Quantum Mechanical studies of p-Azoxyanisole and identification of its Electro-optic Activity

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1. Bond alteration

Table S1: - Bond length alteration for B3LYP functional combined with different basis sets.

Sr. No.	Bond	Bond Length (Å)		
		6-31G**	6-311G	6-311G**
1	C1-C2	1.392974	1.395297	1.391362
2	C1-C6	1.402182	1.401637	1.400274
3	C1-H7	1.082977	1.079030	1.081150
4	C2-C3	1.392963	1.394922	1.390130
5	C2-H8	1.081986	1.077404	1.080050
6	C3-C4	1.397338	1.399777	1.395744
7	C3-N16	1.458148	1.455873	1.462219
8	C4-C5	1.385213	1.387538	1.382937
9	C4-H9	1.082110	1.077442	1.080271
10	C5-C6	1.402986	1.402218	1.401332
11	C5-H10	1.084545	1.079574	1.082672
12	C6-O11	1.360322	1.386997	1.357736
13	O11-C12	1.420785	1.453477	1.422246
14	C12-H13	1.097356	1.091871	1.095531
15	C12-H14	1.090873	1.084274	1.088635
16	C12-H15	1.097366	1.091689	1.095497
17	N16-N17	1.281264	1.294801	1.277810
18	N16-O18	1.263056	1.310720	1.257703
19	N17-C24	1.396218	1.404484	1.395235
20	C19-C20	1.388262	1.389608	1.386612
21	C19-C24	1.409054	1.410843	1.406853
22	C19-H25	1.085059	1.080318	1.083236
23	C20-C21	1.402121	1.402938	1.400684

24	C20-H26	1.083309	1.079394	1.081479
25	C21-C22	1.401988	1.401031	1.400019
26	C21-O29	1.362199	1.387433	1.359429
27	C22-C23	1.386272	1.388333	1.383805
28	C22-H27	1.085210	1.080153	1.083435
29	C23-C24	1.416771	1.418625	1.415895
30	C23-H28	1.078050	1.073838	1.075990
31	O29-C30	1.419798	1.452869	1.421291
32	C30-H31	1.090814	1.084428	1.088625
33	C30-H32	1.097295	1.091954	1.095650
34	C30-H33	1.097260	1.091813	1.095554

Table S2: - Bond length alteration for M06L functional combined with different basis sets.

Sr. No.	**Bond**	**Bond Length (Å)**		
		6-31G**	**6-311G**	**6-311G****
1	C1-C2	1.3887	1.3927	1.39
2	C1-C6	1.3997	1.4022	1.4006
3	C1-H7	1.0844	1.0835	1.0861
4	C2-C3	1.3914	1.3955	1.3921
5	C2-H8	1.0827	1.0816	1.0843
6	C3-C4	1.3953	1.3995	1.3962
7	C3-N16	1.4517	1.4509	1.4545
8	C4-C5	1.3822	1.3865	1.3834
9	C4-H9	1.0831	1.0819	1.0849
10	C5-C6	1.4005	1.4024	1.4013
11	C5-H10	1.085	1.0831	1.0866
12	C6-O11	1.3564	1.3832	1.3558
13	O11-C12	1.4136	1.4492	1.4130
14	C12-H13	1.0974	1.0954	1.0992
15	C12-H14	1.0894	1.0873	1.0909
16	C12-H15	1.0973	1.0954	1.0992
17	N16-N17	1.2895	1.3062	1.2884
18	N16-O18	1.258	1.304	1.2517
19	N17-C24	1.3883	1.3984	1.3892
20	C19-C20	1.3845	1.3879	1.3857
21	C19-C24	1.4076	1.4113	1.4084
22	C19-H25	1.0861	1.0846	1.0877
23	C20-C21	1.3994	1.4027	1.4004
24	C20-H26	1.0843	1.0834	1.0861

25	C21-C22	1.3995	1.4016	1.4004
26	C21-O29	1.3581	1.3839	1.3575
27	C22-C23	1.3832	1.3872	1.3843
28	C22-H27	1.0859	1.0840	1.0875
29	C23-C24	1.4161	1.4195	1.4171
30	C23-H28	1.0791	1.0787	1.0809
31	O29-C30	1.4123	1.4486	1.4117
32	C30-H31	1.0898	1.0876	1.0913
33	C30-H32	1.0976	1.0955	1.0995
34	C30-H33	1.0977	1.0955	1.0995

Table S3: - Bond length alteration for M06-2X functional combined with different basis sets.

