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IR Spectra of Dye Molecules Calculated Using Density Functional Theory

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14. ABSTRACT Calculations of IR absorption spectra for energy-minimized dye molecules using density function theory (DFT) are presented. These calculations can provide interpretation of absorption spectra with respect to isolated molecular structure for excitation by electromagnetic waves at IR frequencies. The absorption spectra corresponding to excitation states of isolated molecules are to be associated with molecular-level response modes that are uncoupled to other molecules at zero temperature, in contrast to that of bulk systems at finite temperature. DFT-calculated absorption spectra represent quantitative estimates that can be correlated with additional information obtained from laboratory measurements. The DFT software GAUSSIAN was used for calculations of vibrational excitation states presented here.						
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Introduction

This report presents calculations of IR spectra using density functional theory (DFT) for a set of dye molecules as isolated structures and within solvent backgrounds. The dye molecules whose spectra are considered, designated according to wavelength (nm) of maximum IR absorption, are triarylamine (Dye 978), tetraaryldiamine (Dye 949), transition metal dithiolene (Dye 836) and indolium iodide (Dye 775) (see reference [1]). References [2,3] describe the formalism underlying DFT calculations of IR absorption spectra corresponding to vibrational states of molecules.

The DFT software GAUSSIAN (G09 for this study) can be used to compute approximations of IR absorption spectra for a single molecule or molecule within a solvent background [2,3]. For IR spectra, this program calculates vibrational frequencies by determining second derivatives of the energy with respect to the Cartesian nuclear coordinates, and then transforming to mass-weighted coordinates at a stationary point of the geometry. The IR absorption spectrum is obtained using DFT to compute ground state electronic structure in the Born-Oppenheimer approximation using Kohn-Sham DFT [4-9]. GAUSSIAN uses specified orbital basis functions to describe the electronic wavefunctions and electronic charge density. For a given set of nuclear positions, the calculation directly gives the electronic charge density of the molecule, the potential energy V , and the displacements in Cartesian coordinates of each atom. The procedure for vibrational analysis used in GAUSSIAN is described in reference [3], and is reviewed in reference [9].

Energy-Minimized Structures and Their IR Spectra

Results of a computational investigation using DFT concerning dye molecules 775, 836-Metals, 949 and 978 [1] are presented. These results include the energy-minimized configuration of these molecules, their ground-state oscillation frequencies and their IR intensities. The DFT calculations have resulted in molecular geometries corresponding to energetically stable structures. For these calculations, geometry energy optimization and vibrational analysis was effected using DFT model B3LYP [10,11] and orbital basis functions indicated below, for each molecule [12,13]. These basis functions are described in reference [14]. Graphical representations of stable molecular geometries for dyes 775, 836-Metals, 949 and 978 and their IR spectra are shown in Figs. (1) through (24). IR intensities as a function of frequency, for molecules and IR spectra shown in Figs. (1) through (24), are given in Tables 1 through 12.

Conclusion

The DFT calculated absorption spectra given here provide information concerning the molecular level dielectric response of certain dye molecules for the IR range of frequencies. The calculations of IR spectra associated with these dye molecules are meant to serve as reasonable estimates of molecular level response characteristics, providing interpretation of dielectric response features. The calculated spectra reported here can complement measured and calculated absorption spectra outside the IR range of frequencies.

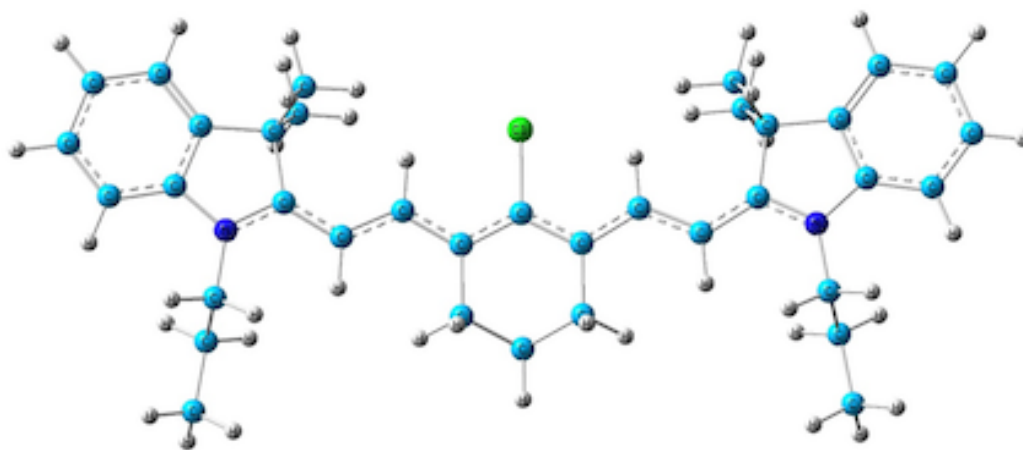


Figure 1. Dye 775, $C_{36}H_{44}ClN_2I$, DFT model and basis function rB3LYP/6-311+G(d,p) after geometry optimization.

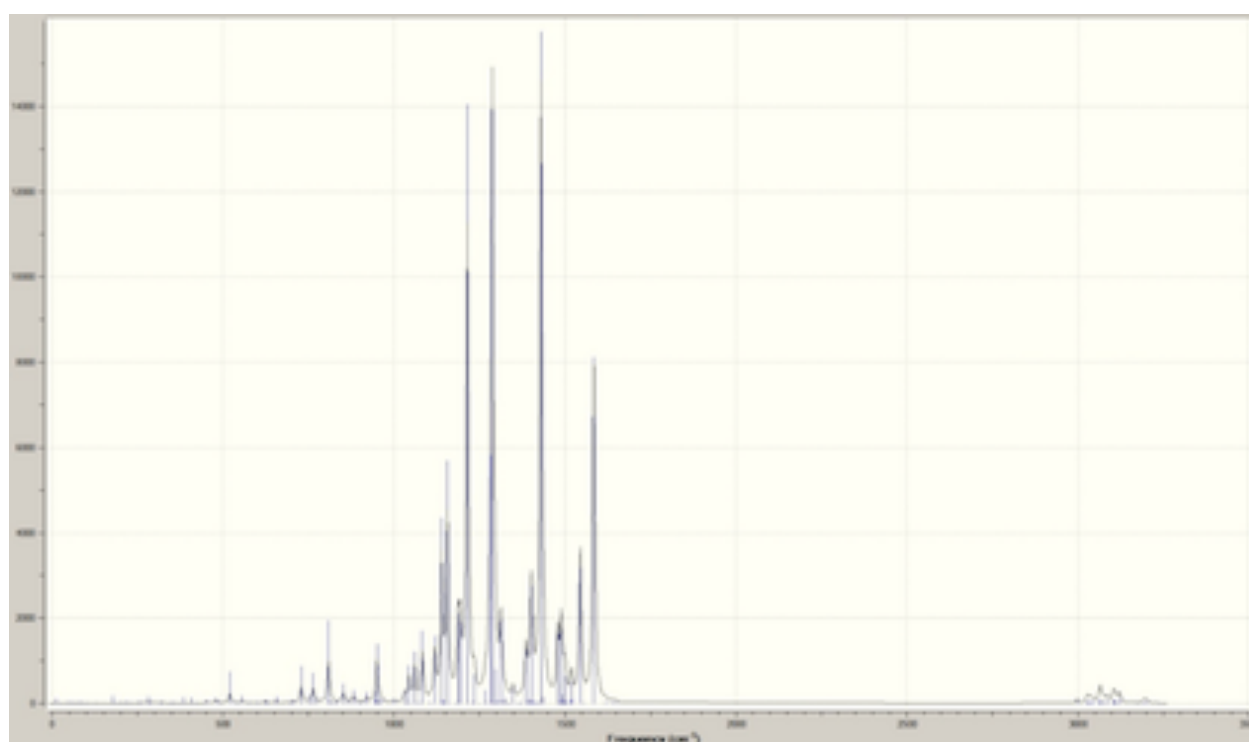


Figure 2. DFT calculated IR spectrum (arbitrary units) of dye 775, $C_{36}H_{44}ClN_2I$.

Table 1. DFT calculated IR spectrum of dye 775, $C_{36}H_{44}ClN_2I$.

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	9.4567	0.0112	82	824.7212	4.1345	163	1416.9139	7.1389
2	12.1251	0.2685	83	830.4839	0.0677	164	1421.8176	0.9953
3	19.6115	0.0217	84	834.8111	6.6054	165	1421.891	9.1974
4	28.3942	0.072	85	852.1771	72.0445	166	1429.9424	4229.936
5	35.2145	0.0249	86	864.1001	18.1636	167	1437.0118	40.6121
6	39.2141	0.0308	87	873.3529	1.3002	168	1437.329	14.239
7	42.5043	0.0236	88	873.3636	0.0212	169	1479.1251	443.7982
8	48.7502	0.4627	89	881.6921	51.1737	170	1485.1501	0.1457
9	53.2141	0.0629	90	894.0351	1.11	171	1485.2104	0.0523

10	61.64	0.4677	91	894.3845	5.6354	172	1487.6304	0
11	70.8031	0.1329	92	901.6247	0.2283	173	1487.663	7.2812
12	81.8835	0.8071	93	905.4065	6.5056	174	1489.2465	480.234
13	89.9974	0.07	94	921.1189	43.9731	175	1489.3271	4.0887
14	91.994	0.2127	95	943.7053	14.3484	176	1492.1862	52.7639
15	101.5364	0.0979	96	948.4443	49.4709	177	1495.3282	3.26
16	101.6806	0.4589	97	949.1132	3.8707	178	1495.3376	8.644
17	128.0692	0.5136	98	950.4308	247.2545	179	1498.7605	5.3475
18	130.9439	0.1117	99	950.6448	3.4958	180	1500.0032	177.3886
19	137.8527	0.0492	100	956.795	0.2693	181	1500.5416	16.2705
20	151.3806	0.2164	101	957.0065	6.7044	182	1501.6263	11.4556
21	177.6881	5.8438	102	961.9655	9.1205	183	1501.6827	0.1337
22	187.6469	0.6349	103	963.4648	20.5279	184	1504.1985	2.7291
23	199.1127	1.0809	104	1000.2446	14.5749	185	1504.5083	0.9545
24	206.9856	0.4728	105	1001.6823	0.1846	186	1504.7104	12.7
25	216.5962	1.7011	106	1001.6871	0.0559	187	1504.9167	1.8585
26	218.8459	0.0072	107	1031.783	61.177	188	1516.2813	15.3317
27	228.2614	0.7428	108	1032.2283	0.2595	189	1516.5211	10.5635
28	228.9215	0.0621	109	1035.7904	0.0978	190	1519.6024	138.3388
29	229.6261	0.0103	110	1035.8462	1.3059	191	1520.6841	28.196
30	242.1845	0.2424	111	1044.3439	175.3732	192	1544.6617	1045.1788
31	242.3497	0.0283	112	1044.9344	1.4161	193	1554.8232	6.3923
32	251.1725	2.1081	113	1061.269	242.7891	194	1584.5188	2416.9038
33	252.4301	0.2113	114	1064.1139	4.7564	195	1620.7073	14.7853
34	261.0562	1.3441	115	1076.4146	1.6911	196	1637.6516	10.4351
35	261.5704	0.0751	116	1082.5298	344.3254	197	1637.8892	5.316
36	281.9508	8.5352	117	1105.5442	5.1664	198	1650.4781	10.7123
37	283.1093	0.3824	118	1106.6439	4.9542	199	1651.8005	1.5796
38	287.5904	0.2189	119	1119.2986	334.4565	200	2998.134	4.7704
39	291.5413	0.1343	120	1120.3209	4.1903	201	2998.6248	24.4029
40	318.6769	0.2234	121	1140.1068	932.467	202	3026.7639	10.1237
41	320.0809	3.3926	122	1142.5996	15.7917	203	3026.7979	28.3893
42	344.6857	0.162	123	1147.1764	3.1434	204	3030.636	18.1637
43	344.7163	0.8905	124	1147.2509	2.6916	205	3033.7778	0.0052
44	352.2668	0.7303	125	1156.6722	1235.9312	206	3033.7854	28.2688
45	353.4232	1.7743	126	1161.0535	0.2475	207	3042.1804	0.0952
46	370.1685	0.9618	127	1179.825	4.0869	208	3042.2034	25.1477
47	384.3889	10.4705	128	1187.8248	474.1443	209	3044.3696	0.8554
48	405.6241	9.7449	129	1188.8768	0.1031	210	3044.4521	15.866
49	414.8471	0.1204	130	1194.542	433.3192	211	3060.2952	4.7804
50	424.6401	1.057	131	1195.0778	0.7587	212	3060.3037	0.1235
51	451.4264	7.1982	132	1214.7349	3206.5303	213	3065.2314	57.1717
52	451.7339	1.9825	133	1231.3672	8.5892	214	3065.3962	43.5596
53	479.1213	11.004	134	1234.7754	156.6687	215	3066.9785	6.7154
54	479.3818	5.0522	135	1250.7031	1.8811	216	3069.2954	26.9729
55	488.5933	4.4679	136	1266.5468	71.4182	217	3076.9841	28.2231
56	519.9745	72.0338	137	1270.0996	1.9572	218	3087.865	45.3843
57	527.7273	2.3144	138	1284.2281	1403.8739	219	3087.885	0.6015
58	541.417	1.0067	139	1288.0172	3473.9597	220	3104.0942	1.7498
59	556.0339	18.1023	140	1291.9753	5.8316	221	3104.105	36.2792
60	556.5571	1.5692	141	1297.6864	195.7538	222	3106.3301	41.1268
61	575.4516	2.4121	142	1298.6667	5.6447	223	3106.3506	1.3703

