The Effects of Basis Sets on Absorbance Spectra

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Contents

Abstract

The ability to accurately and efficiently model realistic absorbance spectra remains a difficult task with today's theoretical models. In order to explore the extent of the accuracy and predictive qualities of today's theoretical models, Time-Dependent Density Functional Theory (TD-DFT) was used to explore the effect of basis set size on the accuracy of the calculated absorbance spectra. The effects of the Linear Response (LR) Random Phase Approximation (RPA) Pople and Dunning Basis sets 6-31G, 6-31G**, 6-311G**, 6-311G++, cc-pVTZ, cc-PVDZ, aug-cc-pVTZ, aug-cc-pVDZ, and aug-cc-pVQZ were explored and the LR Tamm-Dancoff Approximation (TDA) basis sets aug-cc-pVDZ, aug-cc-PVTZ, aug-cc-PVQZ, and 6-31G+ were also partially explored. On average, the error of all basis sets was acceptable and remained between 1% and 13%. The LR RPA basis sets explored had a general trend of aug-cc-pVTZ > 6-311G++ > aug-cc-pVDZ > cc-pVTZ > 6-311G** > cc-pVDZ > 6-31G** > 6-31G in order of decreasing agreeance with experimental results.

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Introduction

Understanding the accuracy and predictive capabilities of theoretical models in simulation of absorption spectra is important for the design of new light-absorbing devices such as solar cells. DFT based approaches allow for inexpensive simulation of absorption, but the accuracy strongly depends on the basis set and functional used. By exploring the theoretical simulations of absorbance spectra utilizing NWChem, we can understand the nature of absorbance energy shift as it correlates with basis set completeness.[1-3]

Background

Spectroscopic techniques provide invaluable information into the quantum properties of chemical species. When a molecule is irradiated with light, an electron will absorb the light and transition to an excited state. The excitation of electrons is governed by a set of selection rules in which some transitions are allowed and some transitions are forbidden. However, forbidden transitions can still be observed at high pressures. Absorption in the ultraviolet-visible region of the electromagnetic spectrum usually corresponds with electronic transitions, while absorption in the infrared region of the electromagnetic spectra corresponds with molecular vibrations.

The theoretical prediction of absorbance spectra is still a major challenge. Currently, the most widely used method to calculate absorbance spectra is Time Dependent Density Function Theory (TD-DFT) because of its ability to incorporate time-dependent external fields. However, TD-DFT is highly sensitive to the type of functional and basis set used when calculating absorbance spectra.[2]

In this paper, the accuracy and predictive capabilities of a number of popular Linear Response (LR) Pople and Dunning basis sets have been explored with both the Random Phase Approximation (RPA) and Tamm-Dancoff Approximation (TDA). Future work will incorporate different methods

and functionals while also exploring a wider, more comprehensive set of molecules.

Methodology

The geometries for all molecules were optimized at the DFT level using the B3LYP functional and the LANL2DZ basis set by employing Qchem 4.1. Absorbance spectra calculations were performed at the TD-DFT level using the PBE96 functional employing NWchem 6.3.[4]

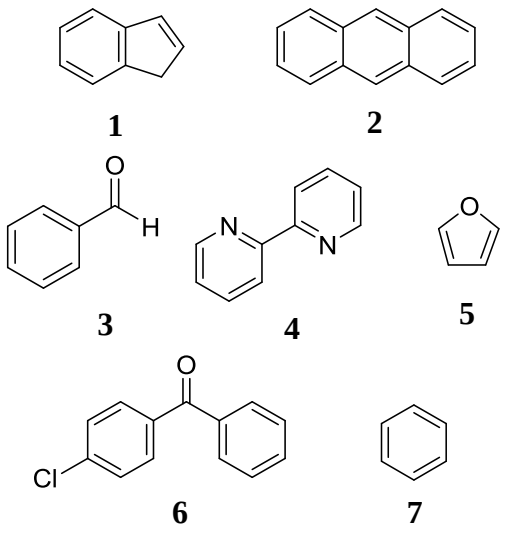

Figure 1. Seven chromophores used to study the basis set effect on absorbance spectra calculations.

The effects of the following Linear Response (LR) Random Phase Approximation (RPA) Pople and Dunning Basis sets were explored: 6-31G, 6-31G**, 6-311G**, 6-311G++, cc-pVTZ, cc-PVDZ, aug-cc-pVTZ, aug-cc-pVDZ, and aug-cc-pVQZ. The effects of the following LR Tamm-Dancoff Approximation (TDA) basis sets were also partially explored: aug-cc-pVDZ, aug-cc-PVTZ, aug-cc-PVQZ, and 6-31G+.[2]

Chromophores **1** – **7** were chosen based on their strong $\pi \rightarrow \pi^*$ transition in the UV-Vis portion of the electromagnetic spectrum. All calculations were performed by following a standard approach: the ground state geometry of each molecule was optimized until the self-consistent field (SCF) energy converged with a DIIS error below 1.0E-08 a.u., the vibrational spectrum was calculated to confirm that all roots were real and the optimized geometry was a true global minimum, and then the excited state energies were computed with TD-DFT.[2,4]

Results

Current theoretical models have several limitations that can result in sizeable discrepancies when compared to experimental results. One such limitation of our theoretical model is the inability to determine vibronic couplings. The computation of Franck-Condon factors that would be necessary to compute the couplings would require the determination of the Hessian for excited states, which,

with today's resources, is not feasible for most systems.

Another limitation that may drastically affect the experimental and theoretical agreement is the molecular interactions between bulk material and solvent. The following calculations were performed on a single, isolated molecule, while experimental results may experience significant solvent interactions as well as other intermolecular interactions with the bulk substance. In realistic conditions, the molecule could be protonated or deprotonated by solvent, the excited states could be stabilized by solvent, or intermolecular interaction within the bulk substance could influence the absorption spectra.

On average, the accuracy of the basis sets was ordered as predicted with increasing basis set size. The error remained between 1% and 13% for all studied basis sets, which represents an acceptable, expected deviation from experimental results. The LR RPA basis sets explored had a general trend of aug-cc-pVTZ > 6-311G++ > aug-cc-pVDZ > cc-pVTZ > 6-311G** > cc-pVDZ > 6-31G** > 6-31G in order of decreasing agreeance with experimental results.

Table 1. Comparison of absorbance peak energies for various Pople and Dunning basis sets (eV)[a]

	Exp.	6-31G	6-31G**	6-311G++	6-311G**	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ
1	4.34	4.89	4.77	4.65	4.73	4.75	4.69	4.65	4.64
3	4.45	5.00	4.96	4.78	4.90	4.94	4.85	4.78	4.77
4	4.13	4.47	4.35	4.22	4.30	4.33	4.26	4.23	4.22
5	5.99	6.47	6.33	5.87	6.21	6.26	6.10	5.85	5.83
6	3.63	3.93	3.91	3.78	3.87	3.87	3.82	3.79	

	Exp.	RPA 6-31G	TDA aug-cc-pVDZ	TDA aug-cc-pVTZ	TDA aug-cc-pVQZ	RPA aug-cc-pVTZ
7	6.97307	7.41642	6.81381	6.78929	6.81381	6.76126

	Exp.	RPA 6-311G**	TDA 6-31G+*	RPA aug-cc-pVQZ	TDA aug-cc-pVQZ
2	4.94	4.97	5.52	4.88	5.29

[a]All experimental results obtained from references 5-11.

However, the order of basis set accuracy for **5** differed slightly, having a trend of cc-pVTZ > 6-311G++ > aug-cc-pVDZ > aug-cc-pVTZ > 6-311G** > cc-pVDZ > 6-31G** > 6-31G in order of decreasing accuracy. The origin of this deviation in order is currently unknown, but will be further explored in future studies by incorporating more physically and chemically similar molecules.

Generally, convergence of absorbance energies was seen for augmented basis sets, which remained within 0.05 eV from each other for all studied molecules. However, in the interest of minimizing computational cost, we have concluded that the most efficient and accurate basis set to calculate absorbance spectra is LR-RPA aug-cc-pVDZ, which remained below 7.5% error for all studied molecules.

In order to gather more statistically meaningful and complete data, future studies will incorporate an extensive list of molecules with diverse physical and chemical properties. Furthermore, the comparative effects of RPA versus TDA will be explored for a wider variety of basis sets, and the effects of Real Time (RT) versus Linear Response (LR) will also be explored.

Since the accuracy of TD-DFT is highly dependent on the type of functional used, future studies will explore the pros and cons of a variety of functionals, including LDA, PW91, PBE, and B3LYP. For a more comprehensive study of the basis set effect on absorbance spectra, the relative accuracies of each studied basis set will be studied with each functional to ensure that the basis set effect is independent of the functional used.

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Acknowledgments

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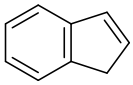
Appendix A: Indene

I. Molecular Structure



DFT/B3LYP

Basis: LANL2DZ

```
17
 ENER      9 -347.68324
C       -0.949362     -1.420274      0.000002
C       -2.173542     -0.729945      0.000002
C       -2.203014      0.672028      0.000000
C       -1.013391      1.413635     -0.000001
C        0.206053      0.728970     -0.000001
C        0.234641     -0.689171      0.000001
C        1.593711      1.215492     -0.000002
H       -0.935479     -2.506713      0.000003
H       -3.105143     -1.287246      0.000003
H       -3.158271      1.188084      0.000000
H       -1.042431      2.499265     -0.000002
C        2.446237      0.165085      0.000000
H        1.870954      2.262826     -0.000003
C        1.681908     -1.146813      0.000001
H        1.923538     -1.761927     -0.879704
H        1.923538     -1.761925      0.879709
H        3.527859      0.218023      0.000000
```

Approximate Ionization Potential[1]: 8.3 eV

II. Analysis

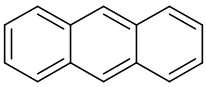
Table 2. Oscillation Strengths (OS) and energy values (eV) for the physically meaningful roots of indene. A continuation of the roots can be found on the page 8.

