SUPPLEMENTARY INFORMATION

Ground-State Electronic Structure in Charge-Transfer Complexes Based on Carbazole and Diarylamine Donors

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Table S1. Calculated adiabatic IP for a set of 30 aromatic amines.

	6-31G(d)				
	LC-ωPBE	ωB97X-D	M06	M06-2X	exp.
9,10-dihydro-acridine	6.861	6.692	6.634	6.851	7.24[1]
4,5-iminophenanthrene	7.191	6.998	6.906	7.193	7.6[2]
1-naphthyl phenyl amine	6.778	6.613	6.560	6.800	7.12[3]
2-naphthyl phenyl amine	6.843	6.677	6.598	6.841	7.15[3]
N-benzyl-N-methylaniline	6.860	6.718	6.729	6.898	7.4[4]
N,N-dimethyl-benzenamine	7.541	6.867	6.881	7.057	7.24[3,5-14]
N,N,N',N'-tetramethyl-[1,1'-biphenyl]-4,4'-diamine	6.190	5.984	5.849	6.057	6.4[15]
N-methylaniline	7.157	7.048	7.068	7.228	7.33[7,9,12,14,16-17]
N-methyl-N-phenyl-benzenamine	6.909	6.745	6.719	6.902	6.94
N-phenylcarbazole	7.197	6.990	6.870	7.124	7.7[2]
N-isopropylcarbazole	7.199	7.000	6.936	7.169	7.6[18-19]
N-methylcarbazole	7.251	7.088	7.033	7.301	7.5[2]
10-methyl-10H-phenothiazine	6.635	6.389	6.335	6.500	6.73[20]
benzidine	6.478	6.283	6.113	6.369	6.88[21]
4-aminobiphenyl	6.951	6.775	6.686	6.911	7.5[22]
1,2-benzocarbazole	7.067	6.880	6.778	7.063	7.1[2]
2,3-benzocarbazole	7.040	6.823	6.692	6.991	7.1[2]
naphtho[2,3-c]carbazole	6.731	6.512	6.372	6.700	7.0[2]
1,2:7,8-dibenzocarbazole	6.970	6.764	6.612	6.956	7.1[2]
1,2:5,6-dibenzocarbazole	7.024	6.827	6.690	7.006	6.9[2]
3,4:5,6-dibenzocarbazole	6.572	6.370	6.226	6.527	7.1[2]
naphtho[2,3-b]carbazole	6.916	6.700	6.548	6.890	7.0[2]
benzo[b]naphtho[2,3-h]carbazole	6.578	6.372	6.214	6.532	7.1[2]
anthra[2,3-b]carbazole	6.388	6.173	6.013	6.346	6.5[2]
anthra[2,3-c]carbazole	6.209	6.014	5.871	6.177	7.3[2]
9H-carbazole	7.470	7.260	7.208	7.437	7.457[2,23-24]
5H-dibenz[b,f]azepine	6.719	6.484	6.379	6.639	6.78[25]
diphenylamine	7.086	6.932	6.845	7.055	7.19[10,14,26]
4,4'-diaminodiphenylamine	5.976	5.819	5.696	5.897	6.2[21]
triphenylamine	6.761		6.495	6.688	6.803[10,14,26]
MSE	0.247	0.461	0.547	0.295	
MUE	0.276	0.461	0.547	0.302	
RMS	0.359	0.519	0.603	0.382	

Table S2. Experimental values for the oxidation potential.

	Oxidation Potential	
R	3	3,6
NMe_2	0.38	
NH_2	0.47	
OCH_3		0.78
CH_3	1.12	
H	1.16	1.16
F	1.23	
Br	1.26	1.37
CN	1.43	1.71
NO_2	1.51	1.84
σ_m	1.03(0.71)	1.28(0.79)
σ_p	0.71(0.92)	0.96(0.99)
σ_p^+	0.48(0.96)	0.68(0.98)

Table S3. Calculated adiabatic EA for a set of 30 aromatic compounds.