62	576.2366	2.973	143	1305.2479	15.8602	224	3109.1721	0.0021
63	599.3418	4.2476	144	1313.0264	512.9307	225	3109.1836	10.0953
64	623.0378	10.2772	145	1317.3264	13.3154	226	3111.6013	12.5035
65	628.8983	6.0933	146	1326.5981	29.091	227	3111.6826	32.5479
66	629.4725	0.2259	147	1331.6843	0.7645	228	3120.7864	0.2847
67	653.5026	0.6054	148	1333.549	1.4457	229	3120.7888	3.4512
68	655.783	20.825	149	1335.197	0.3904	230	3123.0486	65.1245
69	696.078	1.8687	150	1348.3177	84.5914	231	3123.1072	0.4894
70	699.6522	2.1769	151	1359.3114	0.3058	232	3172.9573	2.1524
71	704.5116	11.2548	152	1366.2047	1.4323	233	3172.9768	4.1032
72	728.715	120.3422	153	1371.1379	9.9532	234	3182.8523	3.308
73	746.5762	0.1157	154	1386.2506	330.0995	235	3182.8525	1.1898
74	752.2559	24.619	155	1392.1055	3.9914	236	3194.6575	3.2922
75	753.3333	0.4659	156	1393.0315	2.041	237	3194.6606	13.7311
76	763.2212	0.1978	157	1394.1755	9.1938	238	3195.8518	3.6449
77	763.3028	101.0471	158	1396.1279	23.6782	239	3195.9558	10.9988
78	774.0505	0.5875	159	1401.5497	782.7378	240	3202.7915	25.064
79	774.1697	19.6875	160	1406.3394	0.1279	241	3202.8125	0.2953
80	808.5025	295.1543	161	1406.4272	14.3735	242	3236.9729	0.6754
81	813.4872	9.747	162	1407.7031	6.8984	243	3237.3054	1.0467

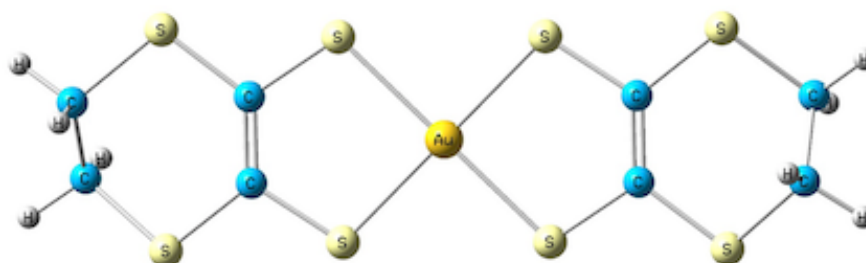


Figure 3. Dye 836-Au, $C_8H_8AuS_8$, DFT model and basis function uB3LYP/QZVP after geometry optimization.

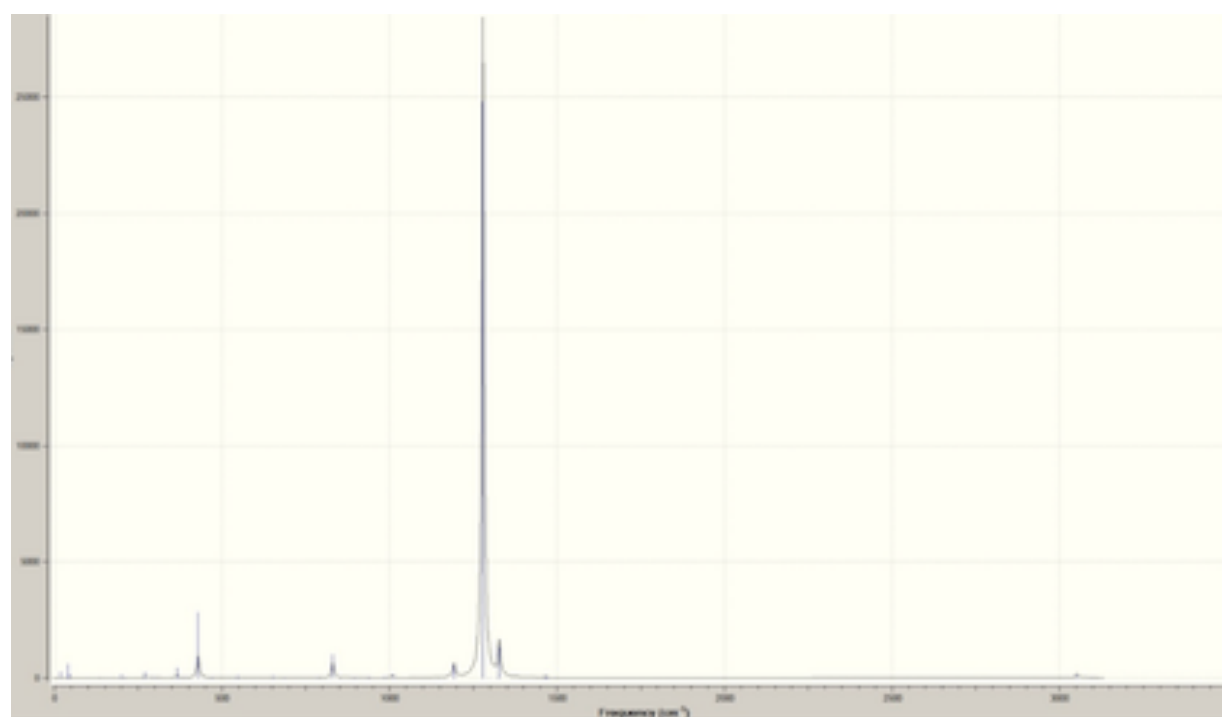


Figure 4. DFT calculated IR spectrum (arbitrary units) of dye FHI83642-Au, $C_8H_8AuS_8$.

Table 2. DFT calculated IR spectrum of dye FHI83642-Au, C₈H₈AuS₈

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	18.9940	1.3540	36	788.9990	0.3840
2	37.0370	0.1650	37	790.8510	7.9160
3	40.1200	5.9770	38	830.5310	211.5050
4	40.9240	0.0000	39	851.7390	0.0000
5	45.9300	1.6060	40	895.2960	3.3170
6	64.9250	0.0800	41	896.9420	2.6320
7	79.5500	0.0200	42	936.7420	0.0490
8	94.8320	0.0000	43	938.0900	0.0000
9	129.0490	0.0000	44	984.9060	11.2830
10	134.9580	0.3830	45	985.4080	0.4250
11	181.9240	0.0020	46	1008.4130	35.1870
12	198.3170	6.9860	47	1008.8020	0.0000
13	209.9140	3.4150	48	1143.4120	0.3530
14	268.3040	0.0000	49	1143.5410	1.7130
15	269.3860	16.4120	50	1192.4430	170.3290
16	289.1970	0.1800	51	1193.6350	0.0000
17	290.0160	0.3460	52	1278.8390	8294.9170
18	303.1790	1.0350	53	1297.1400	0.9540
19	304.3530	0.0000	54	1297.4709	2.7380
20	329.5330	0.0040	55	1321.6770	0.0000
21	342.6550	0.0100	56	1327.5490	444.4170
22	365.2590	40.4320	57	1463.5430	2.8910
23	368.8200	0.0000	58	1463.5540	16.3670
24	382.3900	0.0000	59	1466.3760	0.0000
25	398.4570	0.0210	60	1466.6429	8.9920
26	428.3390	302.7470	61	1471.9240	0.0000
27	441.1130	0.0000	62	3047.4910	1.8970
28	469.0740	0.0390	63	3047.4971	6.8370
29	471.3010	0.2250	64	3052.2510	54.5830
30	544.4500	0.0000	65	3052.3169	0.0080
31	546.3880	10.4660	66	3096.1011	2.6560
32	651.0820	11.5150	67	3096.1411	0.0010
33	651.3170	0.0000	68	3108.8201	2.7230
34	686.2320	0.4680	69	3108.8259	7.0620
35	686.4280	1.2460			

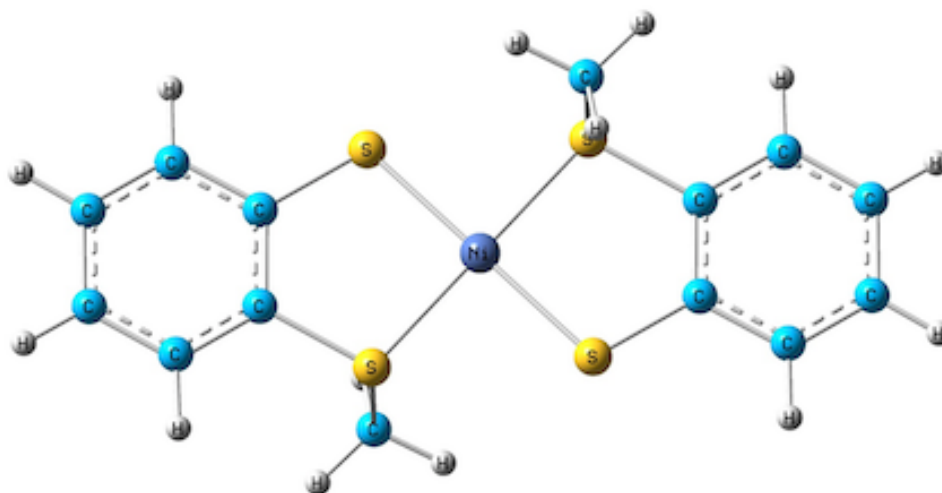


Figure 5. Dye FHI83642-Ni, $C_{14}H_{14}NiS_4$, DFT model and basis function rB3LYP/6-311+G(d,p) after geometry optimization.

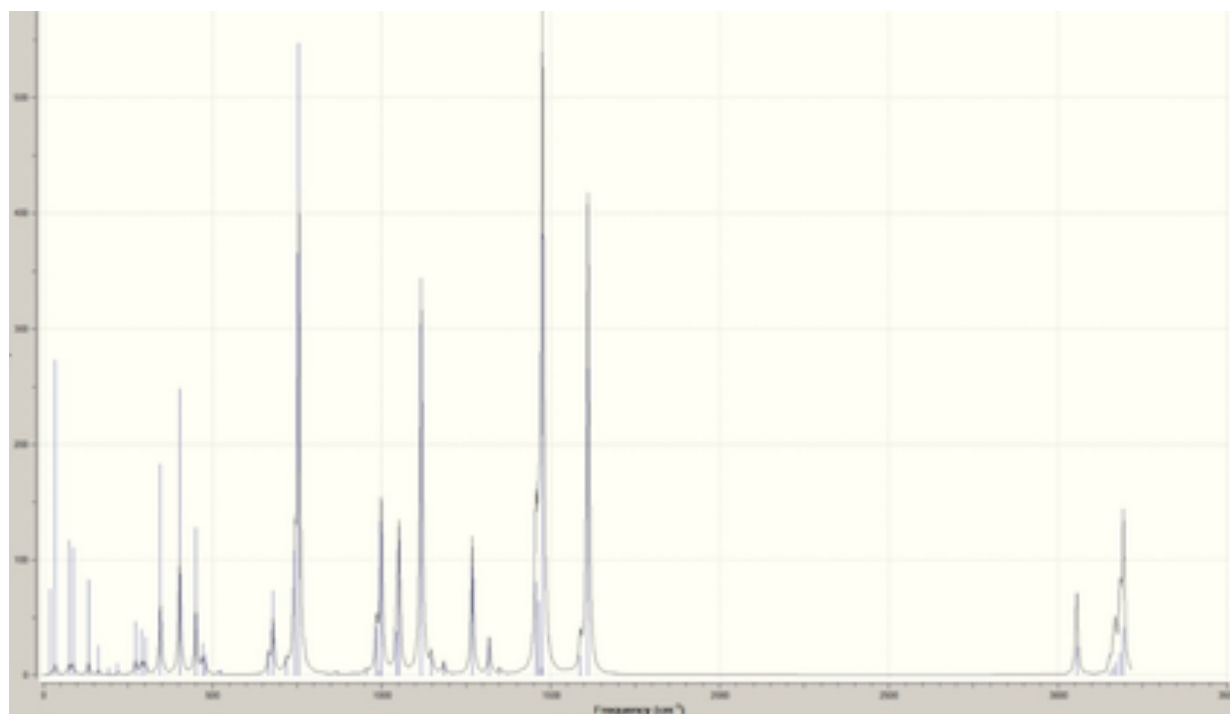


Figure 6. DFT calculated IR spectrum (arbitrary units) of dye FHI83642-Ni, $C_{14}H_{14}NiS_4$.

