

ELECTRONIC SUPPORTING INFORMATION

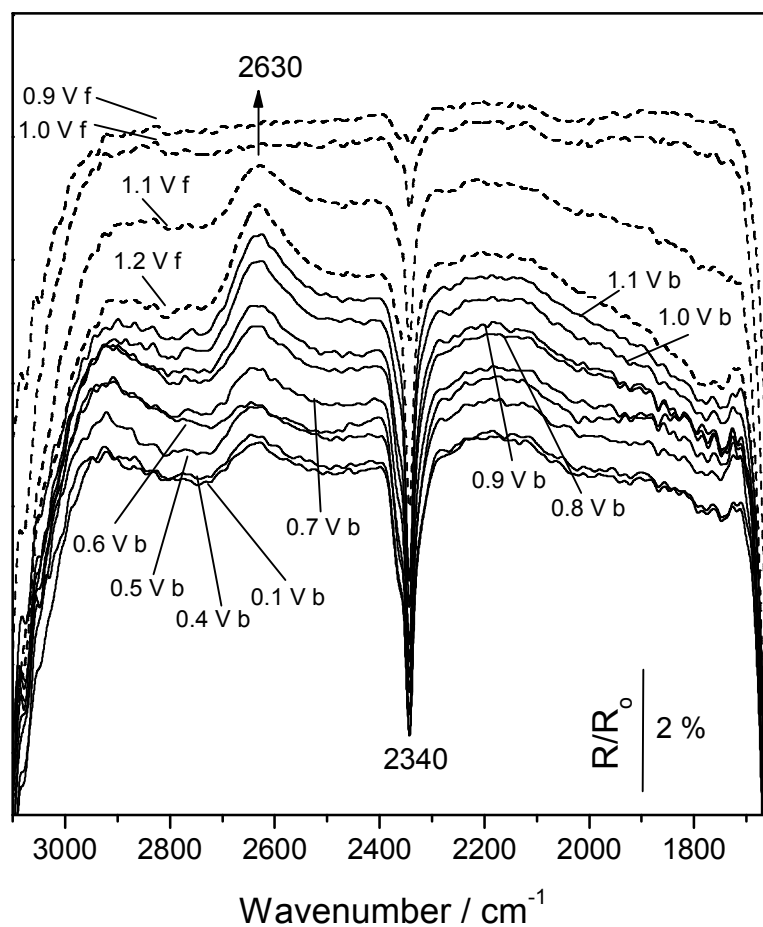


Figure S1. In-situ FTIR spectra acquired during oxidation of aniline (10 mM/0.1 M HClO₄) on polycrystalline Pt. Sample potentials as indicated in the figure (f = forward, b = backward step direction). Reference potential = 0.10 V_{RHE}. Spectra taken with p-polarized light, 128 scans at 8 cm⁻¹ resolution. Same conditions as those described for Figure 1B.

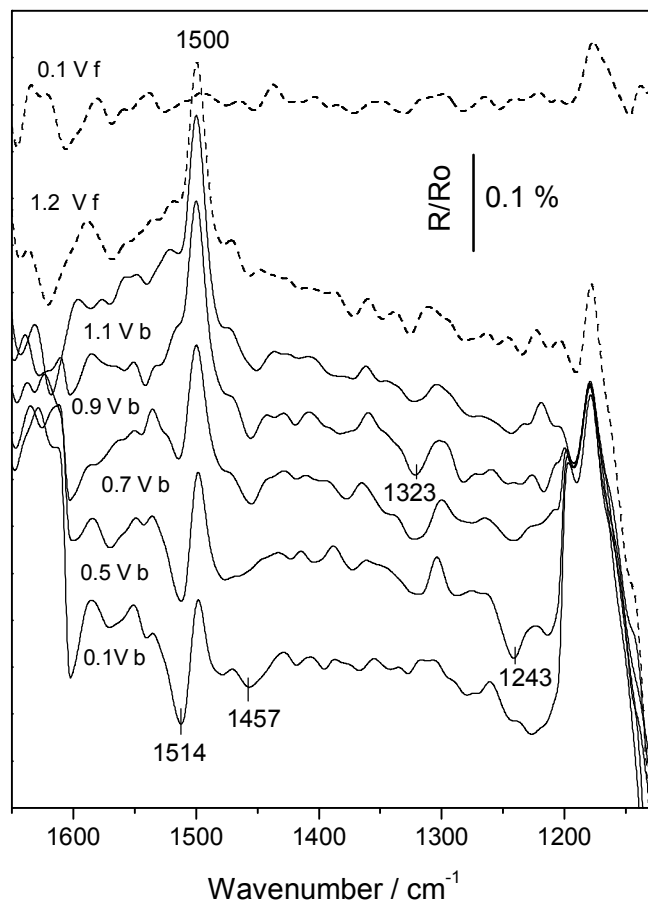
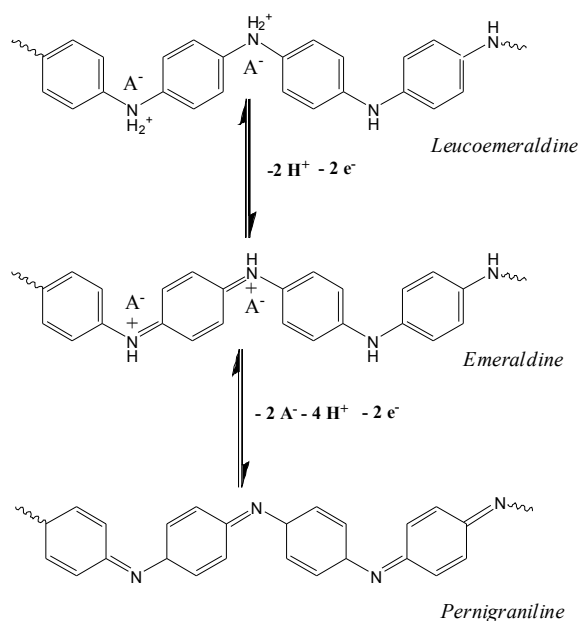