Sr. No.	**Bond**	**Bond Length (Å)**		
		6-31G**	**6-311G**	**6-311G****
1	C1-C2	1.390779	1.392794	1.389405
2	C1-C6	1.397983	1.396580	1.396121
3	C1-H7	1.082583	1.078453	1.080853
4	C2-C3	1.387029	1.388819	1.384491
5	C2-H8	1.082183	1.077414	1.080147
6	C3-C4	1.392913	1.394935	1.390967
7	C3-N16	1.459011	1.452301	1.462217
8	C4-C5	1.382080	1.384247	1.380129
9	C4-H9	1.082153	1.077284	1.080430
10	C5-C6	1.399665	1.397427	1.398082
11	C5-H10	1.083957	1.078812	1.081993
12	C6-O11	1.353704	1.379731	1.351534
13	O11-C12	1.412205	1.442308	1.412799
14	C12-H13	1.096120	1.090884	1.093757
15	C12-H14	1.089128	1.083120	1.087232
16	C12-H15	1.096029	1.090748	1.093946
17	N16-N17	1.264209	1.276771	1.261394
18	N16-O18	1.249089	1.298174	1.244720
19	N17-C24	1.402346	1.408983	1.401779
20	C19-C20	1.385993	1.387150	1.384743
21	C19-C24	1.401956	1.403039	1.400078
22	C19-H25	1.084950	1.079794	1.082949
23	C20-C21	1.397493	1.398101	1.396517
24	C20-H26	1.083003	1.078772	1.080783
25	C21-C22	1.397321	1.395220	1.395231
26	C21-O29	1.356053	1.380603	1.353658
27	C22-C23	1.384433	1.386593	1.382537

28	C22-H27	1.084630	1.079365	1.082809
29	C23-C24	1.410832	1.412137	1.410227
30	C23-H28	1.077565	1.073177	1.075524
31	O29-C30	1.410511	1.441698	1.411976
32	C30-H31	1.089287	1.083305	1.087479
33	C30-H32	1.096508	1.091019	1.094740
34	C30-H33	1.096269	1.090878	1.094806

Table S4: - Bond angle alteration for B3LYP functional combined with different basis sets.

Sr. No.	**Bond**	**Bond Angle (in Degree)**		
		6-31G**	**6-311G**	**6-311G****
1	C6-C1-C2	119.892477	119.707236	119.942180
2	H7-C1-C2	119.088349	119.161638	118.978418
3	H7-C1-C6	121.019114	121.131082	121.079170
4	C3-C2-C1	119.782662	119.714089	119.866903
5	H8-C2-C1	120.758629	120.921521	120.759055
6	H8-C2-C3	119.458706	119.364389	119.374040
7	C4-C3-C2	120.670788	120.766862	120.556320
8	N16-C3-C2	121.594590	121.184420	121.557633
9	N16-C3-C4	117.734607	118.048717	117.886019
10	C5-C4-C3	119.606874	119.538209	119.649597
11	H9-C4-C3	118.873923	118.852369	118.813721
12	H9-C4-C5	121.519185	121.609420	121.536681
13	C6-C5-C4	120.313393	120.122153	120.401163
14	H10-C5-C4	121.096569	121.297037	121.107471
15	H10-C5-C6	118.590006	118.580801	118.491203
16	C5-C6-C1	119.733693	120.151442	119.583730
17	O11-C6-C1	124.669267	124.365065	124.665636
18	O11-C6-C5	115.597009	115.483492	115.750624
19	C12-O11-C6	118.549189	119.384903	118.783698
20	H13-C12-O11	111.594126	111.180295	111.436642
21	H14-C12-O11	105.937725	105.016958	105.722390
22	H14-C12-H13	109.257258	109.712295	109.302506
23	H15-C12-O11	111.555411	111.173704	111.446538
24	H15-C12-H13	109.182559	109.926715	109.540355
25	H15-C12-H14	109.229815	109.719271	109.295076
26	N17-N16-C3	115.445723	116.502259	115.565484
27	O18-N16-C3	116.859953	116.864220	116.840519
28	O18-N16-N17	127.694292	126.633507	127.593682
29	C24-N17-N16	121.425747	122.370526	121.560839
30	C24-C19-C20	122.075484	121.605723	122.044702

