4792110	0.0000000
H	-3.3601991	-1.2403476	0.0000000
H	-3.3601991	1.2403476	0.0000000
H	-1.2336450	2.4792110	0.0000000
H	1.2336450	-2.4792110	0.0000000
H	3.3601991	-1.2403476	0.0000000
H	3.3601991	1.2403476	0.0000000
H	1.2336450	2.4792110	0.0000000

1.2 Anthracene

24

C	3.6364407	0.7092632	0.0000000
C	3.6364407	-0.7092632	0.0000000
C	2.4631842	-1.3986828	0.0000000
C	1.2153155	-0.7171129	0.0000000
C	2.4631842	1.3986828	0.0000000
C	1.2153155	0.7171129	0.0000000
C	0.0000000	-1.3953341	0.0000000
C	-1.2153155	-0.7171129	0.0000000
C	0.0000000	1.3953341	0.0000000
C	-1.2153155	0.7171129	0.0000000
C	-2.4631842	-1.3986828	0.0000000
C	-3.6364407	-0.7092632	0.0000000
C	-3.6364407	0.7092632	0.0000000
C	-2.4631842	1.3986828	0.0000000
H	4.5806137	1.2419122	0.0000000
H	4.5806137	-1.2419122	0.0000000
H	2.4607070	-2.4837541	0.0000000
H	2.4607070	2.4837541	0.0000000
H	0.0000000	-2.4813789	0.0000000
H	0.0000000	2.4813789	0.0000000
H	-2.4607070	-2.4837541	0.0000000
H	-4.5806137	-1.2419122	0.0000000
H	-4.5806137	1.2419122	0.0000000
H	-2.4607070	2.4837541	0.0000000

1.3 Pentacene

36

C	3.6529973	0.7223822	0.0000000
C	3.6529973	-0.7223822	0.0000000
C	4.9087494	1.4023285	0.0000000
C	2.4511437	1.3998934	0.0000000
C	4.9087494	-1.4023285	0.0000000
C	2.4511437	-1.3998934	0.0000000
C	6.0766968	-0.7129337	0.0000000

C	6.0766968	0.7129337	0.0000000
C	1.2179088	0.7231311	0.0000000
C	1.2179088	-0.7231311	0.0000000
C	0.0000000	1.4004123	0.0000000
C	0.0000000	-1.4004123	0.0000000
C	-1.2179088	0.7231311	0.0000000
C	-1.2179088	-0.7231311	0.0000000
C	-2.4511437	1.3998934	0.0000000
C	-2.4511437	-1.3998934	0.0000000
C	-3.6529973	0.7223822	0.0000000
C	-3.6529973	-0.7223822	0.0000000
C	-4.9087494	1.4023285	0.0000000
C	-4.9087494	-1.4023285	0.0000000
C	-6.0766968	0.7129337	0.0000000
C	-6.0766968	-0.7129337	0.0000000
H	4.9070778	2.4873571	0.0000000
H	2.4519296	2.4857769	0.0000000
H	4.9070778	-2.4873571	0.0000000
H	2.4519296	-2.4857769	0.0000000
H	7.0221702	-1.2432185	0.0000000
H	7.0221702	1.2432185	0.0000000
H	0.0000000	2.4861917	0.0000000
H	0.0000000	-2.4861917	0.0000000
H	-2.4519296	2.4857769	0.0000000
H	-2.4519296	-2.4857769	0.0000000
H	-4.9070778	2.4873571	0.0000000
H	-4.9070778	-2.4873571	0.0000000
H	-7.0221702	1.2432185	0.0000000
H	-7.0221702	-1.2432185	0.0000000

1.4 Pyrene

26

C	0.0000000	-3.5011851	0.0000000
C	-1.2032753	-2.8143410	0.0000000
C	-1.2274469	-1.4191301	0.0000000
C	-2.4489890	-0.6763829	0.0000000
C	-2.4489890	0.6763829	0.0000000
C	-1.2274469	1.4191301	0.0000000
C	-1.2032753	2.8143410	0.0000000
C	0.0000000	3.5011851	0.0000000
C	1.2032753	2.8143410	0.0000000
C	1.2274469	1.4191301	0.0000000
C	2.4489890	0.6763829	0.0000000
C	2.4489890	-0.6763829	0.0000000
C	1.2274469	-1.4191301	0.0000000
C	1.2032753	-2.8143410	0.0000000
C	0.0000000	-0.7088804	0.0000000
C	0.0000000	0.7088804	0.0000000
H	-2.1417964	-3.3586003	0.0000000
H	0.0000000	-4.5852884	0.0000000
H	2.1417964	-3.3586003	0.0000000
H	3.3849250	-1.2253485	0.0000000
H	3.3849250	1.2253485	0.0000000
H	2.1417964	3.3586003	0.0000000
H	0.0000000	4.5852884	0.0000000
H	-2.1417964	3.3586003	0.0000000
H	-3.3849250	1.2253485	0.0000000
H	-3.3849250	-1.2253485	0.0000000

2 Ground state vibrational levels

2.1 Naphthalene

2.1.1 PBE0 level

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	171.47	2.72523	YES	NO
8	au	186.44	0.00000	NO	NO
9	b2u	366.42	1.42471	YES	NO
10	b2g	395.37	0.00000	NO	YES
11	b3g	478.74	0.00000	NO	YES
12	b1u	487.32	23.56279	YES	NO
13	b1g	516.17	0.00000	NO	YES
14	ag	521.90	0.00000	NO	YES
15	b3u	630.67	3.56214	YES	NO
16	au	636.04	0.00000	NO	NO
17	b2g	729.22	0.00000	NO	YES
18	ag	785.06	0.00000	NO	YES
19	b3g	792.04	0.00000	NO	YES
20	b1u	802.55	118.16295	YES	NO
21	b2u	810.00	0.19617	YES	NO
22	au	850.47	0.00000	NO	NO
23	b3g	905.33	0.00000	NO	YES
24	b2g	950.53	0.00000	NO	YES
25	b1g	951.80	0.00000	NO	YES
26	b1u	966.71	2.71297	YES	NO
27	au	973.09	0.00000	NO	NO
28	b3g	978.95	0.00000	NO	YES
29	b3u	1048.77	8.39391	YES	NO
30	ag	1059.63	0.00000	NO	YES
31	b2u	1156.18	5.60379	YES	NO
32	b3u	1173.45	0.79595	YES	NO
33	b1g	1176.34	0.00000	NO	YES
34	ag	1187.74	0.00000	NO	YES
35	b3u	1245.73	1.29969	YES	NO
36	b1g	1272.11	0.00000	NO	YES
37	b2u	1295.30	6.80341	YES	NO
38	b3u	1414.36	1.12458	YES	NO
39	b2u	1420.02	5.77858	YES	NO
40	ag	1434.41	0.00000	NO	YES
41	ag	1497.95	0.00000	NO	YES
42	b1g	1500.53	0.00000	NO	YES
43	b3u	1566.09	9.56669	YES	NO
44	ag	1640.72	0.00000	NO	YES
45	b2u	1662.20	3.82249	YES	NO
46	b1g	1697.14	0.00000	NO	YES
47	b1g	3178.60	0.00000	NO	YES
48	b2u	3179.72	4.62961	YES	NO
49	b3u	3182.91	0.48509	YES	NO
50	ag	3185.41	0.00000	NO	YES
51	b1g	3197.67	0.00000	NO	YES
52	b2u	3198.50	41.58391	YES	NO
53	b3u	3210.71	29.92416	YES	NO
54	ag	3211.46	0.00000	NO	YES