Figure S2. In-situ FTIR spectra taken during oxidation of aniline (10 mM/0.1 M HClO_4) on polycrystalline Pt (reference spectrum taken at 0.1 V_{RHE}). Spectra taken with s-polarized light, 256 scans at 8 cm^{-1} resolution. Sample potentials as indicated in the figure (f = forward, b = backward step direction).



Scheme S1. Changes of chemical structures during oxidation/reduction of PANI in acid media. A^- are the anions present in the electrolyte (ClO_4^- in this work).

Table 1. Assignment of vibrational bands observed during ANI oxidation (Figure 1B). The wavenumber values calculated by DFT to the vibrations described in the table are shown between parentheses.[⊗]

Wavenumber/ cm^{-1}	Sense	Vibration	Species
1551 (1582)	+	C=C str.	ANI ^a
1536 (1535)	+	NH ₂ plane bending	ANI ^a
1500	+	C=C aromat. str.	See text
1514 (1536)	-	C=C aromat. str.	4ADA ^b
1475 (1483)	-	Bending secondary N-H	4ADA ^a
1457 (1462)	-	C=C arom. str.	4ADA ^c & BZ ^c
1323 (1341)	-	C-N str.ar.sec.amines ^d	4ADA ^b
1293 (1335)	+	C-N symmetric str.	ANI ^a
1243 (1240)	-	C-N str	4ADA ^c & BZ ^c

^a E. Pretsch, P. Bühlmann, C. Affolder, Structure Determination of Organic Compounds, Springer, Berlin, 2000.
^b P. Sett, A.K. De, S. Chattopadhyay, P.K. Mallick, Chemical Physics, 2002, 276, 211-224.
^c S. Akyüz, T. Akyüz, N.M. Ozer, J. Mol. Struct., 2001, 565, 493-496.
^d R. Buvanewari, A. Gopalan, T. Vasudevan, H-L. Wang,; T-C. Wen, Thin Solid Films, 2004, 458, 77-85.

[⊗] Note that in ref. c the spectrum of adsorbed benzidine is described.

Table 2. Assignment of vibrational bands of the isolated adsorbate produced during ANI oxidation (Figure 3B). The wavenumber values calculated by DFT to the vibrations described in the table are shown between parentheses.

Wavenumber/ cm ⁻¹	Sense	Vibration	Species
1582 (1590)	-	C=N str. ^a	4ADAOx
1511(1536)	+	C=C arom. str. ^b	4ADA
1417 (1436)	-	C-C str. ^c	4ADAOx
1367 (1382)	-	C-N stretching in a quinonimine ring. ^d	4ADAOx
1313 (1309)	+	C-N stretching ^b	4ADA
1243 (1245)	-	C-N str. in C-N=C ^e	4ADAOx
1218 (1221)	-	-NH bend ^e	4ADAOx

^a S. Quillard, G. Louarn, J.P. Buisson, M. Boyer, S. Lefrant, M. Lapkowski, A. Pron, Synth. Met., 1997, 84, 805.
^b P. Sett, A.K. De, S. Chattopadhyay, P.K. Mallick, Chemical Physics, 2002, 276, 211-224.
^c E. Pretsch, P. Bühlmann, C. Affolder, Structure Determination of Organic Compounds, Springer, Berlin, 2000.
^d L. Brožová, P. Holler, J. Kovářová, J. Stejskal, M. Trchová, Polymer Degradation and Stability, 2008, 93, 592-600.
^e S. Quillard, G. Louarn, S. Lefrant, A.G. MacDiarmid, Phys Rev B, 1994, 50,12496-12508

Table 3. Assignment of vibrational bands observed during 0.05 and 0.1 M PANI oxidation (Figures 4 and 5). The wavenumber values calculated by DFT to the vibrations described in the text are shown between parentheses.