Table 3. DFT calculated IR spectrum of dye FHI83642-Ni, $C_{14}H_{14}NiS_4$

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	20.3797	0.4477	32	665.3619	0.0000	63	1268.1902	34.7742
2	35.2344	2.8118	33	665.6519	4.3234	64	1318.3732	9.6472
3	46.4497	0.0000	34	678.5626	0.0000	65	1318.4813	0.0000
4	75.6208	2.5852	35	678.5955	14.5039	66	1348.8486	1.5395
5	87.7651	2.8366	36	718.1993	2.7275	67	1349.4901	0.0000
6	96.6678	0.0000	37	718.7481	0.0000	68	1455.7532	0.0000
7	133.3376	3.2041	38	743.1390	0.0000	69	1456.3553	34.4685
8	140.4414	0.0000	39	743.2125	25.7914	70	1464.2178	0.0000
9	153.7205	0.0000	40	754.6133	0.0000	71	1464.4418	27.3499

10	162.7047	1.2157	41	754.9072	120.8704	72	1471.4747	0.0000
11	169.4489	0.0000	42	866.8618	0.0000	73	1471.4968	2.6904
12	192.8835	0.3438	43	867.0222	0.8058	74	1476.0098	164.8259
13	193.3936	0.0000	44	953.5806	0.0000	75	1477.0765	0.0000
14	209.8123	0.0000	45	953.6574	1.1943	76	1587.8877	7.8553
15	219.2784	0.6613	46	982.4346	0.0000	77	1588.1593	0.0000
16	272.4839	3.7080	47	985.1256	12.0855	78	1610.1339	125.1094
17	283.7149	0.0000	48	994.7195	0.0000	79	1610.3269	0.0000
18	289.7251	3.3211	49	994.7797	1.0195	80	3055.4890	21.5872
19	301.2722	2.9075	50	997.3572	0.0000	81	3055.5591	0.0000
20	328.7405	0.0000	51	999.0436	44.3881	82	3152.3606	3.0295
21	346.3013	18.5320	52	1044.4352	11.7520	83	3152.4067	0.0000
22	364.6656	0.0000	53	1044.6180	0.0000	84	3163.3855	1.4531
23	402.9933	29.2206	54	1051.4095	35.9075	85	3163.4160	0.0000
24	446.8901	0.0000	55	1051.8074	0.0000	86	3164.3240	6.0346
25	451.0126	16.8627	56	1117.4246	99.4586	87	3164.3369	0.0000
26	451.9783	0.0000	57	1118.6274	0.0000	88	3170.5264	10.2067
27	470.4206	3.8394	58	1146.9913	0.0000	89	3170.5308	0.0000
28	477.0362	0.0000	59	1147.4969	4.8491	90	3183.7617	0.0000
29	479.4927	2.5502	60	1183.9507	3.1004	91	3183.7700	18.2387
30	522.3286	0.0000	61	1184.0103	0.0000	92	3193.6003	38.6800
31	523.0005	0.7208	62	1267.2614	0.0000	93	3193.6641	0.0000

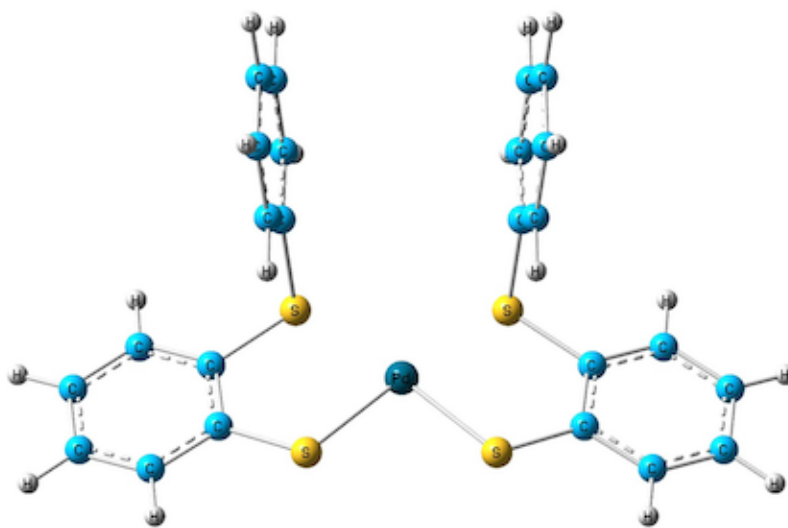


Figure 7. Dye FHI83642-Pd, $C_{24}H_{18}PdS_4$, DFT model and basis function rB3LYP/DGDZVP after geometry optimization.

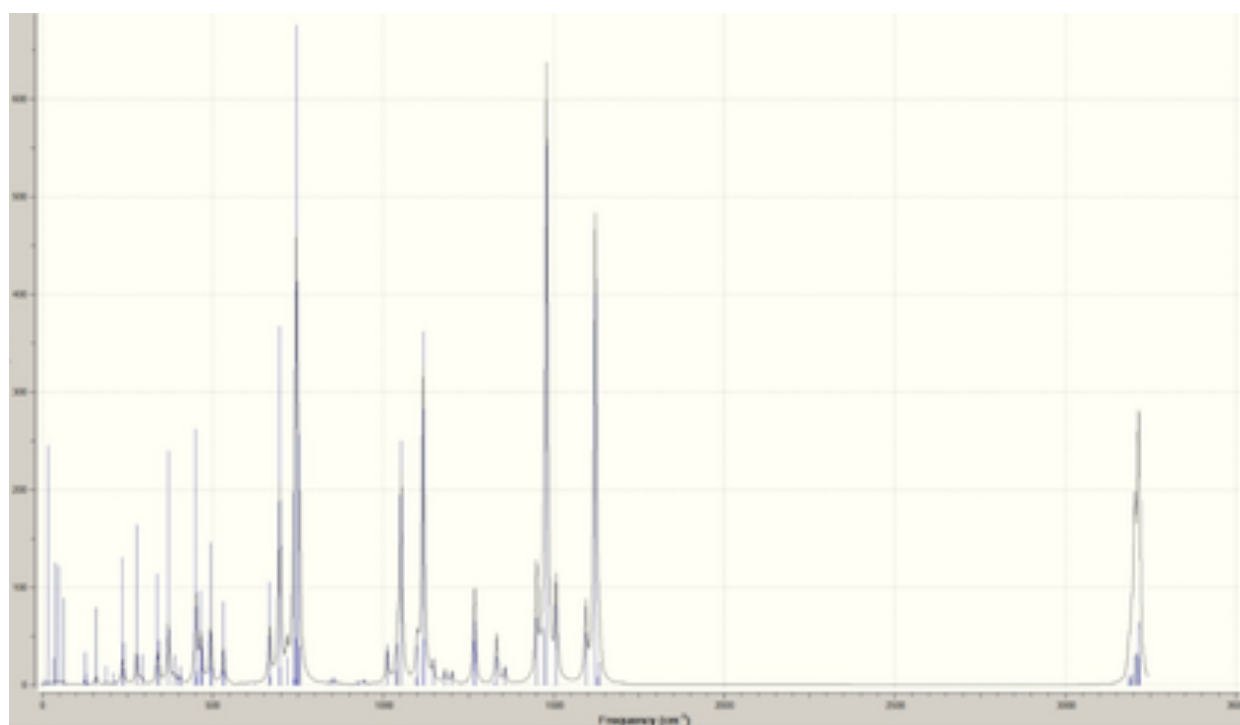


Figure 8. DFT calculated IR spectrum (arbitrary units) of dye FHI83642-Pd, C₂₄H₁₈PdS₄.

Table 4. DFT calculated IR spectrum of dye FHI83642-Pd, C₂₄H₁₈PdS₄

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	6.3048	0.0074	46	696.1108	54.9176	91	1181.3604	3.0002
2	17.6309	0.9278	47	697.9897	0.6902	92	1199.8413	0.5654
3	19.6591	0.0079	48	698.6606	1.1196	93	1201.0345	3.1398
4	32.3385	0.1089	49	699.0326	2.6638	94	1267.2964	12.2059
5	32.4477	0.1946	50	717.9789	4.4165	95	1267.6232	17.7683
6	38.2716	1.0281	51	718.6847	4.2710	96	1324.5114	0.0486
7	48.5852	0.0773	52	738.8888	36.3571	97	1324.7893	1.0301
8	48.7627	1.2705	53	739.4968	0.9946	98	1332.2520	6.3516
9	62.9026	1.2005	54	744.7755	7.6523	99	1332.2614	8.4078
10	65.7927	0.0114	55	745.0501	108.1652	100	1356.0997	0.0000
11	125.2183	0.4356	56	752.3147	44.1050	101	1356.4688	4.9692
12	126.1313	0.8976	57	754.9876	6.4366	102	1449.4880	21.3363
13	127.3633	0.3239	58	842.7895	0.0018	103	1449.9777	12.0290
14	130.3705	0.0632	59	847.1698	1.1139	104	1470.0641	1.7655
15	158.7695	2.7089	60	856.9464	0.0686	105	1470.6002	18.4431
16	188.0754	0.7855	61	856.9949	1.2999	106	1478.5682	175.3909
17	188.5711	0.3591	62	926.9130	0.6153	107	1479.7600	5.7856
18	207.8915	0.5521	63	929.5234	0.2303	108	1506.4550	2.4319
19	219.6976	0.1838	64	943.7401	0.3327	109	1506.8966	26.5761
20	235.4700	6.6097	65	943.7484	1.1876	110	1594.1523	18.2608
21	239.6052	2.2187	66	979.6998	0.0322	111	1594.2650	3.7073
22	276.7849	9.7294	67	981.4834	0.0369	112	1621.2947	139.5760
23	292.7748	1.9556	68	981.5140	0.0073	113	1622.6556	2.0425
24	337.2703	8.2390	69	981.9238	0.0981	114	1628.6246	0.0257
25	342.1329	3.3547	70	997.8617	0.0020	115	1628.7966	2.8930
26	369.8502	19.0033	71	998.7551	0.0533	116	1632.6118	0.2173

27	387.7435	2.5545	72	1011.2414	1.0024	117	1633.0096	8.2128
28	401.2880	0.9348	73	1011.6947	9.0518	118	3185.2197	6.8453
29	404.2271	1.6288	74	1036.5696	3.3728	119	3185.2322	0.4302
30	408.2024	0.0664	75	1036.7432	0.0180	120	3186.3479	0.0556
31	409.6767	0.0136	76	1042.2867	1.9310	121	3186.6252	0.4316
32	448.6181	0.8128	77	1042.7164	9.5280	122	3192.3328	4.8450
33	450.8152	25.3657	78	1052.1237	56.4718	123	3192.3467	2.4405
34	451.4446	1.4091	79	1052.6519	4.7970	124	3194.7544	0.0201
35	464.3410	9.6141	80	1095.0226	1.8399	125	3195.1736	7.7436
36	466.1976	1.8280	81	1095.0452	1.1654	126	3202.7605	0.4525
37	467.8935	4.1321	82	1100.1400	0.0862	127	3202.7781	20.8756
38	493.0394	15.4063	83	1100.6359	9.5278	128	3203.2190	1.6014
39	495.5623	1.9790	84	1116.5345	86.7102	129	3203.7468	20.7072
40	531.4868	9.7751	85	1118.5979	11.1124	130	3211.3125	0.2522
41	532.9739	1.7050	86	1146.4023	5.1874	131	3211.6616	22.4548
42	624.1030	0.0017	87	1146.8669	0.7822	132	3214.3911	44.4883
43	624.3860	0.2222	88	1179.0496	0.0019	133	3214.4485	3.7533
44	667.3155	15.1375	89	1179.3768	0.1079	134	3217.2854	1.6318
45	667.9200	1.3935	90	1181.3046	0.8885	135	3217.4402	19.5434

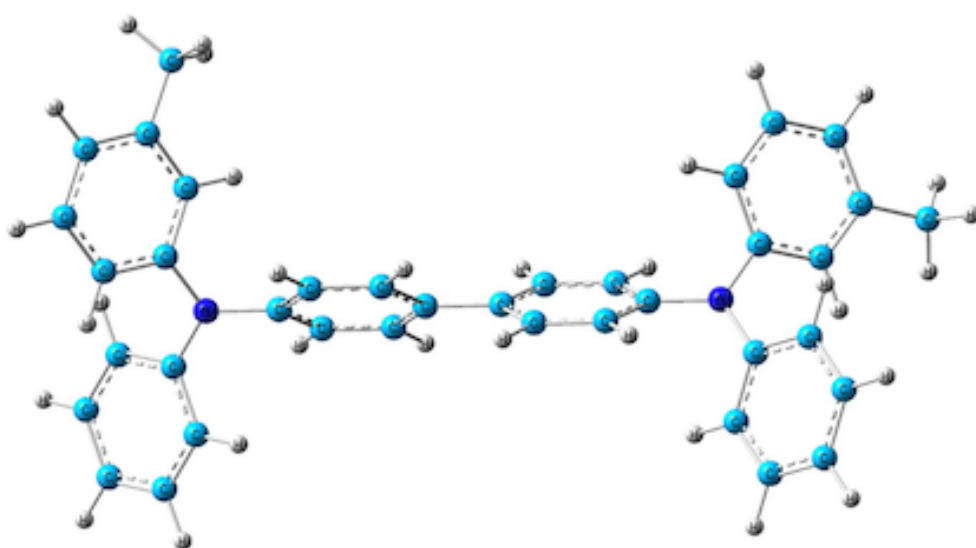


Figure 9. Dye FH94931, $C_{38}H_{32}N_2$, DFT model and basis function rB3LYP/6-311+G(d,p) after geometry optimization.

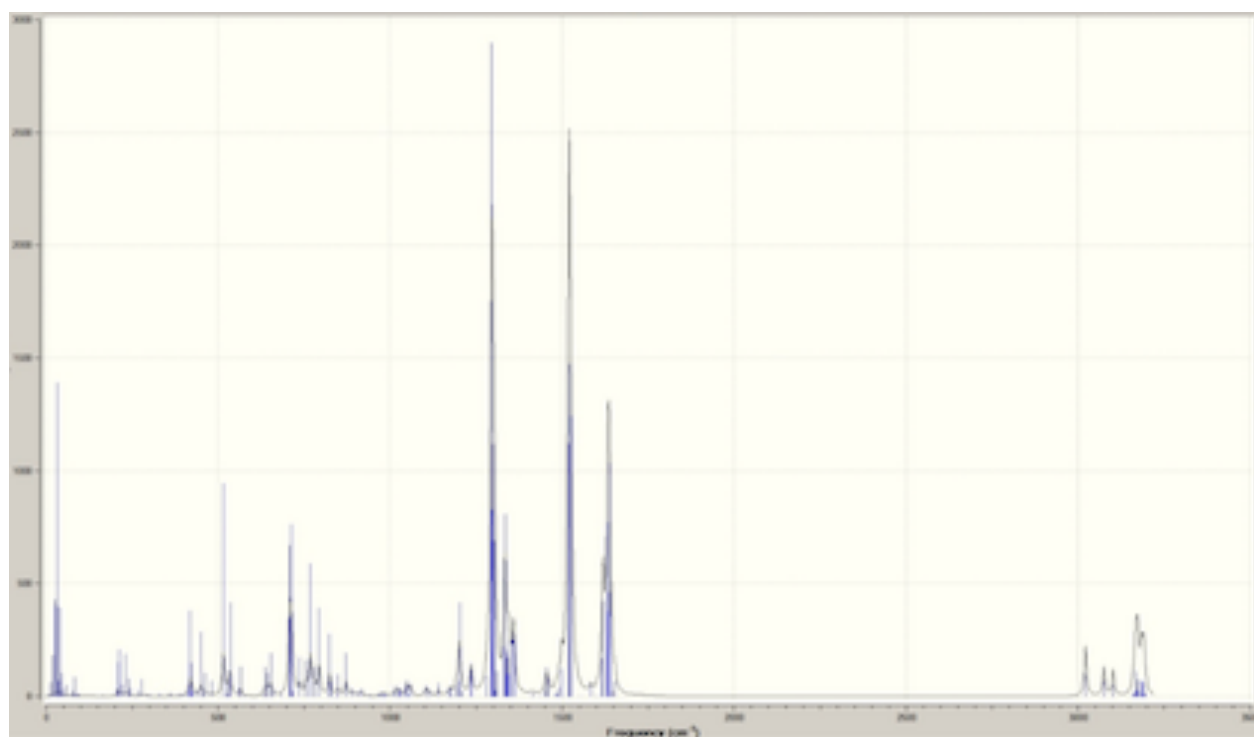


Figure 10. DFT calculated IR spectrum (arbitrary units) of dye FH94931, C₃₈H₃₂N₂.

