

# Computational study of Linear carbon chain based organic dyes for Dye sensitized solar cells.

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Electronic supplementary information (ESI) available

## Electronic Supplementary Information:

Optimized geometry and frequencies of dyes at B3LYP-6-311+G(3df,3pd)/SMD level

### BZ-S

C	-2.75121100	-0.81802800	0.11794400
C	-3.18092300	-2.13409200	0.24263600
S	-4.11163500	0.25237100	-0.01185100
C	-4.56587700	-2.26938300	0.23542200
H	-2.50466800	-2.96848300	0.34243700
C	-5.25475500	-1.06595500	0.10408200
H	-5.08388900	-3.21358900	0.32519100
C	-6.66239900	-0.97852500	0.07402700
H	-7.15027300	-1.94100300	0.16191500
C	-7.50476800	0.09798000	-0.04541700
C	-7.04356200	1.43287400	-0.17021400
C	-8.96950700	-0.04949600	-0.05428800
O	-9.38236100	-1.32535300	0.06639900
H	-10.35319100	-1.32469400	0.04837500
O	-9.74476700	0.87761300	-0.15945700
N	-6.66561300	2.51920100	-0.27180400
C	2.66392600	1.11787300	0.02669100
C	3.12304900	2.41535000	0.04757200
S	4.02973200	0.01360300	-0.05348600
C	4.52364100	2.54380800	-0.00556000
H	2.46448500	3.26989200	0.09897300
C	5.17031900	1.32653900	-0.05617500
H	5.05371600	3.48491100	0.00643000
H	7.06341300	1.98899000	0.12909500
C	7.23763500	-0.03400600	-0.18579500
C	6.93691800	-1.16376500	-0.90160400
S	8.74755300	-0.22420900	0.67027600
C	7.93167100	-2.17342100	-0.77207400
H	6.06463300	-1.26259000	-1.52805300
C	8.97568500	-1.80941100	0.02157500
H	7.87691900	-3.12715200	-1.27672500
H	9.87120100	-2.36102100	0.25603400
N	6.53074600	1.14947300	-0.05095300
C	-1.38669700	-0.32173900	0.09085800
C	-0.29811000	-1.21058500	0.10605200
C	-1.09171700	1.05307100	0.04919400
C	1.00296800	-0.75034900	0.08589600
H	-0.46820500	-2.27715000	0.13234900
C	0.20745300	1.51371200	0.02608000

H	-1.89179100	1.78183500	0.03681200
C	1.30084500	0.62465600	0.04582000
H	1.80231700	-1.47945900	0.10488600
H	0.37852300	2.57981900	-0.00931100

Frequencies --	10.3096	22.8701	27.1546
Frequencies --	31.3853	33.6537	44.3940
Frequencies --	45.8370	57.3989	62.1386
Frequencies --	76.4805	97.2163	112.0247
Frequencies --	135.2229	146.5442	162.6517
Frequencies --	182.2577	204.6744	225.2564
Frequencies --	246.3113	270.5411	290.4176
Frequencies --	315.5824	336.8531	351.3191
Frequencies --	365.3909	403.1363	406.2141
Frequencies --	418.4799	435.9986	445.9758
Frequencies --	458.0285	487.5888	495.3677
Frequencies --	497.0479	509.0535	535.2828
Frequencies --	557.2483	565.9529	586.4534
Frequencies --	595.5336	611.9866	612.4679
Frequencies --	619.8949	643.2819	644.7499
Frequencies --	669.4517	680.4394	690.0661
Frequencies --	698.8137	728.5618	732.5705
Frequencies --	733.2883	752.5668	762.4402
Frequencies --	777.1484	791.7631	815.3613
Frequencies --	824.3091	826.0924	827.2027
Frequencies --	830.2936	849.1755	854.0201
Frequencies --	909.1556	923.9098	937.0505
Frequencies --	957.4252	966.7320	971.2477
Frequencies --	977.3004	991.6781	1023.8495
Frequencies --	1062.1958	1069.6122	1079.5959
Frequencies --	1099.4356	1100.5188	1143.6250
Frequencies --	1147.9360	1151.4005	1206.6317
Frequencies --	1221.1317	1229.6842	1255.7915
Frequencies --	1261.0217	1272.4535	1299.2182
Frequencies --	1307.8571	1324.9940	1328.5889
Frequencies --	1345.9547	1362.5156	1381.9211
Frequencies --	1394.0030	1401.1249	1434.8405
Frequencies --	1454.3448	1473.9582	1481.3126
Frequencies --	1513.2426	1518.8215	1550.2706
Frequencies --	1567.7488	1570.8065	1583.7440
Frequencies --	1588.5053	1633.3931	1726.1663
Frequencies --	2300.0722	3173.9971	3175.5526
Frequencies --	3185.3102	3199.1890	3202.3379
Frequencies --	3204.5207	3205.0912	3209.3819
Frequencies --	3216.8620	3226.7341	3230.7583
Frequencies --	3249.6238	3577.5957	3715.7607

## BZ-N

C	2.44619000	-0.83858800	-0.09179100
C	2.89289400	-2.15275000	-0.18351800
S	3.79421100	0.25110200	0.01157800
C	4.27871700	-2.27091500	-0.17222800
H	2.22703000	-2.99778800	-0.26154700
C	4.95390300	-1.05603700	-0.07053300
H	4.80817700	-3.21081300	-0.23732200
C	6.35916500	-0.94988700	-0.04133200
H	6.86001300	-1.90742200	-0.10588300
C	7.18828600	0.14056600	0.05393900
C	6.71019300	1.47184700	0.14742100

C	8.65399600	0.01249800	0.06882700
O	9.08500500	-1.26020700	-0.02381600
H	10.05561600	-1.24465400	-0.00298000
O	9.41732000	0.95170100	0.15574500
N	6.31889300	2.55570600	0.22311400
C	-2.98621000	1.04301500	-0.05723300
C	-3.45843200	2.33814400	-0.07438600
S	-4.34570400	-0.07235100	-0.01278700
C	-4.85747300	2.45532000	-0.04607000
H	-2.80599600	3.19838800	-0.10636500
C	-5.49883700	1.22987700	-0.01695700
H	-5.39519300	3.39212900	-0.05514800
H	-7.39199500	1.89663200	-0.11660600
C	-7.57389600	-0.12998600	0.08221300
C	-7.24740500	-1.40756700	0.50081900
C	-8.43478300	-2.19060700	0.39112500
H	-6.29512000	-1.74320600	0.86880300
C	-9.43407400	-1.37757500	-0.07800000
H	-8.53206500	-3.23436200	0.63996500
H	-10.47012100	-1.57048800	-0.29377300
N	-6.85093300	1.04746200	-0.02423300
C	1.07776800	-0.35762600	-0.07807100
C	-0.00295400	-1.25707400	-0.09489500
C	0.76786300	1.01498600	-0.04834800
C	-1.30819400	-0.80993800	-0.08750200
H	0.17775100	-2.32214300	-0.11246200
C	-0.53507900	1.46301600	-0.03958100
H	1.56072400	1.75165300	-0.03369100
C	-1.62134500	0.56327700	-0.06137400
H	-2.10022800	-1.54707600	-0.10451900
H	-0.71659200	2.52771000	-0.01446100
H	-9.39639100	0.67335100	-0.62770700
N	-8.89682700	-0.12571800	-0.26853100

Frequencies --	9.8653	23.1121	24.7332
Frequencies --	30.0490	39.8869	47.1055
Frequencies --	54.0485	58.6543	62.6880
Frequencies --	76.2508	102.3952	112.0315
Frequencies --	141.8900	148.7075	164.5376
Frequencies --	184.1428	215.8562	227.0680
Frequencies --	262.9904	274.0184	304.8090
Frequencies --	314.5477	334.6980	361.6451
Frequencies --	370.8035	393.7625	408.1269
Frequencies --	415.5194	437.4314	446.1985
Frequencies --	469.7384	476.0149	486.8332
Frequencies --	495.1670	509.5292	534.1522
Frequencies --	556.6276	588.9586	612.3235
Frequencies --	618.1844	620.0230	624.2370
Frequencies --	642.8580	644.8231	650.0700
Frequencies --	668.8022	672.9583	698.4166
Frequencies --	706.5654	727.8636	732.8803
Frequencies --	750.4633	759.1844	762.6935
Frequencies --	776.7569	785.8287	797.4171
Frequencies --	825.9547	827.1310	830.3600
Frequencies --	853.5342	869.0674	898.8215
Frequencies --	909.9502	936.3132	956.9374
Frequencies --	966.1529	969.1602	978.0306
Frequencies --	992.1028	993.5261	1022.1294
Frequencies --	1047.2368	1068.4793	1080.4208
Frequencies --	1100.4519	1116.9095	1127.6019
Frequencies --	1143.2186	1148.9761	1203.9720