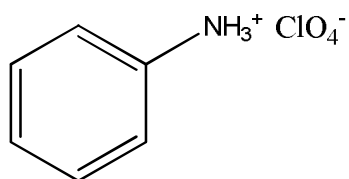
Wavenumber/ cm ⁻¹	Sense	Vibration ^a	Species ^{&}	
P005 [#]	P01 [#]			
1581 (1588)	1581	-	N=Q=N* str. ^b	EM
1512 (1546)	1512	+	C=C arom. str. N-B-N	LE
1475 (1462)	1487	-	C=C arom. str. N-B-N	PN
1450 (1422)	-	-	C=C arom. str. N-B-N	PN
1423 (1433)	-	+	C-N str.	LE
1377 (1381)	1360	-	C-N str. ^c	EM and PN
1342 (1309)	-	-	C-C str., N-H o.o.p. bend	EM
1288 (1277)		+	C-N str. sec. aromatic amine ^d	LE
1238	1268	-	C-N stretch, C-C-C ring i.p. def.	EM
1218 (1213)	-	+	-NH ₂ ⁺ bend.	LE
1157 (1154)	1189	-	N=Q=N ^e C-H in plane bending ^e	EM

^{*} Q = quinonoid unit, B= benzenoid unit,
[&] LE = leucoemeraldine unit, EM = emeraldine unit, PN = pernigraniline unit
[#] P005= PANI produced in 0.05 M ANI, P01 = PANI produced in 0.1 M ANI
^a E.P. Pretsch, P. Bühlmann, C. Affolder, Structure Determination of Organic Compounds, Springer, Berlin, 2000.
^b C. Yang, C. Chen, Y. Zeng, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2007, 66,37-41.
^c L. Brožová, P. Holler, J. Kovářová, J. Stejskal, M. Trchová, Polymer Degradation and Stability, 2008, 93, 592-600.
^d S. Kazim, V. Ali, M. Zulfeqar, M. Mazharul Haq, M. Husai, Current Applied Physics, 2007, 7, 68-75.
^e R. Singh, V. Arora, R.P. Tandon, S. Chandra, N. Kumar, A. Mansingh, Polymer, 1997, 38, 4897.

Table 4. Assignment of vibrational bands observed after degradation of PANI and its comparison with hydroquinone. (Figure 6). The wavenumber values calculated by DFT to the vibrations described in the table are shown between parentheses.

Wavenumber/ cm ⁻¹	Sense	Vibration ^a	Species ^k
2800 ^a (2795)	-		<i>IN</i>
2622 ^a (2618)	+		<i>IN</i>
2340 ^a (2345)	-	asym. str.	<i>CO</i> ₂
1656 ^b (1654)	-	C=O stretching	<i>BQ</i>
1515 ^c (1518)	+	C=C ar. str.	<i>HQ</i>
1471 (1426)	+		<i>HQ</i>
1315 (1309)	-		<i>BQ</i>
1242 ^d (1237)	+	C-O-H sym. str.	<i>HQ</i>
1223 ^d (1225)	+	C-O-H asym. str.	<i>HQ</i>

^k *HQ* = hydroquinone, *BQ* = benzoquinone, *IN* = indophenol.
^a E.P. Pretsch, P. Bühlmann, C. Affolder, Structure Determination of Organic Compounds, Springer, Berlin, 2000.
^b D. Lin-Vien, N.B. Colthup, W.G. Fateley, J.G. Grasselli, The Handbook of Infrared and Raman Characteristic Frequencies of Organic Molecules, Academic Press, San Diego, USA, 1991.
^c G. Socrates, Infrared Characteristic Group Frequencies, Wiley, New York, 1980.
^d L.J. Bellamy, Advances in infrared group frequencies, Halsted Press, London, 1975.



ANI = aniline protonated

----- GAMESS Interface -----

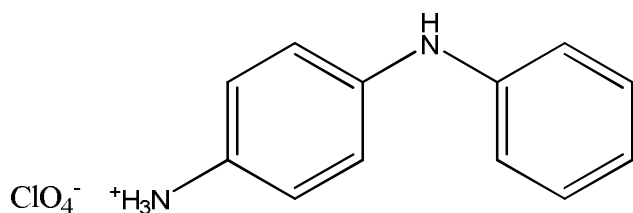
GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%) Wavenumbers

-----	-----
100.00	5.9300
100.00	9.4700
99.96	13.1000
99.11	30.7300
99.87	33.7300
99.13	43.9400
99.87	51.7800
99.88	69.4700
99.44	185.5000
98.25	260.8600
99.22	382.1000
100.00	424.8000
99.78	445.4900
99.44	471.8100
98.87	571.8200
99.93	668.5100
99.34	718.8000
97.82	782.8700
99.74	859.3600
99.96	883.6400
99.99	962.7500
99.09	1018.7400
99.99	1022.7400
99.91	1053.2100
100.00	1060.9200
99.84	1079.4800
99.71	1136.3300
99.06	1146.2000
99.97	1226.4600
99.92	1231.9200
99.99	1335.4000
99.97	1394.0000
99.78	1404.9900
99.86	1535.0600
90.06	1582.6700
84.25	1605.5800
96.28	1661.2300
98.39	1662.3200
99.77	1691.4700
99.96	1702.6900

0.00	2722.5700
99.83	3173.2600
99.92	3180.2200
99.71	3189.2900
99.55	3201.3000
99.62	3214.7600
98.71	3460.4800
97.29	3547.4100



4ADA = 4-aminodiphenylamine monoprotonated

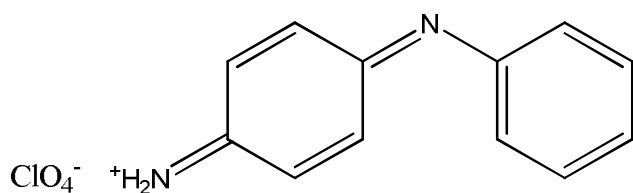
GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%) Wavenumbers

