

## Supplementary Material

### First principle study of electronic and non-linear optical properties of triphenylamine dyes: Interactive design computation of new NLO compounds

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#### Optimized Cartesian Coordinates

Dye 1

Symbol	X	Y	Z
C	2.201819	2.183373	-1.06588
C	2.577269	1.261278	-0.07853
C	2.803381	3.439755	-1.11167
C	3.570272	1.607213	0.847817
C	3.795541	3.782602	-0.19107
C	4.178418	2.859607	0.783976
N	1.972918	-0.03428	-0.02727
C	2.833444	-1.17284	0.059741
C	2.609044	-2.16284	1.027316
C	3.927592	-1.29181	-0.80801
C	3.46151	-3.26227	1.111489
C	4.78397	-2.38666	-0.7062
C	4.553439	-3.37843	0.248968
C	0.582447	-0.18265	-0.07235

C	-0.27233	0.843305	0.391617
C	-0.00807	-1.35951	-0.58127
C	-1.64725	0.705582	0.345712
C	-1.38411	-1.48883	-0.62028
C	-2.25092	-0.46842	-0.16461
H	1.441184	1.911485	-1.79031
H	2.503737	4.147118	-1.87914
H	4.101569	-0.52398	-1.55457
H	5.628697	-2.46842	-1.38372
H	0.157101	1.749611	0.801601
H	0.62067	-2.15895	-0.95447
H	-2.26005	1.51375	0.723934
H	-1.81374	-2.39987	-1.02866
H	3.278659	-4.02263	1.864997
H	4.946077	3.117779	1.50734
H	3.859115	0.892309	1.611061
H	1.769916	-2.06408	1.708086
H	5.219591	-4.23237	0.322559
H	4.266527	4.759671	-0.23396
C	-3.67058	-0.71319	-0.26136
H	-3.92682	-1.68201	-0.68098
C	-4.75691	0.048533	0.074797
C	-6.14205	-0.44262	-0.13365
O	-7.14353	0.184199	0.143263
O	-6.19302	-1.68868	-0.67674
H	-7.13869	-1.8917	-0.76199
C	-4.67911	1.357287	0.643676
N	-4.59606	2.422444	1.106499

#### Dye 2

Symbol	X	Y	Z
C	2.979341	2.216106	-1.0714
C	3.405489	1.319743	-0.08024
C	3.50473	3.50605	-1.11923
C	4.372742	1.729132	0.848376
C	4.471543	3.911287	-0.19701
C	4.905168	3.015264	0.782026
N	2.879059	-0.00721	-0.02566
C	3.796389	-1.09466	0.104273
C	3.584286	-2.09454	1.064877
C	4.931493	-1.15771	-0.71609
C	4.489797	-3.14655	1.189723
C	5.840181	-2.20469	-0.57295

C	5.622722	-3.20571	0.37561
C	1.498138	-0.23819	-0.11201
C	0.572714	0.723512	0.353616
C	0.994013	-1.4347	-0.66138
C	-0.78855	0.498531	0.265956
C	-0.37208	-1.65085	-0.73731
C	-1.30613	-0.69626	-0.2831
H	2.240201	1.897214	-1.79892
H	3.166269	4.191277	-1.89075
H	5.095647	-0.38412	-1.45887
H	6.715953	-2.24241	-1.21401
H	0.937417	1.64405	0.794093
H	1.681552	-2.18449	-1.03458
H	-1.46464	1.257585	0.64589
H	-0.73502	-2.57751	-1.17458
H	4.315381	-3.91442	1.937647
H	5.653459	3.320722	1.507341
H	4.70176	1.035946	1.615336
H	2.71247	-2.04046	1.708557
H	6.329786	-4.02262	0.481041
H	4.883552	4.914546	-0.24178
C	-2.72063	-0.97798	-0.39736
H	-2.96461	-1.94949	-0.82796
C	-3.76372	-0.17921	-0.03514
H	-3.58942	0.802428	0.396879
C	-5.11886	-0.59132	-0.2068
H	-5.2962	-1.57105	-0.64205
C	-6.22864	0.140379	0.128663
C	-6.10565	1.441529	0.707838
N	-5.94521	2.495194	1.176224
C	-7.60761	-0.35205	-0.07969
O	-8.61457	0.264086	0.202321
O	-7.64467	-1.59502	-0.6328
H	-8.58784	-1.80833	-0.72094