Frequencies --	1216.4983	1223.4266	1229.7775
Frequencies --	1255.7147	1269.2620	1297.6333
Frequencies --	1301.4453	1309.7021	1325.1969
Frequencies --	1340.2584	1345.0585	1369.7192
Frequencies --	1382.1235	1401.2406	1420.2093
Frequencies --	1430.4750	1443.3498	1457.5018
Frequencies --	1477.1568	1507.1531	1511.8374
Frequencies --	1524.2758	1556.1943	1566.2291
Frequencies --	1583.6088	1597.7596	1607.2644
Frequencies --	1633.8136	1724.6051	2298.4601
Frequencies --	3173.6895	3174.8638	3185.1666
Frequencies --	3197.4850	3201.2658	3204.2645
Frequencies --	3208.9712	3215.9960	3230.5186
Frequencies --	3237.1945	3267.1437	3271.4196
Frequencies --	3565.6395	3625.4646	3715.8777

#### PY-4S

C	-4.26104700	-1.12322200	-0.00083200
C	-3.06220600	-0.85332200	-0.00171600
C	-1.75938400	-0.56007600	-0.00192500
C	-0.55859900	-0.28590100	-0.00319800
C	0.74140200	0.01329000	-0.00331900
C	1.93959100	0.29054800	-0.00416300
C	3.24432000	0.59358300	-0.00355000
C	4.43536600	0.87284700	-0.00329700
C	5.79175600	1.18213300	-0.00224900
C	6.38302400	2.44184500	-0.00119700
S	6.99879200	-0.09057800	-0.00187500
C	7.77957000	2.38496800	0.00002400
H	5.80350000	3.35458000	-0.00123100
C	8.29996000	1.09209300	-0.00007300
H	8.42156700	3.25684000	0.00104500
C	9.69531300	0.82018700	0.00134900
H	10.30461700	1.71780200	0.00251100
C	10.38298800	-0.36445600	0.00158400
C	9.74618500	-1.63484800	0.00017400
C	11.86196200	-0.41677000	0.00334200
O	12.43678300	0.80091500	0.00440900
H	13.40221400	0.67761000	0.00565400
O	12.50189500	-1.44832600	0.00382200
N	9.22319700	-2.66712000	-0.00104000
C	-5.61081100	-1.40808400	-0.00024500
C	-6.25433700	-2.64125300	0.00017000
S	-6.81348500	-0.09689200	0.00016300
C	-7.64884700	-2.56166600	0.00069700
H	-5.70325200	-3.57257000	0.00004700
C	-8.12461200	-1.25145900	0.00071400
H	-8.31316500	-3.41606100	0.00103300
H	-10.06379500	-1.72690400	0.00147900
C	-10.06467600	0.32250400	0.00120900
C	-9.54867000	1.59621100	0.00112400
S	-11.82299600	0.35361100	0.00142600
C	-10.56775500	2.59822500	0.00124100
H	-8.49827600	1.84308400	0.00103500
C	-11.83289800	2.09626000	0.00141400
H	-10.35136400	3.65892800	0.00120700
H	-12.77743400	2.61931700	0.00154600
N	-9.44842300	-0.92051000	0.00114600

Frequencies --	16.6769	23.6803	31.2298
Frequencies --	36.2900	45.6578	56.3790
Frequencies --	65.2539	68.5903	76.6821
Frequencies --	77.3461	86.5522	101.5304
Frequencies --	114.2791	125.9067	136.6550
Frequencies --	155.6479	164.0544	187.7441
Frequencies --	206.8391	209.7054	248.2797
Frequencies --	255.1617	270.8977	276.1139
Frequencies --	296.0014	309.8628	336.7639
Frequencies --	341.7770	408.6150	413.1090
Frequencies --	427.9235	443.8281	444.9124
Frequencies --	486.3947	488.8713	504.2243
Frequencies --	511.7497	523.6897	530.7507
Frequencies --	546.8093	551.7404	564.1262
Frequencies --	568.4072	574.9359	587.5088
Frequencies --	598.2876	603.6518	624.0219
Frequencies --	628.2569	630.7623	652.3027
Frequencies --	664.5209	673.0946	689.0921
Frequencies --	693.5739	698.4219	714.4608
Frequencies --	719.3784	738.4099	756.1474
Frequencies --	782.0647	794.6111	808.2564
Frequencies --	809.7351	820.9604	831.4875
Frequencies --	836.1847	851.8219	916.7622
Frequencies --	930.0411	934.8962	956.0954
Frequencies --	989.5653	1049.3379	1069.4415
Frequencies --	1074.9847	1091.0368	1096.4596
Frequencies --	1130.2130	1137.5842	1155.7120
Frequencies --	1196.4184	1230.0638	1247.0804
Frequencies --	1266.7765	1277.7977	1287.3719
Frequencies --	1338.8969	1359.1847	1372.5232
Frequencies --	1386.0108	1398.7415	1426.5594
Frequencies --	1444.1531	1473.2996	1474.6026
Frequencies --	1514.1901	1541.6171	1560.2415
Frequencies --	1579.4571	1595.5580	1718.9269
Frequencies --	2083.7280	2112.0289	2214.3600
Frequencies --	2235.3060	2284.0270	3173.5684
Frequencies --	3187.9699	3190.9842	3194.8250
Frequencies --	3204.2127	3214.4157	3224.6613
Frequencies --	3232.1995	3525.4368	3681.1013

#### PY-4N

C	-4.70318300	-1.09139700	0.00077300
C	-3.50031400	-0.83105900	0.00075900
C	-2.19728600	-0.54724600	0.00071400
C	-0.99368600	-0.27914800	0.00065300
C	0.30632900	0.01437900	0.00063400
C	1.50635800	0.28792200	0.00057200
C	2.81088000	0.58846100	0.00058700
C	4.00289500	0.86616800	0.00057000
C	5.35898100	1.17365100	0.00055800
C	5.95241200	2.43303800	0.00100500
S	6.56521700	-0.10040500	-0.00006800
C	7.34841000	2.37466800	0.00087100
H	5.37390700	3.34642100	0.00141700
C	7.86831200	1.08114000	0.00029800
H	7.99122800	3.24597500	0.00117000
C	9.26250700	0.80810200	0.00009500
H	9.87270400	1.70512300	0.00053400
C	9.94999800	-0.37749900	-0.00056400
C	9.31258800	-1.64735100	-0.00132700
C	11.42831600	-0.43040900	-0.00059100

O	12.00409700	0.78719900	0.00010500
H	12.96934900	0.66284600	0.00004500
O	12.06857000	-1.46202000	-0.00116900
N	8.78920900	-2.67953700	-0.00196600
C	-6.05260800	-1.36190700	0.00072400
C	-6.71073500	-2.59061200	0.00107300
S	-7.24595900	-0.03752200	0.00014100
C	-8.10182700	-2.49973800	0.00090400
H	-6.16757800	-3.52671700	0.00144200
C	-8.56783900	-1.18207200	0.00038800
H	-8.77413400	-3.34783100	0.00112000
H	-10.52472600	-1.60998600	0.00013400
C	-10.45871300	0.43545300	-0.00040600
C	-9.94473000	1.72419900	-0.00029500
C	-11.06411900	2.61063000	-0.00102000
H	-8.90895600	2.01754300	0.00032800
C	-12.20859500	1.84794100	-0.00192100
H	-11.01949500	3.68924200	-0.00104000
H	-13.25140600	2.12067000	-0.00274100
N	-9.87726700	-0.82787600	0.00006500
H	-12.46224800	-0.26342900	-0.00156200
N	-11.82826100	0.52479200	-0.00150400