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
1	4.6035	0.0071	4.5145	0.0077	4.4622	0.0070	4.3793	0.0058	4.4807	0.0070	4.4299	0.0071	4.3842	0.0057	4.3793	0.0060
2	4.8895	0.1619	4.7740	0.1462	4.7289	0.1512	4.6476	0.1633	4.7487	0.1494	4.6894	0.1509	4.6541	0.1647	4.6441	0.1629
3	5.4352	0.1457	5.3214	0.1401	5.2425	0.1416	5.0073	0.0057	5.2670	0.1395	5.1873	0.1414	4.9741	0.0058	4.9719	0.0057
4	5.8413	0.0014	5.7443	0.0009	5.6814	0.0004	5.1056	0.1454	5.7038	0.0005	5.6376	0.0007	5.1052	0.1421	5.0979	0.1412
5	6.3590	0.1534	6.2304	0.1717	6.1030	0.1845	5.2933	0.0001	6.1473	0.1797	6.0315	0.1836	5.2469	0.0001	5.2434	0.0001
6	6.5552	0.0002	6.4032	0.0002	6.2264	0.0014	5.4407	0.0002	6.3434	0.0002	6.1200	0.0013	5.3836	0.0003	5.3713	0.0003
7	6.6318	0.1408	6.4958	0.1137	6.3570	0.0002	5.5524	0.0042	6.4392	0.1099	6.2805	0.0002	5.5533	0.0048	5.5445	0.0054
8	7.0388	0.0004	6.8749	0.0003	6.4079	0.1035	5.6764	0.0011	6.5912	0.0007	6.3579	0.1025	5.6437	0.0012	5.6418	0.0012
9	7.2367	0.0020	7.0615	0.0018	6.4920	0.0001	5.8605	0.1661	6.8184	0.0004	6.3684	0.0000	5.8088	0.0081	5.7932	0.0074
10	7.3307	0.0001	7.2535	0.0001	6.8212	0.0002	5.8775	0.0085	6.8935	0.0001	6.6935	0.0002	5.8535	0.1559	5.8412	0.1387
11	7.4827	0.2816	7.3342	0.2714	6.8302	0.0003	5.9433	0.0007	6.9670	0.0023	6.7519	0.0004	5.8748	0.0010	5.8533	0.0007
12	7.5213	0.0001	7.3551	0.0001	6.8973	0.0012	5.9675	0.0011	7.2350	0.2883	6.7899	0.0009	5.9208	0.0010	5.8840	0.0289
13	7.6413	0.0593	7.4587	0.0002	6.9688	0.0027	6.0778	0.0100	7.2603	0.0001	6.8683	0.0031	5.9614	0.0142	5.9171	0.0010
14	7.6490	0.0002	7.5076	0.0723	7.1674	0.0000	6.1096	0.0050	7.2671	0.0011	7.0462	0.0000	6.0527	0.0047	6.0412	0.0044
15	7.7722	0.4087	7.6081	0.3627	7.1769	0.2906	6.2743	0.1207	7.2846	0.0001	7.0829	0.2977	6.2534	0.0005	6.1847	0.0027
16	7.8011	0.0002	7.7683	0.0001	7.2847	0.0000	6.2873	0.0002	7.3701	0.0001	7.1582	0.0053	6.2680	0.0023	6.2520	0.0005
17	8.0221	0.0001	7.8368	0.0005	7.3305	0.0058	6.3835	0.0032	7.4432	0.1810	7.2061	0.0000	6.2735	0.1081	6.2643	0.1034
18	8.0420	0.0008	7.8679	0.0027	7.3706	0.0006	6.5412	0.0000	7.5220	0.2514	7.2687	0.0003	6.4737	0.0000	6.4597	0.0000
19	8.0622	0.0027	7.9474	0.0001	7.4017	0.2843	6.6131	0.0084	7.5726	0.0004	7.3153	0.3979	6.5439	0.0079	6.5230	0.0074
20	8.2158	0.0001	8.1834	0.0001	7.4741	0.1451	6.7011	0.0001	7.7438	0.0052	7.3158	0.0000	6.5948	0.0001	6.5272	0.0000
21	8.4061	0.0738	8.2768	0.0709	7.4757	0.0001	6.7305	0.1036	7.7509	0.0008	7.3642	0.0020	6.6348	0.0895	6.5345	0.0587
22	8.4528	0.0080	8.2887	0.0008	7.4945	0.0023	6.7541	0.0001	7.7971	0.0017	7.4172	0.0319	6.6483	0.0004	6.5721	0.0003
23	8.4659	0.0004	8.3050	0.0108	7.7463	0.0004	6.7665	0.0012	7.9316	0.0001	7.6502	0.0006	6.7354	0.0005	6.5821	0.0379
24	8.4982	0.0042	8.4030	0.0001	7.8022	0.0027	6.8373	0.0036	7.9368	0.0008	7.7216	0.0025	6.7776	0.0203	6.7228	0.0005
25	8.6210	0.0001	8.4567	0.0040	7.8909	0.0321	6.8530	0.0785	8.1062	0.0606	7.7682	0.0343	6.8082	0.0038	6.7665	0.0544
26			8.5597	0.0002	7.9659	0.0006	6.8749	0.0004	8.1796	0.0008	7.7941	0.0002	6.8408	0.0003	6.7972	0.0039
27			8.5945	0.0004	8.0925	0.0017	6.9572	0.1729	8.2073	0.0089	7.9357	0.0005	6.9147	0.2314	6.8386	0.0004
28			8.6827	0.0000	8.1537	0.0058	7.0608	0.0000	8.3120	0.0004	7.9823	0.0000	6.9366	0.0000	6.8608	0.0000
29					8.1548	0.0157	7.1594	0.0047	8.3741	0.0007	7.9971	0.0069	7.1020	0.1876	6.9015	0.2011
30					8.1572	0.0000	7.1633	0.3673	8.4576	0.0018	8.0491	0.0015	7.1119	0.0046	7.1090	0.0045
31					8.1734	0.0025	7.2067	0.0004	8.5158	0.0002	8.0803	0.0165	7.1754	0.2252	7.1098	0.3353
32					8.3132	0.0003	7.2396	0.0001	8.5477	0.0353	8.2047	0.0000	7.1895	0.0006	7.1687	0.0000
33					8.3332	0.0474	7.2587	0.0420	8.5554	0.0002	8.2176	0.0001	7.2106	0.0001	7.1766	0.0009
34					8.3594	0.0000	7.3020	0.0153	8.6089	0.0038	8.2204	0.0468	7.2433	0.0148	7.1931	0.0001
35					8.4351	0.0002	7.3708	0.0000			8.2298	0.0000	7.2633	0.0000	7.2012	0.0000
36					8.5629	0.0006	7.3822	0.0024			8.4825	0.0002	7.3199	0.0007	7.2205	0.0001
37					8.6129	0.0003	7.4287	0.0009			8.5035	0.0015	7.3770	0.0003	7.2325	0.0141
38							7.5288	0.0074			8.5172	0.0728	7.4215	0.0001	7.2447	0.0006
39							7.5343	0.0001			8.5585	0.0091	7.4620	0.0076	7.3356	0.0347
40							7.6140	0.0010			8.5801	0.0003	7.5007	0.0013	7.3446	0.0000
41							7.6535	0.0362			8.6054	0.0007	7.5686	0.0412	7.3983	0.0374

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
42							7.7242	0.0024					7.5956	0.0012	7.4353	0.0003
43							7.7366	0.0000					7.6666	0.0000	7.4386	0.0133
44							7.8058	0.0016					7.7063	0.0018	7.4550	0.0109
45							7.8096	0.0117					7.7283	0.0110	7.5307	0.0053
46							7.8233	0.0014					7.7292	0.0022	7.5798	0.0047
47							7.8378	0.0010					7.7374	0.0005	7.5799	0.0010
48							7.8657	0.0039					7.7427	0.0025	7.6532	0.0000
49							7.9215	0.0004					7.7646	0.0001	7.6656	0.0047
50							7.9424	0.0525					7.7653	0.0008	7.6844	0.0003
51							7.9457	0.0023					7.7911	0.0000	7.6931	0.0024
52							7.9653	0.0292					7.8502	0.0542	7.7142	0.0014
53							8.0682	0.0034					7.8822	0.0015	7.7202	0.0092
54							8.1097	0.0448					7.8980	0.0192	7.7329	0.0005
55							8.1698	0.0212					7.9089	0.0017	7.7893	0.0294
56							8.1734	0.0009					7.9535	0.0009	7.7926	0.0001
57							8.2012	0.0012					7.9996	0.0003	7.8338	0.0492
58							8.2098	0.0028					8.0632	0.0745	7.8420	0.0006
59							8.2550	0.0005					8.0845	0.0048	7.8833	0.0063
60							8.2612	0.0049					8.0918	0.0039	7.8855	0.0032
61							8.3489	0.0068					8.0945	0.0016	7.8950	0.0269
62							8.3491	0.0008					8.1276	0.0003	7.8967	0.0000
63							8.3764	0.0092					8.1592	0.0001	7.9498	0.0001
64							8.3837	0.0337					8.1694	0.0010	8.0143	0.0030
65							8.3945	0.0073					8.1761	0.0001	8.0357	0.0210
66							8.4024	0.0117					8.1790	0.0064	8.0525	0.0004
67							8.4071	0.0000					8.2018	0.0160	8.0646	0.0410
68							8.4412	0.0007					8.2751	0.0023	8.1085	0.0006
69							8.4619	0.0001					8.3030	0.0057	8.1409	0.0000
70							8.4855	0.0011					8.3259	0.0382	8.1673	0.0033
71							8.5045	0.0000					8.3374	0.0000	8.1954	0.0001
72							8.5106	0.0000					8.3610	0.0073	8.2391	0.0003
73							8.5623	0.0009					8.3705	0.0003	8.2512	0.0028
74							8.5788	0.0009					8.3976	0.0049	8.2741	0.0019
75							8.5846	0.0000					8.4274	0.0001	8.2952	0.0019
76							8.5928	0.0000					8.4359	0.0061	8.3098	0.0289
77							8.5999	0.0009					8.4574	0.0006	8.3191	0.0074
78							8.6206	0.0001					8.4638	0.0025	8.3399	0.0034
79													8.4830	0.0001	8.3501	0.0035
80													8.4981	0.0032	8.3604	0.0003
81													8.5080	0.0000	8.3664	0.0053
82													8.5465	0.0005	8.3914	0.0003
83													8.5591	0.0001	8.3938	0.0078
84													8.5834	0.0008	8.3989	0.0062
85													8.5988	0.0020	8.4325	0.0000
86													8.6331	0.0136	8.4357	0.0028
87															8.4594	0.0010
88															8.4629	0.0022
89															8.4634	0.0020
90															8.4699	0.0013
91															8.5440	0.0007
92															8.5809	0.0017
93															8.6151	0.0306

Appendix B: Anthracene

I. Molecular Structure



DFT/B3LYP (?)

Basis: 6-31G+* (?)

No Coordinate Data

Approximate Ionization Potential[2]: 7.4 eV

II. Analysis

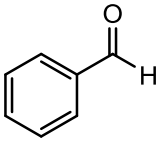
Table 3. Oscillation Strengths (OS) and energy values (eV) for the physically meaningful roots of anthracene. A continuation of the roots can be found on the page 10.