Dye 3

Symbol	X	Y	Z
C	5.100008	2.215214	-1.08817
C	5.53663	1.310338	-0.10843
C	5.677185	3.480253	-1.18025
C	6.566891	1.690587	0.764583
C	6.706902	3.854555	-0.31477
C	7.150265	2.951095	0.653076

N	4.951696	0.014026	-0.0062
C	5.805579	-1.11848	0.138096
C	5.516092	-2.11498	1.083009
C	6.956082	-1.24083	-0.65531
C	6.358228	-3.21675	1.219158
C	7.80168	-2.33741	-0.49944
C	7.506654	-3.33334	0.433428
C	3.551913	-0.14469	-0.06124
C	2.693109	0.835892	0.477916
C	2.972064	-1.28349	-0.64896
C	1.317744	0.685149	0.420294
C	1.59262	-1.42822	-0.68951
C	0.722475	-0.45143	-0.1666
H	4.311243	1.921402	-1.7728
H	5.329102	4.170113	-1.94353
H	7.181539	-0.47356	-1.38834
H	8.689024	-2.41826	-1.12051
H	3.118683	1.714192	0.950072
H	3.609166	-2.04943	-1.07647
H	0.694864	1.457941	0.859585
H	1.170869	-2.31521	-1.1556
H	6.121842	-3.97977	1.955121
H	7.946916	3.231581	1.33593
H	6.904633	0.994086	1.524669
H	4.632708	-2.01907	1.705461
H	8.164277	-4.18936	0.548091
H	7.159241	4.838127	-0.3945
C	-0.71606	-0.66153	-0.25546
H	-1.00058	-1.61863	-0.68948
C	-1.69549	0.190966	0.12672
H	-1.41771	1.157119	0.54273
C	-3.13155	-0.03536	0.033197
C	-4.01072	0.994792	0.435
C	-3.71265	-1.23319	-0.43838
C	-5.38695	0.856239	0.371728
H	-3.59118	1.92669	0.803969
C	-5.08599	-1.37635	-0.50439
H	-3.08233	-2.05854	-0.75194
C	-5.96574	-0.34187	-0.10417
H	-6.01391	1.678427	0.691473
H	-5.50637	-2.30903	-0.87152
C	-7.38462	-0.60488	-0.21797
C	-8.48135	0.155382	0.077626

H	-7.62433	-1.58872	-0.61126
C	-9.86043	-0.35724	-0.13636
O	-10.8701	0.268876	0.107706
O	-9.88965	-1.61844	-0.64155
H	-10.8312	-1.83669	-0.73514
C	-8.42812	1.481975	0.607738
N	-8.36927	2.561503	1.039313

Dye 4

Symbol	X	Y	Z
C	5.302971	2.20391	-1.10517
C	5.684895	1.285794	-0.11516
C	5.961609	3.426768	-1.21746
C	6.743653	1.607722	0.74672
C	7.019036	3.743398	-0.36237
C	7.408268	2.825497	0.615026
N	5.014661	0.032517	0.007741
C	5.79279	-1.15298	0.159852
C	5.452775	-2.10988	1.128316
C	6.918053	-1.36734	-0.64984
C	6.219079	-3.26498	1.270496
C	7.688646	-2.51707	-0.48803
C	7.342074	-3.47423	0.467509
C	3.607446	-0.03161	-0.02004
C	2.827104	1.016519	0.507749
C	2.946057	-1.14451	-0.57683
C	1.442987	0.955464	0.474424
C	1.561715	-1.20769	-0.59911
C	0.775837	-0.15882	-0.0769
H	4.491779	1.953831	-1.7809
H	5.655027	4.128185	-1.98793
H	7.182441	-0.62978	-1.40018
H	8.557171	-2.66973	-1.12203
H	3.317002	1.876709	0.949288
H	3.528542	-1.95626	-0.99738
H	0.858346	1.768769	0.891744
H	1.069588	-2.0694	-1.03816
H	5.944046	-3.99704	2.024209
H	8.226153	3.061713	1.289443
H	7.039435	0.900169	1.514058
H	4.58981	-1.94218	1.764094
H	7.940994	-4.37174	0.586461
H	7.534642	4.6939	-0.45763