Frequencies --	16.9330	24.3009	32.6342
Frequencies --	36.2940	44.2662	66.2517
Frequencies --	66.3862	74.1610	77.1938
Frequencies --	80.4987	87.0041	101.9666
Frequencies --	114.2175	126.3697	141.7071
Frequencies --	155.4598	164.8660	188.3296
Frequencies --	206.8911	216.5370	251.0628
Frequencies --	275.1225	280.6259	291.9822
Frequencies --	310.0324	313.3363	339.8602
Frequencies --	349.7302	408.8889	422.7348
Frequencies --	428.3836	440.2960	445.9810
Frequencies --	478.0526	491.1800	493.5942
Frequencies --	507.6965	512.7712	525.4163
Frequencies --	542.8377	552.0484	561.1465
Frequencies --	595.2420	597.3840	600.2352
Frequencies --	618.0113	627.1929	627.6886
Frequencies --	630.9905	651.3748	655.0226
Frequencies --	655.7090	664.0300	686.2134
Frequencies --	693.8288	698.1310	718.8969
Frequencies --	736.8206	755.7357	763.3423
Frequencies --	781.8690	791.1358	802.0499
Frequencies --	817.5947	821.0093	850.8065
Frequencies --	880.3159	896.4600	917.2241
Frequencies --	933.3738	955.4928	988.1339
Frequencies --	988.9444	1048.1901	1054.9323
Frequencies --	1071.8046	1091.4440	1116.4214
Frequencies --	1123.0738	1130.9770	1154.8820
Frequencies --	1193.9671	1206.1835	1233.1410
Frequencies --	1258.5247	1269.9140	1286.6731
Frequencies --	1299.9893	1347.5710	1367.5667
Frequencies --	1377.4634	1398.4381	1416.6077
Frequencies --	1422.5064	1442.9314	1447.4213
Frequencies --	1474.3714	1492.5466	1513.8071
Frequencies --	1547.0717	1578.4051	1589.5622
Frequencies --	1609.8259	1717.7784	2066.1980
Frequencies --	2106.2130	2209.8810	2230.7511
Frequencies --	2282.9635	3173.3718	3189.8530
Frequencies --	3194.3282	3202.9718	3214.1099
Frequencies --	3219.6520	3250.6060	3256.1193

Frequencies -- 3524.4638            3589.9375            3681.6034

**PY-3S**

C	-3.00017600	0.90628800	0.05381100
C	-1.82524500	0.56118200	0.04554900
C	-0.53888300	0.19834600	0.03427200
C	0.64370900	-0.12542600	0.02299100
C	1.93664700	-0.47297500	0.00871300
C	3.11526900	-0.78919700	-0.00610200
C	4.46152100	-1.13168500	-0.02551100
C	5.02202000	-2.40343700	-0.06878900
S	5.69128500	0.09904000	0.00230700
C	6.41406600	-2.37707100	-0.08114700
H	4.42279200	-3.30035800	-0.09068300
C	6.96122200	-1.09728400	-0.04689200
H	7.03639700	-3.25965200	-0.11411000
C	8.35771800	-0.85601700	-0.05564900
H	8.94700400	-1.76298900	-0.09764700
C	9.06754100	0.31171700	-0.02051800
C	8.45360500	1.58958900	0.04340200
C	10.54356300	0.33983100	-0.04323700
O	11.10160800	-0.88116800	-0.10108500
H	12.06644100	-0.76631500	-0.11317000
O	11.19767500	1.35929700	-0.01358400
N	7.94841800	2.62578100	0.09679600
C	-4.32455900	1.29250600	0.06199000
C	-4.85853900	2.57242400	0.05360100
S	-5.62209100	0.09564300	0.10597000
C	-6.25291700	2.60852500	0.08594700
H	-4.23309500	3.45248000	0.02661100
C	-6.82856700	1.34504800	0.10623900
H	-6.84424900	3.51214600	0.08191700
H	-8.74491800	1.92166600	-0.04727700
C	-8.81096500	-0.12945400	0.13927800
C	-8.48371100	-1.25510800	0.84751200
S	-10.24349100	-0.38810800	-0.82138000
C	-9.39735000	-2.32254200	0.62518700
H	-7.65150900	-1.31375000	1.53155400
C	-10.40667400	-2.00116700	-0.23020100
H	-9.31385600	-3.28544900	1.10753200
H	-11.24463000	-2.60358600	-0.54064700
N	-8.16865900	1.10150600	0.08609800

Frequencies --	4.1226	9.8592	16.5726
Frequencies --	23.6488	29.0259	40.4774
Frequencies --	49.2838	57.0939	64.8257
Frequencies --	74.8395	84.1917	101.9825
Frequencies --	123.5895	133.3437	141.4136
Frequencies --	162.2691	179.9222	215.0264
Frequencies --	228.8573	230.1970	263.2160
Frequencies --	267.2092	296.1155	325.9388
Frequencies --	335.7370	351.5437	401.3957
Frequencies --	412.0105	430.2687	441.7721
Frequencies --	463.7468	468.0354	494.6731
Frequencies --	497.9163	507.3869	511.0092
Frequencies --	518.3610	544.7422	566.2399
Frequencies --	572.7317	577.7656	592.3824
Frequencies --	601.4417	609.7049	617.2009
Frequencies --	622.4801	656.7547	670.7776
Frequencies --	682.2350	692.4416	701.7104

Frequencies --	722.8563	739.9058	750.5211
Frequencies --	777.9823	778.5329	787.4811
Frequencies --	801.2510	802.6171	813.7585
Frequencies --	826.3235	839.6579	840.4566
Frequencies --	850.7874	928.3436	928.4715
Frequencies --	946.3576	977.0563	1019.0219
Frequencies --	1061.7521	1068.3125	1088.7107
Frequencies --	1099.9016	1108.7474	1146.2875
Frequencies --	1156.1242	1189.8011	1223.6364
Frequencies --	1247.5624	1268.7960	1272.7489
Frequencies --	1291.7455	1331.8396	1352.1437
Frequencies --	1376.8239	1392.3808	1401.7885
Frequencies --	1426.0406	1444.4455	1473.1923
Frequencies --	1480.4924	1512.1376	1543.6806
Frequencies --	1572.0954	1578.5673	1590.4699
Frequencies --	1733.5210	2132.6045	2188.6608
Frequencies --	2253.5667	2306.8568	3190.7160
Frequencies --	3206.8475	3211.0386	3214.3208
Frequencies --	3223.9968	3225.2232	3234.3689
Frequencies --	3247.8409	3568.4988	3701.4648

**PY-3N**

C	3.39517500	0.91862700	-0.02823800
C	2.21232700	0.59581200	-0.02857400
C	0.92262900	0.25049400	-0.02642100
C	-0.26303700	-0.06628900	-0.02267800
C	-1.55520000	-0.41326000	-0.01599700
C	-2.73318200	-0.73479200	-0.00777700
C	-4.07543500	-1.08947300	0.00489800
C	-4.62336200	-2.36802000	0.03182000
S	-5.31873700	0.12838100	-0.00990100
C	-6.01500400	-2.35656000	0.04191000
H	-4.01470700	-3.25877200	0.04400400
C	-6.57666300	-1.08225700	0.02228000
H	-6.62788800	-3.24611600	0.06305100
C	-7.97468900	-0.85648000	0.03135400
H	-8.55430300	-1.77026500	0.05932300
C	-8.69771900	0.30450200	0.01164900
C	-8.09747200	1.58952700	-0.03098200
C	-10.17325700	0.31651200	0.03151200
O	-10.71926600	-0.91116800	0.06767300
H	-11.68509700	-0.80554900	0.07977500
O	-10.83868800	1.32924800	0.01744000
N	-7.60336800	2.63192600	-0.06703300
C	4.72821300	1.26331200	-0.02595000
C	5.30949500	2.52577000	-0.02653700
S	5.98589300	0.02198000	-0.03191200
C	6.70117600	2.51375600	-0.03645600
H	4.71455000	3.42714300	-0.02000000
C	7.23657500	1.22760200	-0.02999900
H	7.32374200	3.39620600	-0.03696500
H	9.16923900	1.74844600	0.07350400
C	9.18592700	-0.29617500	-0.02335000
C	8.77819200	-1.54926400	-0.44231400
C	9.87661800	-2.42970500	-0.22343800
H	7.83293700	-1.80808300	-0.88415400
C	10.90634400	-1.69437800	0.30743200
H	9.89928300	-3.48384900	-0.44411400
H	11.90097000	-1.97324900	0.60772700
N	8.56062900	0.94286100	0.00093800