	RPA 6-311G**		TDA 6-31G+*		RPA aug-cc-pVQZ		TDA aug-cc-pVQZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS
1	2.9205	0.0380	3.2049	0.0624	2.8961	0.0336	3.1054	0.0535
2	3.6063	0.0005	3.6808	0.0008	3.5968	0.0002	3.6088	0.0001
3	3.9031	0.0000	3.9677	0.0000	3.8858	0.0000	3.8891	0.0000
4	4.5744	0.0000	4.8463	0.0000	4.5058	0.0000	4.5151	0.0000
5	4.8186	0.0000	4.9356	0.0000	4.5148	0.0000	4.5994	0.0000
6	4.9696	1.7171	5.1926	0.0000	4.5871	0.0000	4.6756	0.0000
7	5.1082	0.0000	5.2505	0.0000	4.6854	0.0000	4.6857	0.0000
8	5.1515	0.0000	5.3548	0.0000	4.7547	0.0013	4.7552	0.0013
9	5.2981	0.0001	5.5194	2.5638	4.8855	1.7693	5.1142	0.0000
10	5.3362	0.0027	5.5490	0.0005	5.1013	0.0000	5.1448	0.0000
11	5.4708	0.0000	5.5746	0.0000	5.1266	0.0000	5.1547	0.0000
12	5.5434	0.0000	5.6100	0.0000	5.1542	0.0000	5.1905	0.0000
13	5.6066	0.1125	5.8781	0.0000	5.1902	0.0000	5.2249	0.0001
14	5.7149	0.0000	6.0023	0.1808	5.2018	0.0001	5.2769	0.0000
15	5.8006	0.0000	6.2229	0.0026	5.2215	0.0001	5.2894	2.6154
16	5.8153	0.0000	6.4693	0.0000	5.4141	0.0000	5.4594	0.0000
17	5.9187	0.0001	6.5060	0.0000	5.4524	0.0562	5.4692	0.0000
18	6.0628	0.0021	6.5140	0.0119	5.4636	0.0000	5.5457	0.0000
19	6.3342	0.0000	6.6248	0.0000	5.5441	0.0000	5.5994	0.0227
20	6.3844	0.0000	6.6668	0.0000	5.6530	0.0068	5.6536	0.0069
21	6.3867	0.0002	6.6897	0.3045	5.6779	0.0000	5.6785	0.0000
22	6.4093	0.1481	6.7112	0.0000	5.6849	0.0000	5.6851	0.0000
23	6.5138	0.1016	6.7891	0.0000	5.7367	0.0000	5.7404	0.0000
24	6.5332	0.0000	6.8724	0.0003	5.7566	0.0891	5.8222	0.0391
25	6.6106	0.0000	6.9286	0.0426	5.7977	0.0071	5.8537	0.0077
26	6.6222	0.0000	6.9489	0.1581	5.8534	0.0075	5.8555	0.1597
27	6.6351	0.0000	6.9780	0.0013	5.8692	0.0000	5.8711	0.0000
28	6.7985	0.0027	7.0261	0.0000	5.9257	0.0000	5.9259	0.0000
29	6.8032	0.0006	7.0461	0.0000	5.9296	0.0000	5.9350	0.0000
30	6.8798	0.0000	7.1325	0.0000	5.9962	0.0000	5.9965	0.0000
31	6.9121	0.0013	7.2251	0.0000	6.0788	0.0000	6.0960	0.0000
32	6.9300	0.0000	7.2849	0.0000	6.1656	0.0000	6.1673	0.0000
33	6.9634	0.0013	7.3943	0.0000	6.1670	0.0000	6.1677	0.0000
34	6.9634	0.0010	7.4250	0.0000	6.2345	0.0000	6.2350	0.0000
35	7.0102	0.0000	7.5422	0.1656	6.2350	0.0900	6.2609	0.0000
36	7.0394	0.0000	7.5620	0.0013	6.2600	0.0000	6.2628	0.0000
37	7.0742	0.0000	7.6288	0.0000	6.2622	0.0000	6.3222	0.0000
38	7.1527	0.0000	7.7801	0.0000	6.3215	0.0000	6.3635	0.0000
39	7.1825	0.0000			6.3283	0.0071	6.3669	0.0000
40	7.2199	0.0000			6.3566	0.0000	6.3818	0.0187
41	7.2497	0.0065			6.3633	0.0000	6.4245	0.0699
42	7.2718	0.0000			6.4367	0.0000	6.4397	0.0000
43	7.3579	0.0000			6.4812	0.0701	6.4966	0.1371
44	7.3689	0.1043			6.5300	0.0000	6.5348	0.0000
45	7.3855	0.0000			6.5829	0.0000	6.5832	0.0000
46	7.4203	0.0000			6.5897	0.0000	6.5902	0.0000
47	7.4557	0.0021			6.5988	0.0000	6.5989	0.0000
48	7.5521	0.0000			6.6117	0.0171	6.6342	0.1003
49	7.5736	0.0000			6.6339	0.0000	6.6343	0.0000
50	7.6109	0.0000			6.6732	0.0148	6.6736	0.0154
51	7.7114	0.0000					6.7089	0.0007

	RPA 6-311G**		TDA 6-31G+*		RPA aug-cc-pVQZ		TDA aug-cc-pVQZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS
52							6.7146	0.0000
53							6.7518	0.0002
54							6.8048	0.0000
55							6.8145	0.0821
56							6.8232	0.0000
57							6.8408	0.0001
58							6.8419	0.0025
59							6.8675	0.0000
60							6.9052	0.0306
61							6.9214	0.0011
62							6.9413	0.0000
63							6.9589	0.0000
64							6.9652	0.0000
65							6.9966	0.0000
66							7.0268	0.0000
67							7.0271	0.0000
68							7.0278	0.0000
69							7.0408	0.0070
70							7.0757	0.0000
71							7.1117	0.0000
72							7.1314	0.0000
73							7.1410	0.0086
74							7.1584	0.0000
75							7.1662	0.0000
76							7.1951	0.0000
77							7.2320	0.0000
78							7.2348	0.0212
79							7.2434	0.0000
80							7.2657	0.1274
81							7.2970	0.0000
82							7.3027	0.0000
83							7.3034	0.0000
84							7.3098	0.0000
85							7.3367	0.0040
86							7.3507	0.0400
87							7.3747	0.0000
88							7.3780	0.0000
89							7.4009	0.0045
90							7.4076	0.0000
91							7.4198	0.0110
92							7.4261	0.0000
93							7.4303	0.0000
94							7.4520	0.0006
95							7.4732	0.0527
96							7.4790	0.0000
97							7.5128	0.0000
98							7.5339	0.0023
99							7.5639	0.0746
100							7.5951	0.0000

Appendix C: Benzaldehyde

I. Molecular Structure



DFT/B3LYP

Basis: LANL2DZ

```
   14
 ENER     10 -345.48477
C         1.732695    -1.064719     0.000002
C         2.218034     0.249332     0.000002
C         1.326752     1.333494    -0.000001
C         0.354620    -1.295409    -0.000002
C        -0.048818     1.104687    -0.000004
C        -0.542118    -0.213360    -0.000005
C        -1.993009    -0.466959    -0.000010
O        -2.864960     0.418014     0.000010
H        -2.285042    -1.533786     0.000012
H        -0.032067    -2.311418    -0.000002
H        -0.759383     1.924369    -0.000007
H         1.708661     2.349199     0.000000
H         2.424945    -1.900255     0.000004
H         3.288509     0.429331     0.000005
```

Approximate Ionization Potential[3]: 9.5 eV

II. Analysis

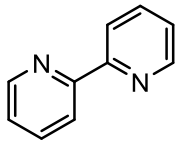
Table 4. Oscillation Strengths (OS) and energy values (eV) for the physically meaningful roots of benzaldehyde. A continuation of the roots can be found on the page 14.

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
1	3.1354	0.0000	3.1011	0.0000	3.0641	0.0001	3.0842	0.0000	3.0572	0.0000	3.0683	0.0000	3.0513	0.0001	3.0560	0.0001
2	4.3092	0.0158	4.2430	0.0000	4.1777	0.0000	4.1889	0.0000	4.1469	0.0000	4.1768	0.0000	4.1622	0.0000	4.1696	0.0000
3	4.3479	0.0000	4.2961	0.0152	4.1892	0.0154	4.2703	0.0154	4.3008	0.0149	4.2378	0.0151	4.1937	0.0150	4.1951	0.0151
4	5.0032	0.2486	4.9647	0.2327	4.7773	0.2301	4.9050	0.2270	4.9435	0.2245	4.8536	0.2290	4.7763	0.2276	4.7757	0.2276
5	5.6182	0.0007	5.5797	0.0005	5.3591	0.0150	5.5289	0.0005	5.5042	0.0005	5.4927	0.0005	5.3137	0.0167	5.3221	0.0150
6	5.9199	0.0000	5.8490	0.0000	5.4217	0.0009	5.8038	0.0000	5.8068	0.0000	5.7199	0.0000	5.3988	0.0010	5.4048	0.0010
7	5.9989	0.0569	5.9285	0.0657	5.7069	0.0001	5.8522	0.0696	5.8800	0.0707	5.8040	0.0737	5.6719	0.0138	5.6746	0.0137
8	6.3354	0.0002	6.2449	0.0003	5.7103	0.0280	6.2042	0.0003	6.2073	0.0003	6.1211	0.0004	5.6783	0.0001	5.6758	0.0001
9	6.6438	0.2300	6.5328	0.2547	5.7953	0.0842	6.2742	0.0142	6.4229	0.1178	6.2441	0.0251	5.7744	0.0954	5.7704	0.0940
10	6.7301	0.0647	6.5964	0.0459	6.0300	0.0008	6.5104	0.1874	6.5448	0.0353	6.4496	0.2517	5.9527	0.0002	5.9444	0.0001
11	7.3726	0.1036	7.2479	0.1112	6.1105	0.0005	6.5498	0.2081	6.6876	0.2625	6.5031	0.1362	6.0842	0.0005	6.0778	0.0005
12	7.4147	0.0019	7.2599	0.0018	6.2045	0.0034	6.9063	0.0090	7.1369	0.0425	6.8442	0.0077	6.1772	0.0034	6.1747	0.0035
13	7.4207	0.1910	7.3031	0.1558	6.2973	0.0001	7.1647	0.0029	7.1603	0.0023	7.0711	0.0032	6.2702	0.0001	6.2682	0.0001
14	7.6278	0.0028	7.5254	0.0006	6.3069	0.3465	7.2032	0.2172	7.3351	0.1580	7.1339	0.2301	6.3070	0.3284	6.2961	0.3282
15	7.7210	0.0000	7.5708	0.0005	6.4113	0.0221	7.2239	0.0014	7.4434	0.0003	7.1799	0.0013	6.3338	0.0257	6.3315	0.0225
16	7.7897	0.1127	7.6617	0.0742	6.4323	0.0171	7.3195	0.0001	7.5291	0.0017	7.2765	0.0001	6.4290	0.0220	6.4174	0.0162
17	8.0396	0.0001	7.9044	0.0001	6.6081	0.0007	7.4500	0.0005	7.5474	0.0001	7.3633	0.0005	6.5038	0.0029	6.4721	0.0096
18	8.1102	0.0004	7.9672	0.0682	6.6286	0.0003	7.5076	0.0318	7.6146	0.0844	7.4002	0.0195	6.5891	0.0002	6.5342	0.0021
19	8.2214	0.0009	8.0551	0.0008	6.7200	0.0176	7.5470	0.0008	7.6334	0.0001	7.4924	0.0006	6.6799	0.0179	6.5800	0.0002
20	8.2599	0.2044	8.1083	0.0828	6.8543	0.0023	7.5889	0.0677	7.8628	0.0001	7.5247	0.0798	6.7239	0.0014	6.6709	0.0164
21	8.2870	0.0001	8.1721	0.0001	6.9098	0.0104	7.7618	0.0059	7.8944	0.0141	7.6568	0.0059	6.8503	0.0097	6.7443	0.0236
22	8.3746	0.0000	8.2674	0.0000	6.9434	0.2303	7.7875	0.0000	7.9525	0.2202	7.7127	0.0000	6.8588	0.0215	6.8298	0.0090
23	8.4346	0.1560	8.2885	0.2115	6.9716	0.0772	7.8498	0.0005	8.0228	0.0010	7.7628	0.0003	6.9371	0.2869	6.9107	0.2761
24	8.5405	0.0001	8.4512	0.0000	7.0033	0.0017	7.8973	0.0090	8.1255	0.0597	7.8209	0.0076	6.9439	0.0016	6.9233	0.0014
25	8.6342	0.0009	8.5696	0.0007	7.0645	0.0022	7.9254	0.2499	8.1637	0.0000	7.8528	0.2309	7.0359	0.0024	7.0249	0.0025
26	8.7257	0.0010	8.6451	0.0006	7.3006	0.0005	8.0146	0.0006	8.1672	0.0548	7.9344	0.0006	7.2380	0.0004	7.1773	0.0219
27	8.7794	0.0000	8.6926	0.0001	7.3447	0.0749	8.0807	0.0624	8.2786	0.0050	7.9886	0.0609	7.2437	0.0307	7.2042	0.0011
28	8.9416	0.0016	8.8139	0.0011	7.3609	0.0003	8.3622	0.0006	8.3722	0.0002	8.2337	0.0031	7.3243	0.0002	7.2227	0.0005
29	8.9816	0.0000	8.8250	0.0011	7.3866	0.0006	8.4114	0.0049	8.4269	0.0008	8.2533	0.0007	7.3345	0.0006	7.3093	0.0002
30	8.9944	0.0018	8.9518	0.0019	7.4146	0.0237	8.4425	0.0020	8.5917	0.0005	8.2938	0.0042	7.3807	0.0627	7.3216	0.0007
31	9.0034	0.0006	8.9525	0.0000	7.4834	0.0006	8.4450	0.0018	8.6448	0.0000	8.3354	0.0017	7.3966	0.0004	7.3375	0.0426
32	9.0586	0.0297	9.0121	0.0199	7.5084	0.0009	8.5039	0.0020	8.7476	0.0003	8.3868	0.0013	7.4296	0.0015	7.3460	0.0003
33	9.0901	0.0001	9.0661	0.0002	7.5687	0.0010	8.5962	0.0004	8.7568	0.0018	8.5313	0.0001	7.4950	0.0008	7.4112	0.0001
34	9.3701	0.0154	9.2266	0.0000	7.5987	0.0003	8.6368	0.0001	8.8004	0.0038	8.5602	0.0010	7.5112	0.0000	7.4516	0.0007
35	9.3842	0.0001	9.2736	0.0161	7.6299	0.0723	8.6852	0.0013	8.8751	0.0032	8.5760	0.0005	7.5939	0.0404	7.4690	0.0003
36	9.5181	0.0000	9.2943	0.0000	7.7444	0.0001	8.7189	0.0013	8.9732	0.0015	8.6241	0.0131	7.6386	0.0155	7.4797	0.0397
37	9.6584	0.0001	9.3966	0.0001	7.7866	0.0095	8.7500	0.0018	8.9887	0.0192	8.6378	0.0017	7.6802	0.0192	7.5077	0.0120
38	9.6864	0.0011	9.5998	0.0009	7.8062	0.0021	8.7505	0.0182	9.0933	0.0003	8.6537	0.0005	7.7245	0.0002	7.5483	0.0152
39	9.7741	0.0182	9.7158	0.0176	7.8552	0.0004	8.7692	0.0004	9.1581	0.0002	8.6798	0.0052	7.7327	0.0001	7.6381	0.0001
40					7.8788	0.0002	9.1545	0.0001	9.1768	0.0006	9.0684	0.0000	7.7668	0.0001	7.6560	0.0089
41					7.9086	0.0579	9.1747	0.0083	9.2256	0.0087	9.0822	0.0073	7.8498	0.0007	7.6876	0.0043
42					7.9176	0.0013	9.2048	0.0000	9.2275	0.0001	9.1088	0.0000	7.8695	0.0348	7.7185	0.0001
43					7.9444	0.0001	9.2376	0.0035	9.3094	0.0001	9.1301	0.0001	7.9135	0.0007	7.7229	0.0006
44					8.0747	0.0629	9.3070	0.0001	9.5493	0.0046	9.1307	0.0033	7.9879	0.0216	7.8337	0.0181
45					8.1341	0.0023	9.3430	0.0001	9.7390	0.0000	9.2144	0.0002	8.0010	0.0470	7.8767	0.1212
46					8.1804	0.0000	9.4589	0.0006			9.2471	0.0004	8.0700	0.0020	7.8943	0.0009
47					8.2522	0.0007	9.5015	0.0057			9.4541	0.0033	8.1382	0.0005	7.9456	0.0197
48					8.3008	0.0220	9.5891	0.0321			9.4841	0.0296	8.1441	0.0427	8.0617	0.0006
49					8.3469	0.0005	9.6712	0.0003			9.5290	0.0005	8.1515	0.0004	8.0635	0.0016
50					8.4806	0.0214	9.7687	0.0005			9.5843	0.0053	8.2409	0.0005	8.0960	0.0002
51					8.4872	0.0066					9.6285	0.0006	8.2516	0.0025	8.1298	0.0169
52					8.5003	0.0087					9.6503	0.0774	8.3097	0.0002	8.1358	0.0000
53					8.5084	0.0020					9.8417	0.0000	8.3395	0.0247	8.1596	0.0004