Table 5. DFT calculated IR spectrum of dye FH94931, C₃₈H₃₂N₂.

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	8.5171	0.0052	71	793.0877	36.2589	141	1334.106	126.224
2	12.7889	0.0918	72	794.3326	4.0707	142	1337.5575	31.2132
3	18.6322	0.3939	73	823.553	26.478	143	1342.5583	26.9794
4	26.4526	1.3218	74	828.2077	6.1246	144	1344.9778	15.2652
5	29.8646	1.405	75	838.9373	0.2752	145	1345.0957	9.2406
6	31.873	5.1889	76	840.071	0.2667	146	1348.4156	38.7761
7	37.2671	0.1686	77	846.4379	0.3312	147	1358.1749	39.5638
8	37.6752	0.3124	78	846.6476	0.222	148	1359.9363	49.5207
9	40.4687	1.8689	79	850.0138	9.5686	149	1413.9948	1.2304
10	45.6957	0.5567	80	871.6786	19.6384	150	1414.0121	2.0119
11	48.6195	0.1698	81	889.4105	2.9058	151	1432.6368	0.5033
12	59.4721	0.3414	82	889.9269	3.4698	152	1449.1198	4.9551
13	72.5953	0.0361	83	904.4282	2.2116	153	1454.7035	21.5581
14	76.4994	0.2167	84	905.2351	1.4055	154	1460.9286	13.5765
15	82.8238	0.8182	85	916.981	3.6224	155	1482.9185	2.4446
16	90.6586	0.0817	86	917.7034	2.5264	156	1484.2144	2.0167
17	94.5716	0.1509	87	941.5331	0.4521	157	1490.2773	6.1414
18	149.2803	0.0194	88	943.9577	0.1669	158	1490.2856	7.0691
19	167.0486	0.0949	89	966.4723	1.0791	159	1498.5887	20.2769
20	203.9834	0.8134	90	970.4154	1.1665	160	1498.9337	21.1746
21	210.5049	3.7414	91	978.6958	1.944	161	1518.9761	198.8834
22	212.4134	5.1168	92	978.9499	2.1955	162	1518.984	191.6613
23	220.4211	1.3204	93	981.9863	0.4723	163	1521.4919	262.3142
24	231.2178	5.0698	94	982.1146	0.1871	164	1522.8295	90.3796
25	239.4807	2.216	95	983.9683	0.5231	165	1526.1527	221.5224
26	243.6738	1.0113	96	983.9953	0.6958	166	1550.9888	0.1159

27	266.0486	0.8721	97	987.5876	0.5807	167	1583.283	8.825
28	278.4355	2.4914	98	987.8889	0.2697	168	1602.7356	0.3178
29	296.7482	0.33	99	997.1897	0.0815	169	1615.4323	31.54
30	323.4844	0.0367	100	997.2686	0.0739	170	1616.9073	21.7638
31	329.3716	0.5093	101	1012.72	0.9345	171	1619.7065	79.9948
32	359.3066	0.6053	102	1012.7819	0.9841	172	1620.5938	36.1678
33	389.1202	0.5148	103	1013.4291	1.5916	173	1632.1992	147.1507
34	401.0262	0.3174	104	1013.6484	1.7334	174	1633.2712	71.835
35	412.8531	2.0386	105	1017.5029	5.3164	175	1635.9264	88.1552
36	418.9425	18.6355	106	1027.8073	3.3667	176	1638.1581	197.6801
37	420.1354	1.2989	107	1028.7914	4.2158	177	1646.0643	4.2708
38	423.0822	7.3781	108	1032.125	1.4605	178	1651.1675	13.0434
39	426.1276	1.0992	109	1047.7017	5.979	179	3020.8589	33.8816
40	437.1487	1.3418	110	1048.6641	8.4046	180	3020.8733	31.8261
41	449.7941	14.955	111	1051.2467	1.0984	181	3074.9871	11.4395
42	455.2391	0.9529	112	1060.0707	6.3517	182	3075.0022	25.6238
43	462.7526	5.6598	113	1060.168	6.7061	183	3101.4531	17.5975
44	480.7242	3.9968	114	1104.0148	5.8939	184	3101.5198	15.8938
45	515.3894	56.9726	115	1104.2289	4.3311	185	3158.4497	3.872
46	525.4308	0.6431	116	1115.1091	3.8471	186	3158.4575	4.8609
47	528.7568	3.4968	117	1115.3492	2.5343	187	3161.7019	5.3834
48	531.124	7.044	118	1140.1417	7.6397	188	3161.7544	4.8788
49	535.5703	26.0036	119	1141.2094	0.3477	189	3167.6094	39.9999
50	559.1248	2.1933	120	1173.6451	5.0376	190	3167.6758	11.5644
51	565.6974	8.5486	121	1174.2628	4.2556	191	3169.1401	10.3469
52	575.63	0.3461	122	1179.8669	0.5611	192	3169.2268	9.6741
53	631.0884	0.4029	123	1179.8846	0.328	193	3172.3982	0.1728
54	631.2802	0.7509	124	1191.3457	6.1794	194	3173.249	2.8767
55	636.8101	9.7136	125	1191.3612	4.8209	195	3173.3418	23.258
56	643.0227	2.4066	126	1198.1219	9.5723	196	3173.353	27.1223
57	643.7934	7.7936	127	1198.5596	9.8801	197	3175.3674	7.9653
58	653.4352	14.7364	128	1202.425	58.3866	198	3175.3789	8.3322
59	659.6861	2.0749	129	1207.7723	2.8251	199	3184.0464	25.1335
60	684.3468	0.9351	130	1234.3167	16.9722	200	3184.1565	26.3882
61	708.0124	55.3525	131	1236.2965	21.048	201	3189.4209	1.1839
62	708.242	32.5781	132	1281.4468	13.8844	202	3190.1377	21.8297
63	711.9629	29.9624	133	1294.7164	3.42	203	3190.3872	6.3145
64	714.4976	63.7536	134	1295.0582	438.8489	204	3190.4919	11.1423
65	717.2775	1.8574	135	1297.5007	125.4556	205	3190.5996	10.1314
66	738.1232	15.03	136	1300.7502	169.992	206	3191.9641	0.2267
67	755.3679	0.7477	137	1302.0121	105.0675	207	3193.1877	5.0472
68	756.0401	14.2495	138	1307.4788	4.1712	208	3193.1914	6.0987
69	768.3858	52.8149	139	1310.5839	17.3868	209	3194.0144	3.675
70	778.833	11.9474	140	1330.5861	33.9128	210	3194.1824	3.9782

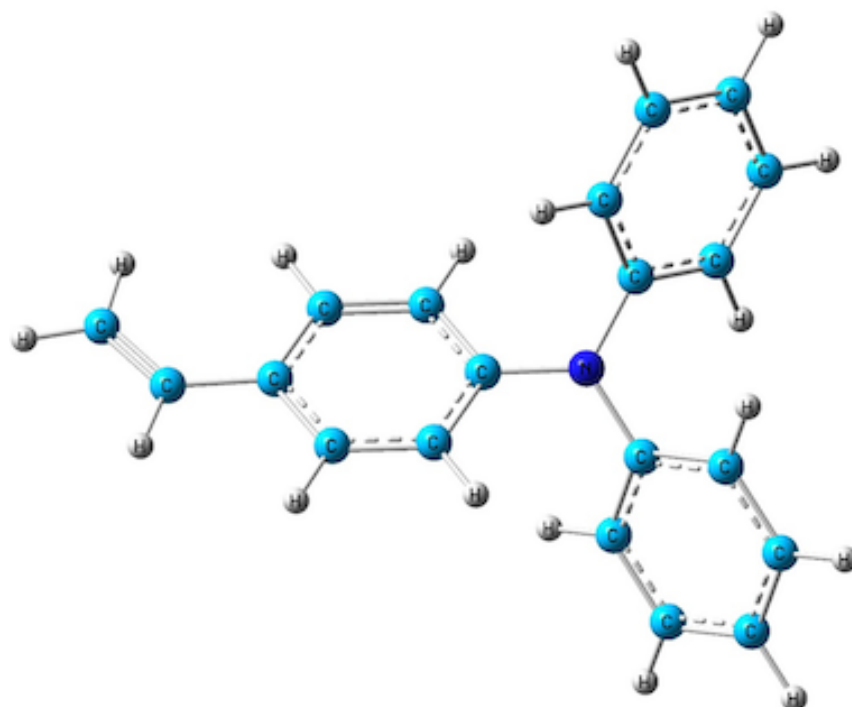


Figure 11. Dye FHI97811, $C_{20}H_{17}N$, DFT model and basis function rB3LYP/6-311+G(d,p) after geometry optimization.

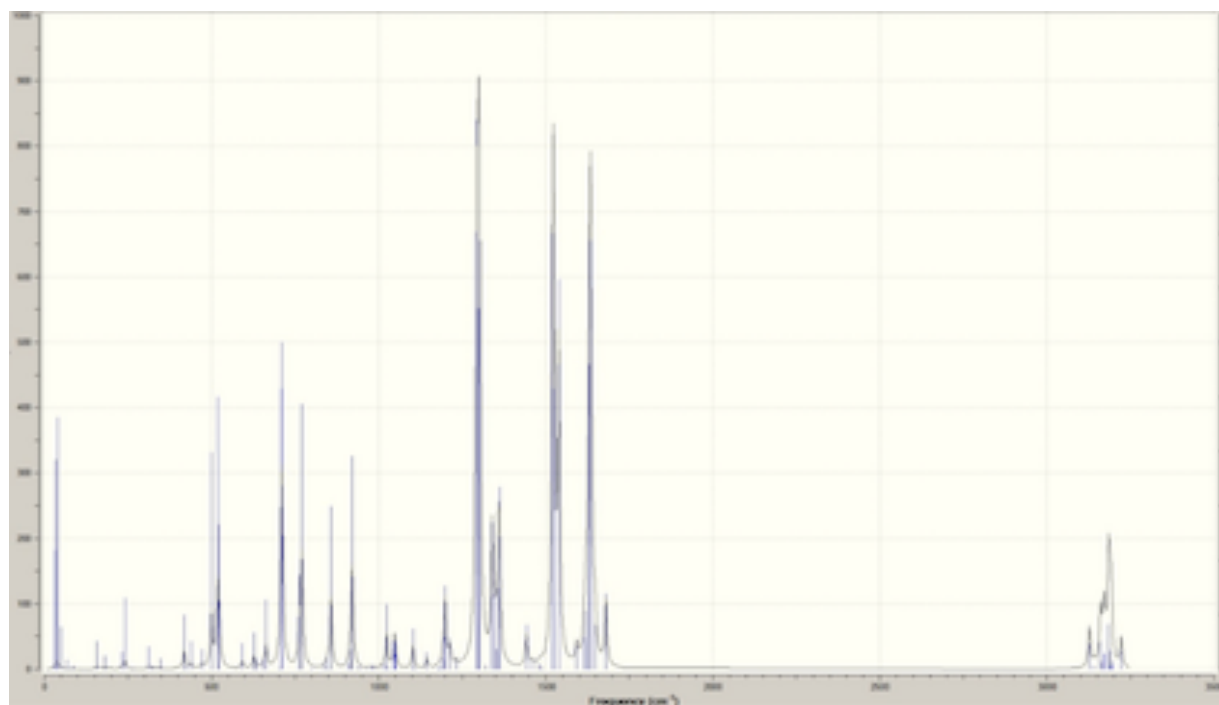


Figure 12. DFT calculated IR spectrum of dye FHI97811, $C_{20}H_{17}N$.