C	-0.64115	-0.2217	-0.10488
C	-1.85869	-0.27299	-0.12761
C	-3.27411	-0.33002	-0.15353
C	-3.94482	-1.44486	-0.70264
C	-4.05017	0.729717	0.370202
C	-5.3277	-1.48657	-0.72222
H	-3.36445	-2.26635	-1.10837
C	-5.43328	0.6831	0.348302
H	-3.54533	1.590759	0.794664
C	-6.11065	-0.4305	-0.20091
H	-5.82811	-2.35177	-1.14861
H	-5.99147	1.514195	0.759206
C	-7.54988	-0.58405	-0.27625
H	-7.8739	-1.51368	-0.73525
C	-8.57636	0.223821	0.122886
C	-8.40981	1.497156	0.751499
N	-8.25983	2.532148	1.262522
C	-9.99662	-0.17407	-0.0732
O	-10.9482	0.50022	0.258653
O	-10.1337	-1.38649	-0.67008
H	-11.091	-1.53275	-0.74217

Dye 5

Symbol	X	Y	Z
C	5.131259	-1.91613	1.28487
C	5.454537	-1.00513	0.267684
C	5.942422	-3.02559	1.51495
C	6.608112	-1.21782	-0.50178
C	7.093163	-3.23298	0.75176
C	7.422582	-2.32065	-0.25262
N	4.631241	0.133783	0.025504
C	5.251503	1.407648	-0.14166
C	4.864712	2.255884	-1.1903
C	6.266552	1.818983	0.734466
C	5.475636	3.498414	-1.34704
C	6.884116	3.055924	0.55905
C	6.49007	3.904149	-0.47748
C	3.229722	0.007121	-0.0273
C	2.62945	-1.16748	-0.5292
C	2.388943	1.046059	0.413617
C	1.252086	-1.29604	-0.57687
C	1.010331	0.909298	0.35146

C	0.397235	-0.26215	-0.13752
H	4.246758	-1.74805	1.890246
H	5.680253	-3.72219	2.305944
H	6.56547	1.165779	1.547443
H	7.668334	3.36194	1.24529
H	3.258141	-1.97433	-0.88841
H	2.824082	1.956029	0.81045
H	0.832828	-2.21274	-0.97986
H	0.383887	1.723621	0.706092
H	5.16593	4.145284	-2.16265
H	8.312581	-2.47271	-0.85627
H	6.859337	-0.51554	-1.28958
H	4.087395	1.936383	-1.87654
H	6.968481	4.869947	-0.60685
H	7.726731	-4.09438	0.938775
C	-1.05264	-0.34306	-0.16217
H	-1.56258	0.550725	0.19642
C	-1.81483	-1.38886	-0.57067
H	-1.33879	-2.29825	-0.93092
C	-3.25259	-1.43636	-0.57868
C	-4.02936	-2.51342	-0.9983
S	-4.26463	-0.11234	-0.04371
C	-5.40673	-2.28164	-0.89239
H	-3.59286	-3.43426	-1.36777
C	-5.7332	-1.02336	-0.38958
H	-6.16812	-3.0025	-1.17031
C	-7.06935	-0.57472	-0.19638
H	-7.82235	-1.30545	-0.4783
C	-7.5607	0.613347	0.281758
C	-6.72433	1.690942	0.700309
N	-6.02058	2.556269	1.035812
C	-9.0158	0.862156	0.398166
O	-9.51068	1.889745	0.812637
O	-9.76959	-0.19418	-0.01277
H	-10.6912	0.085932	0.109089

Dye 6

Symbol	X	Y	Z
C	5.424128	-1.91083	1.253573
C	5.673707	-0.96332	0.249286
C	6.321642	-2.95502	1.468669