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
54					8.5089	0.0018							8.3878	0.0232	8.1701	0.0420
55					8.5443	0.0239							8.4219	0.0150	8.2383	0.0001
56					8.5520	0.0011							8.4497	0.0005	8.2452	0.0001
57					8.5773	0.0011							8.4677	0.0214	8.3258	0.0061
58					8.5917	0.0080							8.4761	0.0112	8.3408	0.0019
59					8.6296	0.0014							8.4843	0.0005	8.3943	0.0006
60					8.6611	0.0000							8.4902	0.0173	8.3998	0.0036
61					8.6677	0.0243							8.4959	0.0010	8.4068	0.0004
62					8.7119	0.0052							8.5219	0.0015	8.4216	0.0094
63					8.7535	0.0008							8.5503	0.0011	8.4482	0.0074
64					8.7598	0.0052							8.5887	0.0014	8.4635	0.0276
65					8.8025	0.0050							8.6165	0.0011	8.4635	0.0077
66					8.8118	0.0097							8.6229	0.0015	8.4696	0.0022
67					8.8393	0.0002							8.7157	0.0099	8.4874	0.0009
68					8.8813	0.0110							8.7231	0.0000	8.5216	0.0030
69					8.9091	0.0171							8.7432	0.0002	8.5423	0.0028
70					8.9133	0.0011							8.7650	0.0003	8.5809	0.0001
71					8.9179	0.0012							8.7816	0.0047	8.5841	0.0007
72					9.0557	0.0000							8.8240	0.0226	8.5907	0.0014
73					9.0925	0.0044							8.8745	0.0000	8.6354	0.0011
74					9.1042	0.0000							8.8775	0.0020	8.6734	0.0008
75					9.1178	0.0068							8.9693	0.0005	8.6771	0.0066
76					9.1400	0.0032							8.9954	0.0001	8.7037	0.0090
77					9.1778	0.0023							8.9955	0.0224	8.7325	0.0168
78					9.1990	0.0009							9.0139	0.0015	8.7911	0.0169
79					9.2065	0.0123							9.0449	0.0078	8.8055	0.0195
80					9.2101	0.0001							9.0480	0.0000	8.8606	0.0030
81					9.2184	0.0101							9.0826	0.0029	8.8817	0.0004
82					9.2321	0.0009							9.0985	0.0001	8.8945	0.0001
83					9.2362	0.0017							9.1055	0.0020	8.9263	0.0117
84					9.3773	0.0118							9.1162	0.0016	8.9681	0.0009
85					9.3941	0.0092							9.1372	0.0231	8.9848	0.0015
86					9.4098	0.0003							9.1448	0.0060	9.0014	0.0003
87					9.4826	0.0092							9.1957	0.0000	9.0278	0.0000
88					9.5384	0.0190							9.2174	0.0013	9.0451	0.0010
89					9.5428	0.0014							9.2189	0.0016	9.0710	0.0000
90					9.5572	0.0330							9.2291	0.0001	9.0820	0.0010
91					9.5877	0.0016							9.2602	0.0128	9.0821	0.0180
92					9.6099	0.0043							9.2898	0.0004	9.0923	0.0030
93					9.6275	0.0003							9.3034	0.0076	9.1151	0.0064
94					9.6358	0.0002							9.3204	0.0027	9.1151	0.0011
95					9.6443	0.0001							9.4155	0.0013	9.1784	0.0006
96					9.6871	0.0019							9.4163	0.0164	9.2223	0.0022
97					9.7148	0.0099							9.4234	0.0023	9.2256	0.0250
98													9.4600	0.0304	9.2387	0.0013
99													9.4981	0.0000	9.2909	0.0003
100													9.5051	0.0127	9.2998	0.0000

Appendix D: Bipyridyl

I. Molecular Structure



DFT/B3LYP

Basis: LANL2DZ

```
   20
 ENER      9 -495.25214
C        3.498559    -0.084824     0.000028
C        2.857317     1.159780    -0.000083
C        1.462481     1.208472    -0.000095
C        0.740852     0.003593     0.000007
N        1.360912    -1.204290     0.000111
C        2.707832    -1.238597     0.000122
C       -0.740841    -0.003579    -0.000001
C       -1.462471    -1.208458    -0.000067
C       -2.857306    -1.159767    -0.000073
C       -3.498549     0.084837    -0.000013
C       -2.707822     1.238610     0.000047
N       -1.360902     1.204303     0.000053
H        4.580209    -0.161608     0.000042
H        3.436405     2.077557    -0.000161
H        0.917249     2.143298    -0.000172
H        3.159580    -2.225611     0.000208
H       -0.917238    -2.143284    -0.000103
H       -3.436395    -2.077544    -0.000125
H       -4.580199     0.161622    -0.000014
H       -3.159570     2.225625     0.000094
```

Approximate Ionization Potential[4]: 8.6 eV

II. Analysis

Table 5. Oscillation Strengths (OS) and energy values (eV) for the physically meaningful roots of bipyridyl. A continuation of the roots can be found on the page 17.