Table 6. DFT calculated IR spectrum of dye FHI97811, $C_{20}H_{17}N$

	Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)
1	32.8196	2.3686	37	835.2083	2.457	73	1335.2072	90.5788
2	34.7648	4.0442	38	846.1968	3.7348	74	1339.9154	35.2548
3	38.784	1.8269	39	847.3837	0.4423	75	1349.7922	7.6213

4	50.7588	0.4812	40	856.2754	69.8494	76	1355.2328	44.5593
5	73.0631	0.0736	41	910.6174	0.7372	77	1358.9897	89.4801
6	74.693	0.0783	42	916.072	9.9682	78	1439.1365	27.4177
7	85.1549	0.1479	43	923.0887	73.6564	79	1458.9932	4.7701
8	157.7725	1.5662	44	939.2264	1.1463	80	1477.1211	2.6932
9	181.6922	0.6694	45	946.1809	0.1608	81	1484.2267	3.078
10	232.0841	1.6466	46	969.2593	0.1677	82	1517.0909	251.3532
11	241.8385	6.6268	47	984.703	0.6828	83	1519.4257	197.4772
12	263.8616	0.267	48	989.0797	0.3423	84	1535.5632	219.265
13	310.27	2.9781	49	989.2073	0.336	85	1589.7644	14.8935
14	322.7112	0.7631	50	1003.0457	0.1384	86	1612.5459	22.6706
15	347.1926	1.6519	51	1003.6806	0.0867	87	1617.6925	47.0463
16	418.0091	9.6442	52	1011.8355	1.1492	88	1624.7629	174.7303
17	419.5652	4.0326	53	1012.3617	2.7738	89	1628.6329	256.5144
18	424.8287	0.6001	54	1024.5619	0.8084	90	1643.0577	30.3562
19	437.9391	6.0814	55	1029.2695	25.7512	91	1672.6844	49.5361
20	472.2316	4.0733	56	1043.7933	13.3845	92	3129.0364	30.5652
21	499.4503	46.8484	57	1045.5737	15.2892	93	3138.5698	5.0683
22	518.2068	62.9041	58	1047.4928	7.1276	94	3163.8716	27.8929
23	522.0201	29.327	59	1099.9053	19.6824	95	3165.6958	5.9288
24	591.2336	8.6347	60	1102.0089	2.0827	96	3166.3955	4.744
25	626.189	9.482	61	1142.9413	8.6664	97	3172.6467	12.8478
26	628.9759	0.1414	62	1174.0294	0.9929	98	3173.135	10.7688
27	632.553	4.2777	63	1175.6469	0.9036	99	3175.5391	18.877
28	653.5999	4.5737	64	1188.046	4.4835	100	3184.7444	36.5764
29	663.0852	20.6713	65	1192.8455	15.1634	101	3185.3677	30.0369
30	700.0047	0.1016	66	1194.9817	47.7766	102	3190.6194	25.8161
31	708.1754	87.4602	67	1209.9989	24.4106	103	3190.9104	20.9451
32	709.6434	100.4371	68	1230.5298	8.19	104	3192.8218	17.8796
33	762.7201	29.7238	69	1286.6422	309.5323	105	3194.0405	5.6264
34	769.3446	17.2609	70	1294.527	362.3179	106	3195.1145	6.2116
35	770.4581	64.9233	71	1298.157	166.066	107	3195.6394	6.5024
36	799.0041	0.1693	72	1317.3455	1.3968	108	3219.5007	17.9438

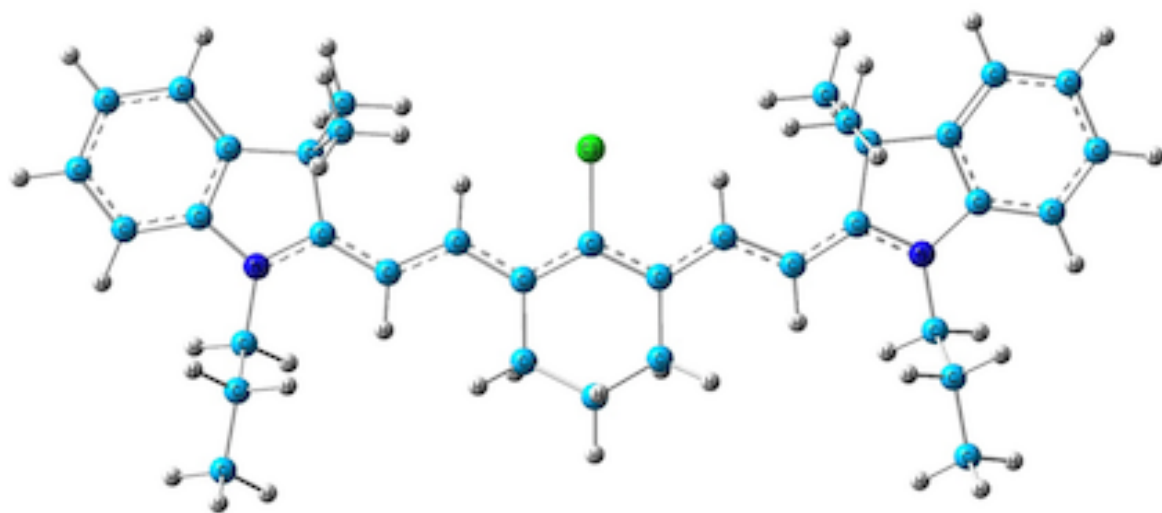


Figure 13. Dye ADS775PI, $C_{36}H_{44}ClN_2I$, in solvent MeOH (Methanol), DFT model and basis function rB3LYP/6-311+G(d,p) after geometry optimization.

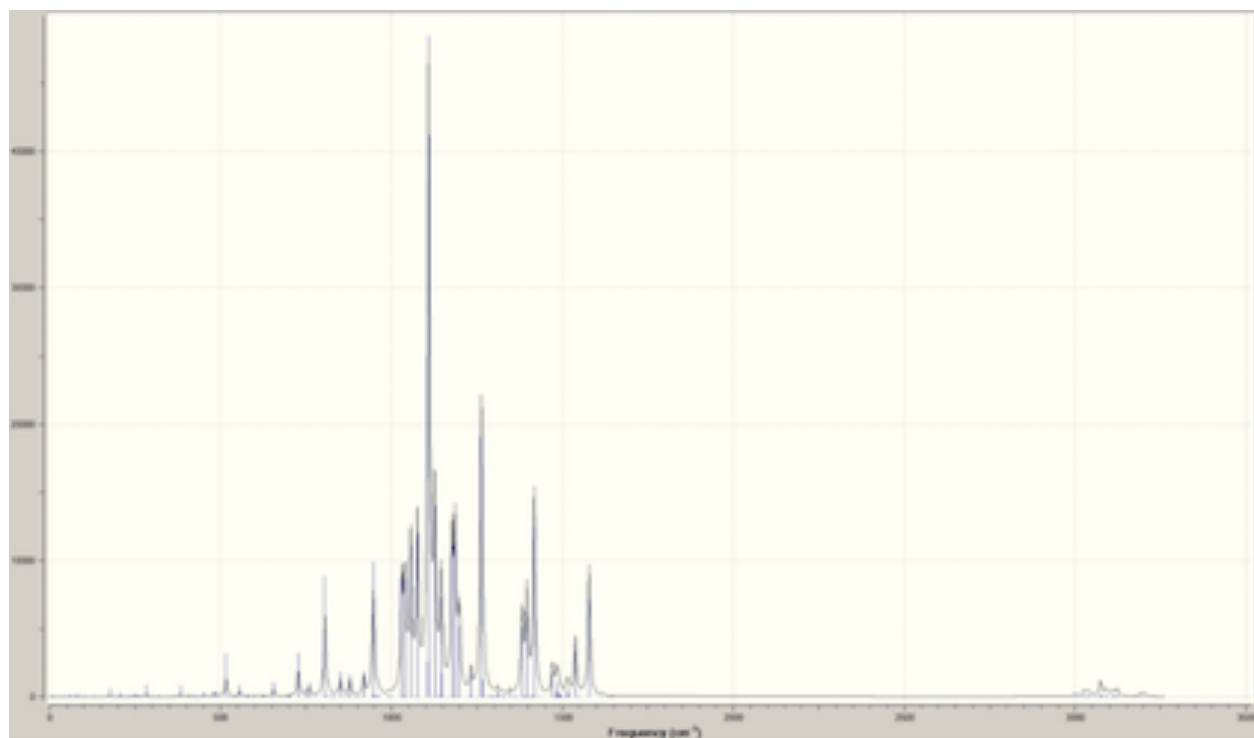


Figure 14. DFT calculated IR spectrum (arbitrary units) of dye ADS775PI, C₃₆H₄₄ClN₂I, in MeOH.

Table 7. DFT calculated IR spectrum of dye ADS775PI, C₃₆H₄₄ClN₂I, in MeOH.

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	8.8267	0.0358	82	823.025	10.3954	163	1412.3279	4.894
2	9.9129	0.2303	83	829.849	5.9711	164	1412.3339	1.7761
3	18.6123	0.0397	84	833.459	13.1116	165	1415.547	30.6734
4	28.0799	0.1426	85	850.6297	384.1437	166	1417.3994	4401.8311
5	35.0448	0.1404	86	863.6824	46.253	167	1432.5433	10.6482
6	39.2931	0.3762	87	874.1691	11.9853	168	1432.6815	15.9506
7	41.9875	0.0389	88	874.194	0.1255	169	1471.1394	659.1326
8	50.6485	0.8785	89	878.5798	339.2716	170	1478.3665	0.6241
9	50.6621	0.4843	90	893.9829	22.11	171	1478.3774	0.3316
10	61.2277	2.4591	91	895.0735	12.0157	172	1480.8022	21.8595
11	69.8883	0.1477	92	900.1298	0.0179	173	1480.8643	7.6779
12	79.0838	4.9043	93	904.402	12.0434	174	1481.0663	15.4975
13	86.2298	0.0837	94	919.006	425.4835	175	1481.6628	147.567
14	87.5399	0.6218	95	943.7295	25.6835	176	1482.4009	5.1948
15	103.9867	1.0599	96	946.8925	2351.9424	177	1485.1871	410.77
16	104.1437	0.5094	97	948.9444	0.0821	178	1488.4265	96.3064
17	127.357	0.8729	98	949.4573	14.3893	179	1491.0786	1.1873
18	129.8152	0.1787	99	949.8768	20.7433	180	1492.0123	1.1609
19	137.5684	0.0142	100	957.563	4.8312	181	1492.3123	0.531
20	152.0425	0.2176	101	957.9246	27.2156	182	1493.8202	84.0703
21	175.812	26.2561	102	960.8158	34.8292	183	1494.316	26.7708
22	191.3601	1.19	103	961.9032	25.6862	184	1497.8296	6.2073
23	203.8269	2.6265	104	991.4557	33.4685	185	1498.6281	22.3454
24	206.1166	14.5664	105	999.4404	2.5296	186	1499.0939	1.3317
25	216.3599	3.1676	106	999.4461	0.0982	187	1499.1071	5.8648
26	217.3109	0.6251	107	1030.137	2277.627	188	1512.4821	109.3355

27	224.7686	0.6037	108	1032.4412	0.1113	189	1512.6554	46.6813
28	236.6391	0.0804	109	1035.1342	7.5832	190	1516.1268	237.1221
29	237.1184	0.5427	110	1035.1979	2.1116	191	1518.8344	42.6927
30	242.2687	2.8624	111	1039.4861	2312.6821	192	1537.8644	1288.2122
31	245.6991	0.0043	112	1042.0909	7.0606	193	1549.1873	28.7494
32	251.7715	0.4113	113	1055.7686	3330.3894	194	1577.786	2807.0085
33	252.3381	11.6868	114	1062.0135	6.7366	195	1613.8026	39.8954
34	263.3866	4.6311	115	1074.0948	3.612	196	1635.4722	3.057
35	264.0257	0.0598	116	1075.7802	3772.5334	197	1635.5876	19.2113
36	282.4169	61.2922	117	1104.3522	7.5272	198	1646.6483	12.3586
37	284.1251	0.463	118	1105.3049	714.9792	199	1648.0729	3.9834
38	284.2703	0.5971	119	1108.2928	13470.277	200	3000.9563	17.6146
39	292.4079	0.2367	120	1120.7928	5.422	201	3001.8418	53.843
40	318.2309	0.2751	121	1126.1351	4170.1372	202	3025.1045	22.0973
41	319.5456	8.4411	122	1139.0063	40.8703	203	3025.1282	77.0582
42	345.1318	2.0625	123	1145.1215	2099.9355	204	3027.7759	50.3646
43	345.1847	1.5949	124	1147.4396	7.4056	205	3034.7056	13.1204
44	352.9783	1.5462	125	1147.8715	492.7639	206	3034.7354	44.0435
45	353.868	2.5679	126	1159.026	2.8848	207	3041.3347	0.5932
46	368.8124	2.9173	127	1174.9609	4.8709	208	3041.3406	64.5053
47	383.219	75.2333	128	1176.8015	3226.4636	209	3043.9868	9.5493
48	405.8888	17.4579	129	1181.1038	0.4641	210	3044.1221	38.5509
49	415.6039	6.411	130	1186.2439	3380.6628	211	3062.3352	3.6491
50	423.7376	1.3993	131	1194.4558	2.3814	212	3062.3359	1.0207
51	450.7764	35.5802	132	1198.2803	1554.4313	213	3070.8557	22.6234
52	451.4773	3.0542	133	1230.187	23.9353	214	3072.4141	58.304
53	481.0987	50.457	134	1232.6866	476.0256	215	3072.9338	143.3823
54	481.4956	21.0141	135	1248.8805	6.6136	216	3073.1792	76.2579
55	487.777	22.3126	136	1262.9576	6271.3472	217	3075.8484	60.3552
56	516.0611	412.269	137	1266.6511	393.8004	218	3087.738	147.5085
57	525.8298	4.8324	138	1270.272	5.1487	219	3087.7468	3.9315
58	540.4931	3.8173	139	1284.4658	30.0169	220	3096.2173	1.5944
59	555.6278	120.0587	140	1289.0596	12.5297	221	3096.2207	89.4727
60	556.4201	2.5382	141	1295.5875	5.2716	222	3108.3298	0.2291
61	578.2608	9.9364	142	1297.2729	31.0967	223	3108.334	28.2003
62	579.1438	5.0046	143	1303.9624	24.0533	224	3110.3708	7.4598
63	598.7701	4.9999	144	1310.5369	142.6451	225	3110.4004	80.6587
64	622.4181	21.4914	145	1315.4045	34.794	226	3115.0361	44.6054
65	627.9104	14.7397	146	1325.2878	55.8954	227	3115.0403	4.0675
66	628.5796	3.3636	147	1329.5413	0.8408	228	3121.822	30.1134
67	651.1243	2.0395	148	1332.8461	1.7071	229	3121.8245	4.2107
68	654.6298	174.1015	149	1334.4318	1.4253	230	3124.0598	127.8642
69	695.1699	3.1528	150	1347.2642	128.9069	231	3124.0825	4.7969
70	699.1975	16.709	151	1357.3956	1.3972	232	3173.0183	8.2506
71	703.8327	21.5986	152	1363.4148	4.264	233	3173.0415	2.2456
72	727.2622	589.0742	153	1365.6484	38.992	234	3180.9829	13.0431
73	745.0547	0.4274	154	1382.0494	1768.8016	235	3180.9836	7.8716
74	751.1358	96.1841	155	1388.1353	0.2866	236	3193.6621	43.5127
75	752.0848	1.5316	156	1389.6479	14.6206	237	3193.6743	38.3195
76	759.6286	4.7925	157	1390.4135	1.8881	238	3201.186	17.24
77	759.7265	191.9318	158	1392.3086	1.6923	239	3201.3145	8.5206
78	775.754	2.3615	159	1395.578	2190.7898	240	3203.9734	60.5395