2.1.2 MP2 level

mode	symmetry	wave number	IR intensity	selection rules
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		cm** (-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	au	220.75	0.00000	NO	NO
8	b1u	235.86	2.89398	YES	NO
9	b2u	406.38	2.16221	YES	NO
10	b2g	461.99	0.00000	NO	YES
11	b3g	544.23	0.00000	NO	YES
12	ag	547.33	0.00000	NO	YES
13	b1g	551.04	0.00000	NO	YES
14	b1u	557.55	20.83089	YES	NO
15	b3u	671.17	4.26894	YES	NO
16	au	693.27	0.00000	NO	NO
17	ag	811.90	0.00000	NO	YES
18	b2u	855.01	2.10513	YES	NO
19	b2g	858.63	0.00000	NO	YES
20	b3g	861.10	0.00000	NO	YES
21	b1u	921.57	147.55860	YES	NO
22	au	978.36	0.00000	NO	NO
23	b3g	1019.95	0.00000	NO	YES
24	b1g	1020.07	0.00000	NO	YES
25	b3u	1038.74	1.54568	YES	NO
26	b2g	1094.72	0.00000	NO	YES
27	ag	1105.09	0.00000	NO	YES
28	b3u	1110.36	4.43512	YES	NO
29	b1u	1111.66	3.22295	YES	NO
30	au	1113.77	0.00000	NO	NO
31	b3g	1117.84	0.00000	NO	YES
32	b2u	1224.77	3.34018	YES	NO
33	b1g	1240.58	0.00000	NO	YES
34	ag	1279.82	0.00000	NO	YES
35	b3u	1305.67	0.31378	YES	NO
36	b1g	1369.92	0.00000	NO	YES
37	b2u	1380.35	5.64191	YES	NO
38	ag	1400.00	0.00000	NO	YES
39	b3u	1417.02	1.33583	YES	NO
40	b2u	1541.19	3.61459	YES	NO
41	b1g	1599.00	0.00000	NO	YES
42	ag	1611.26	0.00000	NO	YES
43	b3u	1668.62	13.63637	YES	NO
44	ag	1710.85	0.00000	NO	YES
45	b2u	1723.94	8.37673	YES	NO
46	b1g	1782.79	0.00000	NO	YES
47	b1g	3213.29	0.00000	NO	YES
48	b2u	3216.60	4.16077	YES	NO
49	b3u	3217.16	0.56059	YES	NO
50	ag	3223.23	0.00000	NO	YES
51	b1g	3234.44	0.00000	NO	YES
52	b2u	3236.55	61.33126	YES	NO
53	b3u	3250.37	50.91482	YES	NO
54	ag	3251.52	0.00000	NO	YES

2.2 Anthracene

2.2.1 PBE0 level

mode	symmetry	wave number	IR intensity	selection rules	
		cm** (-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-

3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	89.87	1.38624	YES	NO
8	au	121.09	0.00000	NO	NO
9	b2g	234.35	0.00000	NO	YES
10	b2u	236.67	1.41686	YES	NO
11	b3g	269.77	0.00000	NO	YES
12	b1u	388.45	0.04965	YES	NO
13	b1g	395.56	0.00000	NO	YES
14	ag	401.42	0.00000	NO	YES
15	b1u	479.71	26.64079	YES	NO
16	b2g	486.08	0.00000	NO	YES
17	au	506.28	0.00000	NO	NO
18	b1g	532.87	0.00000	NO	YES
19	b3g	594.95	0.00000	NO	YES
20	b3u	615.36	8.75019	YES	NO
21	ag	636.84	0.00000	NO	YES
22	b2u	663.02	0.66288	YES	NO
23	b1u	741.08	84.72216	YES	NO
24	au	766.77	0.00000	NO	NO
25	b2g	772.62	0.00000	NO	YES
26	ag	774.87	0.00000	NO	YES
27	b3g	792.99	0.00000	NO	YES
28	b3u	836.57	0.04969	YES	NO
29	b3g	846.93	0.00000	NO	YES
30	au	872.07	0.00000	NO	NO
31	b1u	902.30	56.66165	YES	NO
32	b2u	920.03	1.76347	YES	NO
33	b3g	926.15	0.00000	NO	YES
34	b1g	930.81	0.00000	NO	YES
35	b2g	960.79	0.00000	NO	YES
36	b1u	965.82	5.78731	YES	NO
37	b3g	976.12	0.00000	NO	YES
38	au	976.15	0.00000	NO	NO
39	b3u	1039.98	7.81022	YES	NO
40	ag	1044.12	0.00000	NO	YES
41	b1g	1136.64	0.00000	NO	YES
42	b3u	1164.85	1.69914	YES	NO
43	b2u	1177.58	7.92495	YES	NO
44	ag	1191.32	0.00000	NO	YES
45	b3u	1197.00	2.12805	YES	NO
46	b1g	1212.14	0.00000	NO	YES
47	b2u	1295.56	4.66382	YES	NO
48	b1g	1300.93	0.00000	NO	YES
49	ag	1307.18	0.00000	NO	YES
50	b2u	1350.58	7.03677	YES	NO
51	b3u	1398.15	3.60752	YES	NO
52	b1g	1416.34	0.00000	NO	YES
53	b3u	1446.18	2.35139	YES	NO
54	ag	1461.77	0.00000	NO	YES
55	b3u	1490.41	1.73757	YES	NO
56	b2u	1498.99	1.68459	YES	NO
57	ag	1531.05	0.00000	NO	YES
58	b3u	1603.18	7.38992	YES	NO
59	ag	1622.17	0.00000	NO	YES
60	b1g	1646.11	0.00000	NO	YES
61	b2u	1694.44	5.40552	YES	NO
62	b1g	1695.84	0.00000	NO	YES
63	b2u	3175.91	9.36066	YES	NO
64	ag	3177.75	0.00000	NO	YES

65	b1g	3180.14	0.00000	NO	YES
66	b2u	3180.46	7.27746	YES	NO
67	b3u	3184.94	0.03732	YES	NO
68	ag	3185.84	0.00000	NO	YES
69	b1g	3199.08	0.00000	NO	YES
70	b2u	3199.27	43.59042	YES	NO
71	b3u	3211.46	38.16447	YES	NO
72	ag	3211.76	0.00000	NO	YES