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
1	3.3319	0.0011	3.4594	0.0007	3.4229	0.0007	3.4339	0.0007	3.4226	0.0006	3.4113	0.0005	3.4033	0.0006	3.3966	0.0006
2	3.6628	0.0000	3.7988	0.0000	3.7636	0.0000	3.7726	0.0000	3.7642	0.0000	3.7544	0.0000	3.7451	0.0000	3.7398	0.0000
3	3.9684	0.0000	4.0701	0.0000	3.9772	0.0000	4.0177	0.0000	4.0193	0.0000	3.9773	0.0000	3.9588	0.0000	3.9519	0.0000
4	4.2099	0.0000	4.3470	0.0001	4.2201	0.3771	4.2999	0.3633	4.3007	0.0001	4.2634	0.3692	4.2269	0.3767	4.2168	0.3768
5	4.4661	0.0062	4.3484	0.3549	4.2763	0.0007	4.3050	0.0003	4.3304	0.3642	4.2766	0.0004	4.2570	0.0006	4.2537	0.0006
6	4.4662	0.3593	4.4479	0.0000	4.3099	0.0000	4.3893	0.0000	4.4185	0.0000	4.3497	0.0000	4.3180	0.0000	4.3128	0.0000
7	4.5648	0.0000	4.5529	0.0040	4.4705	0.0030	4.5074	0.0035	4.5030	0.0034	4.4689	0.0029	4.4513	0.0030	4.4417	0.0029
8	4.7440	0.0000	4.8567	0.0000	4.8004	0.0000	4.8232	0.0000	4.8114	0.0000	4.7967	0.0000	4.7807	0.0000	4.7729	0.0000
9	5.0338	0.1773	4.9240	0.1665	4.8044	0.1354	4.8773	0.1555	4.8913	0.1587	4.8451	0.1483	4.8096	0.1335	4.8037	0.1335
10	5.1125	0.0000	4.9791	0.0000	4.8605	0.0000	4.9305	0.0000	4.9595	0.0000	4.8966	0.0000	4.8690	0.0000	4.8597	0.0000
11	5.2137	0.0000	5.3239	0.0228	5.2003	0.0249	5.2728	0.0221	5.2941	0.0218	5.2369	0.0218	5.2074	0.0249	5.2013	0.0251
12	5.4533	0.0264	5.3718	0.0000	5.2733	0.0000	5.3195	0.0000	5.3087	0.0000	5.2890	0.0000	5.2514	0.0000	5.2499	0.0000
13	5.5188	0.0000	5.4034	0.0000	5.2954	0.0000	5.3597	0.0000	5.3791	0.0000	5.3306	0.0000	5.3011	0.0000	5.2959	0.0000
14	5.5873	0.0000	5.5007	0.0821	5.3713	0.1163	5.4482	0.0971	5.4725	0.0908	5.4103	0.1059	5.3139	0.0000	5.3145	0.0000
15	5.6220	0.0741	5.6517	0.0000	5.3813	0.0000	5.5965	0.0000	5.6140	0.0000	5.5607	0.0000	5.3778	0.1149	5.3714	0.1154
16	5.7640	0.0000	5.7444	0.0000	5.5195	0.0000	5.6923	0.0000	5.6834	0.0000	5.6667	0.0000	5.4734	0.0005	5.4720	0.0005
17	6.3002	0.0608	6.1835	0.0665	5.5411	0.0008	6.1152	0.0713	6.1426	0.0672	6.0718	0.0744	5.5245	0.0000	5.5212	0.0000
18	6.3526	0.0000	6.2276	0.0000	5.5837	0.0000	6.1618	0.0000	6.1908	0.0000	6.1167	0.0000	5.5417	0.0000	5.5404	0.0000
19	6.5656	0.0012	6.4035	0.0008	5.6509	0.0001	6.3589	0.0009	6.3515	0.0009	6.2855	0.0008	5.6304	0.0001	5.6290	0.0001
20	6.6268	0.0000	6.4723	0.0000	5.7340	0.0069	6.3936	0.0000	6.4238	0.0000	6.3451	0.0000	5.6937	0.0070	5.6901	0.0069
21	6.9531	0.5232	6.8032	0.5037	5.7663	0.0310	6.5098	0.0000	6.7501	0.0000	6.4525	0.0000	5.6993	0.0286	5.6999	0.0277
22	6.9633	0.0000	6.8081	0.0000	5.9042	0.0384	6.6197	0.0277	6.7526	0.5073	6.5499	0.0228	5.8207	0.0356	5.8085	0.0325
23	7.1172	0.0000	6.9339	0.0000	5.9185	0.0000	6.7206	0.4651	6.8314	0.0000	6.6605	0.4780	5.8519	0.0000	5.8508	0.0000
24	7.4264	0.0000	7.2723	0.0001	6.0221	0.0800	6.7458	0.0000	6.8694	0.0000	6.6767	0.0000	6.0276	0.0792	6.0219	0.0807
25	7.4275	0.0000	7.3438	0.0236	6.0577	0.0000	6.7539	0.0000	6.9360	0.0115	6.6890	0.0000	6.0488	0.0059	6.0342	0.0057
26	7.4782	0.0005	7.3504	0.0001	6.1052	0.0058	6.8499	0.0020	7.1036	0.0000	6.7738	0.0000	6.0489	0.0000	6.0358	0.0000
27	7.5136	0.0001	7.4343	0.0021	6.1375	0.0000	6.8640	0.0000	7.1869	0.0011	6.7760	0.0020	6.0626	0.0000	6.0527	0.0000
28	7.5375	0.1021	7.4868	0.0000	6.2071	0.0000	6.8961	0.0970	7.2209	0.0757	6.8431	0.0861	6.1079	0.0000	6.0956	0.0000
29	7.6057	0.0031	7.5567	0.0000	6.2777	0.0000	6.9808	0.0000	7.2217	0.0001	6.9161	0.0000	6.1985	0.0000	6.1860	0.0000
30	7.6330	0.0000	7.5631	0.3389	6.2929	0.0000	7.2204	0.0000	7.2657	0.0000	7.1515	0.0000	6.2720	0.0009	6.2551	0.0009
31	7.6955	0.0042	7.6296	0.0000	6.2975	0.0010	7.2777	0.0270	7.2850	0.0000	7.1990	0.0301	6.2781	0.0000	6.2630	0.0000
32	7.7188	0.0000	7.6971	0.2067	6.3385	0.0000	7.2873	0.0000	7.3133	0.0504	7.2038	0.0001	6.2962	0.0000	6.2861	0.0000
33	7.7507	0.2593	7.7003	0.0000	6.4128	0.0000	7.3482	0.1052	7.3642	0.0025	7.2683	0.1099	6.3372	0.0000	6.3221	0.0000
34	7.8317	0.1259	7.7219	0.0149	6.5090	0.0372	7.3616	0.0029	7.4557	0.0000	7.2769	0.0028	6.4272	0.0128	6.4151	0.0115
35	7.8502	0.0000	7.8240	0.0000	6.5306	0.0006	7.4071	0.0000	7.5849	0.4880	7.3389	0.0000	6.4743	0.0498	6.4609	0.0550
36	7.8894	0.2321	7.8376	0.0026	6.5475	0.2390	7.4836	0.0000	7.5906	0.0000	7.3687	0.0000	6.4880	0.0007	6.4783	0.0013
37	7.9560	0.0000	7.8394	0.0000	6.6271	0.2809	7.5387	0.4881	7.6430	0.0000	7.4380	0.0033	6.5914	0.4074	6.4864	0.0008
38	7.9816	0.0000	7.8769	0.0000	6.6814	0.0000	7.5623	0.0039	7.6555	0.0800	7.4669	0.4829	6.6240	0.0990	6.5663	0.4065
39	7.9874	0.0000	7.9130	0.0000	6.6842	0.0000	7.6114	0.0000	7.7494	0.0942	7.4851	0.0000	6.6419	0.0000	6.5788	0.0000
40	8.0070	0.0000	7.9944	0.1011	6.7292	0.0154	7.6248	0.0683	7.7634	0.0000	7.5621	0.0000	6.6448	0.0000	6.5960	0.0714
41	8.0243	0.0000	8.0344	0.0000	6.7647	0.0000	7.6352	0.0000	7.7717	0.0019	7.5699	0.0542	6.6621	0.0000	6.6380	0.0000
42	8.1286	0.0000	8.0682	0.0000	6.7726	0.0000	7.6911	0.0000	7.8437	0.0000	7.6058	0.0000	6.7346	0.0014	6.6460	0.0000
43	8.2124	0.0000	8.1102	0.0005	6.8049	0.0000	7.7245	0.0000	7.9874	0.0000	7.6291	0.0000	6.7471	0.0000	6.7279	0.0205
44	8.3619	0.0006	8.2144	0.0000	6.9115	0.0011	7.7621	0.0000	7.9985	0.0026	7.6745	0.0000	6.7623	0.0000	6.7325	0.0000
45	8.4102	0.0000	8.2500	0.0000	6.9209	0.0156	7.7675	0.0019	8.0070	0.0000	7.6848	0.0000	6.7910	0.0112	6.7580	0.0151
46	8.4979	0.0594	8.3280	0.0588	6.9410	0.0021	7.7933	0.0000	8.0451	0.0001	7.7057	0.0012	6.8591	0.0009	6.7628	0.0000
47	8.5080	0.0000	8.3518	0.0000	6.9560	0.0054	7.8225	0.0000	8.0556	0.0004	7.7194	0.0000	6.8746	0.0000	6.8061	0.0000
48	8.5256	0.0000	8.3584	0.0000	6.9645	0.0000	7.8361	0.0000	8.1309	0.0000	7.7289	0.0000	6.9148	0.0064	6.8292	0.0007
49	8.5312	0.0001	8.3661	0.0002	7.0492	0.0000	7.9368	0.0000	8.1497	0.0000	7.7502	0.0000	6.9768	0.0297	6.8374	0.0000
50	8.5392	0.1241	8.6436	0.0000	7.0798	0.0126	7.9619	0.0649	8.1510	0.0000	7.8284	0.0827	6.9926	0.0000	6.8598	0.0000
51	8.7794	0.0000	8.6857	0.0000	7.0990	0.0000	7.9629	0.0000	8.1815	0.0000	7.9043	0.0000	6.9947	0.0000	6.9131	0.0064
52	8.8149	0.0000	8.6890	0.1628	7.1036	0.0887	7.9698	0.0000	8.2618	0.0000	7.9157	0.0000	7.0036	0.0002	6.9573	0.0002
53			8.7245	0.0000	7.1059	0.0004	8.0529	0.0009	8.2824	0.0000	7.9580	0.0000	7.0235	0.0023	6.9577	0.0029
54			8.7517	0.0665	7.1422	0.0018	8.0640	0.0021	8.2866	0.0252	7.9744	0.0009	7.0373	0.0133	6.9692	0.0000
55			8.7715	0.0001	7.1558	0.0000	8.1430	0.0000	8.2974	0.0009	7.9934	0.0020	7.1042	0.0000	6.9777	0.0000
56			8.8078	0.0011	7.1852	0.0000	8.1694	0.0000	8.3109	0.0000	8.0730	0.0136	7.1165	0.0000	7.0352	0.0134

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
57					7.2001	0.0003	8.1817	0.0000	8.3112	0.0000	8.0847	0.0000	7.1175	0.0000	7.0523	0.0000
58					7.2124	0.0891	8.2446	0.0069	8.3868	0.0972	8.0865	0.0000	7.1407	0.0000	7.0851	0.0000
59					7.2300	0.0000	8.2523	0.0178	8.3989	0.0010	8.0964	0.0080	7.1767	0.0003	7.0910	0.0108
60					7.2413	0.0000	8.2573	0.0210	8.4149	0.0000	8.1801	0.0056	7.1812	0.0183	7.1211	0.0000
61					7.2587	0.0000	8.2841	0.0000	8.5717	0.0000	8.1990	0.0000	7.1890	0.0000	7.1628	0.0003
62					7.2765	0.0096	8.2873	0.0000	8.6015	0.0037	8.2115	0.0003	7.2128	0.1234	7.1840	0.0000
63					7.2875	0.0044	8.2934	0.0002	8.6131	0.0046	8.2444	0.0782	7.2159	0.0000	7.2000	0.1555
64					7.2914	0.0000	8.3326	0.0688	8.6171	0.0000	8.2557	0.0000	7.2233	0.0097	7.2008	0.0000
65					7.3226	0.0132	8.3501	0.0000	8.6534	0.1346	8.2731	0.0000	7.2530	0.0038	7.2084	0.0104
66					7.3524	0.2349	8.5131	0.0000	8.6551	0.0000	8.3374	0.0016	7.2669	0.0110	7.2195	0.0002
67					7.3573	0.0014	8.5240	0.0019	8.6866	0.0000	8.3874	0.0000	7.2820	0.0022	7.2370	0.0029
68					7.3914	0.0000	8.5573	0.0000	8.7090	0.0000	8.4634	0.0000	7.3168	0.0000	7.2396	0.0000
69					7.4048	0.1817	8.6035	0.0000	8.7199	0.0013	8.4683	0.1276	7.3699	0.4061	7.2536	0.0108
70					7.5001	0.0000	8.6071	0.1643	8.8152	0.0295	8.4862	0.0000	7.3746	0.0000	7.2664	0.0010
71					7.5085	0.0584	8.6417	0.0000			8.5082	0.0000	7.3942	0.0000	7.2939	0.0000
72					7.5549	0.0000	8.6515	0.0000			8.5731	0.0000	7.4031	0.0056	7.3054	0.0000
73					7.5568	0.0000	8.7197	0.0016			8.5800	0.0000	7.4428	0.0000	7.3122	0.0055
74					7.5617	0.0000	8.7634	0.0006			8.6192	0.0045	7.4867	0.0003	7.3366	0.3707
75					7.5697	0.0065	8.7871	0.0158			8.6357	0.0008	7.4957	0.0000	7.4409	0.0000
76					7.5956	0.0000	8.8364	0.0000			8.6597	0.0097	7.5067	0.0551	7.4776	0.0683
77					7.6143	0.0015					8.6778	0.0219	7.5386	0.0000	7.4787	0.0000
78					7.6209	0.0000					8.7306	0.0006	7.5479	0.0000	7.4832	0.0000
79					7.6287	0.0000					8.8035	0.0095	7.5550	0.0000	7.5117	0.0154
80					7.6393	0.0004							7.5682	0.0000	7.5190	0.0000
81					7.6773	0.0000							7.5821	0.0016	7.5243	0.0000
82					7.7421	0.0000							7.6137	0.0000	7.5368	0.0000
83					7.7608	0.0000							7.6595	0.0000	7.5431	0.0000
84					7.7764	0.0000							7.6844	0.0000	7.5638	0.0040
85					7.8265	0.0000							7.7260	0.0000	7.5820	0.0013
86					7.8323	0.0008							7.7623	0.0821	7.6426	0.0000
87					7.8485	0.0000							7.7712	0.0011	7.6488	0.0000
88					7.8837	0.0000							7.8020	0.0000	7.6739	0.0027
89					7.9037	0.0018							7.8202	0.0000	7.6839	0.0000
90					7.9174	0.0027							7.8245	0.0000	7.6846	0.0776
91					7.9410	0.0759							7.8276	0.0015	7.7062	0.0000
92					7.9774	0.0008							7.8297	0.0068	7.7074	0.0000
93					7.9894	0.0000							7.8391	0.0000	7.7395	0.0225
94					7.9957	0.0000							7.8445	0.0116	7.7543	0.0009
95					8.0004	0.0046							7.9492	0.0000	7.7573	0.0035
96					8.0570	0.0000							7.9695	0.0000	7.7723	0.0000
97					8.0743	0.0000							7.9696	0.0013	7.7730	0.0000
98					8.1216	0.0000							7.9819	0.0000	7.8015	0.0000
99					8.1538	0.0001							7.9950	0.0028	7.8123	0.0012
100					8.1707	0.0577							8.0247	0.0000	7.8674	0.0000

Appendix E: Furan

I. Molecular Structure

DFT/B3LYP

Basis: LANL2DZ

```
    9
 ENER      8 -229.95201
C        1.120015     -0.328711      0.000001
C        0.721886      0.976317      0.000000
C       -1.120011     -0.328716     -0.000001
C       -0.721888      0.976314     -0.000001
O        0.000003     -1.161322     -0.000003
H        2.072862     -0.827253      0.000002
H       -2.072857     -0.827262     -0.000003
H        1.365072      1.842372      0.000000
H       -1.365078      1.842366     -0.000001
```

Approximate Ionization Potential[5]: 8.8 eV

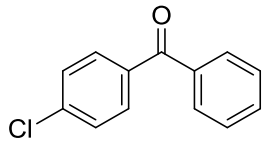
II. Analysis

Table 6 Oscillation Strengths (OS) and energy values (eV) for the physically meaningful roots of furan.