79	775.8385	23.7074	160	1402.2091	12.588	241	3204.0073	4.4046
80	805.0196	1790.9379	161	1402.2178	4.8618	242	3235.377	0.9276
81	810.0037	33.5812	162	1405.9489	11.0027	243	3235.6931	1.9537

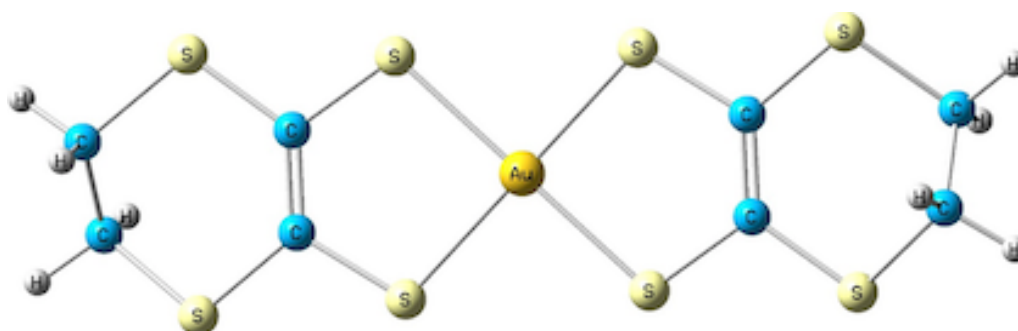


Figure 15. Dye FHI83642-Au, $C_8H_8AuS_8$, DFT model and basis function uB3LYP/QZVP after Geometry Optimization, in solvent CH_2Cl_2 .

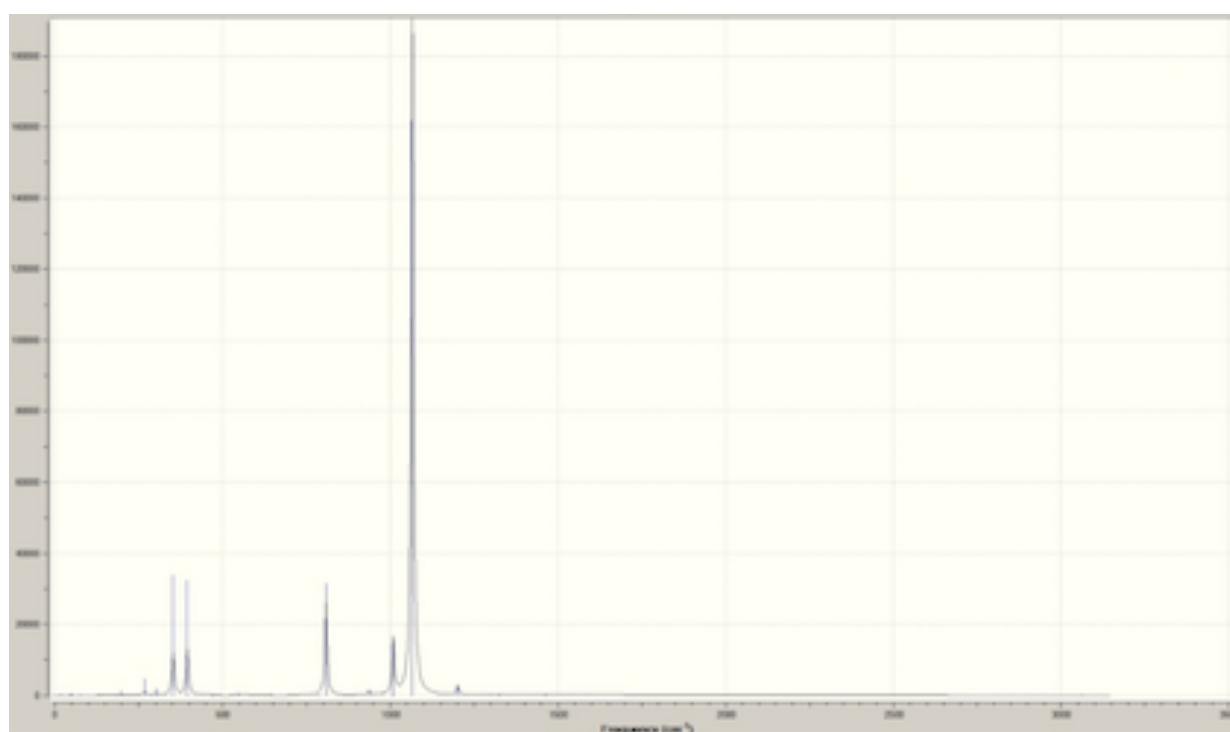


Figure 16. DFT calculated IR spectrum (arbitrary units) of dye FHI83642-Au, $C_8H_8AuS_8$, in solvent CH_2Cl_2 .

Table 8. DFT calculated IR spectrum of dye FHI83642-Au, $C_8H_8AuS_8$, in CH_2Cl_2 .

	Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)
1	18.9770	1.4690	36	786.8420	1.0250
2	40.3240	0.0000	37	788.6710	24.8440
3	44.6570	0.6600	38	808.0430	7997.0161
4	47.4200	2.7100	39	844.0240	0.0000
5	49.3520	11.2160	40	894.0110	6.5930
6	64.3280	0.0930	41	895.3400	8.4830
7	77.4880	1.7540	42	936.6630	364.1360

8	91.8280	0.0000	43	938.7810	0.0000
9	128.5820	0.0000	44	978.1380	15.1440
10	135.6200	0.8810	45	979.2320	1.0210
11	181.9940	0.0140	46	1008.7490	4610.5298
12	197.1650	75.2470	47	1012.6170	0.0000
13	209.6380	7.4210	48	1066.0750	57518.3594
14	267.2030	400.7140	49	1144.6680	0.2720
15	267.9650	0.0000	50	1144.7780	3.2210
16	288.7280	0.4040	51	1198.8440	0.0000
17	288.8420	0.5230	52	1201.2679	839.6620
18	301.8240	190.0070	53	1300.8540	0.2880
19	304.1030	0.0000	54	1301.1720	4.9650
20	328.8290	0.0050	55	1321.8530	0.0000
21	341.9640	0.3210	56	1325.6689	82.5640
22	352.4210	3732.4519	57	1459.4139	6.0110
23	368.4180	0.0020	58	1459.4240	24.9000
24	381.6980	0.0000	59	1461.9611	0.0000
25	395.0240	4017.1609	60	1462.1370	8.4720
26	398.0330	0.1480	61	1470.6331	0.0000
27	440.7340	0.0000	62	3059.2610	7.7670
28	469.0050	0.0430	63	3059.2671	2.1580
29	471.3740	0.9390	64	3062.6899	59.0680
30	546.3060	0.0000	65	3062.7229	0.1660
31	547.4650	112.8930	66	3109.3779	9.1190
32	647.0150	115.2500	67	3109.4319	0.0000
33	647.4640	0.0000	68	3121.3911	2.6730
34	683.3850	0.9520	69	3121.3989	8.0320
35	683.5770	3.2320			

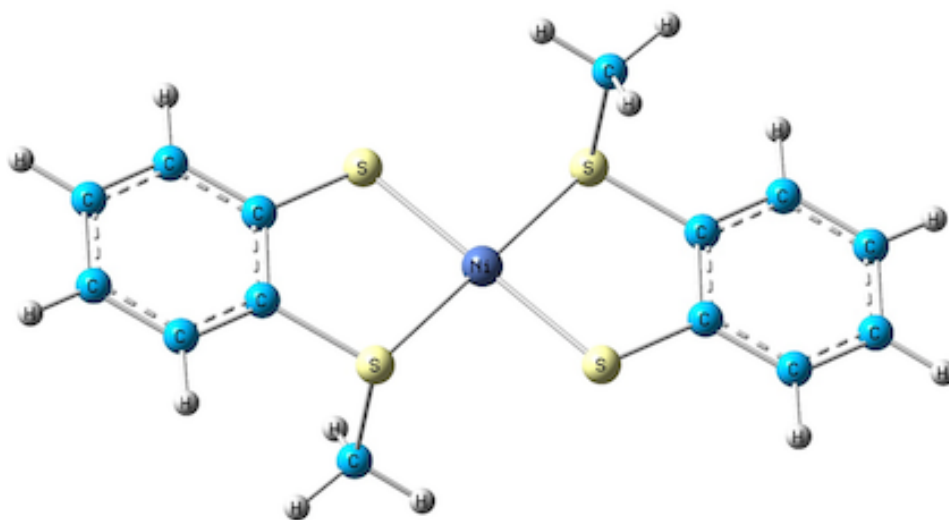


Figure 17. Dye FHI83642-Ni, $C_{14}H_{14}NiS_4$, DFT model and basis function rB3LYP/6-311+G(d,p) after Geometry Optimization, in solvent CH_2Cl_2 .

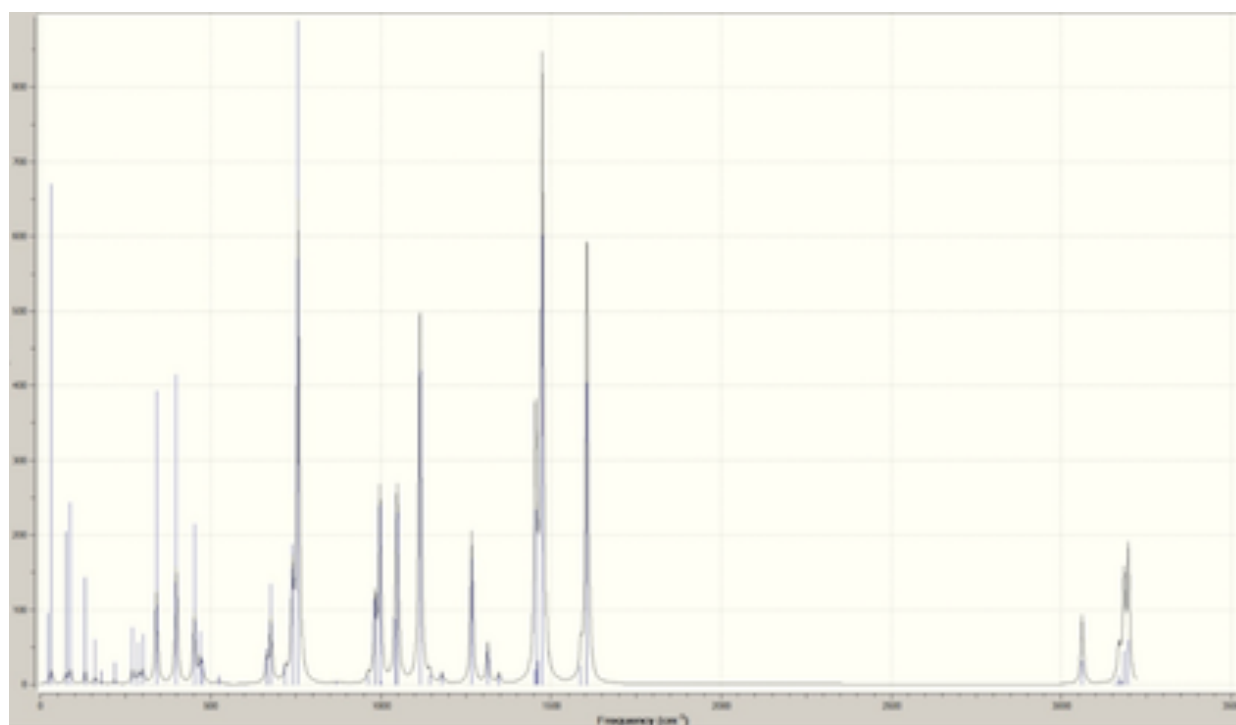


Figure 18. DFT calculated IR spectrum (arbitrary units) of dye FHI83642-Ni, C₁₄H₁₄NiS₄, in solvent CH₂Cl₂.

Table 9. DFT calculated IR spectrum of dye FHI83642-Ni, C₁₄H₁₄NiS₄, in solvent CH₂Cl₂.