-----	-----
89.79	4.9000
98.16	7.3400
88.30	11.4100
98.87	17.3400
99.76	20.3000
99.16	30.0700
98.71	33.3900
97.75	39.7200
99.38	47.2700
92.26	67.3000
86.11	92.2400
94.54	121.5600
97.54	195.4700
99.59	246.4000
98.18	269.0100
85.75	316.9200
95.63	329.2600
96.22	354.5700
96.39	356.8000
97.49	362.8000
69.58	444.8600
40.79	499.6400
86.78	518.0200
92.80	569.2400
39.58	571.2400
96.56	627.5500
93.21	630.3500
76.27	643.8400
98.35	659.0200
86.94	682.0400
0.00	773.9800
82.24	803.5800
98.90	837.6700
97.45	839.5800
21.82	867.5300
84.75	886.5000
85.98	926.8200
99.97	970.6500
94.74	975.9100
96.81	979.8100
92.18	993.4500
96.25	1013.0800

77.32	1046.2000
47.22	1050.9700
26.63	1065.2400
97.30	1097.8400
2.22	1107.1800
31.63	1123.0600
97.49	1153.4800
75.13	1158.9600
81.21	1163.4800
93.11	1181.5600
38.52	1216.8200
27.04	1228.8700
12.23	1240.0800
96.29	1282.6400
58.63	1309.5200
61.79	1341.4600
75.57	1357.7200
22.40	1385.0100
94.86	1388.4900
94.96	1462.2400
25.72	1536.6300
36.35	1550.2800
88.80	1550.8500
73.41	1586.2800
63.03	1612.3100
73.46	1686.2400
94.03	1759.9300
96.49	1774.1800
94.35	1783.6700
97.93	1790.0600
98.69	2938.3400
95.80	3022.6300
97.78	3036.3100
99.37	3051.1900
97.98	3052.0900
99.68	3060.0000
95.72	3066.9000
96.33	3072.0800
98.44	3080.6200
98.59	3374.0800
69.32	3417.1900
91.41	3540.0000



4ADAOx = 4-aminodiphenylamine oxidized monoprotonated

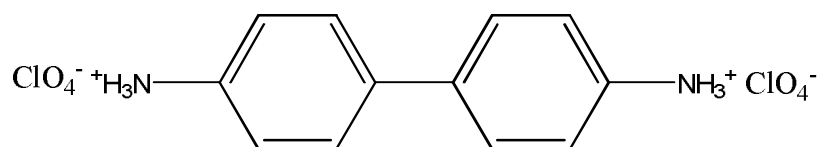
GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%) Wavenumbers

Transmittance (%)	Wavenumbers
100.00	3.7300
99.97	9.5000
99.04	11.3000
100.00	12.8200
99.01	14.2700
99.97	16.7200
99.91	17.7300
98.04	20.4400
99.22	24.1000
98.28	40.4800
99.75	77.8800
99.45	99.6400
99.92	202.7800
98.52	214.4500
99.17	227.7800
99.08	332.9200
99.91	353.6300
99.95	358.6700
89.27	415.0800
74.66	443.0900
81.46	462.6200
56.93	468.2600
96.95	525.2200
92.79	532.4500
48.23	584.9700
99.65	598.3700
99.53	627.3200
88.62	627.8300
84.52	668.5100
99.92	711.5800
95.79	771.6500
68.50	774.4600
83.08	817.8200
100.00	844.0400
99.01	857.4300
99.32	879.0900
0.00	886.1000
95.01	937.8700
94.98	951.3200
99.99	974.9900
99.68	992.6800
71.87	993.5800

99.28	1015.2500
97.01	1017.4100
44.88	1051.9900
42.64	1102.2500
52.20	1124.5300
77.19	1133.5000
99.44	1153.1200
98.78	1159.0100
71.67	1165.3300
91.36	1181.3800
98.41	1221.6900
85.19	1245.2000
99.96	1300.2100
39.81	1314.7300
52.73	1382.2200
95.26	1436.2000
98.89	1514.7800
75.79	1540.7900
72.73	1590.6100
97.01	1771.6100
99.69	1788.0700
99.84	1832.8700
93.80	1846.1700
98.65	1862.9400
99.01	1874.1100
87.86	2306.5700
99.50	3006.7800
97.88	3027.1200
99.74	3042.7800
99.90	3043.5400
98.52	3052.0100
98.37	3061.5000
98.51	3062.6400
98.37	3067.7600
98.84	3083.9700
98.72	3470.4000



BZ = Benzidine diprotonated

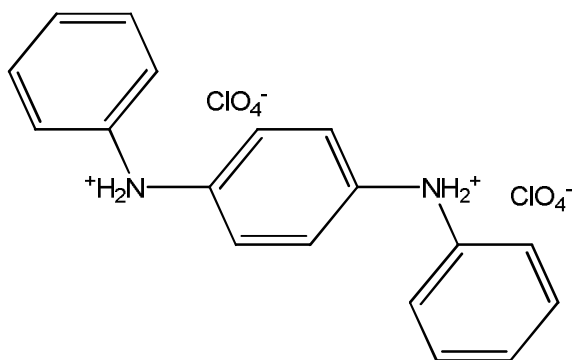
GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%) Wavenumbers