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
1	6.4736	0.1455	6.3255	0.1381	5.4237	0.0000	5.4237	0.0000	6.2580	0.1435	6.0953	0.1479	5.3638	0.0000	5.3571	0.0000
2	6.5750	0.0020	6.4670	0.0010	5.8723	0.1622	5.8723	0.1622	6.4191	0.0005	6.3208	0.0003	5.8138	0.0259	5.7907	0.0236
3	7.9569	0.0000	7.8276	0.0000	5.8745	0.0250	5.8745	0.0250	7.1300	0.0000	6.6934	0.0000	5.8539	0.1637	5.8319	0.1644
4	8.2446	0.0030	8.2964	0.0000	6.0476	0.0000	6.0476	0.0000	7.8423	0.0000	7.3854	0.0135	5.9607	0.0000	5.9339	0.0000
5	8.4072	0.0000	8.2980	0.0014	6.2106	0.0000	6.2106	0.0000	7.9780	0.0084	7.4281	0.0000	6.2088	0.0000	6.2034	0.0000
6	8.6712	0.3479	8.4835	0.3322	6.5509	0.0008	6.5509	0.0008	8.2269	0.0019	7.8073	0.0015	6.4255	0.0000	6.4167	0.0000
7	8.8197	0.1096	8.6693	0.1037	6.5675	0.0155	6.5675	0.0155	8.2395	0.0011	7.8317	0.0036	6.5022	0.0181	6.5064	0.0177
8	9.0160	0.0010	8.8658	0.0009	6.6642	0.0000	6.6642	0.0000	8.3300	0.0013	8.1378	0.3484	6.6172	0.0000	6.5478	0.0000
9			8.9725	0.0001	7.0199	0.0000	7.0199	0.0000	8.3640	0.3382	8.1496	0.0005	6.9551	0.0000	6.6862	0.0043
10			9.0518	0.0004	7.1129	0.0135	7.1129	0.0135	8.5512	0.1098	8.1774	0.0000	6.9630	0.0090	6.9427	0.0000
11					7.1683	0.0066	7.1683	0.0066	8.8709	0.0006	8.3865	0.1117	7.0806	0.0063	7.0354	0.0000
12					7.3785	0.0000	7.3785	0.0000	8.9467	0.0019	8.4918	0.0000	7.1940	0.0000	7.0665	0.0055
13					7.6927	0.0000	7.6927	0.0000	8.9490	0.0000	8.4963	0.0026	7.5627	0.0000	7.4718	0.0142
14					7.7246	0.3257	7.7246	0.3257	9.0378	0.0000	8.8162	0.0022	7.6873	0.2967	7.5641	0.0000
15					7.7870	0.0001	7.7870	0.0001			8.9637	0.0000	7.7337	0.0000	7.6461	0.2381
16					7.9912	0.0000	7.9912	0.0000			9.1734	0.0000	7.8211	0.0006	7.6681	0.0011
17					8.0332	0.0001	8.0332	0.0001					7.8317	0.0021	7.6872	0.0017
18					8.1211	0.0009	8.1211	0.0009					8.0497	0.0428	7.7517	0.0000
19					8.1286	0.1108	8.1286	0.1108					8.0507	0.0000	7.7717	0.0000
20					8.2223	0.0258	8.2223	0.0258					8.0944	0.1036	7.7767	0.0690
21					8.2902	0.0000	8.2902	0.0000					8.0951	0.0015	7.7772	0.0201
22					8.3799	0.0004	8.3799	0.0004					8.1940	0.0098	7.8162	0.0034
23					8.5497	0.0537	8.5497	0.0537					8.2430	0.0000	8.0587	0.0000
24					8.6840	0.0319	8.6840	0.0319					8.2548	0.0012	8.0588	0.0026
25					8.7501	0.0000	8.7501	0.0000					8.3467	0.0460	8.1026	0.0950
26					8.7698	0.0008	8.7698	0.0008					8.4655	0.0000	8.1967	0.0384
27					8.7846	0.0016	8.7846	0.0016					8.4969	0.0008	8.3571	0.0000
28					8.9672	0.0000	8.9672	0.0000					8.6031	0.0276	8.5762	0.0230
29					9.0840	0.0004	9.0840	0.0004					8.7425	0.0005	8.6133	0.0000
30													8.9227	0.0010	8.6406	0.0529
31													8.9627	0.0000	8.7237	0.0098
32													9.0150	0.0529	8.7853	0.0021
33															8.8242	0.0000
34															8.8689	0.0000
35															8.8812	0.0059
36															8.9164	0.0079
37															8.9603	0.0000
38															9.0110	0.0013

Appendix F: Chlorobenzophenone

I. Molecular Structure



DFT/B3LYP

Basis: LANL2DZ

```
   24
 ENER    11 -590.83080
C       -0.957043    -1.195735    -0.007657
C       -2.146349    -0.295115    -0.028611
C        0.430913    -0.641175     0.004659
C        0.752446     0.603921     0.575760
C        2.078458     1.046481     0.622148
C        2.792001    -1.009494    -0.480212
C        1.467455    -1.446350    -0.505319
C        3.072809     0.234302     0.084291
H       -0.025715     1.220928     1.009110
H        1.215141    -2.417376    -0.915529
H        3.589561    -1.620895    -0.883820
Cl       4.801326     0.813338     0.128329
H        2.331674     1.998348     1.072054
O       -1.118598    -2.439023     0.002268
C       -3.353367    -0.783060     0.508796
C       -2.129649     0.979082    -0.627303
C       -3.292992     1.753954    -0.671471
C       -4.508159    -0.001657     0.478668
C       -4.480469     1.270035    -0.110837
H       -1.219080     1.351202    -1.083095
H       -5.429783    -0.381596     0.907434
H       -3.361812    -1.776849     0.942087
H       -5.380771     1.875616    -0.138837
H       -3.272856     2.729077    -1.147239
```

Approximate Ionization Potential[6]: 9.7 eV

II. Analysis

Table 7. Oscillation Strengths (OS) and energy values (eV) for the physically meaningful roots of chlorobenzophenone. A continuation of the roots can be found on the page 22.

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
1	3.0269	0.0010	2.9806	0.0010	2.9605	0.0014	2.9851	0.0010	2.9685	0.0010	2.9668	0.0010	2.9516	0.0013
2	3.8835	0.0305	3.8521	0.0387	3.7654	0.1792	3.8266	0.0735	3.8346	0.1409	3.7978	0.1690	3.7752	0.1720
3	3.9255	0.1823	3.8847	0.1279	3.7956	0.0177	3.8497	0.0969	3.8753	0.0048	3.8316	0.0106	3.8038	0.0173
4	4.1005	0.0345	4.0111	0.0594	3.9534	0.0418	3.9816	0.0625	3.9631	0.0701	3.9613	0.0511	3.9423	0.0498
5	4.2021	0.0167	4.1380	0.0230	4.0507	0.0162	4.1075	0.0193	4.1025	0.0150	4.0804	0.0146	4.0576	0.0159
6	4.2278	0.0159	4.1622	0.0052	4.0818	0.0221	4.1347	0.0084	4.1514	0.0047	4.1111	0.0128	4.0860	0.0166
7	4.3263	0.0408	4.2360	0.0471	4.1735	0.0471	4.2107	0.0487	4.2086	0.0524	4.1922	0.0509	4.1684	0.0499
8	4.4782	0.0075	4.3706	0.0110	4.3316	0.0085	4.3545	0.0096	4.3247	0.0178	4.3353	0.0103	4.3222	0.0093
9	4.7757	0.0001	4.7050	0.0016	4.5980	0.0002	4.7190	0.0002	4.6607	0.0001	4.6186	0.0002	4.6163	0.0002
10	4.8821	0.0010	4.7650	0.0001	4.6668	0.0016	4.7281	0.0013	4.8120	0.0013	4.7852	0.0011	4.7037	0.0017
11	5.0320	0.0060	4.9295	0.0058	4.8163	0.0125	4.8726	0.0083	4.8932	0.0085	4.8452	0.0113	4.8213	0.0125
12	5.0750	0.0017	4.9729	0.0018	4.8389	0.0063	4.9113	0.0029	4.9214	0.0048	4.8706	0.0057	4.8427	0.0056
13	5.1223	0.0104	5.0170	0.0093	4.8896	0.0054	4.9465	0.0103	4.9632	0.0052	4.9186	0.0056	4.8904	0.0062
14	5.2564	0.0017	5.1589	0.0023	5.0182	0.0011	5.0973	0.0019	5.0911	0.0033	5.0493	0.0020	5.0281	0.0012
15	5.2892	0.0039	5.1965	0.0035	5.0881	0.0125	5.1443	0.0048	5.1680	0.0046	5.1251	0.0072	5.0951	0.0108
16	5.3694	0.0825	5.2722	0.1092	5.1020	0.0993	5.2030	0.1130	5.1997	0.1069	5.1466	0.1045	5.1140	0.1014
17	5.5480	0.0820	5.4716	0.0147	5.2685	0.0049	5.4165	0.0044	5.4196	0.0079	5.3645	0.0026	5.2235	0.0035
18	5.6320	0.0370	5.5044	0.0766	5.3290	0.0022	5.4498	0.0891	5.4559	0.0921	5.4015	0.0952	5.3393	0.0029
19	5.6961	0.0244	5.5802	0.0027	5.3651	0.0997	5.5547	0.0099	5.5752	0.0122	5.5104	0.0146	5.3739	0.0915
20	5.7355	0.0263	5.6174	0.0017	5.4569	0.0080	5.5845	0.0179	5.6144	0.0384	5.5463	0.0410	5.4678	0.0130
21	5.7888	0.0092	5.6355	0.0387	5.4627	0.0079	5.6072	0.0118	5.7208	0.0019	5.6180	0.0008	5.5008	0.0360
22	5.8168	0.0180	5.6636	0.0185	5.5103	0.0055	5.6231	0.0181	5.7359	0.0011	5.6588	0.0035	5.5151	0.0037
23	5.8822	0.0033	5.6738	0.0171	5.5280	0.0261	5.6440	0.0191	5.7729	0.0020	5.6934	0.0191	5.5533	0.0003
24	5.8921	0.0072	5.8081	0.0033	5.5496	0.0269	5.7729	0.0022	5.7799	0.0222	5.7197	0.0080	5.5740	0.0053
25	5.9533	0.0225	5.8530	0.0192	5.6144	0.0003	5.8040	0.0192	5.8070	0.0213	5.7548	0.0174	5.6023	0.0222
26	6.0647	0.0091	5.9112	0.0123	5.6751	0.0043	5.8834	0.0492	5.8305	0.0016	5.7770	0.0024	5.6613	0.0041
27	6.0769	0.0612	5.9806	0.0049	5.7207	0.0270	5.8923	0.0109	5.8975	0.0749	5.8259	0.0750	5.7054	0.0179
28	6.1260	0.0111	5.9893	0.0662	5.7561	0.0121	5.9193	0.0238	5.9886	0.0006	5.9428	0.0006	5.7643	0.0318
29	6.2158	0.0004	6.1274	0.0004	5.7661	0.0461	6.0507	0.0007	6.0398	0.0009	5.9456	0.0016	5.7721	0.0030
30	6.2370	0.0056	6.1338	0.0035	5.7934	0.0039	6.0839	0.0153	6.0905	0.0030	6.0127	0.0040	5.8006	0.0546
31	6.2954	0.0918	6.2081	0.1041	5.8627	0.0201	6.1365	0.0944	6.1598	0.0681	6.0863	0.1058	5.8511	0.0019
32	6.4197	0.0055	6.3240	0.0051	5.9182	0.0010	6.2479	0.0059	6.1772	0.0422	6.1330	0.0038	5.8825	0.0036
33	6.4345	0.0997	6.3446	0.1148	5.9444	0.0117	6.2690	0.0406	6.3278	0.1249	6.2127	0.0160	5.9230	0.0078
34	6.5940	0.0203	6.4946	0.1529	5.9525	0.0017	6.3375	0.1563	6.4363	0.2834	6.2874	0.2190	5.9360	0.0015
35	6.6459	0.2730	6.5086	0.1692	5.9862	0.0469	6.4120	0.3124	6.4528	0.0026	6.3513	0.2801	5.9777	0.0272
36	6.7324	0.1040	6.6005	0.0971	6.0321	0.0490	6.4651	0.0090	6.5297	0.1222	6.3767	0.0046	6.0218	0.0601
37	6.7857	0.0596	6.6625	0.0708	6.1135	0.0300	6.5193	0.0814	6.5516	0.0198	6.4579	0.0842	6.0646	0.0002
38	6.8341	0.0052	6.7548	0.0007	6.1248	0.0358	6.5840	0.0923	6.6110	0.1264	6.5185	0.1062	6.0977	0.0625
39	6.9196	0.0227	6.7909	0.0093	6.1478	0.0057	6.6769	0.0005	6.6876	0.0005	6.6121	0.0015	6.1295	0.0075
40	6.9459	0.1259	6.8151	0.0996	6.1584	0.0062	6.7168	0.0105	6.7169	0.0203	6.6503	0.0052	6.1336	0.0011
41	7.0059	0.0155	6.8801	0.0190	6.2179	0.2572	6.7368	0.0801	6.7625	0.0729	6.6791	0.0797	6.2197	0.2521
42	7.1248	0.0065	6.9804	0.0114	6.2810	0.0028	6.8046	0.0149	6.8065	0.0317	6.7386	0.0049	6.2388	0.0021
43	7.1667	0.0107	7.0108	0.0130	6.2947	0.2328	6.8597	0.0196	6.9129	0.0115	6.7666	0.0340	6.2588	0.0453
44	7.2627	0.0231	7.0922	0.0021	6.3361	0.0113	6.9093	0.0180	6.9383	0.0130	6.8419	0.0148	6.3034	0.2212