2.3 Pentacene

2.3.1 PBE0 level

mode	symmetry	wave number	IR intensity	selection rules	
		cm ⁻¹	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	36.63	0.42833	YES	NO
8	au	71.05	0.00000	NO	NO
9	b2g	100.63	0.00000	NO	YES
10	b2u	119.68	1.05808	YES	NO
11	b3g	148.78	0.00000	NO	YES
12	b1u	191.84	1.26152	YES	NO
13	b1g	238.49	0.00000	NO	YES
14	au	240.96	0.00000	NO	NO
15	ag	266.29	0.00000	NO	YES
16	b2g	293.06	0.00000	NO	YES
17	b3g	351.50	0.00000	NO	YES
18	b2u	362.07	0.14598	YES	NO
19	b1u	382.33	0.03381	YES	NO
20	b1g	453.11	0.00000	NO	YES
21	b1u	471.00	38.82299	YES	NO
22	b2g	472.68	0.00000	NO	YES
23	b1u	479.90	2.49957	YES	NO
24	b2g	483.75	0.00000	NO	YES
25	b3u	493.77	9.87480	YES	NO
26	b1g	510.58	0.00000	NO	YES
27	au	527.38	0.00000	NO	NO
28	b3g	557.93	0.00000	NO	YES
29	b2u	578.35	3.12427	YES	NO
30	ag	614.42	0.00000	NO	YES
31	b3u	635.44	5.26015	YES	NO
32	ag	642.17	0.00000	NO	YES
33	b1g	727.92	0.00000	NO	YES
34	au	729.20	0.00000	NO	NO
35	b1u	746.34	79.25251	YES	NO
36	b2g	753.38	0.00000	NO	YES
37	b3u	756.59	3.42937	YES	NO
38	b3g	765.34	0.00000	NO	YES
39	ag	774.06	0.00000	NO	YES
40	au	782.26	0.00000	NO	NO
41	b3g	788.66	0.00000	NO	YES
42	ag	810.69	0.00000	NO	YES
43	b2u	841.81	0.12853	YES	NO
44	b3g	842.87	0.00000	NO	YES
45	b1u	845.86	19.21280	YES	NO
46	au	850.53	0.00000	NO	NO
47	b3g	882.68	0.00000	NO	YES
48	b2g	896.24	0.00000	NO	YES
49	b3u	904.72	0.27379	YES	NO

50	au	914.16	0.00000	NO	NO
51	b2u	923.35	2.34608	YES	NO
52	b1u	929.07	82.95683	YES	NO
53	b3g	932.09	0.00000	NO	YES
54	b1g	937.34	0.00000	NO	YES
55	b2g	965.72	0.00000	NO	YES
56	b1u	966.32	7.07698	YES	NO
57	au	976.60	0.00000	NO	NO
58	b3g	976.62	0.00000	NO	YES
59	b3u	1029.79	10.09649	YES	NO
60	ag	1032.40	0.00000	NO	YES
61	b3u	1143.73	1.41106	YES	NO
62	b2u	1152.87	8.79958	YES	NO
63	b1g	1164.88	0.00000	NO	YES
64	ag	1186.61	0.00000	NO	YES
65	b3u	1191.55	0.16832	YES	NO
66	b1g	1201.17	0.00000	NO	YES
67	b2u	1213.58	2.66927	YES	NO
68	ag	1215.90	0.00000	NO	YES
69	b1g	1254.70	0.00000	NO	YES
70	b3u	1265.14	1.50679	YES	NO
71	b2u	1299.33	0.03279	YES	NO
72	b1g	1302.45	0.00000	NO	YES
73	b1g	1319.42	0.00000	NO	YES
74	b2u	1331.06	19.56249	YES	NO
75	ag	1353.40	0.00000	NO	YES
76	b3u	1374.28	12.14354	YES	NO
77	b2u	1383.55	4.09383	YES	NO
78	b1g	1422.70	0.00000	NO	YES
79	ag	1442.58	0.00000	NO	YES
80	b3u	1450.09	1.84013	YES	NO
81	b3u	1452.21	4.94179	YES	NO
82	ag	1465.62	0.00000	NO	YES
83	b3u	1489.61	0.12355	YES	NO
84	b2u	1493.41	0.55610	YES	NO
85	ag	1504.88	0.00000	NO	YES
86	b3u	1564.40	3.27224	YES	NO
87	ag	1585.90	0.00000	NO	YES
88	ag	1602.13	0.00000	NO	YES
89	b3u	1605.26	4.12006	YES	NO
90	b1g	1615.78	0.00000	NO	YES
91	b1g	1663.30	0.00000	NO	YES
92	b2u	1665.48	0.58644	YES	NO
93	b1g	1697.12	0.00000	NO	YES
94	b2u	1699.97	9.08810	YES	NO
95	b2u	3176.53	2.89420	YES	NO
96	b1g	3177.55	0.00000	NO	YES
97	ag	3178.12	0.00000	NO	YES
98	b3u	3179.31	4.06902	YES	NO
99	b2u	3179.94	10.27873	YES	NO
100	b1g	3180.84	0.00000	NO	YES
101	b2u	3181.15	23.65402	YES	NO
102	ag	3182.43	0.00000	NO	YES
103	b3u	3185.70	3.74485	YES	NO
104	ag	3186.03	0.00000	NO	YES
105	b1g	3199.80	0.00000	NO	YES
106	b2u	3199.82	44.86627	YES	NO
107	b3u	3211.88	55.58837	YES	NO
108	ag	3211.99	0.00000	NO	YES

2.4 Pyrene

2.4.1 PBE0 level

mode	symmetry	wave number	IR intensity	selection rules	
		cm** (-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	98.35	0.62579	YES	NO
8	au	151.48	0.00000	NO	NO
9	b1u	213.48	10.38792	YES	NO
10	b2g	250.03	0.00000	NO	YES
11	b3g	262.64	0.00000	NO	YES
12	b3u	360.80	1.64130	YES	NO
13	au	404.01	0.00000	NO	NO
14	ag	412.86	0.00000	NO	YES
15	b1g	463.05	0.00000	NO	YES
16	b1u	501.22	2.12059	YES	NO
17	b2u	508.22	2.86536	YES	NO
18	b1g	509.27	0.00000	NO	YES
19	b3g	518.42	0.00000	NO	YES
20	b2g	542.34	0.00000	NO	YES
21	b3u	551.21	2.51201	YES	NO
22	b3g	591.46	0.00000	NO	YES
23	ag	606.74	0.00000	NO	YES
24	au	699.51	0.00000	NO	NO
25	b2u	707.23	0.04890	YES	NO
26	b1u	736.63	49.41843	YES	NO
27	b1g	750.92	0.00000	NO	YES
28	b1u	758.25	20.97654	YES	NO
29	b3g	789.58	0.00000	NO	YES
30	ag	816.58	0.00000	NO	YES
31	b2g	818.93	0.00000	NO	YES
32	b2u	837.96	4.57780	YES	NO
33	b1u	868.88	95.33423	YES	NO
34	b3g	892.10	0.00000	NO	YES
35	au	903.44	0.00000	NO	NO
36	b2g	917.12	0.00000	NO	YES
37	b3g	959.04	0.00000	NO	YES
38	b1u	962.21	0.75808	YES	NO
39	au	968.48	0.00000	NO	NO
40	b3g	973.33	0.00000	NO	YES
41	b3u	993.01	0.00003	YES	NO
42	b2u	1022.97	1.71247	YES	NO
43	ag	1102.90	0.00000	NO	YES
44	b2u	1123.86	8.11749	YES	NO
45	b1g	1134.13	0.00000	NO	YES
46	b3u	1169.70	0.34905	YES	NO
47	ag	1172.44	0.00000	NO	YES
48	b1g	1204.37	0.00000	NO	YES
49	b3u	1211.96	15.77181	YES	NO
50	b3u	1244.48	0.01526	YES	NO
51	b1g	1266.66	0.00000	NO	YES
52	b2u	1273.12	2.90748	YES	NO
53	ag	1280.69	0.00000	NO	YES
54	ag	1367.92	0.00000	NO	YES
55	b3u	1370.00	5.26462	YES	NO
56	b1g	1428.50	0.00000	NO	YES
57	b1g	1443.09	0.00000	NO	YES
58	ag	1457.01	0.00000	NO	YES