C	6.839755	-1.072	-0.52232
C	7.485007	-3.05867	0.703401
C	7.740154	-2.10948	-0.28819
N	4.764249	0.112811	0.023401
C	5.290469	1.432093	-0.12058
C	4.874639	2.254223	-1.1785
C	6.244695	1.911855	0.788037
C	5.397346	3.53906	-1.31298
C	6.774881	3.191619	0.635429
C	6.351702	4.013484	-0.41089
C	3.379737	-0.1201	-0.06282
C	2.881137	-1.33833	-0.56868
C	2.455736	0.860349	0.35367
C	1.517198	-1.5669	-0.64934
C	1.092313	0.633773	0.262951
C	0.589064	-0.58632	-0.23814
H	4.529033	-1.82219	1.860334
H	6.116504	-3.68136	2.249652
H	6.565826	1.277537	1.607566
H	7.513068	3.551055	1.346333
H	3.574343	-2.10073	-0.90457
H	2.818028	1.799447	0.75551
H	1.152223	-2.50759	-1.04856
H	0.396462	1.397156	0.595049
H	5.066519	4.165537	-2.13613
H	8.639367	-2.18151	-0.89297
H	7.033719	-0.34082	-1.29993
H	4.144654	1.881592	-1.88957
H	6.76174	5.012328	-0.52286
H	8.185532	-3.86905	0.879306
C	-0.80548	-0.81537	-0.32361
C	-2.00776	-1.01251	-0.39618
C	-3.39038	-1.21256	-0.46795
C	-4.07422	-2.34159	-0.91342
C	-5.46554	-2.19586	-0.84556
H	-3.56309	-3.22693	-1.26968
C	-5.88985	-0.96271	-0.35096
H	-6.16965	-2.96408	-1.14651
S	-4.5018	0.043964	0.040303
C	-7.26205	-0.60907	-0.1999
H	-7.95332	-1.38951	-0.50555
C	-7.84642	0.540827	0.262523
C	-9.31896	0.692224	0.333801



O	-9.89186	1.684282	0.732814
O	-9.98673	-0.41069	-0.10027
H	-10.9288	-0.19434	-0.0077
C	-7.09654	1.670674	0.706956
N	-6.46159	2.579164	1.0645

Dye 7

Symbol	X	Y	Z
C	7.145533	-2.33449	-0.76189
C	7.560414	-0.99611	-0.84772
C	7.797291	-3.32061	-1.49967
C	8.645616	-0.67086	-1.67657
C	8.881357	-2.99558	-2.31731
C	9.302733	-1.66683	-2.39613
N	6.894921	0.017189	-0.10156
C	7.660106	1.006545	0.577569
C	7.273502	2.355801	0.544269
C	8.816661	0.646952	1.287297
C	8.023297	3.318272	1.217253
C	9.570399	1.619457	1.94121
C	9.177708	2.958999	1.915641
C	5.479497	0.036596	-0.03187
C	4.700007	-0.29145	-1.15387
C	4.822173	0.383252	1.160465
C	3.310345	-0.27923	-1.07772
C	3.431817	0.406244	1.221167
C	2.645963	0.072266	0.107444
H	6.312951	-2.59371	-0.11651
H	7.463335	-4.35132	-1.42191
H	9.118528	-0.39446	1.321169
H	10.46254	1.323647	2.485722
H	5.188507	-0.55728	-2.085
H	5.406155	0.635534	2.038839
H	2.727752	-0.53655	-1.95757
H	2.945169	0.67735	2.153605
H	7.709625	4.357637	1.181441
H	10.14077	-1.39812	-3.03283
H	8.968226	0.362228	-1.7506
H	6.385478	2.642176	-0.00917
H	9.763465	3.712798	2.432428
H	9.391429	-3.76766	-2.88489

C	1.152095	0.091122	0.177967
C	0.428957	1.141372	-0.43304
C	0.46005	-0.93742	0.856383
C	1.095253	2.225703	-1.09033
C	-1.01461	1.136532	-0.40576
C	-0.98555	-0.91745	0.936987
C	1.162829	-2.02084	1.478418
C	0.395738	3.224987	-1.71251
H	2.178497	2.243238	-1.08661
C	-1.70091	2.181268	-1.10337
C	-1.71559	0.103562	0.272259
C	-1.62046	-1.9244	1.73429
H	2.24106	-2.05772	1.380674
C	0.505972	-2.98832	2.189066
C	-1.02376	3.194883	-1.72953
H	0.924772	4.037588	-2.20137
H	-2.78325	2.160354	-1.15237
C	-0.90487	-2.9229	2.340057
H	-2.6924	-1.87686	1.874943
H	1.062958	-3.79733	2.652271
H	-1.57394	3.975926	-2.24604
H	-1.418	-3.66539	2.944216
C	-3.18778	0.149081	0.285276
H	-3.62559	1.121276	0.504701
C	-4.0196	-0.8735	-0.00691
H	-3.58501	-1.82414	-0.3089
C	-5.48142	-0.82895	-0.01497
C	-6.19391	-1.90376	-0.58097
C	-6.23314	0.233195	0.532533
C	-7.5796	-1.90532	-0.61779
H	-5.64502	-2.74684	-0.99095
C	-7.61609	0.246109	0.474887
H	-5.72415	1.051595	1.031087
C	-8.32831	-0.81716	-0.12122
H	-8.10181	-2.75441	-1.05031
H	-8.15501	1.072769	0.916593
C	-9.77802	-0.93313	-0.18603
H	-10.1119	-1.96705	-0.26002
C	-10.8083	-0.03549	-0.15657
C	-10.7915	1.455763	-0.19448
O	-11.7419	2.141874	0.11427
O	-9.63777	1.984148	-0.66613
H	-9.77691	2.946535	-0.67146