	6-31G		6-31G**		6-311G++		6-311G**		cc-pVDZ		cc-pVTZ		aug-cc-pVDZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
45	7.2752	0.0835	7.1339	0.0283	6.3751	0.0299	6.9371	0.0189	7.0685	0.0308	6.8648	0.0194	6.3652	0.0296
46	7.3351	0.0722	7.1821	0.0990	6.3893	0.0112	7.0197	0.0014	7.0869	0.0077	6.9207	0.0044	6.3711	0.0031
47	7.3601	0.0109	7.2356	0.0260	6.4116	0.0305	7.0319	0.0036	7.1250	0.1155	6.9697	0.0026	6.4052	0.0147
48	7.3835	0.1477	7.2382	0.0194	6.4590	0.0369	7.0760	0.0483	7.1603	0.0098	7.0067	0.0284	6.4297	0.0275
49	7.4055	0.0161	7.2575	0.0974	6.4743	0.0440	7.1112	0.0924	7.1811	0.0682	7.0487	0.1057	6.4561	0.0100
50	7.4388	0.1318	7.2919	0.0926	6.5032	0.0065	7.1401	0.0507	7.2070	0.0239	7.0654	0.0312	6.4669	0.0594
51	7.5040	0.0033	7.3142	0.0019	6.5125	0.0123	7.1702	0.0259	7.2431	0.0557	7.0936	0.0227	6.4809	0.0134
52	7.5347	0.1263	7.3761	0.0260	6.5311	0.0030	7.1918	0.0565	7.2859	0.0183	7.1113	0.0310	6.5135	0.0114
53	7.5525	0.0372	7.3897	0.1393	6.6206	0.0601	7.1965	0.0239	7.3055	0.0314	7.1256	0.0450	6.5377	0.0089
54	7.5704	0.0150	7.4012	0.0309	6.6295	0.0018	7.2179	0.0753	7.3231	0.1007	7.1451	0.0776	6.5859	0.0043
55	7.5992	0.0150	7.5007	0.0019	6.6313	0.0370	7.2308	0.0038	7.3612	0.0446	7.1553	0.0033	6.5993	0.0033
56	7.6866	0.0061	7.5289	0.0068	6.6429	0.0208	7.2722	0.0024	7.3741	0.0073	7.1942	0.0209	6.6201	0.0235
57	7.7113	0.0622	7.5436	0.0251	6.7106	0.0050	7.2909	0.0217	7.4400	0.0135	7.2073	0.0205	6.6264	0.0196
58	7.7590	0.0013	7.5610	0.0309	6.7161	0.0135	7.3043	0.0190	7.4798	0.0165	7.2402	0.1506	6.6386	0.0569
59	7.7627	0.0018	7.6429	0.0480	6.7188	0.0093	7.3316	0.1334	7.5065	0.0170	7.2742	0.0039	6.6622	0.0165
60	7.7930	0.0497	7.6842	0.0063	6.7329	0.0044	7.3500	0.0133	7.5223	0.0072	7.2818	0.0137	6.6888	0.0011
61	7.8403	0.0065	7.7028	0.0090	6.7500	0.0045	7.4429	0.0182	7.5483	0.0263	7.3601	0.0195	6.6982	0.0054
62	7.8611	0.0017	7.7048	0.0002	6.7544	0.0169	7.4715	0.0287	7.5580	0.0150	7.3792	0.0027	6.7198	0.0184
63	7.8936	0.0055	7.7247	0.0137	6.7872	0.0343	7.4733	0.0151	7.5867	0.0141	7.4055	0.0331	6.7314	0.0150
64	7.9584	0.0220	7.7275	0.0010	6.7889	0.0091	7.5086	0.0018	7.5909	0.0146	7.4404	0.0132	6.7370	0.0223
65	7.9636	0.0112	7.8003	0.0400	6.8173	0.0001	7.5106	0.0240	7.6083	0.0020	7.4535	0.0084	6.7561	0.0002
66	8.0100	0.0410	7.8972	0.0308	6.8239	0.0054	7.5634	0.0424	7.6219	0.0103	7.4741	0.0089	6.7877	0.0132
67	8.0460	0.0010	7.9138	0.0206	6.8437	0.0160	7.5957	0.0032	7.6293	0.0244	7.4996	0.0168	6.8058	0.0166
68	8.0844	0.0538	7.9331	0.0209	6.8507	0.0221	7.6158	0.0077	7.6611	0.0048	7.5133	0.0033	6.8292	0.0158
69	8.1178	0.0018	7.9721	0.0334	6.8746	0.0019	7.6341	0.0045	7.6993	0.0456	7.5158	0.0039	6.8378	0.0038
70	8.1273	0.0219	8.0038	0.0048	6.9520	0.0494	7.6383	0.0006	7.7290	0.0431	7.5282	0.0077	6.9231	0.0154
71	8.1804	0.0074	8.0174	0.0011	6.9664	0.0865	7.6470	0.0011	7.7821	0.0012	7.5515	0.0234	6.9300	0.0241
72	8.2091	0.0807	8.0349	0.0386	6.9796	0.0930	7.6646	0.0289	7.8032	0.0045	7.5843	0.0071	6.9378	0.0469
73	8.2259	0.0044	8.0552	0.0281	6.9844	0.0413	7.6966	0.0088	7.8335	0.0347	7.6151	0.0012	6.9468	0.0494
74	8.2885	0.0005	8.0725	0.0190	7.0034	0.0074	7.7126	0.0023	7.8660	0.0316	7.6489	0.0301	6.9538	0.0458
75	8.2921	0.0021	8.1712	0.0022	7.0136	0.0068	7.7420	0.0288	7.9059	0.0143	7.6686	0.0136	6.9836	0.0244
76	8.3230	0.0005	8.1828	0.0345	7.0438	0.0617	7.7702	0.0141	7.9564	0.0390	7.6973	0.0055	6.9980	0.0769
77	8.3741	0.0462	8.1904	0.0422	7.0567	0.0541	7.8356	0.0259	7.9684	0.0036	7.7391	0.0042	7.0292	0.0604
78	8.4358	0.0158	8.2075	0.0050	7.0903	0.0036	7.8646	0.0261	7.9709	0.0009	7.7593	0.0300	7.0646	0.0228
79	8.4493	0.0026	8.3038	0.0114	7.1031	0.0390	7.9012	0.0181	8.0248	0.0272	7.7862	0.0084	7.0736	0.0383
80	8.4984	0.0470	8.3784	0.0114	7.1247	0.0102	7.9255	0.0057	8.0514	0.0096	7.8012	0.0199	7.0850	0.0271
81	8.5271	0.0130	8.4247	0.0039	7.1285	0.0090	7.9625	0.0046	8.1231	0.0520	7.8368	0.0091	7.1153	0.0129
82	8.5567	0.0079	8.4561	0.0030	7.1692	0.0049	7.9757	0.0433	8.1310	0.0113	7.8755	0.0030	7.1278	0.0089
83	8.5767	0.0332	8.4616	0.0545	7.1812	0.0131	8.0071	0.0092	8.1562	0.0188	7.8905	0.0348	7.1536	0.0060
84	8.6044	0.0204	8.4729	0.0055	7.1837	0.0052	8.0243	0.0013	8.1803	0.0080	7.8936	0.0039	7.1759	0.0039
85	8.6180	0.0291	8.5298	0.0035	7.2073	0.0079	8.0291	0.0018	8.2495	0.0067	7.8998	0.0096	7.1828	0.0045
86	8.6581	0.0032	8.5447	0.0259	7.2367	0.0110	8.0605	0.0024	8.2699	0.0205	7.9451	0.0169	7.2039	0.0180
87	8.6979	0.0041	8.5690	0.0023	7.2708	0.0146	8.0694	0.0010	8.2961	0.0036	7.9741	0.0013	7.2177	0.0190
88	8.7247	0.0042	8.5903	0.0042	7.2771	0.0001	8.0748	0.0058	8.3361	0.0075	8.0111	0.0076	7.2328	0.0148
89	8.7650	0.0044	8.5941	0.0482	7.3002	0.0047	8.1142	0.0111	8.3728	0.0093	8.0358	0.0123	7.2464	0.0023
90	8.7829	0.0135	8.6332	0.0447	7.3441	0.0260	8.1229	0.0607	8.3936	0.0318	8.0566	0.0245	7.2639	0.0099
91	8.7962	0.0107	8.6689	0.0032	7.3589	0.0253	8.1526	0.0221	8.4105	0.0041	8.0719	0.0233	7.2893	0.0005
92	8.8232	0.0133	8.6928	0.0020	7.3800	0.0001	8.2147	0.0040	8.4324	0.0041	8.0869	0.0021	7.3254	0.0202
93	8.8421	0.0236	8.7167	0.0095	7.3823	0.0091	8.2328	0.0004	8.4371	0.0020	8.1002	0.0033	7.3316	0.0032
94	8.8734	0.0666	8.7347	0.0145	7.3884	0.0037	8.2420	0.0138	8.4558	0.0002	8.1332	0.0008	7.3504	0.0112
95	8.9015	0.0016	8.7633	0.0124	7.3967	0.0065	8.2641	0.0042	8.4761	0.0019	8.1606	0.0147	7.3690	0.0255
96	8.9167	0.0071	8.7941	0.0009	7.4256	0.0021	8.3121	0.0075	8.4931	0.0031	8.1723	0.0009	7.3804	0.0002
97	8.9318	0.0043	8.8175	0.0003	7.4330	0.0046	8.3664	0.0134	8.5126	0.0070	8.1909	0.0103	7.4091	0.0129
98	8.9489	0.0050	8.8191	0.0128	7.4525	0.0164	8.3781	0.0070	8.5244	0.0069	8.2419	0.0118	7.4104	0.0031
99	8.9593	0.0179	8.8482	0.0138	7.4690	0.0086	8.3970	0.0035	8.5404	0.0090	8.2536	0.0074	7.4193	0.0042
100	9.0101	0.0025	8.8638	0.0545	7.4809	0.0027	8.4055	0.0123	8.5779	0.0104	8.3079	0.0547	7.4272	0.0016