59	b2u	1469.81	7.23890	YES	NO
60	b3u	1472.79	4.25160	YES	NO
61	b2u	1505.38	3.72298	YES	NO
62	b3u	1541.11	2.50792	YES	NO
63	b1g	1551.12	0.00000	NO	YES
64	ag	1616.64	0.00000	NO	YES
65	b1g	1655.02	0.00000	NO	YES
66	b2u	1660.74	13.11492	YES	NO
67	b3u	1669.63	2.74141	YES	NO
68	ag	1698.98	0.00000	NO	YES
69	b2u	3178.81	1.70290	YES	NO
70	b1g	3178.90	0.00000	NO	YES
71	ag	3181.62	0.00000	NO	YES
72	b2u	3181.73	0.00084	YES	NO
73	b3u	3189.73	15.99051	YES	NO
74	b1g	3190.10	0.00000	NO	YES
75	b3u	3198.22	45.05284	YES	NO
76	ag	3198.40	0.00000	NO	YES
77	b2u	3207.58	41.44902	YES	NO
78	ag	3207.82	0.00000	NO	YES

3 Excited state vibrational levels

3.1 Naphthalene

3.1.1 PBE0 level

mode	symmetry	wave number	IR intensity	selection rules	
		cm** (-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	au	158.49	0.00000	NO	NO
8	b1u	165.43	3.44991	YES	NO
9	b2g	268.89	0.00000	NO	YES
10	b2u	358.82	1.40528	YES	NO
11	b1u	379.19	10.49039	YES	NO
12	b3g	469.19	0.00000	NO	YES
13	b1g	472.17	0.00000	NO	YES
14	au	475.70	0.00000	NO	NO
15	ag	507.14	0.00000	NO	YES
16	b3u	559.94	162.63094	YES	NO
17	b2g	688.98	0.00000	NO	YES
18	b1u	690.20	133.68196	YES	NO
19	b3g	730.46	0.00000	NO	YES
20	au	741.11	0.00000	NO	NO
21	ag	768.95	0.00000	NO	YES
22	b2u	798.68	7.99019	YES	NO
23	b2g	823.87	0.00000	NO	YES
24	b1u	851.07	15.35174	YES	NO
25	b3g	856.20	0.00000	NO	YES
26	au	891.44	0.00000	NO	NO
27	b3g	894.16	0.00000	NO	YES
28	b1g	920.64	0.00000	NO	YES
29	b3u	1024.18	36.50517	YES	NO
30	b1g	1058.15	0.00000	NO	YES
31	ag	1070.62	0.00000	NO	YES
32	b2u	1092.71	0.92734	YES	NO
33	b3u	1180.45	1.69956	YES	NO
34	ag	1180.46	0.00000	NO	YES
35	b3u	1235.25	1.50715	YES	NO
36	b1g	1251.18	0.00000	NO	YES

37	b2u	1296.09	11.09135	YES	NO
38	b2u	1410.89	16.40048	YES	NO
39	b1g	1425.47	0.00000	NO	YES
40	ag	1433.39	0.00000	NO	YES
41	b3u	1470.87	0.05449	YES	NO
42	ag	1491.93	0.00000	NO	YES
43	b1g	1505.13	0.00000	NO	YES
44	b2u	1507.64	5.78497	YES	NO
45	b3u	1592.04	40.22458	YES	NO
46	ag	1634.47	0.00000	NO	YES
47	b1g	3186.21	0.00000	NO	YES
48	b3u	3188.65	41.13414	YES	NO
49	b2u	3189.00	17.19251	YES	NO
50	ag	3192.55	0.00000	NO	YES
51	b1g	3204.27	0.00000	NO	YES
52	b2u	3206.07	17.27017	YES	NO
53	b3u	3222.47	24.50920	YES	NO
54	ag	3223.35	0.00000	NO	YES

3.1.2 CC2 level

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
				IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	au	165.10	0.00000	NO	NO
8	b1u	186.01	2.28482	YES	NO
9	b2g	259.10	0.00000	NO	YES
10	b2u	341.68	4.45656	YES	NO
11	b3g	345.99	0.00000	NO	YES
12	b1u	369.12	7.11276	YES	NO
13	au	399.93	0.00000	NO	NO
14	b3g	479.18	0.00000	NO	YES
15	ag	497.32	0.00000	NO	YES
16	b3u	534.50	228.56820	YES	NO
17	au	645.07	0.00000	NO	NO
18	b1g	671.26	0.00000	NO	YES
19	b1u	705.99	141.57704	YES	NO
20	b2g	708.92	0.00000	NO	YES
21	ag	747.28	0.00000	NO	YES
22	b2u	774.31	7.35261	YES	NO
23	b3g	781.03	0.00000	NO	YES
24	b2g	796.16	0.00000	NO	YES
25	b1u	803.87	8.09310	YES	NO
26	au	861.46	0.00000	NO	NO
27	b3g	870.37	0.00000	NO	YES
28	b3u	1003.44	50.86038	YES	NO
29	b1g	1004.74	0.00000	NO	YES
30	ag	1047.94	0.00000	NO	YES
31	b2u	1072.80	1.41021	YES	NO
32	b1g	1130.32	0.00000	NO	YES
33	ag	1168.36	0.00000	NO	YES
34	b3u	1172.50	2.69213	YES	NO
35	b3u	1237.32	1.75995	YES	NO
36	b1g	1254.45	0.00000	NO	YES
37	b2u	1276.72	15.81732	YES	NO
38	b2u	1393.87	18.74775	YES	NO
39	b1g	1409.29	0.00000	NO	YES
40	ag	1450.45	0.00000	NO	YES
41	ag	1478.10	0.00000	NO	YES

42	b2u	1480.03	8.20089	YES	NO
43	b3u	1568.64	45.33410	YES	NO
44	b3u	1587.79	16.39472	YES	NO
45	ag	1620.02	0.00000	NO	YES
46	b1g	1678.16	0.00000	NO	YES
47	b2u	3182.08	28.23349	YES	NO
48	b3u	3186.50	28.94424	YES	NO
49	ag	3188.23	0.00000	NO	YES
50	b1g	3188.78	0.00000	NO	YES
51	b2u	3209.03	10.36476	YES	NO
52	b3u	3227.58	33.93089	YES	NO
53	ag	3228.40	0.00000	NO	YES
54	b1g	3241.00	0.00000	NO	YES