-----	-----
98.86	6.5200
100.00	7.5100
99.93	9.7100
99.80	13.0600
98.23	23.0300
98.33	26.4200
98.82	32.9400
99.16	35.7400
99.60	37.4400
99.62	39.1400
97.33	49.3400
99.27	55.8400
98.91	73.9400
99.23	148.5300
99.17	168.3300
97.06	193.7100
99.01	226.8200
96.36	256.2800
99.42	279.7200
96.45	288.5600
99.12	351.2100
99.98	358.3500
98.22	364.3600
99.88	387.3900
85.68	456.9300
85.93	466.1200
87.00	533.9800
96.30	542.3500
77.64	547.7200
80.58	561.1600
59.88	574.1100
44.55	618.2100
79.28	623.8300
88.36	638.5100
99.43	649.6600
98.32	675.5900
98.58	702.0000
98.44	713.5100
98.92	844.1000
99.74	847.9600
46.52	854.5800
99.86	867.9900
88.84	883.4800
99.93	958.6800
99.98	976.4400

99.95	979.1800
99.98	986.4100
98.56	1000.2700
74.93	1040.9800
99.75	1053.5000
91.57	1103.4400
93.08	1107.1700
0.00	1120.6000
86.40	1130.0100
82.63	1137.9800
93.18	1160.8200
94.93	1162.6000
95.53	1170.1300
84.87	1175.4700
97.13	1226.3700
99.42	1228.5000
99.81	1262.5200
99.95	1316.1900
98.05	1324.6300
75.47	1362.3400
99.94	1483.3700
91.40	1525.8700
94.47	1550.7400
84.01	1590.3900
98.44	1642.8900
76.67	1650.2500
99.96	1683.2500
99.90	1768.6100
99.97	1776.5600
99.97	1800.3700
99.99	1813.5800
88.27	2181.5000
93.16	2203.0400
99.50	3020.0700
99.30	3032.8400
99.65	3038.5300
98.80	3043.1000
98.69	3053.7900
99.66	3055.5000
98.51	3070.9400
99.70	3071.8300
96.20	3377.3000
96.16	3384.5100
98.90	3510.6700
98.93	3514.7000



LE = model unit of polyaniline, leucomeraldine form protonated

GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

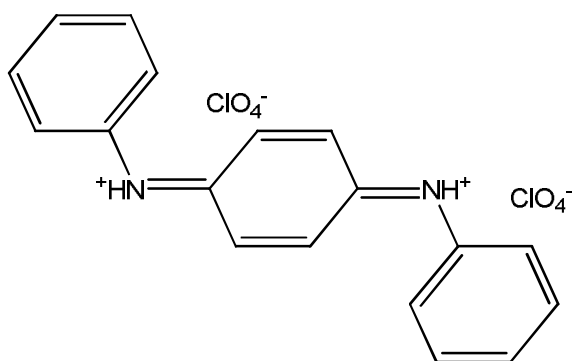
IR Spectrum Species:

Transmittance (%) Wavenumbers

99.83	8.4800
99.71	9.4600
99.93	11.8900
99.44	16.4600
97.21	25.4600
99.81	26.7700
99.96	33.0000
99.80	34.2500
100.00	36.4300
99.64	39.4000
99.41	43.3900
99.42	48.6700
99.62	50.0400
99.67	55.8700
97.26	59.5100
99.93	73.4300
99.35	126.2700
100.00	186.3100
98.46	198.0400
99.99	241.3000
98.55	259.6200
99.69	268.4800
100.00	312.2200
100.00	335.7100
99.86	354.1000
99.90	357.6300
99.99	357.8500
99.97	428.4500
93.34	468.1000
61.24	482.9500
98.60	495.9100
95.17	501.6300
98.72	528.3000
0.00	540.3200
99.66	564.6800
98.91	570.6800
4.04	575.9800
93.59	589.2100
96.47	603.9500
99.93	628.9300
97.62	631.4700
99.84	647.3400
99.58	654.2700
62.06	661.4300
99.98	719.0400
40.16	762.1700
99.76	786.2300
80.68	808.4200
99.85	839.9600
99.98	848.3500
99.75	850.1700
96.92	869.8900
96.92	871.7600

82.91	902.2900
99.99	941.2000
88.99	950.8000
99.95	974.0400
99.99	978.2900
99.71	980.6700
99.99	981.6700
99.88	1003.2200
97.99	1019.9600
99.85	1021.8700
58.56	1040.0500
39.13	1044.3900
99.98	1046.2700
99.83	1047.6000
52.46	1063.2700
20.85	1107.4600
98.74	1107.9900
67.81	1117.5800
55.78	1119.4100
84.92	1149.0300
95.58	1151.0300
92.31	1154.1800
99.01	1164.2000
93.78	1166.2200
99.85	1177.6800
27.39	1208.1600
99.69	1213.8000
92.41	1228.5500
99.59	1232.4100
92.44	1264.3600
99.98	1277.6300
99.12	1311.8600
99.98	1321.1100
74.00	1336.9400
100.00	1358.5800
91.24	1372.8800
100.00	1432.6200
62.65	1546.6400
93.97	1547.4400
91.64	1552.5200
87.21	1583.8700
77.80	1586.0900
88.69	1607.6700
100.00	1773.4600
99.08	1777.0400
98.83	1778.8400
99.89	1789.2400
99.71	1790.3000
100.00	1797.3300
88.78	2207.1700
94.68	2234.9000
98.96	3003.0800
99.33	3024.5500
98.70	3031.7700
99.33	3034.2300
99.76	3042.4600
97.88	3044.1600
98.96	3052.2100
99.05	3053.8900
99.65	3056.8400
98.67	3060.8700