H	11.01261400	0.36435200	0.81290700
N	10.47301000	-0.39710800	0.43012100

Frequencies --	6.4961	12.0490	16.9096
Frequencies --	23.1332	29.3361	38.7165
Frequencies --	55.0916	58.9337	66.8496
Frequencies --	77.2608	86.0857	107.3646
Frequencies --	125.4938	137.3716	144.6340
Frequencies --	165.2310	181.5946	218.8675
Frequencies --	230.9148	243.8819	266.8684
Frequencies --	277.9817	311.2368	325.6839
Frequencies --	338.5406	365.8770	402.1395
Frequencies --	414.8344	429.4387	442.1770
Frequencies --	466.3488	476.1100	489.4353
Frequencies --	499.5172	505.7673	511.0162
Frequencies --	516.2315	543.1488	571.8983
Frequencies --	575.5024	595.6796	608.0561
Frequencies --	621.8703	622.5615	624.6925
Frequencies --	644.1828	660.8332	670.7682
Frequencies --	675.0220	701.4338	711.3522
Frequencies --	729.3199	749.3527	764.7485
Frequencies --	767.9371	776.0241	778.3268
Frequencies --	790.6016	797.7854	805.4864
Frequencies --	826.5955	840.6955	875.1467
Frequencies --	898.6569	928.6075	947.5267
Frequencies --	978.9905	993.3348	1019.2620
Frequencies --	1049.8039	1068.0577	1088.9241
Frequencies --	1109.8682	1115.2958	1127.7637
Frequencies --	1153.0350	1187.8799	1211.6404
Frequencies --	1227.3248	1256.8725	1276.1972
Frequencies --	1288.4753	1301.6763	1333.9792
Frequencies --	1367.1469	1380.8266	1400.8099
Frequencies --	1420.8426	1425.7897	1431.5029
Frequencies --	1458.5654	1479.0588	1502.4975
Frequencies --	1514.9418	1556.0843	1587.1993
Frequencies --	1594.6008	1606.1950	1732.1649
Frequencies --	2121.0828	2180.9598	2249.1511
Frequencies --	2305.4760	3189.3731	3209.9229
Frequencies --	3214.2820	3223.5537	3233.9561
Frequencies --	3239.6871	3266.0437	3271.6088
Frequencies --	3559.3098	3622.4836	3702.4895

**PY-2S**

C	1.74465000	0.72886800	0.04718000
C	0.59326700	0.31820000	0.03262300
C	-0.67502500	-0.12070500	0.01275000
C	-1.82804600	-0.51918000	-0.00702500
C	-3.14746300	-0.95168200	-0.03198400
C	-3.62419400	-2.25811500	-0.08702100
S	-4.45650600	0.19423700	0.00451600
C	-5.01403800	-2.32402800	-0.10121900
H	-2.96718800	-3.11349600	-0.11586900
C	-5.64705500	-1.08336800	-0.05687500
H	-5.57634800	-3.24569700	-0.14301400
C	-7.05366700	-0.93282600	-0.06484900
H	-7.58369400	-1.87527100	-0.11491800
C	-7.84069300	0.18651900	-0.02028900
C	-7.31311300	1.50130200	0.05373100
C	-9.31356200	0.11647600	-0.04213300
O	-9.79099400	-1.13864300	-0.11514000

H	-10.76089900	-1.08624900	-0.12493400
O	-10.03561700	1.08922900	0.00033300
N	-6.87850600	2.56893300	0.11457800
C	3.04972000	1.18230100	0.06109500
C	3.52113100	2.48536500	0.05538100
S	4.40205800	0.04905300	0.10813000
C	4.91363900	2.58848200	0.09164600
H	2.85473800	3.33489400	0.02742700
C	5.54816100	1.35453900	0.11296000
H	5.46090900	3.51942100	0.08997100
H	7.44229500	2.00939200	-0.04396000
C	7.58597400	-0.03810800	0.15648000
C	7.32349400	-1.15227900	0.90806700
S	8.98699000	-0.28026900	-0.85360000
C	8.26143600	-2.19684900	0.67963800
H	6.51913200	-1.21528800	1.62450700
C	9.22589900	-1.86876900	-0.22408200
H	8.22907400	-3.14699700	1.19244200
H	10.07125500	-2.45308300	-0.54889600
N	6.89848400	1.16856300	0.09606700

Frequencies --	9.6882	16.2229	19.7414
Frequencies --	26.5948	36.6849	43.2294
Frequencies --	52.3134	60.0910	71.0224
Frequencies --	87.7510	99.4964	113.1578
Frequencies --	146.4071	154.9468	165.3096
Frequencies --	192.7867	218.9306	232.0950
Frequencies --	247.3364	258.0659	308.5822
Frequencies --	318.8531	338.5119	349.0858
Frequencies --	401.4012	426.0903	434.0850
Frequencies --	442.7372	467.1368	485.9954
Frequencies --	498.0204	499.9786	504.0760
Frequencies --	524.0964	529.1815	547.0644
Frequencies --	566.6895	590.1717	598.2994
Frequencies --	599.0976	611.6058	619.6318
Frequencies --	635.5658	641.9871	665.6870
Frequencies --	675.0208	684.0809	692.6984
Frequencies --	701.4018	729.0028	746.5589
Frequencies --	755.3032	777.6712	797.9236
Frequencies --	813.1193	827.4323	833.7384
Frequencies --	840.3423	851.2069	910.1649
Frequencies --	923.8431	927.4353	940.1621
Frequencies --	972.0733	1057.8301	1062.6755
Frequencies --	1074.4963	1093.8432	1099.2275
Frequencies --	1143.3783	1148.6771	1164.6455
Frequencies --	1212.2672	1237.0602	1260.5622
Frequencies --	1269.4160	1286.3656	1319.0115
Frequencies --	1351.1335	1368.6280	1389.2607
Frequencies --	1402.7609	1415.3937	1444.4099
Frequencies --	1471.8499	1477.4711	1509.2013
Frequencies --	1529.2553	1572.2624	1578.5958
Frequencies --	1589.6392	1730.1544	2193.5371
Frequencies --	2217.1761	2304.0351	3184.2981
Frequencies --	3206.6661	3209.7545	3212.9080
Frequencies --	3222.8469	3224.6192	3232.5699
Frequencies --	3246.6218	3571.4854	3708.8761

**PY-2N**

C	2.09672800	0.66599400	0.01801100
C	0.93889200	0.26926800	0.02424700

C	-0.33349000	-0.15348000	0.03119600
C	-1.49194100	-0.53948300	0.03798500
C	-2.81435500	-0.95884600	0.04598500
C	-3.30434200	-2.26206200	0.08696000
S	-4.11379300	0.19889500	0.00203400
C	-4.69389700	-2.31566500	0.08443200
H	-2.65527500	-3.12341900	0.11756400
C	-5.31690000	-1.06918800	0.04080200
H	-5.26453800	-3.23274700	0.11331700
C	-6.72080500	-0.90732900	0.03228300
H	-7.25908300	-1.84575800	0.06871600
C	-7.49913300	0.21949700	-0.01450600
C	-6.96037000	1.53020800	-0.07249100
C	-8.97167000	0.16117500	-0.01288200
O	-9.46069900	-1.09072900	0.04622800
H	-10.43008700	-1.02942700	0.04141200
O	-9.68643200	1.13953100	-0.05939500
N	-6.51710700	2.59512300	-0.12026200
C	3.40561600	1.10004700	0.01115300
C	3.89941100	2.39814300	0.00761300
S	4.74320900	-0.05256600	-0.00851600
C	5.28946700	2.48050800	-0.01497000
H	3.24528500	3.25751900	0.02030700
C	5.91077000	1.23425100	-0.01762700
H	5.85089100	3.40303900	-0.02016100
H	7.80460000	1.88541200	0.05933400
C	7.96097200	-0.15246500	-0.04940100
C	7.62208200	-1.43772600	-0.43163000
C	8.79092900	-2.23506100	-0.26292300
H	6.67537200	-1.77074000	-0.81654300
C	9.79206300	-1.42126700	0.20352700
H	8.87670300	-3.28817400	-0.47284600
H	10.81841600	-1.62439300	0.45355800
N	7.25233200	1.03951800	-0.00345000
H	9.77802800	0.64652600	0.68084500
N	9.27419100	-0.15587800	0.33470700

Frequencies --	11.2343	18.1946	20.1677
Frequencies --	23.3009	37.8958	44.2628
Frequencies --	58.2560	60.0872	73.3998
Frequencies --	92.5703	101.8898	122.8859
Frequencies --	147.7316	157.6131	166.2534
Frequencies --	202.7762	220.5367	235.0394
Frequencies --	257.9468	273.7253	316.1609
Frequencies --	325.4619	331.9950	365.7666
Frequencies --	403.6416	430.6483	436.6865
Frequencies --	444.6858	468.8193	479.5855
Frequencies --	497.5242	498.9173	504.6699
Frequencies --	522.5905	536.8703	544.8932
Frequencies --	593.1178	595.8909	609.4270
Frequencies --	617.7817	623.4216	625.7355
Frequencies --	641.2072	649.5282	666.6404
Frequencies --	674.5064	677.4042	701.2908
Frequencies --	710.6141	742.1339	755.1646
Frequencies --	767.3251	777.3465	793.3573
Frequencies --	796.5295	827.8124	834.0213
Frequencies --	874.3853	898.2210	910.4997
Frequencies --	925.5278	941.6990	973.7053
Frequencies --	994.0168	1049.7874	1061.4162
Frequencies --	1076.0573	1094.8405	1118.0715
Frequencies --	1127.5388	1144.6339	1163.6933
Frequencies --	1209.4371	1213.3488	1245.7328