3.2 Anthracene

3.2.1 PBE0 level

B_{2u}

mode	symmetry	wave number	IR intensity	selection rules	
		cm** (-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	89.53	1.43668	YES	NO
8	au	117.10	0.00000	NO	NO
9	b2u	234.71	1.07368	YES	NO
10	b2g	235.57	0.00000	NO	YES
11	b3g	252.70	0.00000	NO	YES
12	b1u	328.74	1.47703	YES	NO
13	b1g	387.01	0.00000	NO	YES
14	ag	396.47	0.00000	NO	YES
15	b1u	420.16	19.80801	YES	NO
16	b2g	441.98	0.00000	NO	YES
17	au	513.71	0.00000	NO	NO
18	b1g	523.47	0.00000	NO	YES
19	b3g	537.30	0.00000	NO	YES
20	b3u	598.56	23.70841	YES	NO
21	ag	600.96	0.00000	NO	YES
22	b2u	667.24	1.94046	YES	NO
23	b1u	720.84	107.38694	YES	NO
24	b2g	723.69	0.00000	NO	YES
25	au	726.04	0.00000	NO	NO
26	b3g	749.31	0.00000	NO	YES
27	ag	762.81	0.00000	NO	YES
28	b3g	791.76	0.00000	NO	YES
29	b3u	839.82	82.95659	YES	NO
30	au	845.47	0.00000	NO	NO
31	b1u	850.45	26.64342	YES	NO
32	b2g	890.14	0.00000	NO	YES
33	b3g	898.28	0.00000	NO	YES
34	b1u	898.47	29.17846	YES	NO
35	b2u	911.69	0.04566	YES	NO
36	au	915.06	0.00000	NO	NO
37	b3g	918.74	0.00000	NO	YES
38	b1g	919.48	0.00000	NO	YES
39	b3u	1059.37	6.64148	YES	NO
40	ag	1061.36	0.00000	NO	YES
41	b1g	1097.75	0.00000	NO	YES
42	b2u	1132.33	5.11946	YES	NO

43	b3u	1176.76	0.16859	YES	NO
44	ag	1186.79	0.00000	NO	YES
45	b1g	1213.62	0.00000	NO	YES
46	b3u	1218.93	5.13415	YES	NO
47	ag	1282.37	0.00000	NO	YES
48	b1g	1298.87	0.00000	NO	YES
49	b2u	1302.47	13.86669	YES	NO
50	b2u	1305.09	4.91773	YES	NO
51	b3u	1393.67	3.49193	YES	NO
52	b1g	1418.22	0.00000	NO	YES
53	ag	1451.73	0.00000	NO	YES
54	b2u	1468.01	15.01552	YES	NO
55	b3u	1470.62	6.80287	YES	NO
56	b3u	1485.73	77.34025	YES	NO
57	b1g	1543.77	0.00000	NO	YES
58	ag	1546.73	0.00000	NO	YES
59	b1g	1583.24	0.00000	NO	YES
60	b3u	1594.59	8.89424	YES	NO
61	ag	1618.49	0.00000	NO	YES
62	b2u	1628.12	1.47867	YES	NO
63	b2u	3173.84	16.32021	YES	NO
64	ag	3175.37	0.00000	NO	YES
65	b2u	3184.46	17.76450	YES	NO
66	b1g	3185.50	0.00000	NO	YES
67	b3u	3188.17	15.30013	YES	NO
68	ag	3189.06	0.00000	NO	YES
69	b1g	3203.13	0.00000	NO	YES
70	b2u	3203.36	25.30579	YES	NO
71	b3u	3218.80	43.19764	YES	NO
72	ag	3219.17	0.00000	NO	YES

3.3 Pentacene

3.3.1 PBE0 level

B_{2u}

mode	symmetry	wave number	IR intensity	selection rules	
		cm** (-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	39.08	0.43834	YES	NO
8	au	72.24	0.00000	NO	NO
9	b2g	101.97	0.00000	NO	YES
10	b2u	118.88	0.87082	YES	NO
11	b3g	150.76	0.00000	NO	YES
12	b1u	188.70	1.18148	YES	NO
13	b1g	238.50	0.00000	NO	YES
14	au	244.66	0.00000	NO	NO
15	ag	264.73	0.00000	NO	YES
16	b2g	303.30	0.00000	NO	YES
17	b3g	339.81	0.00000	NO	YES
18	b2u	361.87	0.34098	YES	NO
19	b1u	363.00	0.19285	YES	NO
20	b1u	434.30	23.38933	YES	NO
21	b1g	450.47	0.00000	NO	YES
22	b2g	451.51	0.00000	NO	YES
23	b2g	466.85	0.00000	NO	YES
24	b1u	475.40	11.97044	YES	NO
25	b3u	488.69	24.66071	YES	NO

26	b1g	507.27	0.00000	NO	YES
27	au	542.36	0.00000	NO	NO
28	b3g	553.24	0.00000	NO	YES
29	b2u	585.09	0.21256	YES	NO
30	ag	610.31	0.00000	NO	YES
31	ag	620.62	0.00000	NO	YES
32	b3u	627.61	19.78760	YES	NO
33	au	712.88	0.00000	NO	NO
34	b1g	731.23	0.00000	NO	YES
35	b3g	738.73	0.00000	NO	YES
36	b1u	745.90	95.96132	YES	NO
37	b2g	747.04	0.00000	NO	YES
38	b3u	763.63	59.72461	YES	NO
39	ag	767.10	0.00000	NO	YES
40	au	767.68	0.00000	NO	NO
41	b3g	780.37	0.00000	NO	YES
42	b3g	815.31	0.00000	NO	YES
43	ag	818.26	0.00000	NO	YES
44	b1u	839.79	11.99920	YES	NO
45	au	843.02	0.00000	NO	NO
46	b2u	845.61	0.19919	YES	NO
47	b3g	870.88	0.00000	NO	YES
48	b2g	879.85	0.00000	NO	YES
49	au	900.25	0.00000	NO	NO
50	b1u	906.20	72.82689	YES	NO
51	b3u	913.11	0.03402	YES	NO
52	b2u	917.68	0.15274	YES	NO
53	b3g	920.07	0.00000	NO	YES
54	b1g	933.82	0.00000	NO	YES
55	b2g	937.29	0.00000	NO	YES
56	b1u	937.94	18.18848	YES	NO
57	au	952.46	0.00000	NO	NO
58	b3g	952.65	0.00000	NO	YES
59	b3u	1059.68	7.29083	YES	NO
60	ag	1060.25	0.00000	NO	YES
61	b2u	1139.25	6.99432	YES	NO
62	b1g	1148.28	0.00000	NO	YES
63	b3u	1177.53	3.75773	YES	NO
64	ag	1184.15	0.00000	NO	YES
65	b3u	1203.17	22.82480	YES	NO
66	b1g	1206.27	0.00000	NO	YES
67	b2u	1217.11	1.01096	YES	NO
68	ag	1225.94	0.00000	NO	YES
69	b3u	1269.29	0.18244	YES	NO
70	b1g	1272.69	0.00000	NO	YES
71	b2u	1296.95	2.95769	YES	NO
72	b1g	1300.32	0.00000	NO	YES
73	b1g	1306.87	0.00000	NO	YES
74	b2u	1325.98	24.59999	YES	NO
75	ag	1333.55	0.00000	NO	YES
76	b2u	1361.81	8.29230	YES	NO
77	b3u	1376.16	0.06429	YES	NO
78	ag	1417.03	0.00000	NO	YES
79	b1g	1434.04	0.00000	NO	YES
80	b3u	1455.30	9.23143	YES	NO
81	ag	1460.21	0.00000	NO	YES
82	b3u	1461.36	0.16725	YES	NO
83	b3u	1480.06	4.56850	YES	NO
84	b2u	1486.89	5.34210	YES	NO
85	ag	1522.38	0.00000	NO	YES
86	b3u	1541.74	219.29520	YES	NO
87	ag	1560.36	0.00000	NO	YES