31	H25-C19-C20	120.089826	120.539114	120.057071
32	H25-C19-C24	117.834684	117.855161	117.898217
33	C21-C20-C19	119.273498	119.233474	119.417519
34	H26-C20-C19	119.509287	119.547816	119.355804
35	H26-C20-C21	121.217154	121.218684	121.226470
36	C22-C21-C20	119.463193	119.983816	119.309894
37	O29-C21-C20	124.723209	124.348802	124.763565
38	O29-C21-C22	115.813592	115.667376	115.926536
39	C23-C22-C21	121.243373	120.887765	121.295108
40	H27-C22-C21	118.205008	118.302198	118.160869
41	H27-C22-C23	120.551619	120.810035	120.544018
42	C24-C23-C22	120.014321	119.870437	120.095258
43	H28-C23-C22	120.225639	120.590107	120.238080
44	H28-C23-C24	119.760039	119.539455	119.666641
45	C19-C24-N17	112.768693	112.905289	113.022592
46	C23-C24-N17	129.301201	128.675922	129.139888
47	C23-C24-C19	117.930047	118.418777	117.837374
48	C30-O29-C21	118.428887	119.385524	118.717592
49	H31-C30-O29	105.984683	105.039602	105.784168
50	H32-C30-O29	111.643688	111.204777	111.467700
51	H32-C30-H31	109.216996	109.720591	109.296733
52	H33-C30-O29	111.637628	111.208253	111.476716
53	H33-C30-H31	109.167931	109.696737	109.268482
54	H33-C30-H32	109.104740	109.862853	109.453414

Table S5: - Bond angle alteration for M06L functional combined with different basis sets.

Sr. No.	**Bond**	**Bond Angle (in Degree)**		
		6-31G**	**6-311G**	**6-311G****
1	C6-C1-C2	119.8698	119.6103	119.8839
2	H7-C1-C2	119.2246	119.3544	119.2372
3	H7-C1-C6	120.9055	121.0353	120.8789
4	C3-C2-C1	119.8372	119.6188	119.8302
5	H8-C2-C1	120.8379	121.1274	120.8804
6	H8-C2-C3	119.3249	119.2538	119.2894
7	C4-C3-C2	120.5947	120.9643	120.6022
8	N16-C3-C2	121.4826	120.9866	121.5005
9	N16-C3-C4	117.9227	118.0492	117.8973
10	C5-C4-C3	119.6485	119.4667	119.6371
11	H9-C4-C3	118.7832	118.8292	118.7786
12	H9-C4-C5	121.5683	121.7041	121.5842
13	C6-C5-C4	120.2536	119.9588	120.2727

14	H10-C5-C4	121.2292	121.4401	121.2565
15	H10-C5-C6	118.5171	118.601	118.4708
16	C5-C6-C1	119.7962	120.3811	119.7740
17	O11-C6-C1	124.3716	124.0569	124.3934
18	O11-C6-C5	115.8322	115.562	115.8327
19	C12-O11-C6	117.1996	117.6739	117.2047
20	H13-C12-O11	111.6201	111.0461	111.6836
21	H14-C12-O11	106.1687	105.0504	106.2291
22	H14-C12-H13	109.2732	109.9722	109.2334
23	H15-C12-O11	111.6129	111.0443	111.6787
24	H15-C12-H13	108.8196	109.6707	108.7119
25	H15-C12-H14	109.2813	109.9729	109.2393
26	N17-N16-C3	114.8254	115.6391	114.7027
27	O18-N16-C3	117.1746	117.2041	117.2729
28	O18-N16-N17	128.0	127.1567	128.0244
29	C24-N17-N16	120.669	121.4362	120.6471
30	C24-C19-C20	122.2867	121.7611	122.3034
31	H25-C19-C20	120.1964	120.6952	120.2049
32	H25-C19-C24	117.5169	117.5437	117.4917
33	C21-C20-C19	119.1437	119.0025	119.155
34	H26-C20-C19	119.5874	119.6966	119.5822
35	H26-C20-C21	121.2688	121.3009	121.2628
36	C22-C21-C20	119.5144	120.1844	119.4784
37	O29-C21-C20	124.5805	124.1944	124.6131
38	O29-C21-C22	115.9051	115.6212	115.9085
39	C23-C22-C21	121.326	120.8603	121.3535
40	H27-C22-C21	118.1028	118.2418	118.0536
41	H27-C22-C23	120.5712	120.8979	120.5929
42	C24-C23-C22	119.9562	119.763	119.9574
43	H28-C23-C22	119.992	120.4663	120.0184
44	H28-C23-C24	120.0518	119.7708	120.0242
45	C19-C24-N17	112.2347	112.1213	112.2192
46	C23-C24-N17	129.9923	129.4501	130.0284
47	C23-C24-C19	117.773	118.4286	117.7523
48	C30-O29-C21	117.1756	117.7428	117.1924
49	H31-C30-O29	106.2045	105.0608	106.2627
50	H32-C30-O29	111.6893	111.0658	111.7579
51	H32-C30-H31	109.216	109.967	109.1719
52	H33-C30-O29	111.7121	111.0774	111.777
53	H33-C30-H31	109.2129	109.9739	109.1701
54	H33-C30-H32	108.7378	109.6148	108.6324