Frequencies --	1271.0591	1288.1614	1295.6024
Frequencies --	1325.4214	1364.6727	1372.5628
Frequencies --	1401.7789	1410.6847	1424.7804
Frequencies --	1444.3706	1447.9698	1476.6304
Frequencies --	1502.8601	1511.4662	1538.2417
Frequencies --	1587.7814	1596.1604	1606.5131
Frequencies --	1728.4044	2186.9773	2206.7603
Frequencies --	2302.2004	3186.4761	3209.3475
Frequencies --	3212.8336	3222.8142	3232.3039
Frequencies --	3239.2559	3266.5070	3271.5390
Frequencies --	3550.5193	3623.5549	3708.6770

**PY-1S**

C	-0.51583100	0.42498000	0.05598400
C	0.59699200	-0.06818900	0.02732400
C	1.87015900	-0.61987400	-0.00434700
C	2.21988000	-1.96869300	-0.04562000
S	3.28470700	0.39374100	0.00580900
C	3.59442500	-2.16902000	-0.06851500
H	1.48297600	-2.75682100	-0.05793300
C	4.34910300	-0.99592100	-0.04578300
H	4.06355800	-3.14192700	-0.10108800
C	5.75898800	-0.98735200	-0.06303600
H	6.19027500	-1.97960300	-0.09760000
C	6.66082000	0.04725600	-0.04321300
C	6.27247400	1.40969100	0.00237700
C	8.11496300	-0.17849200	-0.06782200
O	8.45553500	-1.48022000	-0.11344800
H	9.42519100	-1.53223700	-0.12795400
O	8.94082500	0.71000000	-0.04970700
N	5.94986900	2.51788500	0.03948000
C	-1.78948900	0.96712900	0.08824300
C	-2.17220600	2.29702800	0.13287800
S	-3.21189300	-0.07450200	0.09810000
C	-3.55568700	2.49074300	0.17902900
H	-1.45127700	3.10134800	0.13408000
C	-4.27037800	1.30217800	0.15708000
H	-4.03924100	3.45566100	0.21465800
H	-6.11704500	2.08830300	0.04182300
C	-6.39899800	0.04894900	0.15709900
C	-6.20161000	-1.11775100	0.84685800
S	-7.83257100	-0.04498100	-0.83231200
C	-7.21478600	-2.08210200	0.58802100
H	-5.39098900	-1.27305900	1.54168900
C	-8.17084800	-1.64306200	-0.27652400
H	-7.23896300	-3.05723400	1.05214700
H	-9.06068000	-2.15041300	-0.61201900
N	-5.63078400	1.20706400	0.13933200

Frequencies --	13.1747	16.7681	24.5927
Frequencies --	26.7891	49.8434	51.6842
Frequencies --	60.1255	61.5362	79.7295
Frequencies --	101.1328	125.0322	135.6725
Frequencies --	153.8347	186.8453	200.2188
Frequencies --	221.2464	249.2967	253.8117
Frequencies --	307.1951	310.0139	329.9528
Frequencies --	372.8237	397.2984	420.9628
Frequencies --	435.1924	448.6047	472.5303
Frequencies --	492.8841	499.0223	506.6551
Frequencies --	529.5773	545.0619	556.5423

Frequencies --	564.5247	572.9732	589.6729
Frequencies --	603.3164	606.0307	617.7001
Frequencies --	646.9505	665.5116	681.4478
Frequencies --	695.5046	697.6430	713.0502
Frequencies --	732.9041	748.8115	769.9419
Frequencies --	776.0406	792.0404	810.8316
Frequencies --	824.9379	826.6341	839.7126
Frequencies --	850.7558	918.3339	927.3339
Frequencies --	933.9692	967.2537	1022.3218
Frequencies --	1062.0158	1069.3766	1087.1219
Frequencies --	1094.8976	1116.5142	1143.6811
Frequencies --	1151.2734	1202.9368	1224.3043
Frequencies --	1252.1373	1269.3804	1281.3180
Frequencies --	1298.1418	1339.1214	1365.2130
Frequencies --	1386.9735	1396.2097	1404.3565
Frequencies --	1424.6291	1472.7360	1481.1726
Frequencies --	1503.6626	1546.6617	1571.5437
Frequencies --	1575.2075	1587.8667	1725.7779
Frequencies --	2216.1320	2299.2565	3189.1848
Frequencies --	3206.4272	3209.0195	3210.2982
Frequencies --	3221.7509	3226.9442	3228.5652
Frequencies --	3245.3200	3572.4756	3710.3516

**PY-1N**

C	-0.84506700	0.42309300	-0.04674200
C	0.27470800	-0.05813600	-0.05855700
C	1.54880800	-0.60343400	-0.07313700
C	1.90239900	-1.95229900	-0.13239100
S	2.96305300	0.41074000	-0.01500600
C	3.27599900	-2.15090000	-0.13333500
H	1.16667200	-2.74051800	-0.17418100
C	4.03064600	-0.97786000	-0.07230600
H	3.74650200	-3.12275400	-0.17602700
C	5.43872300	-0.96956700	-0.05737400
H	5.87037500	-1.96075900	-0.11314100
C	6.34232600	0.06288600	0.02069800
C	5.95558100	1.42323500	0.10944600
C	7.79504000	-0.16570500	0.02801400
O	8.13531200	-1.46496900	-0.07555700
H	9.10460400	-1.51920500	-0.05321600
O	8.62271700	0.71715300	0.11952800
N	5.63574300	2.53071000	0.18221800
C	-2.12737200	0.93847500	-0.03392800
C	-2.54498300	2.26163500	-0.02717200
S	-3.52637400	-0.13598900	-0.00835200
C	-3.92942600	2.42346000	0.00240100
H	-1.84328300	3.08264600	-0.04270700
C	-4.61979500	1.21497900	0.00743100
H	-4.43644500	3.37693900	0.01101600
H	-6.47833000	1.96539500	-0.07033100
C	-6.73923000	-0.06070900	0.06900700
C	-6.47565500	-1.34119500	0.51943100
C	-7.67475000	-2.09039500	0.34358600
H	-5.55934900	-1.69798200	0.95374700
C	-8.61926300	-1.25315100	-0.19430600
H	-7.81872900	-3.12738600	0.59755000
H	-9.64533600	-1.41987200	-0.47118800
N	-5.97062700	1.09254600	-0.00439000
N	-8.03690600	-0.02088900	-0.36330200
H	-8.48738700	0.78697000	-0.76585300

Frequencies --	15.2495	17.2737	29.5608
Frequencies --	44.0689	55.1033	61.8855
Frequencies --	62.8524	73.6022	87.0424
Frequencies --	107.4785	128.9565	145.7375
Frequencies --	155.1992	187.9342	203.4414
Frequencies --	235.3228	252.8052	266.8913
Frequencies --	309.8145	326.9453	336.4900
Frequencies --	390.7037	401.8490	430.6791
Frequencies --	436.2340	449.6635	475.8225
Frequencies --	497.3340	503.0283	506.5580
Frequencies --	528.5116	547.6681	554.3494
Frequencies --	580.9068	593.4119	606.1545
Frequencies --	616.2400	624.0229	643.8974
Frequencies --	655.7705	664.2794	676.9396
Frequencies --	697.2838	711.4003	714.1050
Frequencies --	745.2068	767.6388	774.2387
Frequencies --	779.0866	787.4050	793.5345
Frequencies --	824.6340	826.3087	875.5304
Frequencies --	898.2874	920.1328	932.1854
Frequencies --	963.6824	992.7388	1021.6025
Frequencies --	1048.8615	1069.5144	1087.3784
Frequencies --	1115.8106	1120.2521	1127.3688
Frequencies --	1145.8512	1201.4297	1213.4625
Frequencies --	1227.1641	1260.7228	1281.7188
Frequencies --	1297.5075	1300.7922	1353.2343
Frequencies --	1370.3156	1394.3387	1403.4842
Frequencies --	1416.6125	1426.4359	1451.7583
Frequencies --	1482.0494	1501.7748	1504.7748
Frequencies --	1561.8409	1578.4704	1597.3159
Frequencies --	1607.0954	1723.9112	2206.6556
Frequencies --	2296.4026	3189.0083	3209.2737
Frequencies --	3210.9306	3222.5049	3230.1671
Frequencies --	3239.5277	3266.7073	3271.6718
Frequencies --	3558.1172	3618.9621	3712.8257