88	b1g	1562.03	0.00000	NO	YES
89	b3u	1597.13	16.63430	YES	NO
90	ag	1604.99	0.00000	NO	YES
91	b1g	1621.18	0.00000	NO	YES
92	b2u	1635.98	3.79222	YES	NO
93	b1g	1664.67	0.00000	NO	YES
94	b2u	1665.12	2.68886	YES	NO
95	b2u	3175.16	0.03459	YES	NO
96	ag	3176.18	0.00000	NO	YES
97	b1g	3176.70	0.00000	NO	YES
98	b2u	3177.63	39.06963	YES	NO
99	b3u	3178.22	4.16620	YES	NO
100	ag	3180.59	0.00000	NO	YES
101	b2u	3182.49	9.83720	YES	NO
102	b1g	3182.59	0.00000	NO	YES
103	b3u	3187.04	0.01409	YES	NO
104	ag	3187.17	0.00000	NO	YES
105	b1g	3201.18	0.00000	NO	YES
106	b2u	3201.18	35.44420	YES	NO
107	b3u	3215.36	98.58522	YES	NO
108	ag	3215.71	0.00000	NO	YES

B_{3u}

mode	symmetry	wave number	IR intensity	selection rules	
		cm ⁻¹	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	13.49	0.38238	YES	NO
8	b2g	85.73	0.00000	NO	YES
9	au	108.12	0.00000	NO	NO
10	b2u	121.67	0.53842	YES	NO
11	b3g	169.07	0.00000	NO	YES
12	b1u	175.24	1.17284	YES	NO
13	b1g	238.28	0.00000	NO	YES
14	au	252.79	0.00000	NO	NO
15	ag	265.89	0.00000	NO	YES
16	b2g	281.93	0.00000	NO	YES
17	b3g	342.19	0.00000	NO	YES
18	b1u	352.06	0.10121	YES	NO
19	b2u	360.35	0.45054	YES	NO
20	b1u	429.55	25.49373	YES	NO
21	b1g	448.32	0.00000	NO	YES
22	b2g	452.55	0.00000	NO	YES
23	b2g	459.81	0.00000	NO	YES
24	b1u	469.54	10.78090	YES	NO
25	b3u	489.84	24.10553	YES	NO
26	b1g	506.53	0.00000	NO	YES
27	au	540.12	0.00000	NO	NO
28	b3g	548.84	0.00000	NO	YES
29	b2u	585.44	0.05162	YES	NO
30	ag	603.22	0.00000	NO	YES
31	ag	614.25	0.00000	NO	YES
32	b3u	617.35	21.79197	YES	NO
33	au	718.13	0.00000	NO	NO
34	b1g	731.12	0.00000	NO	YES
35	b3u	731.21	68.50236	YES	NO
36	ag	731.37	0.00000	NO	YES
37	b3g	740.81	0.00000	NO	YES
38	b1u	743.06	96.79589	YES	NO

39	b2g	744.10	0.00000	NO	YES
40	au	768.58	0.00000	NO	NO
41	b3g	782.51	0.00000	NO	YES
42	ag	794.00	0.00000	NO	YES
43	b3g	813.56	0.00000	NO	YES
44	b2u	837.84	0.16133	YES	NO
45	b1u	839.65	10.93200	YES	NO
46	au	841.38	0.00000	NO	NO
47	b3g	869.00	0.00000	NO	YES
48	b2g	880.62	0.00000	NO	YES
49	b3u	881.35	0.03996	YES	NO
50	au	899.42	0.00000	NO	NO
51	b1u	906.46	75.32258	YES	NO
52	b2u	919.06	0.00244	YES	NO
53	b3g	920.20	0.00000	NO	YES
54	b1g	931.48	0.00000	NO	YES
55	b2g	939.77	0.00000	NO	YES
56	b1u	940.32	15.81393	YES	NO
57	au	949.44	0.00000	NO	NO
58	b3g	949.79	0.00000	NO	YES
59	b3u	1019.24	4.85819	YES	NO
60	ag	1021.24	0.00000	NO	YES
61	b2u	1147.64	4.86169	YES	NO
62	b1g	1158.25	0.00000	NO	YES
63	b3u	1177.18	6.20611	YES	NO
64	ag	1182.43	0.00000	NO	YES
65	b3u	1200.23	33.43720	YES	NO
66	b1g	1200.76	0.00000	NO	YES
67	b2u	1216.71	3.18737	YES	NO
68	ag	1222.14	0.00000	NO	YES
69	b3u	1259.83	0.02948	YES	NO
70	b1g	1268.40	0.00000	NO	YES
71	b2u	1298.50	1.83588	YES	NO
72	b1g	1299.86	0.00000	NO	YES
73	b1g	1309.85	0.00000	NO	YES
74	b2u	1322.33	23.84773	YES	NO
75	ag	1346.61	0.00000	NO	YES
76	b3u	1357.84	7.61284	YES	NO
77	b2u	1374.14	8.06422	YES	NO
78	ag	1388.08	0.00000	NO	YES
79	b3u	1404.00	0.00081	YES	NO
80	b1g	1426.06	0.00000	NO	YES
81	ag	1427.25	0.00000	NO	YES
82	b3u	1467.01	1.58384	YES	NO
83	b3u	1487.61	18.81018	YES	NO
84	b2u	1493.33	2.21998	YES	NO
85	ag	1504.82	0.00000	NO	YES
86	b3u	1534.55	216.38057	YES	NO
87	b3u	1555.45	9.71637	YES	NO
88	ag	1562.02	0.00000	NO	YES
89	ag	1570.11	0.00000	NO	YES
90	b1g	1592.83	0.00000	NO	YES
91	b1g	1626.05	0.00000	NO	YES
92	b2u	1655.72	1.51006	YES	NO
93	b2u	1681.37	3.88148	YES	NO
94	b1g	1682.31	0.00000	NO	YES
95	b2u	3175.77	3.19807	YES	NO
96	ag	3176.69	0.00000	NO	YES
97	b1g	3176.79	0.00000	NO	YES
98	b3u	3178.04	4.63913	YES	NO
99	b2u	3179.39	27.23779	YES	NO
100	ag	3181.16	0.00000	NO	YES