Table S6: - Bond angle alteration for M06-2X functional combined with different basis sets.

Sr. No.	Bond	Bond Angle (in Degree)		
		6-31G**	6-311G	6-311G**
1	C6-C1-C2	119.747342	119.593555	119.783732
2	H7-C1-C2	119.138077	119.224132	118.986758
3	H7-C1-C6	121.114360	121.182236	121.229197
4	C3-C2-C1	119.550798	119.496950	119.642615
5	H8-C2-C1	120.931109	121.055283	120.875000
6	H8-C2-C3	119.518090	119.447759	119.482371
7	C4-C3-C2	121.200653	121.204599	121.090448
8	N16-C3-C2	121.192445	120.874701	121.177436
9	N16-C3-C4	117.606902	117.920657	117.732070
10	C5-C4-C3	119.268438	119.252214	119.301620
11	H9-C4-C3	118.995551	118.941963	118.980512
12	H9-C4-C5	121.735996	121.805823	121.717853
13	C6-C5-C4	120.264759	120.080586	120.366730
14	H10-C5-C4	121.358749	121.568261	121.342038
15	H10-C5-C6	118.376401	118.351140	118.291094
16	C5-C6-C1	119.967852	120.372086	119.814765
17	O11-C6-C1	124.389652	124.031036	124.419230
18	O11-C6-C5	115.642493	115.596865	115.765977
19	C12-O11-C6	117.754774	118.760824	117.971819
20	H13-C12-O11	111.269868	110.958798	111.092708
21	H14-C12-O11	106.159277	105.416261	106.027568
22	H14-C12-H13	109.411340	109.765993	109.420613
23	H15-C12-O11	111.296131	110.986209	111.162836
24	H15-C12-H13	109.267249	109.859903	109.580375
25	H15-C12-H14	109.370869	109.76391	109.481408
26	N17-N16-C3	115.568966	116.738901	115.633749
27	O18-N16-C3	116.686440	116.738044	116.689169
28	O18-N16-N17	127.744326	126.523005	127.677075
29	C24-N17-N16	120.808408	122.054605	121.005809
30	C24-C19-C20	122.118915	121.542713	122.089850
31	H25-C19-C20	120.162807	120.682768	120.138410
32	H25-C19-C24	117.718274	117.77450	117.771724
33	C21-C20-C19	119.023390	119.054232	119.170654
34	H26-C20-C19	119.577768	119.625834	119.396192
35	H26-C20-C21	121.398703	121.319894	121.432867
36	C22-C21-C20	119.605470	120.123716	119.448727
37	O29-C21-C20	124.44570	124.033070	124.513281