## TH-S

C	2.37387500	-0.14203800	0.03964000
C	2.46377100	-1.53270100	0.07723600
S	3.95803100	0.57104400	-0.03407000
C	3.77101900	-2.00060900	0.05491900
H	1.60070000	-2.17967800	0.13097000
C	4.73944200	-0.99837400	-0.00154700
H	4.03951000	-3.04700000	0.08369800
C	6.12192100	-1.25713500	-0.02209100
H	6.35825100	-2.31329500	0.00333500
C	7.20605800	-0.41162800	-0.06656300
C	7.08509900	0.99972400	-0.10625000
C	8.58934000	-0.90864600	-0.07356900
O	8.68029300	-2.25259300	-0.03864100
H	9.62388100	-2.48322600	-0.04504200
O	9.56995200	-0.19374000	-0.10547400
N	6.98512300	2.15009100	-0.13965000
C	-2.60558200	1.63864600	0.05946400
C	-3.34970900	2.80020600	0.06936300
S	-3.67290800	0.24521600	0.06867700
C	-4.73843000	2.59671400	0.09008600
H	-2.89688600	3.78087700	0.06630900
C	-5.08728800	1.25974100	0.08230800
H	-5.47358900	3.38803800	0.09806300

H	-7.07563800	1.48213100	-0.10831900
C	-6.78711000	-0.54208500	0.11030700
C	-6.23256300	-1.60814500	0.77011600
S	-8.22169100	-1.02541200	-0.75846800
C	-6.97409900	-2.80880600	0.58649300
H	-5.35699700	-1.53970600	1.39599700
C	-8.07928300	-2.65102400	-0.19188300
H	-6.70070300	-3.74922700	1.04258800
H	-8.82824200	-3.37826700	-0.45900600
N	-6.36659100	0.77622600	0.03566400
C	1.19990600	0.66770400	0.05439200
C	1.08675700	2.04624100	0.12000000
S	-0.39476900	-0.04800400	-0.01038200
C	-0.23088000	2.51321400	0.12643400
H	1.94222400	2.70476100	0.17528300
C	-1.18041500	1.50182000	0.06494700
H	-0.49378900	3.55861800	0.18202800

Frequencies --	11.6212	25.5948	25.8756
Frequencies --	35.3280	41.2350	49.8358
Frequencies --	57.1290	58.5748	67.0752
Frequencies --	79.8516	94.8683	112.1838
Frequencies --	136.0354	149.6303	163.2978
Frequencies --	170.4676	211.1255	226.5050
Frequencies --	243.4640	272.2720	288.4889
Frequencies --	307.2345	323.8471	338.0018
Frequencies --	356.2984	401.5638	404.9089
Frequencies --	415.2742	444.2944	451.7314
Frequencies --	487.3023	497.2468	510.8777
Frequencies --	519.5740	530.3190	555.5160
Frequencies --	566.3294	584.4072	593.2998
Frequencies --	606.6060	610.8483	613.4179
Frequencies --	624.8291	627.3025	661.6393
Frequencies --	672.9659	676.6223	684.9023
Frequencies --	704.6517	732.0228	736.8649
Frequencies --	749.7592	753.4014	776.1388
Frequencies --	793.9839	814.5816	816.0405
Frequencies --	821.4417	824.9805	826.6517
Frequencies --	849.0156	877.0359	914.5027
Frequencies --	919.7620	922.0485	928.9151
Frequencies --	934.0595	969.2795	1060.3002
Frequencies --	1065.0902	1072.9758	1091.4203
Frequencies --	1094.5830	1103.2438	1138.3188
Frequencies --	1149.7099	1178.8059	1210.1996
Frequencies --	1234.1586	1244.2651	1259.8218
Frequencies --	1270.7280	1293.8624	1307.4397
Frequencies --	1329.6575	1350.7562	1361.1864
Frequencies --	1393.6900	1396.9278	1401.8515
Frequencies --	1406.7641	1473.6133	1479.8689
Frequencies --	1480.7237	1502.9016	1517.3061
Frequencies --	1550.6976	1569.4982	1582.2240
Frequencies --	1588.4425	1722.6898	2294.1100
Frequencies --	3185.3975	3200.7053	3205.3672
Frequencies --	3206.0406	3207.3343	3218.7285
Frequencies --	3219.5312	3224.4650	3230.5087
Frequencies --	3251.2616	3568.9850	3706.4108

**TH-N**

C	2.08665800	0.15785000	0.00045500
C	2.20022900	1.54858900	0.01819300
S	3.66103900	-0.58318400	0.00172600

C	3.51397800	1.99405300	0.02843400
H	1.34606000	2.20943600	0.01925200
C	4.46824400	0.97516200	0.02041400
H	3.79948700	3.03627400	0.03975200
C	5.85297400	1.21196600	0.02557100
H	6.10498000	2.26462800	0.03701000
C	6.92659700	0.34938700	0.01837100
C	6.78506600	-1.05993100	0.00520800
C	8.31528200	0.82681600	0.02385300
O	8.42446800	2.17057000	0.03536000
H	9.37119000	2.38745900	0.03794400
O	9.28782000	0.09946900	0.01843600
N	6.66741600	-2.20926000	-0.00522000
C	-2.92431400	-1.52079300	-0.01263300
C	-3.69183900	-2.67014900	-0.01133600
S	-3.96896500	-0.10849500	-0.01785000
C	-5.07365700	-2.44403900	-0.02014900
H	-3.25594200	-3.65855200	-0.00463300
C	-5.40178700	-1.09751100	-0.01489900
H	-5.82269900	-3.22222100	-0.01956900
H	-7.39622200	-1.28861500	0.11227400
C	-7.07885000	0.72773300	-0.03046900
C	-6.46938700	1.88953900	-0.46842600
C	-7.41035000	2.94281700	-0.27505200
H	-5.49112300	1.98084700	-0.90441800
C	-8.54909500	2.39741100	0.26071100
H	-7.25850800	3.98206900	-0.51505500
H	-9.48628500	2.84101100	0.54725200
N	-6.66569800	-0.59503200	0.02140500
C	0.89893100	-0.62626800	-0.01561800
C	0.75598800	-2.00373700	-0.07038900
S	-0.68244800	0.12344300	0.03709600
C	-0.56911200	-2.44357700	-0.07393500
H	1.59815500	-2.68014400	-0.11345200
C	-1.50028800	-1.41162000	-0.02188700
H	-0.85340100	-3.48380400	-0.11838200
N	-8.33400000	1.04826800	0.41169900
H	-8.99363700	0.39304400	0.80244100

Frequencies --	9.0846	19.8293	23.4958
Frequencies --	31.0645	33.9237	45.6800
Frequencies --	49.6132	57.1389	62.4042
Frequencies --	76.1059	87.3439	108.4834
Frequencies --	131.5698	150.8416	162.5263
Frequencies --	169.2015	224.5726	226.0215
Frequencies --	248.5054	251.4390	275.3683
Frequencies --	301.4915	327.7099	333.5580
Frequencies --	357.0186	391.6430	410.1495
Frequencies --	416.4679	444.9076	454.5566
Frequencies --	483.5636	511.5203	519.0553
Frequencies --	533.5339	543.9223	554.7418
Frequencies --	585.7562	603.5275	607.3553
Frequencies --	613.7334	620.0603	625.6176
Frequencies --	636.1719	639.6814	660.9302
Frequencies --	672.8102	679.7408	704.0199
Frequencies --	721.9464	736.3669	749.1772
Frequencies --	750.9066	775.9180	784.9071
Frequencies --	788.9975	816.5695	816.6742
Frequencies --	820.2858	825.4810	876.6342
Frequencies --	885.4605	895.3832	909.7144
Frequencies --	919.4126	926.9116	932.5956
Frequencies --	967.0613	988.2114	1039.3382



Frequencies --	1058.4280	1071.3113	1089.4845
Frequencies --	1102.4235	1112.0391	1130.1906
Frequencies --	1139.3319	1176.5788	1208.6712
Frequencies --	1225.9942	1233.2643	1255.6335
Frequencies --	1264.1259	1286.4005	1294.9019
Frequencies --	1307.6035	1330.2853	1351.1921
Frequencies --	1361.8676	1397.1361	1398.5788
Frequencies --	1407.7032	1427.3832	1442.8039
Frequencies --	1462.4438	1481.7109	1483.0066
Frequencies --	1501.0272	1510.0094	1544.5187
Frequencies --	1570.3534	1587.6994	1608.3155
Frequencies --	1720.9531	2293.7534	3184.0457
Frequencies --	3199.2934	3204.1633	3205.7536
Frequencies --	3216.9117	3219.0009	3224.3184
Frequencies --	3234.2784	3247.4391	3265.9370
Frequencies --	3575.3884	3629.9592	3707.0257

Fig. 1: Calculated absorption spectra of MM6 (TD-CAM-B3LYP/6-311+G(d,p)/SMD), C293 (TD-CAM-B3LYP/6-311+G(d,p)/SMD) and D2 (TD-CAM-B3LYP/6-311+G(3df,3pd)/SMD). The spectra are Gaussianbroadened with 0.3 eV (half width half maximum).