Appendix G: Benzene

I. Molecular Structure

DFT/B3LYP (?)

Basis: 6-31G+* (?)

No Coordinate Data.

Approximate Ionization Potential[7]: 9.2 eV

II. Analysis

Table 8. Oscillation Strengths (OS) and energy values (eV) for the physically meaningful roots of benzene. A continuation of the roots can be found on the page 25.

	RPA 6-31G		TDA aug-cc-pVDZ		TDA aug-cc-pVTZ		TDA aug-cc-pVQZ		RPA aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
1	5.4533	0.0000	5.2234	0.0000	5.2203	0.0000	5.2185	0.0000	5.2179	0.0000
2	6.3845	0.0000	5.8383	0.0000	5.8331	0.0000	5.8289	0.0000	5.8225	0.0000
3	7.4176	0.5514	5.8384	0.0000	5.8332	0.0000	5.8290	0.0000	5.8226	0.0000
4	7.4176	0.5513	5.9614	0.0000	5.9475	0.0000	5.9455	0.0000	5.9449	0.0000
5	7.4189	0.0000	6.3686	0.0000	6.3481	0.0000	6.3412	0.0000	6.3245	0.0001
6	7.5200	0.0000	6.3686	0.0000	6.3481	0.0000	6.3413	0.0001	6.3245	0.0000
7	7.5201	0.0000	6.3749	0.0466	6.3527	0.0438	6.3459	0.0415	6.3289	0.0395
8	7.5495	0.0048	6.3855	0.0000	6.3648	0.0000	6.3572	0.0000	6.3398	0.0000
9	7.9349	0.0000	6.8130	0.5516	6.7885	0.5422	6.7685	0.5140	6.7307	0.4289
10	7.9350	0.0000	6.8131	0.5515	6.7885	0.5421	6.7685	0.5139	6.7308	0.4292
11	8.5743	0.0000	6.9740	0.0000	6.9416	0.0000	6.9214	0.0000	6.8873	0.0000
12	8.5744	0.0000	6.9849	0.0000	6.9517	0.0000	6.9315	0.0000	6.8958	0.0000
13	9.2666	0.0000	6.9849	0.0000	6.9517	0.0000	6.9316	0.0000	6.8959	0.0000
14	9.2927	0.0000	6.9933	0.0000	6.9599	0.0000	6.9399	0.0000	6.9029	0.0000
15	9.2929	0.0000	7.0165	0.0000	7.0065	0.0000	7.0061	0.0000	6.9884	0.1122
16	9.3482	0.0001	7.1147	0.0000	7.1040	0.0000	7.1035	0.0000	6.9885	0.1120
17	9.4945	0.0000	7.1148	0.0000	7.1040	0.0000	7.1036	0.0000	7.0056	0.0000
18	9.5773	0.0000	7.1394	0.0072	7.1269	0.0074	7.1248	0.0306	7.1030	0.0000
19			7.6069	0.0010	7.2989	0.0070	7.1249	0.0306	7.1030	0.0000
20			7.6069	0.0010	7.2991	0.0070	7.1264	0.0074	7.1258	0.0075
21			7.6824	0.0000	7.4208	0.0000	7.3464	0.0000	7.2271	0.0000
22			7.6825	0.0000	7.4209	0.0000	7.3465	0.0000	7.2273	0.0000
23			7.7672	0.0000	7.7478	0.0000	7.6816	0.0000	7.5441	0.0000
24			7.7692	0.0000	7.7479	0.0000	7.6817	0.0000	7.5442	0.0000
25			7.8544	0.0000	7.7577	0.0000	7.7078	0.0000	7.5799	0.0000
26			7.8545	0.0000	7.7597	0.0000	7.7078	0.0000	7.6033	0.0000
27			8.1962	0.0000	7.9325	0.0000	7.7488	0.0000	7.6034	0.0000
28			8.1963	0.0000	7.9325	0.0000	7.7537	0.0000	7.6075	0.0000
29			8.2835	0.0003	7.9826	0.0000	7.7557	0.0000	7.7466	0.0000
30			8.2866	0.0006	8.0521	0.0000	7.7907	0.0000	7.7486	0.0000
31			8.2943	0.0322	8.2480	0.0000	7.9488	0.0000	5.2425	0.0000
32			8.2944	0.0320	8.2480	0.0000	7.9489	0.0000	5.8231	0.0000
33			8.3389	0.0000	8.2597	0.0004	8.1299	0.0007	5.8232	0.0000
34			8.3394	0.0000	8.2628	0.0008	8.1301	0.0000	6.1966	0.0000
35			8.3394	0.0000	8.2689	0.0284	8.1366	0.0000	6.3249	0.0000
36			8.4549	0.0000	8.2689	0.0281	8.1377	0.0124	6.3249	0.0000
37			8.5641	0.0000	8.2963	0.0000	8.1717	0.0000	6.3301	0.0409
38			8.5642	0.0000	8.2964	0.0000	8.1719	0.0000	6.3398	0.0000
39			8.5916	0.0305	8.3088	0.0000	8.2379	0.0000	6.8395	0.1711
40			8.7968	0.0000	8.3088	0.0000	8.2380	0.0000	6.8396	0.1712
41			8.7968	0.0000	8.3165	0.0000	8.2532	0.0004	6.8876	0.0000
42			8.8021	0.0000	8.3186	0.0184	8.2560	0.0012	6.8964	0.0000
43			8.8089	0.0159	8.3574	0.0000	8.2614	0.0273	6.8965	0.0000
44			8.8580	0.0000	8.3575	0.0000	8.2616	0.0266	6.9046	0.0000
45			8.8582	0.0000	8.5901	0.0402	8.4943	0.0000	7.0058	0.0000
46			8.8760	0.0000	8.6719	0.0000	8.5113	0.0000	7.1139	0.0000
47			8.8777	0.0000	8.6900	0.0000	8.5171	0.0000	7.1140	0.0000
48			8.8782	0.0000	8.6952	0.0000	8.5328	0.0000	7.1380	0.0080

	RPA 6-31G		TDA aug-cc-pVDZ		TDA aug-cc-pVTZ		TDA aug-cc-pVQZ		RPA aug-cc-pVTZ	
Roots	Energy	OS	Energy	OS	Energy	OS	Energy	OS	Energy	OS
49			8.8888	0.0000	8.7129	0.0000	8.5837	0.0326	7.2326	0.0000
50			8.9093	0.0000	8.8415	0.0000	8.7323	0.0000	7.2329	0.0000
51			8.9093	0.0000	8.8432	0.0000	8.7781	0.0000	7.3901	0.6106
52			8.9307	0.0000	8.8435	0.0000	8.7783	0.0002	7.3901	0.6107
53			8.9416	0.0000	8.8916	0.0000	8.7811	0.0000	7.5456	0.0000
54			9.0328	0.0000	8.9136	0.0001	8.8190	0.1496	7.5457	0.0000
55			9.1020	0.0000	8.9137	0.0000	8.8218	0.0000	7.5799	0.0000
56			9.1020	0.0000	8.9581	0.1465	8.8226	0.0000	7.6040	0.0000
57			9.1178	0.0000	8.9599	0.0000	8.8228	0.0000	7.6041	0.0000
58			9.1234	0.0000	9.0108	0.0000	8.8264	0.0000	7.6217	0.0000
59			9.1235	0.0000	9.0788	0.0000	8.8359	0.0043	7.7516	0.0000
60			9.1978	0.0000	9.0788	0.0000	8.8360	0.0043	7.7537	0.0000
61			9.1979	0.0000	9.0906	0.0000	8.8650	0.0000	7.7577	0.0000
62			9.2512	0.0000	9.0916	0.0000	8.9552	0.0000	7.7577	0.0000
63			9.2698	0.1879	9.1010	0.0000	8.9573	0.0000	7.8464	0.0000
64			9.4493	0.0000	9.1010	0.0000	9.0088	0.0000	7.8467	0.0013
65			9.4513	0.0000	9.1360	0.0000	9.0745	0.0000	7.8535	0.0000
66			9.5613	0.0000	9.1381	0.0000	9.0746	0.0000	7.8552	0.0138
67					9.1488	0.0000	9.0894	0.0000	8.0327	0.0000
68					9.2176	0.0026	9.0947	0.0000	8.0328	0.0000
69					9.2176	0.0026	9.0949	0.0000	8.2230	0.0000
70					9.3381	0.0000	9.2585	0.0000	8.2385	0.0000
71					9.3399	0.0000	9.2589	0.0000	8.2386	0.0000
72					9.4986	0.0000	9.2631	0.0000	8.2394	0.0004
73					9.4988	0.0000	9.2649	0.0000	8.2417	0.0004
74					9.5851	0.0000	9.3516	0.0000	8.2478	0.0186
75							9.3551	0.0000	8.2479	0.0187
76							9.3558	0.0000	8.2530	0.0000
77							9.3585	0.0000	8.2690	0.0000
78							9.3832	0.0000	8.2690	0.0000
79							9.3833	0.0000	8.4771	0.0000
80							9.5692	0.0319	8.5315	0.0000
81									8.5518	0.0007
82									8.5520	0.0000
83									8.5725	0.0052
84									8.5863	0.1506
85									8.5932	0.0000
86									8.6306	0.0474
87									8.6306	0.0474
88									8.7862	0.0000
89									8.7876	0.0000
90									8.7882	0.0000
91									8.7885	0.0000
92									8.7906	0.0000
93									8.8290	0.0000
94									8.9885	0.0000
95									8.9888	0.0000
96									9.0090	0.0000
97									9.0493	0.0000
98									9.0498	0.0000
99									9.0505	0.0000
100									9.0544	0.0000
101									9.0644	0.0000
102									9.0646	0.0000
103									9.0955	0.0000
104									9.0960	0.0000
105									9.0960	0.0000
106									9.1460	0.0000
107									9.1474	0.0000
108									9.1978	0.0000
109									9.1983	0.0000
110									9.4538	0.0000
111									9.4645	0.0000
112									9.4647	0.0000
113									9.4755	0.0000
114									9.4915	0.0237
115									9.4934	0.0233
116									9.5386	0.0000

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