38	O29-C21-C22	115.948826	115.843203	116.037968
39	C23-C22-C21	121.315475	120.930392	121.370760
40	H27-C22-C21	118.008643	118.098173	117.965445
41	H27-C22-C23	120.675871	120.971428	120.663782
42	C24-C23-C22	119.687473	119.543889	119.777293
43	H28-C23-C22	119.896830	120.375117	119.889024
44	H28-C23-C24	120.415688	120.080994	120.333678
45	C19-C24-N17	112.337816	112.557855	112.511150
46	C23-C24-N17	129.412912	128.637099	129.346254
47	C23-C24-C19	118.249225	118.805035	118.142503
48	C30-O29-C21	117.531692	118.725554	117.719955
49	H31-C30-O29	106.204636	105.447533	106.035560
50	H32-C30-O29	111.371175	110.983124	111.177804
51	H32-C30-H31	109.351542	109.763175	109.453629
52	H33-C30-O29	111.379953	111.020719	111.217687
53	H33-C30-H31	109.350664	109.747429	109.405285
54	H33-C30-H32	109.118828	109.792768	109.477523

2. Ground state dipole moment vs Excited state dipole moment

In the below **Table S7** we compared values of ground state dipole moment and excited state dipole moment that were obtained

Table S7:- Change in the ground state dipole moment and excited state dipole moment.

Parameter	**Method**	**6-31G****	**6-311G**	**6-311G****
Ground state dipole moment **(Debye)**	B3LYP	4.1063	5.0075	4.2086
	M06-2X	4.1393	5.1103	4.2787
	M06L	3.9424	4.8456	3.9891
Excited state dipole moment **(Debye)**	CAM-B3LYP	4.8992	3.8138	4.9748
	M06-2X	5.0339	3.1548	5.0677
	M06L	4.6620	5.3179	4.6377

3. Ground to excited state transition electric dipole moments

3.1 CAM-B3LYP/6-31G**

Table S8: - Ground to excited state transition electric dipole moments for CAM-B3LYP /6-31G**.

State	X	Y	Z	Dip S.
1	0.9764	-0.0234	-3.0054	9.9866
2	0.0323	0.0436	-0.0827	0.0098
3	0.0327	0.0001	0.1915	0.0377
4	-0.5273	0.0059	-0.5816	0.6163

5	0.0528	-0.0003	0.2827	0.0827
6	0.0098	-0.0840	0.0107	0.0073
7	0.8120	-0.0175	0.1513	0.6825
8	0.6135	-0.0003	-0.7445	0.9307
9	0.3522	-0.0069	-0.0463	0.1262
10	0.3044	0.0017	-0.0287	0.0935

3.2 CAM-B3LYP/6-311G

Table S9: - Ground to excited state transition electric dipole moments for CAM-B3LYP /6-311G.

State	X	Y	Z	Dip S.
1	-0.0104	0.0523	0.0377	0.0043
2	1.0272	-0.0225	-3.0382	10.2866
3	-0.3993	0.0047	-0.5174	0.4272
4	-0.3717	0.0036	-0.4246	0.3185
5	0.0034	-0.0992	0.0045	0.0099
6	0.0405	-0.0017	0.0149	0.0019
7	0.8135	-0.0128	-0.0843	0.6691
8	0.1404	0.0004	-0.7647	0.6044
9	0.8522	-0.0119	-0.1721	0.7560
10	0.1328	-0.0002	0.1475	0.0394

3.3 CAM-B3LYP/6-311G**

Table S10: - Ground to excited state transition electric dipole moments for CAM-B3LYP/6-311G**.

State	X	Y	Z	Dip S.
1	0.9890	-0.0220	-3.0143	10.0646
2	-0.0070	0.0403	0.0201	0.0021
3	0.0199	-0.0019	-0.1440	0.0211
4	-0.5716	0.0035	-0.4977	0.5745
5	-0.0917	-0.0024	-0.3820	0.1543
6	0.0092	0.0771	0.0060	0.0061
7	0.8290	-0.0101	0.1772	0.7188
8	0.6259	-0.0133	-0.7778	0.9969
9	0.1693	-0.0007	-0.0289	0.0295
10	0.3210	-0.0110	-0.0897	0.1112

3.4 M06-2X/6-31G**

Table S11: - Ground to excited state transition electric dipole moments for M06-2X/6-31G**.