98.30	3061.7600
98.72	3070.1000
99.32	3075.7000
99.16	3084.2400
98.16	3340.3000
98.22	3373.1600



EM = model unit of polyaniline, emeraldine form protonated

----- GAMESS Interface -----

Model: emeraldine

GAMESS Job: Predict IR/Raman Spectrum DFT

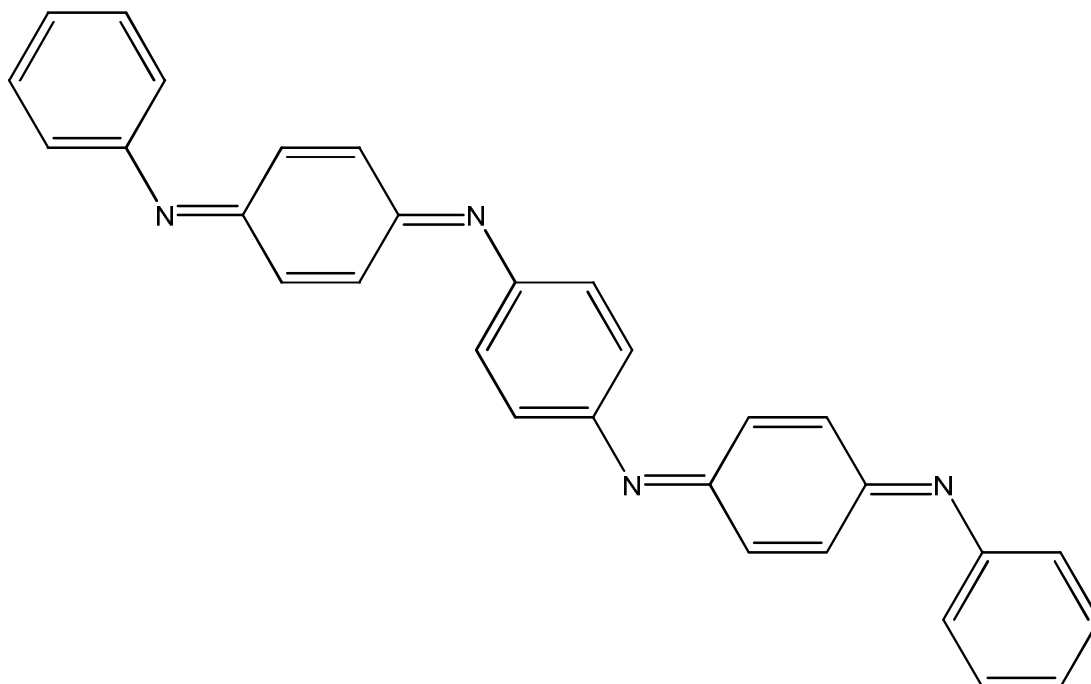
IR Spectrum Species:

Transmittance (%) Wavenumbers

100.00	2.5100
99.97	8.3200
99.98	10.1100
99.66	14.6400
99.94	16.3200
99.99	16.8900
97.77	20.5400
99.97	24.0700
99.66	28.6700
99.93	29.1100
97.83	37.2800
99.47	38.5400
99.79	51.3800
98.87	52.5200
99.98	68.4200
99.68	97.8100
100.00	100.0900
99.78	190.3200
99.94	194.9500
99.99	205.6100
95.68	212.7600
100.00	215.0800
98.05	329.8200
100.00	339.5400
99.82	353.0900
100.00	354.1400
96.61	363.4200
87.60	426.0100
99.93	427.4800
100.00	452.2500
0.00	463.5400
95.86	475.1000
100.00	512.6900
99.99	531.5400

99.00	573.3100
11.95	590.2000
99.37	598.8900
99.94	604.4100
65.18	622.7700
99.97	627.2500
99.69	628.2300
99.91	635.6800
77.07	663.7400
100.00	700.5500
100.00	723.4100
38.04	768.4200
99.80	783.9100
100.00	799.6700
87.02	839.2200
100.00	845.3800
99.97	845.9000
51.61	886.0700
89.06	886.5600
97.25	899.2800
99.95	941.0100
90.21	943.5200
99.99	965.8500
100.00	976.5200
100.00	976.7300
99.26	994.9700
75.88	995.0600
95.78	1017.7400
98.95	1018.5000
100.00	1019.8800
31.56	1049.7800
95.70	1052.6900
59.95	1102.7600
55.03	1103.3300
33.49	1121.7500
99.64	1128.7400
99.54	1151.6300
98.50	1152.6700
88.54	1154.8800
99.22	1158.5600
94.65	1160.2300
99.96	1182.2300
98.82	1221.5700
98.98	1222.1800
99.93	1237.2700
99.95	1298.2700
99.97	1298.3600
56.62	1309.6900
99.96	1371.6400
32.69	1384.2900
93.89	1423.2700
99.99	1496.6000
91.76	1541.3600
71.43	1541.5700
97.81	1588.2200
68.81	1590.3400
98.53	1770.7300
98.05	1771.3300
99.99	1786.9800
99.93	1787.4500
99.99	1832.9100