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	21.7967	0.5770	32	664.1299	0.0000	63	1266.9078	59.1987
2	31.0474	5.7968	33	664.4441	8.7821	64	1313.8447	16.0771
3	45.9036	0.0000	34	676.3306	0.0000	65	1313.9600	0.0000
4	74.4054	4.2372	35	676.4012	25.2811	66	1346.7120	4.0764
5	87.3988	5.9266	36	719.0740	4.7245	67	1347.3011	0.0000
6	96.4767	0.0000	37	719.7017	0.0000	68	1453.5020	0.0000
7	131.0513	5.2134	38	740.1201	0.0000	69	1454.1244	7.6059
8	137.5809	0.0000	39	740.2528	38.7101	70	1454.5688	94.5848
9	153.5194	0.0000	40	756.2852	0.0000	71	1454.7507	0.0000
10	159.4541	2.6350	41	756.5313	187.3974	72	1461.5593	0.0000
11	163.5271	0.0000	42	869.7248	0.0000	73	1461.6849	12.5112
12	177.3976	0.9033	43	869.8355	0.7412	74	1474.1062	246.9626
13	178.7625	0.0000	44	962.0699	0.0000	75	1475.1215	0.0000
14	206.3627	0.0000	45	962.1396	3.1805	76	1587.3235	10.8655
15	217.0938	1.7415	46	980.0832	0.0000	77	1587.6757	0.0000
16	269.9802	5.7165	47	982.8444	31.1680	78	1605.4988	180.7396
17	280.9553	0.0000	48	995.8480	0.0000	79	1605.9114	0.0000
18	286.6656	4.4887	49	996.7775	74.1368	80	3060.8794	26.7954
19	300.3304	5.6119	50	1000.1902	0.8892	81	3060.9463	0.0000
20	323.9084	0.0000	51	1000.2399	0.0000	82	3159.1577	1.8550
21	340.0779	37.2352	52	1043.1078	25.4449	83	3159.1946	0.0000
22	363.9910	0.0000	53	1043.2603	0.0000	84	3168.8481	9.4863
23	399.0269	46.0526	54	1048.2943	67.0273	85	3168.8589	0.0000
24	445.2008	0.0000	55	1048.8461	0.0000	86	3169.2805	2.7837
25	451.8202	27.0081	56	1114.8229	151.4013	87	3169.3032	0.0000

26	452.0459	0.0000	57	1116.0269	0.0000	88	3175.6162	4.0269
27	468.8638	9.2282	58	1143.4316	0.0000	89	3175.6262	0.0000
28	476.2967	0.0000	59	1143.6609	3.9779	90	3184.2852	0.0000
29	476.3809	4.4891	60	1179.4233	4.1034	91	3184.2915	39.6999
30	522.4663	0.0000	61	1179.4641	0.0000	92	3196.7251	52.2901
31	523.0991	1.7071	62	1266.1349	0.0000	93	3196.7720	0.0000

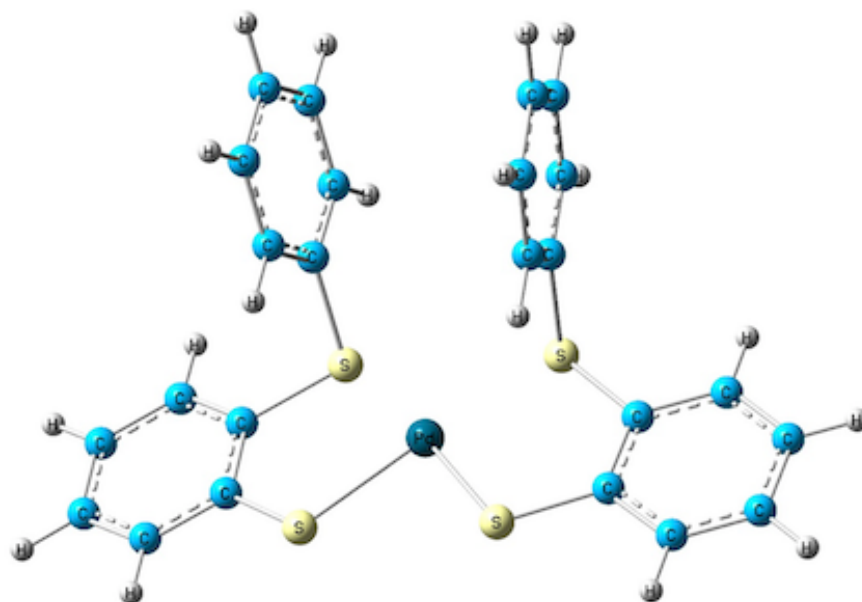


Figure 19. Dye FHI83642-Pd, $C_{24}H_{18}PdS_4$, DFT model and basis function rB3LYP/DGDZVP after Geometry Optimization, in solvent C_2Cl_2 .

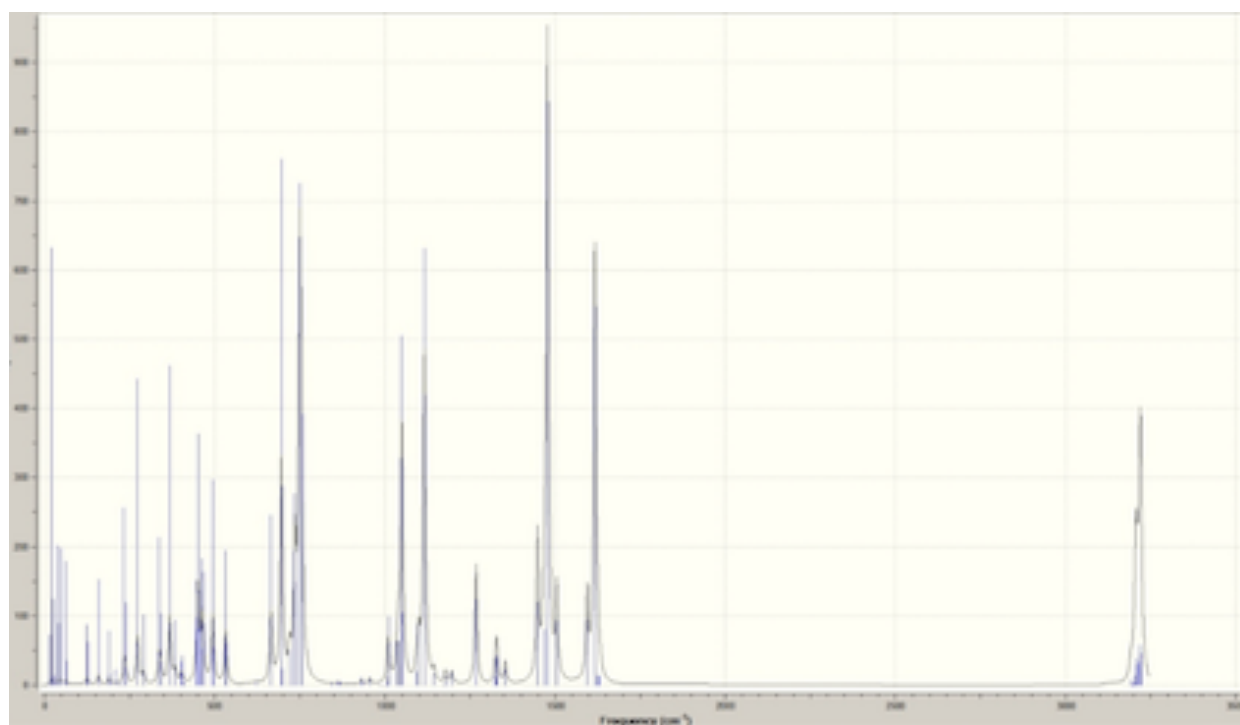


Figure 20. DFT calculated IR spectrum (arbitrary units) of dye FHI83642-Pd, $C_{24}H_{18}PdS_4$, in solvent C_2Cl_2 .

Table 10. DFT calculated IR spectrum of dye FHI83642-Pd, C₂₄H₁₈PdS₄, in solvent C₂Cl₂.

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	14.8977	0.1885	46	695.6668	92.8285	91	1177.8	2.578
2	20.7507	2.3027	47	697.1572	1.187	92	1194.9583	0.9337
3	26.7543	0.584	48	698.0751	2.8613	93	1195.7393	4.5088
4	27.7225	0.0638	49	699.1278	2.8137	94	1267.3698	23.5837
5	38.5394	1.3613	50	720.0753	5.8691	95	1268.2657	27.6125
6	42.1904	0.6554	51	720.5051	6.3558	96	1323.0537	1.6159
7	47.6936	1.6508	52	735.3044	35.6642	97	1323.1932	2.9276
8	48.0762	0.1705	53	736.1883	19.1779	98	1327.54	8.8756
9	62.4738	1.9605	54	749.436	95.382	99	1328.4772	9.8096
10	66.5562	0.4064	55	750.0904	70.5728	100	1353.0962	4.3051
11	123.3971	1.8803	56	755.311	62.2436	101	1353.9167	5.2505
12	126.7291	1.3869	57	755.9428	27.63	102	1448.3848	30.0716
13	127.8388	0.3483	58	843.7829	0.0691	103	1448.7974	30.3431
14	128.2262	0.0652	59	846.0077	0.4694	104	1468.2734	12.3531
15	158.5404	4.2525	60	864.234	0.5348	105	1469.292	20.6364
16	189.3956	2.6038	61	865.0387	0.626	106	1477.8923	224.5424
17	190.5893	0.5328	62	931.0141	1.8013	107	1479.2632	50.6296
18	207.4841	0.8051	63	932.6421	0.4506	108	1504.446	13.6179
19	219.612	0.1482	64	955.5067	1.3829	109	1504.739	24.4916
20	233.4551	10.4786	65	955.7767	1.2083	110	1594.2994	26.2928
21	238.7641	5.0149	66	985.4883	0.0736	111	1594.6434	11.249
22	273.4994	21.2145	67	985.9031	0.0441	112	1616.7482	165.8744
23	290.4815	5.1932	68	990.2077	0.0228	113	1617.7697	24.9553
24	336.5058	12.5877	69	991.1478	0.0458	114	1625.7948	1.5412
25	342.2445	6.2014	70	1005.7092	0.0311	115	1626.0536	3.6487
26	367.8102	29.7876	71	1006.5753	0.0078	116	1628.137	4.1131
27	383.6791	6.3151	72	1009.8314	2.0176	117	1628.726	3.2188
28	401.5134	2.3174	73	1010.14	17.4248	118	3190.8557	4.1996
29	404.3361	3.0079	74	1035.3118	11.4689	119	3191.2341	4.0937
30	409.1491	0.292	75	1035.5787	0.6037	120	3194.9048	0.0941
31	410.2539	0.0756	76	1040.188	11.5164	121	3195.1213	0.1057
32	448.4052	11.9508	77	1040.381	2.9111	122	3198.2732	0.3893
33	450.0289	6.367	78	1049.6173	92.912	123	3198.3972	0.3979
34	451.82	28.7439	79	1049.9894	19.3243	124	3202	1.6021
35	462.6705	14.8409	80	1092.0321	2.9534	125	3202.272	7.4942
36	463.6472	4.2359	81	1092.6525	3.7089	126	3206.3054	21.0932
37	466.086	13.3806	82	1099.0443	0.5882	127	3206.6074	22.0443
38	493.6623	25.6336	83	1099.2668	17.7278	128	3209.7813	6.1178
39	496.0225	4.6812	84	1115.3793	123.596	129	3210.1284	16.5204
40	531.857	18.2077	85	1116.9178	23.0601	130	3216.2192	11.0514
41	532.9803	5.5259	86	1143.678	3.3412	131	3216.8411	18.4689
42	622.5027	0.2384	87	1144.5042	2.2618	132	3219.345	32.5336
43	622.952	0.309	88	1175.7678	0.1154	133	3219.8193	27.8918
44	665.1611	28.6806	89	1177.1733	0.2188	134	3221.6045	13.2691
45	665.6794	1.6096	90	1177.4204	2.3816	135	3221.9202	26.0627

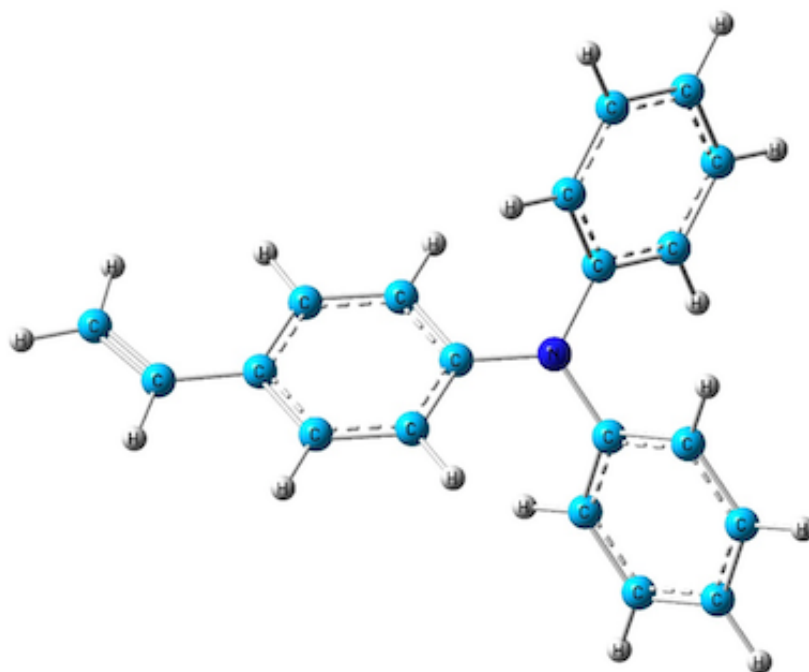


Figure 21. Dye FHI97811, $C_{20}H_{17}N$, DFT model and basis function rB3LYP/6-311+G(d,p) after geometry optimization. in solvent Acetone.

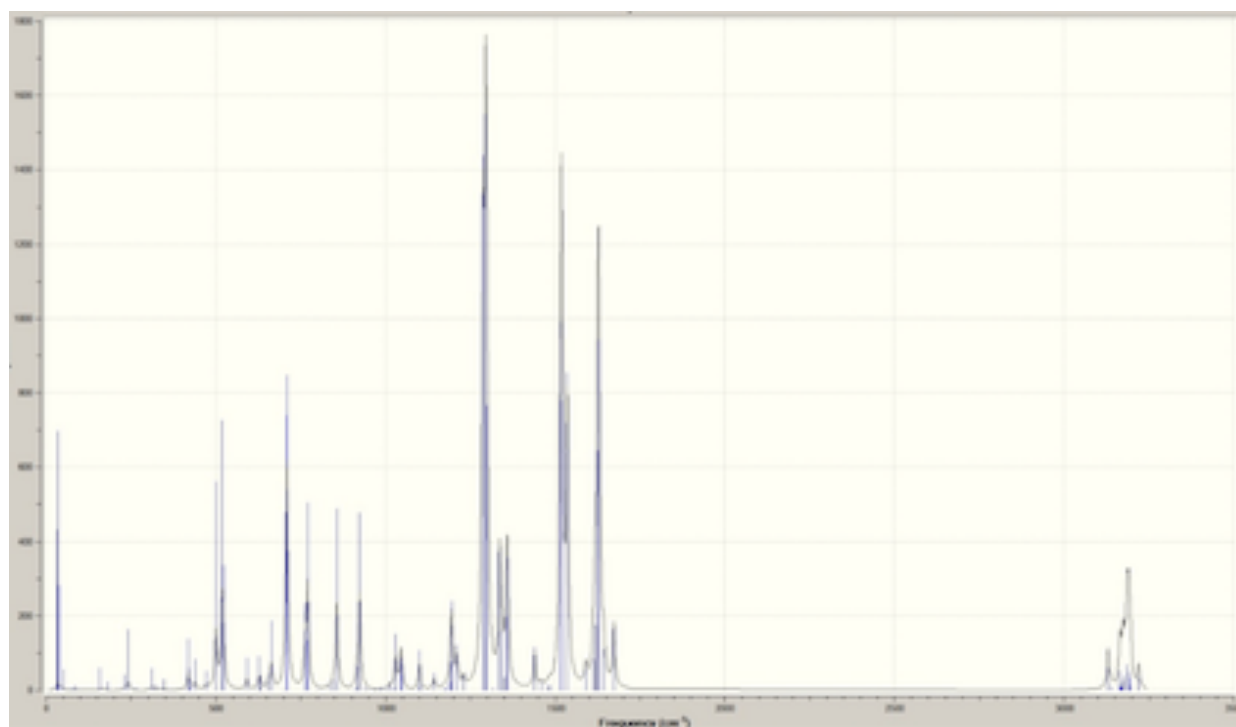


Figure 22. DFT calculated IR spectrum (arbitrary units) of dye FHI97811, $C_{20}H_{17}N$, in solvent Acetone.