101	b2u	3182.05	23.36433	YES	NO
102	b1g	3182.13	0.00000	NO	YES
103	b3u	3185.62	0.07456	YES	NO
104	ag	3185.85	0.00000	NO	YES
105	b2u	3203.84	30.80077	YES	NO
106	b1g	3203.84	0.00000	NO	YES
107	b3u	3217.11	93.72848	YES	NO
108	ag	3217.39	0.00000	NO	YES

3.4 Pyrene

3.4.1 PBE0 level

1B_{2u}

mode	symmetry	wave number	IR intensity	selection rules	
		cm ⁻¹ (-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b1u	99.93	0.63308	YES	NO
8	au	139.62	0.00000	NO	NO
9	b1u	202.48	9.82303	YES	NO
10	b2g	202.94	0.00000	NO	YES
11	b3g	253.50	0.00000	NO	YES
12	b3u	335.65	65.54714	YES	NO
13	au	366.92	0.00000	NO	NO
14	ag	410.89	0.00000	NO	YES
15	b1g	437.27	0.00000	NO	YES
16	b3g	456.17	0.00000	NO	YES
17	b1u	474.96	0.01466	YES	NO
18	b1g	497.09	0.00000	NO	YES
19	b3u	504.27	69.82879	YES	NO
20	b2u	506.09	11.44222	YES	NO
21	b2g	520.90	0.00000	NO	YES
22	b3g	544.35	0.00000	NO	YES
23	ag	605.79	0.00000	NO	YES
24	au	658.41	0.00000	NO	NO
25	b1u	689.45	85.49195	YES	NO
26	b2u	690.68	7.65673	YES	NO
27	b3g	718.12	0.00000	NO	YES
28	b1g	731.06	0.00000	NO	YES
29	b1u	734.51	1.93698	YES	NO
30	b2g	769.09	0.00000	NO	YES
31	ag	813.98	0.00000	NO	YES
32	b2u	817.15	28.86736	YES	NO
33	au	829.03	0.00000	NO	NO
34	b1u	831.94	90.53380	YES	NO
35	b2g	846.51	0.00000	NO	YES
36	b3g	863.38	0.00000	NO	YES
37	b3g	903.42	0.00000	NO	YES
38	au	906.73	0.00000	NO	NO
39	b3g	939.74	0.00000	NO	YES
40	b1u	939.88	0.35447	YES	NO
41	b3u	985.30	0.00096	YES	NO
42	b2u	996.33	7.23864	YES	NO
43	b1g	1091.91	0.00000	NO	YES
44	ag	1097.27	0.00000	NO	YES
45	b2u	1119.97	9.14905	YES	NO
46	b3u	1143.61	24.50934	YES	NO
47	ag	1148.53	0.00000	NO	YES

48	b1g	1178.56	0.00000	NO	YES
49	b3u	1196.73	2.91285	YES	NO
50	b1g	1217.92	0.00000	NO	YES
51	b3u	1234.60	37.14905	YES	NO
52	ag	1260.91	0.00000	NO	YES
53	b2u	1265.13	4.95105	YES	NO
54	b1g	1309.29	0.00000	NO	YES
55	b3u	1314.06	173.06690	YES	NO
56	ag	1371.92	0.00000	NO	YES
57	b3u	1433.23	8.45265	YES	NO
58	b1g	1436.50	0.00000	NO	YES
59	ag	1441.47	0.00000	NO	YES
60	b2u	1452.56	0.33587	YES	NO
61	b3u	1467.22	5.89638	YES	NO
62	b1g	1524.98	0.00000	NO	YES
63	b2u	1525.21	6.56064	YES	NO
64	ag	1551.34	0.00000	NO	YES
65	b1g	1561.05	0.00000	NO	YES
66	b3u	1587.74	90.13686	YES	NO
67	b2u	1593.74	44.45937	YES	NO
68	ag	1641.37	0.00000	NO	YES
69	b2u	3184.32	22.70133	YES	NO
70	b1g	3185.51	0.00000	NO	YES
71	ag	3186.22	0.00000	NO	YES
72	b2u	3186.85	1.94160	YES	NO
73	b3u	3194.64	32.65440	YES	NO
74	b1g	3194.99	0.00000	NO	YES
75	b3u	3201.70	17.89532	YES	NO
76	ag	3202.68	0.00000	NO	YES
77	b2u	3210.81	34.72906	YES	NO
78	ag	3211.03	0.00000	NO	YES

4 Scaled absorption spectra

4.1 Naphthalene

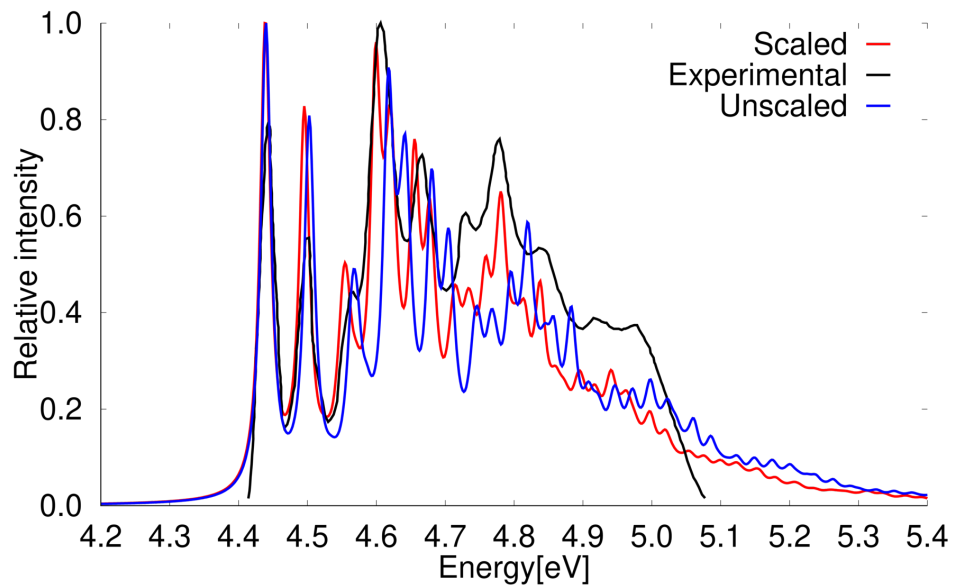


Fig. 1 The absorption spectrum of naphthalene obtained using a scaling factor of 0.9.