State	X	Y	Z	Dip S.
1	0.9615	-0.0192	-2.9385	9.5593

2	-0.0514	0.0449	0.1468	0.0262
3	0.0480	-0.0011	-0.2161	0.0490
4	-0.4717	0.0044	-0.3795	0.3665
5	-0.2499	-0.0001	-0.6684	0.5091
6	-0.0236	-0.0818	-0.0240	0.0078
7	0.8568	-0.0017	0.0910	0.7424
8	0.5181	-0.0163	-0.7920	0.8958
9	0.1742	0.0029	0.0504	0.0329
10	0.0021	-0.0050	0.0331	0.0011

3.5 M06-2X/6-311G

Table S12: - Ground to excited state transition electric dipole moments for M06-2X/6-311G.

State	X	Y	Z	Dip S.
1	-0.0177	0.0455	0.0616	0.0062
2	0.9881	-0.0219	-2.9714	9.8059
3	0.1263	-0.0014	0.4119	0.1856
4	-0.4549	0.0081	-0.7186	0.7234
5	-0.0163	-0.0791	-0.0181	0.0069
6	0.0135	-0.0020	0.2845	0.0811
7	0.8659	-0.0115	-0.0441	0.7519
8	0.3253	-0.0018	-0.7833	0.7195
9	0.5834	-0.0081	-0.1051	0.3515
10	0.2165	0.0010	0.0749	0.0525

3.6 M06-2X/6-311G**

Table S13: - Ground to excited state transition electric dipole moments for M06-2X/6-311G**.

State	X	Y	Z	Dip S.
1	0.9630	-0.0197	-2.9307	9.5167
2	0.0397	0.0433	-0.1074	0.0150
3	0.0655	-0.0031	-0.1960	0.0427
4	-0.4568	0.0011	-0.3335	0.3198
5	-0.2735	-0.0021	-0.7032	0.5694
6	0.0313	-0.0821	0.0265	0.0084
7	0.8574	-0.0193	0.0979	0.7451
8	0.5103	0.0002	-0.7850	0.8766
9	0.1384	-0.0054	0.0607	0.0229
10	-0.0332	0.0036	0.0390	0.0026

3.7 M06L/6-31G**

Table S14: - Ground to excited state transition electric dipole moments for M06L/6-31G**.

State	X	Y	Z	Dip S.
1	0.8388	-0.0195	-3.0559	10.0427
2	-0.0001	0.0271	0.0015	0.0007
3	-0.2624	0.0014	-0.6530	0.4953
4	0.3421	-0.0060	-0.5839	0.4580
5	0.0772	-0.0016	-0.1139	0.0189
6	0.2606	-0.0047	-0.4695	0.2884
7	0.5206	-0.0055	0.1601	0.2966
8	-0.2030	0.0013	0.2617	0.1097
9	0.0066	-0.0543	-0.0082	0.0031
10	-0.0012	0.0341	0.0008	0.0012

3.8 M06L/6-311G

Table S15: - Ground to excited state transition electric dipole moments for M06L/6-311G.

State	X	Y	Z	Dip S.
1	0.8439	-0.0203	-3.1474	10.6184
2	-0.0032	0.0335	0.0100	0.0012
3	-0.4207	0.0046	-0.2910	0.2617
4	-0.0102	-0.0008	-0.1182	0.0141
5	0.1950	-0.0037	-0.3413	0.1545
6	0.3429	-0.0073	-0.6144	0.4951
7	0.0033	0.0825	-0.0019	0.0068
8	0.4102	-0.0034	0.2564	0.2340
9	-0.4621	0.0067	0.2753	0.2893
10	0.0014	0.0245	-0.0001	0.0006

3.9 M06L/6-311G**

Table S16: - Ground to excited state transition electric dipole moments for M06L/6-311G**.

State	X	Y	Z	Dip S.
1	0.8389	-0.0199	-3.0524	10.0211
2	0.0005	0.0267	-0.0002	0.0007
3	-0.2554	0.0013	-0.6610	0.5022
4	0.3458	-0.0062	-0.5816	0.4579
5	0.0778	-0.0016	-0.1091	0.0180
6	0.2598	-0.0046	-0.4651	0.2838
7	0.5187	-0.0054	0.1658	0.2966
8	-0.1793	0.0019	0.2533	0.0963
9	-0.0039	0.0579	0.0048	0.0034
10	-0.0009	0.0263	-0.0002	0.0007