Table 11. DFT calculated IR spectrum of dye FHI97811, $C_{20}H_{17}N$, in solvent Acetone.

	Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)		Freq (cm^{-1})	IR Intensity (KM/Mol)
1	32.8196	2.3686	37	835.2083	2.457	73	1335.2072	90.5788
2	34.7648	4.0442	38	846.1968	3.7348	74	1339.9154	35.2548
3	38.784	1.8269	39	847.3837	0.4423	75	1349.7922	7.6213

4	50.7588	0.4812	40	856.2754	69.8494	76	1355.2328	44.5593
5	73.0631	0.0736	41	910.6174	0.7372	77	1358.9897	89.4801
6	74.693	0.0783	42	916.072	9.9682	78	1439.1365	27.4177
7	85.1549	0.1479	43	923.0887	73.6564	79	1458.9932	4.7701
8	157.7725	1.5662	44	939.2264	1.1463	80	1477.1211	2.6932
9	181.6922	0.6694	45	946.1809	0.1608	81	1484.2267	3.078
10	232.0841	1.6466	46	969.2593	0.1677	82	1517.0909	251.3532
11	241.8385	6.6268	47	984.703	0.6828	83	1519.4257	197.4772
12	263.8616	0.267	48	989.0797	0.3423	84	1535.5632	219.265
13	310.27	2.9781	49	989.2073	0.336	85	1589.7644	14.8935
14	322.7112	0.7631	50	1003.0457	0.1384	86	1612.5459	22.6706
15	347.1926	1.6519	51	1003.6806	0.0867	87	1617.6925	47.0463
16	418.0091	9.6442	52	1011.8355	1.1492	88	1624.7629	174.7303
17	419.5652	4.0326	53	1012.3617	2.7738	89	1628.6329	256.5144
18	424.8287	0.6001	54	1024.5619	0.8084	90	1643.0577	30.3562
19	437.9391	6.0814	55	1029.2695	25.7512	91	1672.6844	49.5361
20	472.2316	4.0733	56	1043.7933	13.3845	92	3129.0364	30.5652
21	499.4503	46.8484	57	1045.5737	15.2892	93	3138.5698	5.0683
22	518.2068	62.9041	58	1047.4928	7.1276	94	3163.8716	27.8929
23	522.0201	29.327	59	1099.9053	19.6824	95	3165.6958	5.9288
24	591.2336	8.6347	60	1102.0089	2.0827	96	3166.3955	4.744
25	626.189	9.482	61	1142.9413	8.6664	97	3172.6467	12.8478
26	628.9759	0.1414	62	1174.0294	0.9929	98	3173.135	10.7688
27	632.553	4.2777	63	1175.6469	0.9036	99	3175.5391	18.877
28	653.5999	4.5737	64	1188.046	4.4835	100	3184.7444	36.5764
29	663.0852	20.6713	65	1192.8455	15.1634	101	3185.3677	30.0369
30	700.0047	0.1016	66	1194.9817	47.7766	102	3190.6194	25.8161
31	708.1754	87.4602	67	1209.9989	24.4106	103	3190.9104	20.9451
32	709.6434	100.4371	68	1230.5298	8.19	104	3192.8218	17.8796
33	762.7201	29.7238	69	1286.6422	309.5323	105	3194.0405	5.6264
34	769.3446	17.2609	70	1294.527	362.3179	106	3195.1145	6.2116
35	770.4581	64.9233	71	1298.157	166.066	107	3195.6394	6.5024
36	799.0041	0.1693	72	1317.3455	1.3968	108	3219.5007	17.9438

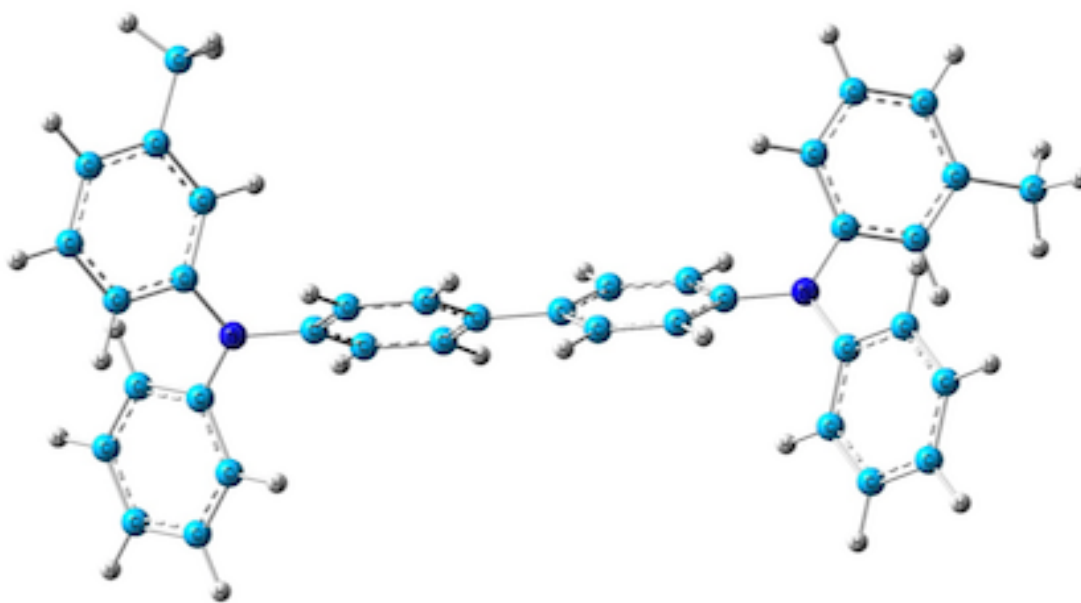


Figure 23. Dye FH94931, $C_{38}H_{32}N_2$, DFT model and basis function rB3LYP/6-311+G(d,p) after geometry optimization, in solvent Acetone.



Figure 24. DFT calculated IR spectrum (arbitrary units) of dye FH94931, $C_{38}H_{32}N_2$, in solvent Acetone.

Table 12. DFT calculated IR spectrum of dye FH94931, $C_{38}H_{32}N_2$, in solvent Acetone.

	Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)		Freq (cm⁻¹)	IR Intensity (KM/Mol)
1	7.875	0.0156	71	793.3276	67.681	141	1330.7762	167.3147
2	11.9781	0.0536	72	794.7222	6.6369	142	1333.8936	48.1031
3	17.9221	0.8016	73	821.8293	63.9726	143	1341.2708	26.1355
4	24.3555	2.2808	74	826.5357	8.4367	144	1342.9167	10.3346
5	28.4583	3.9548	75	836.9133	0.9838	145	1343.8591	28.8872
6	31.0153	5.5469	76	838.4055	2.4728	146	1346.9728	59.6364
7	39.151	1.6538	77	846.9902	1.9319	147	1356.3782	48.7168
8	44.5185	0.8654	78	847.0009	0.489	148	1358.3271	72.2477
9	46.586	0.5508	79	848.6523	23.8472	149	1408.989	2.1242
10	52.1606	0.4996	80	870.2605	40.8286	150	1409.572	1.3546
11	53.1568	0.3473	81	889.9569	9.7712	151	1429.5105	1.5047
12	59.0627	0.4947	82	890.1338	4.2177	152	1444.9554	9.2054
13	72.408	0.0452	83	905.1257	4.0614	153	1448.6241	30.7065
14	75.65	0.4022	84	905.9872	1.8617	154	1456.2666	18.1995
15	83.3204	1.6007	85	917.4728	8.1333	155	1479.7401	7.1359
16	90.2194	0.0827	86	918.8947	4.971	156	1480.4915	0.8712
17	93.4498	0.2269	87	940.8496	0.8723	157	1480.7778	18.5092
18	149.6111	0.0269	88	943.7469	0.151	158	1480.8929	0.3368
19	165.6303	0.0474	89	968.0827	2.3385	159	1490.3202	41.4916
20	203.9294	1.2975	90	971.6823	2.1703	160	1491.5138	52.8446
21	211.194	5.0056	91	978.3459	2.9248	161	1514.6044	208.5862
22	212.0227	10.5081	92	978.9965	3.2585	162	1515.4883	370.7411
23	221.0683	2.0388	93	985.6772	0.0119	163	1517.0453	431.4087
24	231.0843	7.2766	94	985.9974	0.0828	164	1518.8597	122.6392
25	239.0014	3.0922	95	989.0088	0.6593	165	1523.5375	263.3489

26	243.4593	1.3683	96	989.155	0.4238	166	1548.5433	0.3515
27	266.0498	0.9245	97	992.1719	0.6884	167	1581.1719	19.3359
28	278.2318	3.8436	98	993.514	0.2716	168	1600.4771	0.9436
29	296.6282	0.4677	99	1002.5398	0.1836	169	1611.4373	84.8125
30	321.9951	0.0349	100	1002.8723	0.1377	170	1613.2217	43.0171
31	329.0923	1.0178	101	1010.3473	1.3188	171	1614.7401	131.6522
32	359.5123	1.2565	102	1010.8945	1.6582	172	1616.2513	45.121
33	389.0761	1.2724	103	1011.0461	3.3427	173	1626.0837	214.0697
34	400.0413	0.7517	104	1011.4707	3.1529	174	1627.5996	101.7854
35	413.3451	4.734	105	1015.1002	5.2928	175	1630.3627	152.8221
36	419.2488	29.1185	106	1026.5601	3.4556	176	1633.2028	231.4549
37	420.6982	1.1405	107	1028.269	6.1922	177	1641.7081	7.2078
38	423.3269	6.9105	108	1030.4492	4.7171	178	1647.3224	24.0855
39	425.1831	2.9507	109	1044.969	13.4909	179	3022.3518	44.4933
40	437.5656	2.6571	110	1046.3564	18.678	180	3022.4546	41.6101
41	450.7694	26.1915	111	1048.7465	3.0401	181	3076.8442	28.0205
42	456.1637	1.7014	112	1058.6923	13.0169	182	3077.1248	29.1509
43	462.7371	10.8321	113	1059.4034	13.4991	183	3104.3596	28.312
44	479.867	6.649	114	1101.3492	9.4385	184	3104.7715	29.2555
45	515.4787	92.4461	115	1101.6486	11.5781	185	3161.0786	6.318
46	524.9083	1.1653	116	1112.5118	8.0361	186	3161.3076	6.9231
47	527.0881	20.8435	117	1112.906	5.9021	187	3164.9529	6.6575
48	529.8238	19.8157	118	1139.5771	0.2267	188	3165.1021	6.287
49	533.7705	34.0637	119	1141.0074	16.0622	189	3171.8171	20.7001
50	557.3333	2.9701	120	1172.1962	7.4155	190	3171.8979	47.8339
51	565.9102	12.1526	121	1173.3127	7.5097	191	3171.9954	20.989
52	576.3536	0.354	122	1174.4735	1.165	192	3172.1643	6.7261
53	629.4946	0.3784	123	1174.5615	1.1178	193	3174.2791	32.8665
54	629.7595	1.9768	124	1186.5204	9.8178	194	3174.7302	39.2142
55	635.282	20.3967	125	1186.6912	11.3352	195	3176.3245	0.5128
56	641.5599	2.9455	126	1193.4614	16.1443	196	3176.7307	17.0146
57	642.8774	15.5261	127	1194.3593	17.5228	197	3176.9077	9.0768
58	651.6404	26.5093	128	1199.3969	76.1259	198	3177.2615	8.0234
59	658.186	4.5974	129	1207.5419	6.8434	199	3184.822	36.2947
60	683.2867	1.8528	130	1232.1123	29.7493	200	3185.0342	37.9929
61	707.6875	125.5011	131	1234.8639	41.6796	201	3190.7788	1.2285
62	707.9676	33.1721	132	1279.3629	36.5762	202	3190.9673	26.5864
63	711.341	50.0648	133	1290.7047	736.3086	203	3191.4077	27.0095
64	714.2292	116.4277	134	1292.146	65.4507	204	3191.7739	30.9877
65	716.024	4.1356	135	1293.2134	279.4773	205	3192.1257	17.9022
66	736.9101	29.6014	136	1296.4381	298.2312	206	3193.2771	12.3666
67	754.1809	0.8729	137	1298.1106	92.1231	207	3193.3091	10.5366
68	755.5378	27.4286	138	1303.9744	0.3934	208	3193.9697	0.0808
69	768.313	96.0132	139	1308.8066	27.195	209	3195.123	4.8682
70	778.3956	25.0353	140	1327.6962	64.5408	210	3195.2732	4.1469

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