96.05	1839.7000
97.88	1856.9400
100.00	1865.8500
93.13	2266.7200
96.54	2302.4900
99.62	2980.3200
99.79	3008.7800
98.38	3025.6500
99.04	3031.4000
99.87	3041.1100
99.72	3043.2300
99.02	3052.1200
98.89	3055.3400
98.95	3060.6200
99.63	3063.5600
98.86	3068.2700
98.34	3070.6400
99.13	3082.1700
99.19	3083.2700



PN = model unit of polyaniline, pernigraniline form

GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

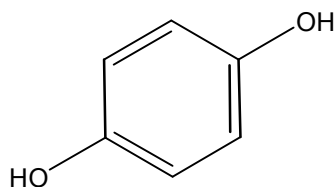
IR Spectrum Species:

Transmittance (%)	Wavenumbers
100.00	3.2000
99.96	7.0400
100.00	8.5000
99.99	9.5600
100.00	9.7500
100.00	11.0900
99.99	13.0700
100.00	13.5800
99.99	14.0300
99.99	15.6100
99.84	16.1500
99.98	16.9700
100.00	18.2200
99.97	43.0000
99.82	48.8800
96.84	57.6400
100.00	70.9800
99.63	92.0800
98.00	92.8700
100.00	99.8000
99.54	140.7400
99.96	176.4800
99.56	198.4700
99.67	202.5400
100.00	218.0500
99.34	268.4200
99.95	269.8200
99.89	316.0600

99.73	343.0100
100.00	350.7300
97.49	351.6000
100.00	353.9600
99.26	355.4800
100.00	366.4000
99.96	382.4600
95.83	416.3500
100.00	435.8600
99.04	451.5600
99.46	463.4500
99.60	476.6200
92.67	494.3700
100.00	497.1300
99.97	534.3900
93.49	549.3300
99.83	551.0000
100.00	562.3600
99.99	598.3000
99.92	599.7100
99.03	614.8300
99.79	616.9900
99.69	627.1400
99.65	628.1300
100.00	641.9000
67.99	648.8100
99.85	667.1100
88.33	677.6900
99.67	689.0400
99.97	712.5500
100.00	713.3200
44.90	768.3900
99.99	771.4100
100.00	791.4000
100.00	791.5500
99.84	797.8400
88.27	807.6100
99.96	837.9300
98.49	840.8200
99.98	845.4800
99.97	845.5000
84.86	864.4000
99.83	876.2200
0.00	876.8700
94.92	885.8000
71.37	897.2800
83.22	935.6500
99.43	937.6200
99.71	948.9400
99.86	957.0500
100.00	969.0700
99.99	975.1500
99.99	975.1600
99.97	987.9800
99.92	988.0300
78.51	989.4800
95.07	990.3000
79.90	995.4600
100.00	1011.4900
100.00	1011.6100
95.06	1013.8900

98.75	1013.9300
93.69	1028.1900
49.18	1050.0400
57.65	1053.4600
65.36	1058.9700
55.87	1102.1100
54.86	1103.9000
67.32	1125.0500
66.74	1128.2500
71.61	1137.5800
68.84	1143.8400
76.48	1145.0600
99.22	1150.0300
99.52	1154.8000
98.86	1159.8400
99.71	1160.5700
99.70	1165.8900
99.96	1175.9100
99.65	1177.1000
99.87	1220.2800
98.73	1222.4700
99.57	1224.9700
99.99	1228.5000
99.97	1228.7800
94.04	1259.0100
99.95	1301.7400
99.95	1301.9000
99.94	1303.1700
22.70	1312.3800
57.32	1326.2700
86.49	1381.5800
37.52	1383.2000
96.13	1422.4000
92.69	1422.5200
91.16	1462.2500
99.99	1506.4000
99.93	1506.9300
93.30	1537.6300
81.39	1540.9500
80.62	1541.2800
78.69	1591.7600
80.06	1595.6300
82.19	1619.3900
100.00	1758.8200
95.06	1771.8300
99.76	1789.5300
99.76	1789.9900
99.34	1794.3800
99.71	1839.3800
99.90	1839.7500
96.10	1847.7600
96.22	1848.0300
98.83	1866.4700
96.97	1868.0800
99.94	1871.9300
99.97	1872.1500
99.60	3013.1300
99.34	3014.0500
99.58	3025.7800
98.57	3033.8000
99.91	3040.3300

99.48	3041.4700
99.60	3043.8500
99.60	3044.1100
98.88	3049.3900
98.71	3055.7800
97.93	3056.4800
98.22	3058.6400
99.75	3058.8300
98.46	3059.2000
98.72	3063.6400
99.78	3063.6800
98.70	3066.0400
99.56	3066.2700
98.48	3076.0100
99.16	3080.2500
98.28	3080.8800
99.18	3093.7900