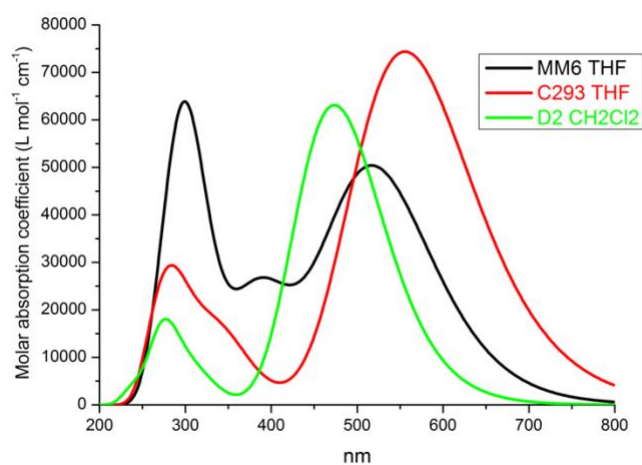
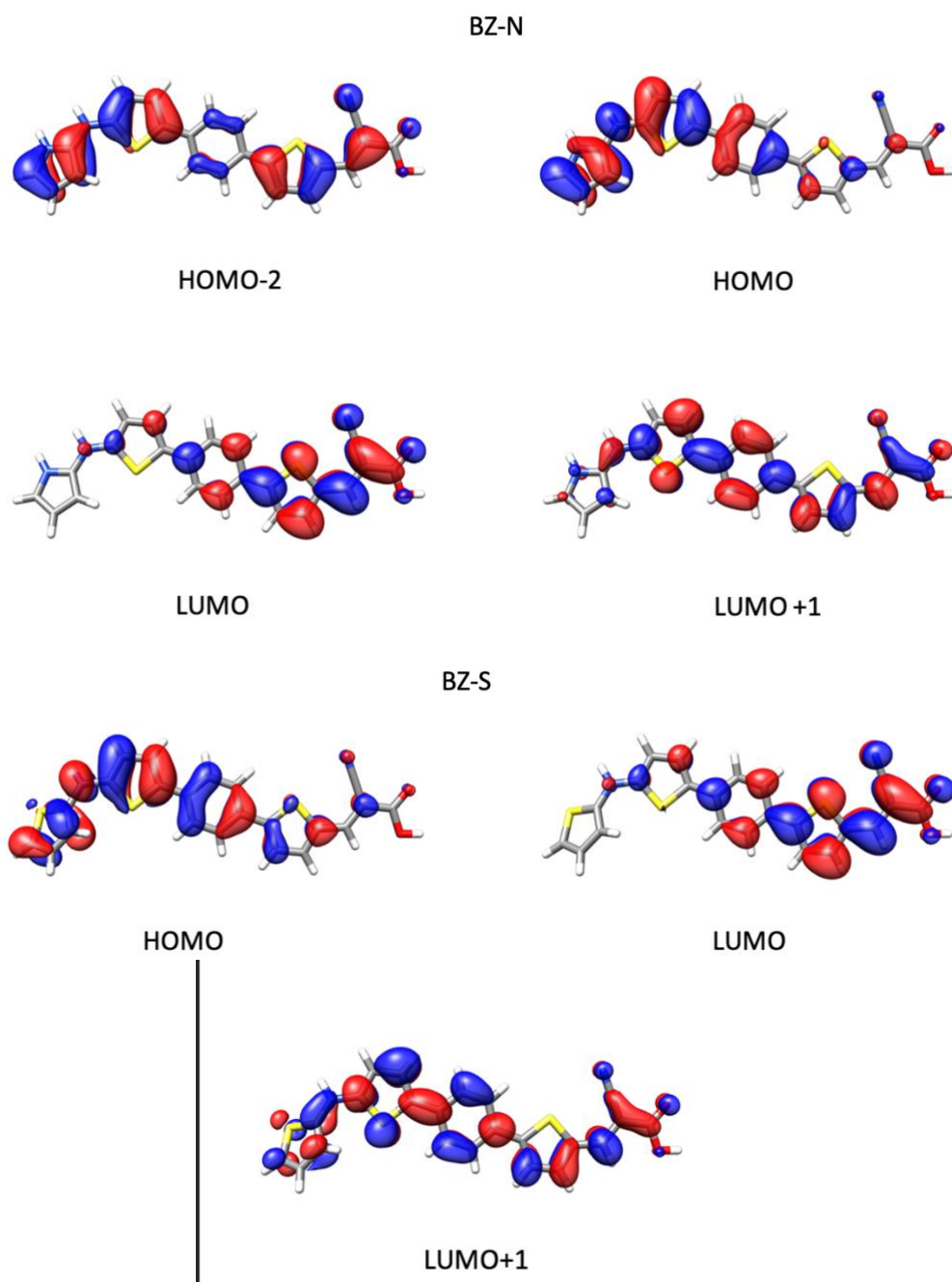
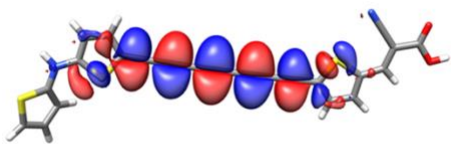


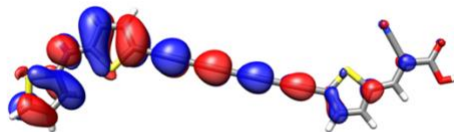
Fig. 2: Main MOs involved in electronic transitions.



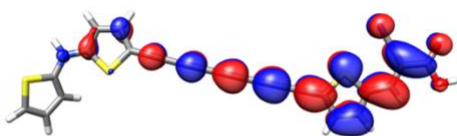
PY-4S



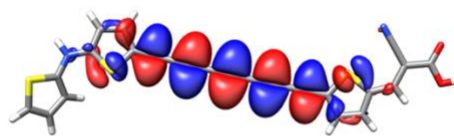
HOMO-2



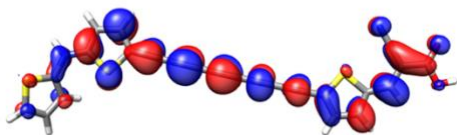
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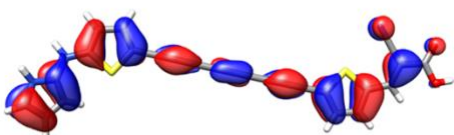
LUMO



LUMO+1

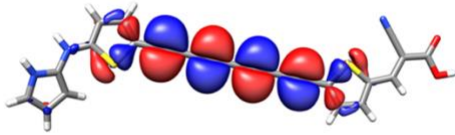


LUMO+2

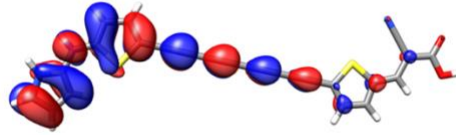


LUMO+3

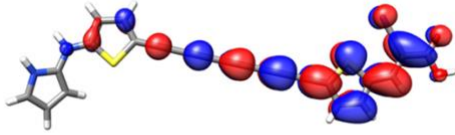
PY-4N



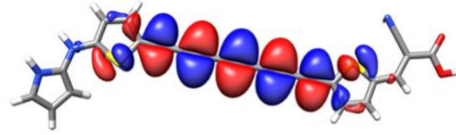
HOMO-2



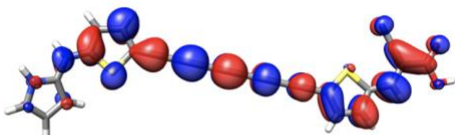
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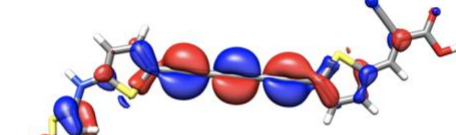
LUMO