4.2 Anthracene

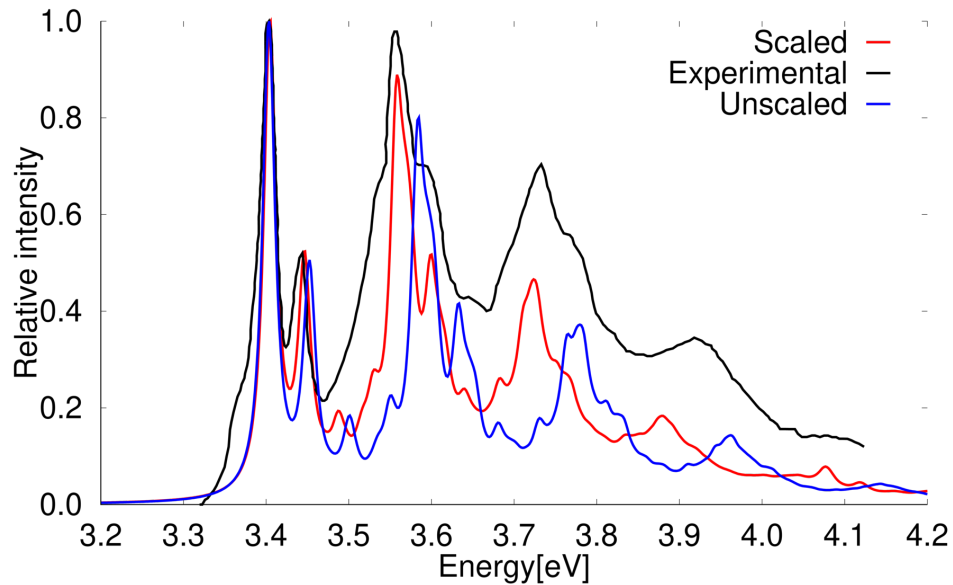


Fig. 2 The absorption spectrum of anthracene obtained using a scaling factor of 0.85.

4.3 Pentacene

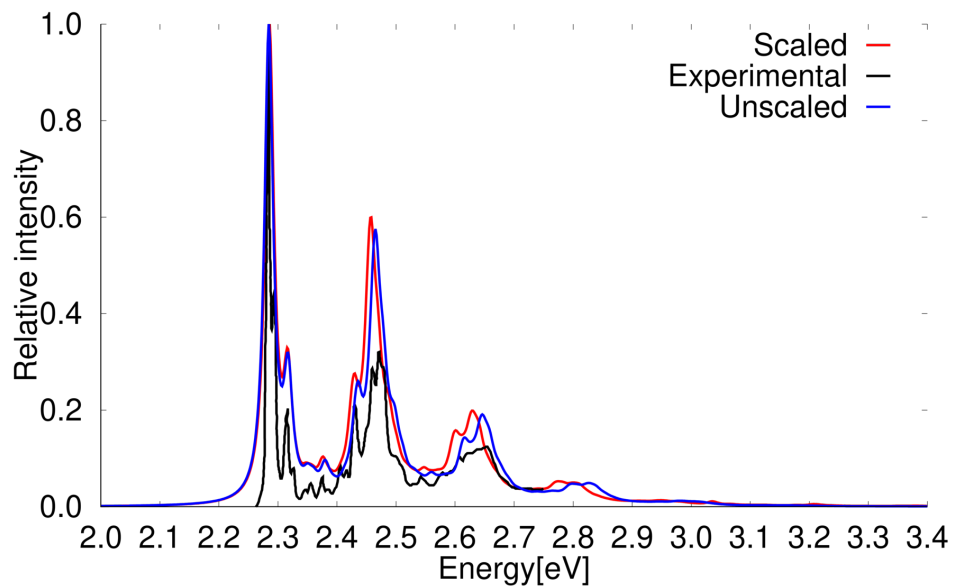


Fig. 3 The absorption spectrum of pentacene obtained using a scaling factor of 0.95.

4.4 Pyrene

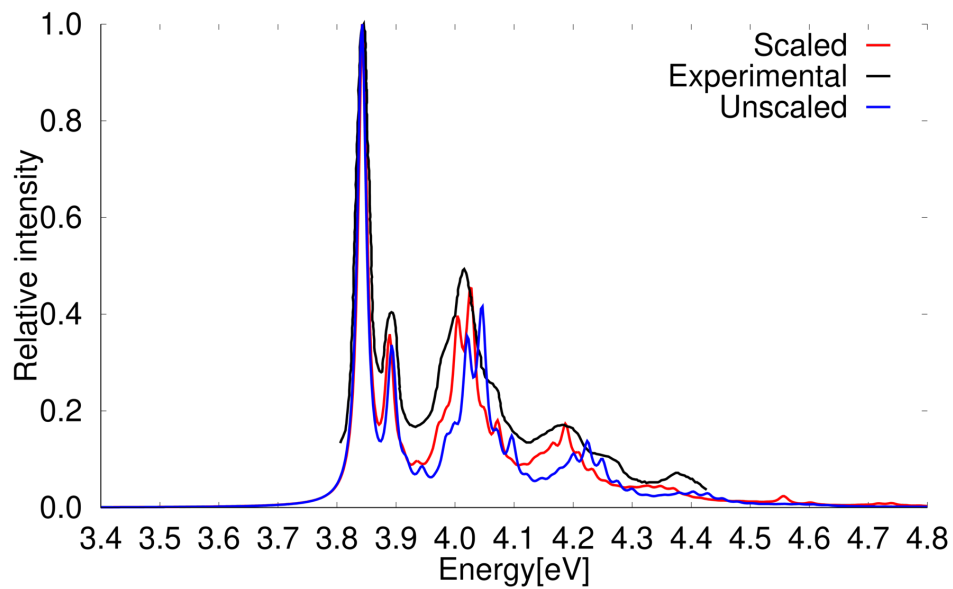


Fig. 4 The absorption spectrum of pyrene obtained using a scaling factor of 0.90.

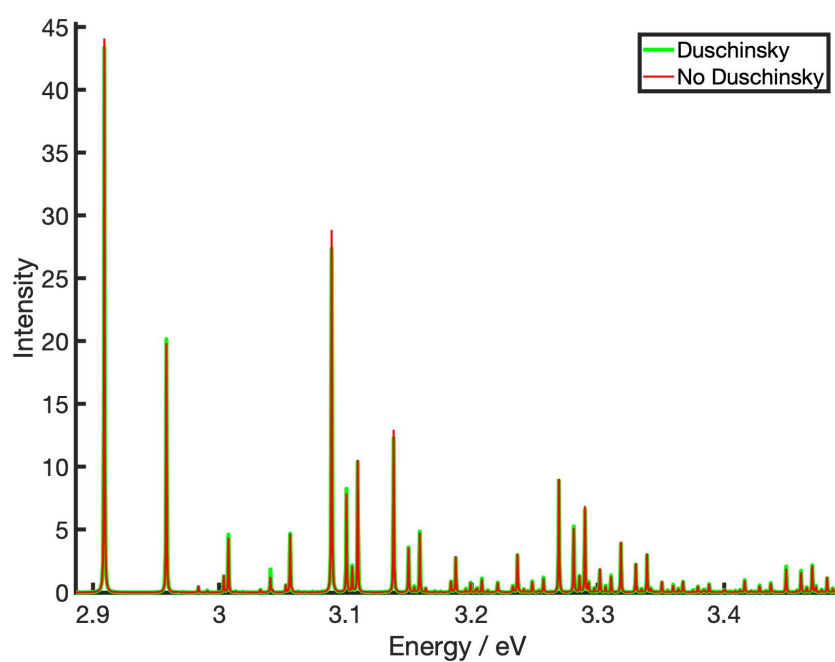


Fig. 5 Comparison of the absorption spectra for anthracene calculated with and without Duschinsky rotation. The spectra have not been shifted to match the experimental 0–0 band.