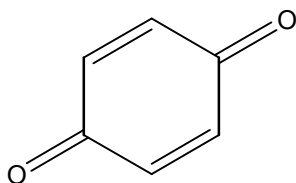


HQ = Hydroquinone

GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%)	Wavenumbers
100.00	2.9700
100.00	11.4200
100.00	14.0300
97.83	55.5200
93.59	68.9800
99.59	77.9500
100.00	83.0500
99.99	265.7400
0.00	298.0400
99.93	313.2800
100.00	356.2100
89.20	425.3300
100.00	433.3500
99.90	475.4100
98.35	519.2900
98.62	667.3500
100.00	713.9300
87.51	792.6800
84.56	805.4100
84.52	868.6400
99.85	889.4200
100.00	914.1400
100.00	990.9900
99.95	1042.1000
97.07	1141.6300
34.59	1220.1700
36.28	1225.6300
98.31	1237.8700
70.29	1349.4700
98.92	1376.3200
74.28	1393.1900
97.06	1426.8000
99.43	1518.8600
27.74	1596.8300
99.88	1696.8800
99.96	1702.6900
97.85	3190.4600
92.73	3206.2000
98.15	3208.9400
95.84	3226.8800
92.94	3760.0500
93.42	3761.3100



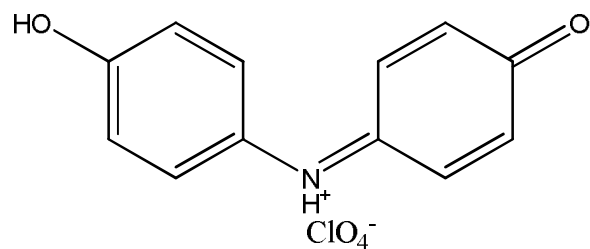
BQ = benzoquinone

GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%) Wavenumbers

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99.37	9.5200
98.28	10.5600
99.14	13.2900
99.99	170.9400
100.00	178.1700
99.99	189.6800
99.98	259.9900
80.42	279.0200
47.02	404.6500
80.27	405.3200
100.00	463.5000
100.00	478.1700
100.00	507.2300
100.00	557.2400
99.83	579.3900
81.85	636.2400
99.87	676.4000
88.41	749.9100
99.97	790.6700
100.00	834.1700
98.33	875.5500
0.00	902.1000
99.70	932.8400
96.83	957.2200
100.00	988.2800
99.92	990.6300
26.69	1055.2800
99.99	1138.9100
98.36	1263.8200
99.93	1276.4400
99.99	1304.5900
71.35	1337.2800
45.32	1654.3200
99.44	3086.6600
99.74	3097.7100
99.29	3112.1200
99.87	3122.8100



IN = indophenol

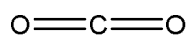
GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%) Wavenumbers

99.97	4.6500
99.98	5.5900
99.95	7.6200
99.72	11.1600
99.98	11.6800
99.93	13.3700
97.25	18.2700
99.09	37.1200
99.80	69.7200
97.72	83.2000
99.82	84.3900
99.45	134.6200
68.57	141.9900
98.64	164.8700
99.97	235.4200
99.47	246.3000
99.89	283.4200
92.19	300.2700
48.13	307.9700
99.99	342.4000
94.39	356.0000
99.89	384.7200
93.94	441.8400
97.57	480.6400
56.65	484.4400
80.71	500.6400
96.71	503.2400
99.22	555.6400
99.95	609.1700
99.65	629.2600
99.12	649.6500
99.08	676.6100
98.74	724.9500
98.91	771.2600
96.55	824.4000
96.63	828.9100
97.01	833.6200
98.24	877.5700
0.00	885.7000
99.96	929.3700
98.98	957.7000
78.10	968.3300
99.31	984.7100
98.32	999.1400

97.74	1019.4900
92.27	1024.9000
55.22	1052.8500
89.59	1125.9800
70.99	1142.1300
97.00	1159.6000
95.82	1193.1100
98.95	1204.5000
98.99	1246.2100
77.78	1272.4200
13.27	1314.7100
94.81	1361.5400
66.84	1391.0900
90.33	1440.5000
95.79	1455.9600
86.64	1502.5900
85.51	1562.7500
90.99	1629.4900
95.22	1764.4500
97.15	1782.0200
99.36	1826.0000
95.53	1854.1900
99.68	1866.1600
92.83	1966.9200
96.56	2189.8900
95.43	2618.2500
98.76	2795.4300
99.66	3004.3800
99.51	3007.2300
99.80	3032.3500
97.18	3040.5200
99.78	3049.3500
98.83	3052.2800
98.08	3069.7300
99.68	3117.4800
94.62	3858.0500



Carbon dioxide

GAMESS Job: Predict IR/Raman Spectrum B3LYP/6-31G

IR Spectrum Species:

Transmittance (%)	Wavenumbers
100.00	0.0400
100.00	0.8500
100.00	19.8100
100.00	102.6100
100.00	102.6400
94.66	541.0200
94.66	542.4100
100.00	1314.9600
0.00	2345.4100