LUMO+1

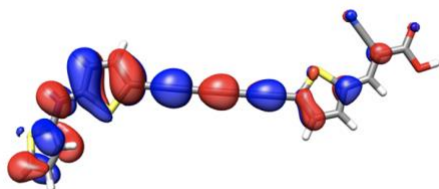


LUMO+2

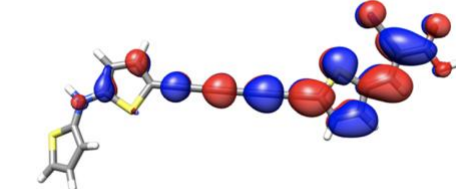


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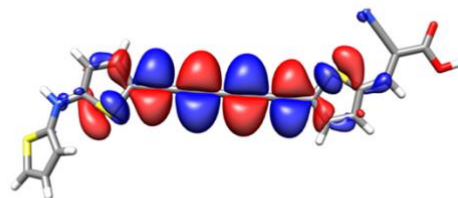
PY-3S



HOMO

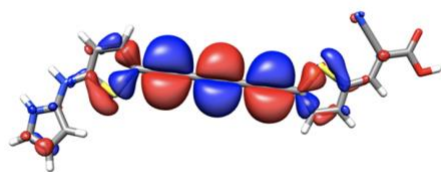


LUMO

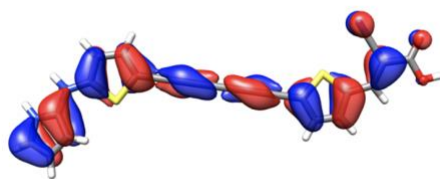


LUMO+1

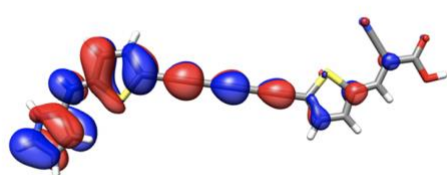
PY-3N



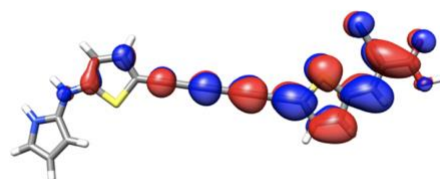
HOMO-3



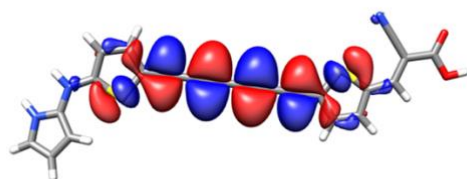
HOMO-2



HOMO

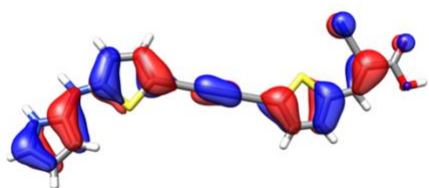


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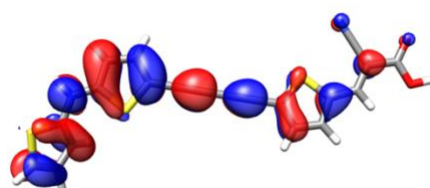


LUMO+1

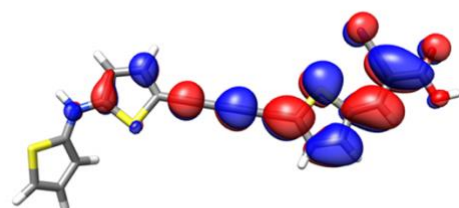
PY-2S



HOMO-6

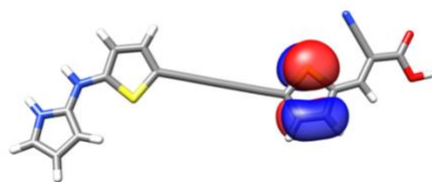


HOMO

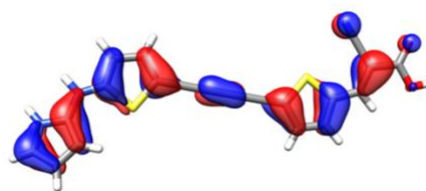


LUMO

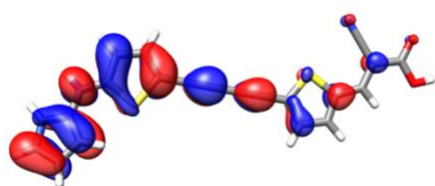
PY-2N



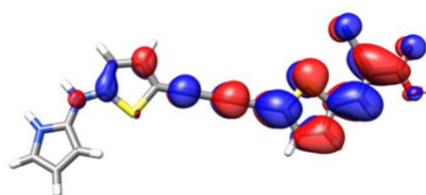
HOMO-6



HOMO-2

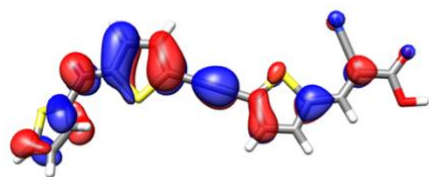


HOMO

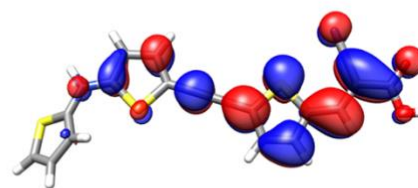


LUMO

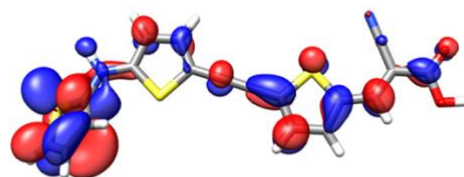
PY-1S



HOMO

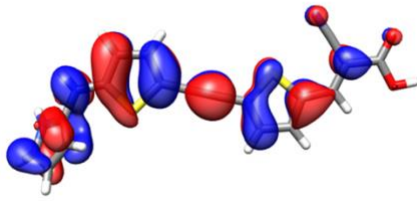


LUMO

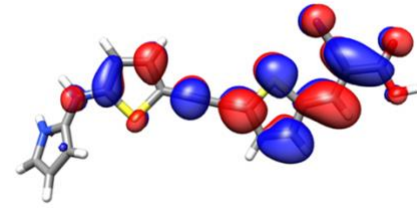


LUMO +2

PY-1N

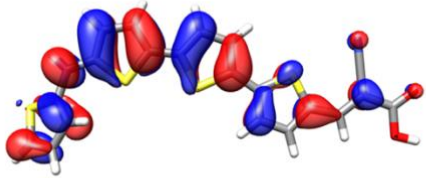


HOMO

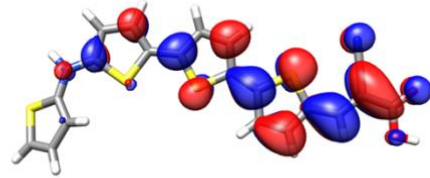


LUMO

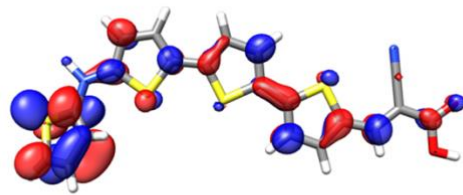
TH-S



HOMO



LUMO

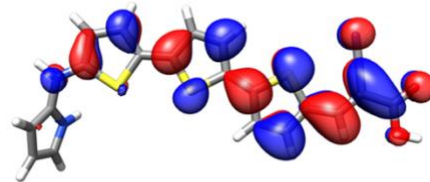


LUMO +2

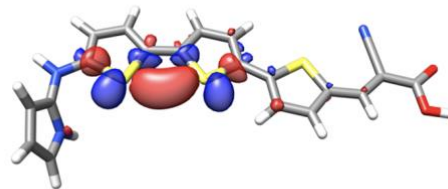
TH-N



HOMO



LUMO



LUMO +3

Table 1: Carbon-Carbon lengths ( $\text{\AA}$ ) for LCCs

PY-4N	PY-4S	PY-3N	PY-3S	PY-2N	PY-2S	PY-N	PY-S
1,228	1,226	1,226	1,225	1,224	1,223	1,219	1,218
1,335	1,334	1,335	1,337	1,341	1,342		
1,230	1,229	1,227	1,226	1,221	1,220		
1,334	1,332	1,338	1,339	<b>1,262</b>	<b>1,262</b>		
1,228	1,227	1,221	1,220				
1,340	1,338	1,269	1,269				
1,221	1,220						
1,274	1,272						

Fig. 3: absorption spectra of I—Dye@ $(\text{TiO}_2)_{14}$  at TD-M062X/6-31G(d)/LANL2DZ/SDDALL level. The spectra are Gaussianbroadened with 0.3 eV (half width half maximum).