C	-12.1374	-0.57937	-0.1184
N	-13.196	-1.06132	-0.09432

Dye 8

Symbol	X	Y	Z
C	-7.24293	2.5495	-0.06123
C	-7.67765	1.272352	-0.44881
C	-7.90559	3.686071	-0.52037
C	-8.79291	1.158672	-1.2933
C	-9.01959	3.569981	-1.35403
C	-9.46035	2.300349	-1.73227
N	-7.00278	0.10647	0.012995
C	-7.7633	-1.0072	0.469028
C	-7.41488	-2.31384	0.09202
C	-8.88008	-0.81157	1.296578
C	-8.16295	-3.39861	0.545074
C	-9.63296	-1.90127	1.729147
C	-9.27781	-3.20064	1.361928
C	-5.5876	0.053879	0.010638
C	-4.84721	0.64713	-1.02608
C	-4.88935	-0.59215	1.045129
C	-3.45651	0.601078	-1.01868
C	-3.49914	-0.65079	1.031866
C	-2.75254	-0.0526	0.004741
H	-6.38724	2.643259	0.599092
H	-7.55669	4.667107	-0.21098
H	-9.15218	0.195509	1.594153
H	-10.4944	-1.73234	2.368801
H	-5.36745	1.141558	-1.83904
H	-5.44175	-1.04582	1.860683
H	-2.90532	1.063374	-1.83239
H	-2.98084	-1.15252	1.843826
H	-7.87992	-4.40314	0.243818
H	-10.322	2.19502	-2.38517
H	-9.13096	0.17429	-1.59927
H	-6.55911	-2.47132	-0.55589
H	-9.86257	-4.04763	1.706999
H	-9.53787	4.457399	-1.70371
C	-1.25939	-0.10983	-0.00057
C	-0.59886	-1.32208	-0.3165
C	-0.50532	1.048453	0.3082

C	-1.32427	-2.50803	-0.66206
C	0.841742	-1.38462	-0.31945
C	0.935868	1.001745	0.293912
C	-1.13499	2.285608	0.661826
C	-0.67905	-3.67794	-0.96445
H	-2.40635	-2.46391	-0.6855
C	1.474086	-2.62296	-0.63624
C	1.597467	-0.21804	-0.01836
C	1.663811	2.188197	0.603909
H	-2.21701	2.323277	0.697135
C	-0.39941	3.402795	0.957241
C	0.739979	-3.73819	-0.94564
H	-1.25229	-4.56277	-1.22455
H	2.557569	-2.66179	-0.62977
C	1.019802	3.355271	0.922518
H	2.74693	2.145829	0.585152
H	-0.90077	4.328308	1.224042
H	1.243122	-4.67055	-1.1843
H	1.594995	4.246265	1.156049
C	3.013737	-0.26939	-0.03195
C	4.233336	-0.30865	-0.04563
C	5.649376	-0.34844	-0.06311
C	6.338674	-1.54433	-0.36242
C	6.408992	0.810946	0.218089
C	7.722008	-1.56757	-0.37741
H	5.773264	-2.44386	-0.58032
C	7.79251	0.782675	0.201129
H	5.892172	1.735976	0.449783
C	8.487815	-0.41189	-0.09859
H	8.23596	-2.49637	-0.60957
H	8.336996	1.691558	0.421306
C	9.929784	-0.55417	-0.14497
H	10.27004	-1.55642	-0.38905
C	10.94114	0.340138	0.060935
C	10.75139	1.718045	0.392364
N	10.58242	2.837722	0.661756
C	12.36895	-0.06538	-0.04869
O	13.30714	0.683406	0.121843
O	12.52826	-1.37681	-0.3633
H	13.48805	-1.51864	-0.40582