	6-31G(d)				exp.
	LC-ωPBE	ωB97X-D	M06	M06-2X	exp.
2,3-dichloro-1,4-naphthalenedione	2.119	2.040	2.057	2.085	2.210[27]
2,3,5,6-tetramethyl-p-benzoquinone	1.464	1.366	1.416	1.439	1.613[27-28]
2-tertbutylanthraquinone	1.411	1.346	1.423	1.434	1.557[27]
2,3,5,6-tetrachloro-p-benzoquinone	2.815	2.743	2.722	2.759	2.686[27-29]
1,4-benzoquinone	1.685	1.628	1.650	1.666	1.825[27-28,30-32]
1,4-naphthalenedione	1.571	1.505	1.539	1.566	1.807[28,33]
tetrabromo-1,2-benzoquinone	2.831	2.759	2.764	2.790	2.440[34]
o-benzoquinone	1.698	1.640	1.678	1.677	1.620[31]
phenyl-p-benzoquinone	1.853	1.793	1.832	1.828	2.042[27]
2-methyl-p-benzoquinone	1.619	1.560	1.583	1.602	1.852[27-28]
2,5-di-t-butyl-p-benzoquinone	1.736	1.665	1.712	1.721	1.870[27]
2-methyl-5-chloro-p-benzoquinone	1.974	1.917	1.932	1.944	2.112[28]
2-methyl-1,4-naphthalenedione	1.495	1.428	1.468	1.482	1.759[27-28]
2,6-dimethyl-p-benzoquinone	1.555	1.491	1.517	1.537	1.763[27-28]
2,6-dimethoxy-p-benzoquinone	1.570	1.490	1.499	1.559	1.717[27]
2,6-dichloro-p-benzoquinone	2.383	2.328	2.339	2.347	2.482[27-28]
2,5-dichloro-p-benzoquinone	2.384	2.330	2.339	2.348	2.404[27-28]
2,5-dimethyl- p-benzoquinone	1.548	1.488	1.501	1.521	1.761[27]
trichlorobenzoquinone	2.608	2.547	2.539	2.557	2.611[28]
2,3-dimethoxy-5-methyl-p-benzoquinone	1.653	1.469	1.516	1.530	1.856[27]
2,3,5-trimethyl-p-benzoquinone	1.486	1.404	1.452	1.450	1.687[28]
tetrafluoro-p-benzoquinone	2.455	2.406	2.410	2.456	2.583[42-144]
methyltrichloro-p-benzoquinone	2.508	2.442	2.435	2.459	2.545[28]
TCNE	3.310	3.185	3.207	3.115	3.17[35]
9,10-anthracenedione	1.345	1.276	1.349	1.370	1.591[27]
2-ethyl-9,10-anthracenedione	1.315	1.256	1.319	1.341	1.557[27]
1-chloro-9,10-anthracenedione	1.508	1.447	1.524	1.530	1.709[27]
1,2,4,5-tetracyanobenzene	2.465	2.356	2.447	2.321	2.20[36]
1,3,5-trinitrobenzene	1.957	1.980	2.218	2.014	2.628[37]
tetracyanoquinodimethane (TCNQ)	3.654	3.521	3.495	3.489	2.80[38-39]
MSE	0.083	0.156	0.120	0.118	
MUE	0.206	0.240	0.212	0.203	
RMS	0.265	0.283	0.245	0.247	

Table S4. The evolution of the bond distances due to ionization for the acceptor molecules using M06-2X/6-31G(d).

Acceptor		Bond a	Bond b	Bond c
PCHL	Neutral	1.203	1.501	1.343
	Anion	1.240	1.460	1.367
	Δ	-0.037	0.041	-0.024
TCNQ	Neutral	1.372	1.453	1.347
	Anion	1.419	1.425	1.369
	Δ	-0.047	0.028	-0.022
F_4-TCNQ	Neutral	1.370	1.451	1.349
	Anion	1.413	1.422	1.368
	Δ	-0.043	0.029	-0.019
F_2-HCNQ	Neutral	1.371	1.459	1.358
	Anion	1.410	1.438	1.379
	Δ	-0.039	0.021	-0.021

Table S5. The relative energies for these two motifs for PCHL and F_4-TCNQ with a reduced set of 2,7- and 3,6-disubstituted carbazole donors

	R						
	NH_2	OH	OCH_3	H	F	CN	NO_2
PCHL: 2,7 Substitution							
Config. I	-0.884	-0.762	-0.792	-0.695	-0.671	-0.599	-0.592
Config. II.	-0.751	-0.662	-0.683	-0.643	-0.604	-0.576	-0.569
Δ	-0.133	-0.100	-0.109	-0.052	-0.067	-0.023	-0.023
PCHL: 3,6 Substitution							
Config. I	-0.843	-0.749	-0.765	-0.695	-0.662	-0.622	-0.633
Config. II.	-0.866	-0.683	-0.679	-0.643	-0.612	-0.548	-0.535
Δ	0.023	-0.066	-0.086	-0.052	-0.050	-0.074	-0.098
F_4-TCNQ: 2,7 Substitution							
Config. I	-1.528	-1.096	-1.172	-0.997	-0.867	-0.702	-0.639
Config. II.	-1.179	-1.097	-0.882	-0.807	-0.654	-0.507	-0.504
Δ	-0.349	0.001	-0.290	-0.190	-0.213	-0.195	-0.135
F_4-TCNQ: 3,6 Substitution							
Config. I	-1.295	-1.079	-1.118	-0.997	-0.833	-0.661	-0.645
Config. II.	-1.207	-0.894	-1.005	-0.807	-0.698	-0.556	-0.616
Δ	-0.088	-0.185	-0.113	-0.190	-0.135	-0.105	-0.029

Table S6. Intermolecular distance using M06-2X/6-31G(d) for different substitutions with varying acceptors.

	Acceptor			
R	PCHL	TCNQ	F_4-TCNQ	F_2-HCNQ
H	3.058	3.176	3.100	3.090
2,7-$N(CH_3)_2$	2.941	3.048	3.005	2.994
2,7-NH_2	2.952	3.062	3.015	3.008
2,7-OH	3.001	3.122	3.053	3.037
2,7-OCH_3	2.992	3.122	3.067	3.041
2,7-$N(Ph)_2$	2.988	3.106	3.034	3.015
2,7-t-Bu	3.027	3.192	3.101	3.100
2,7-CH_3	3.007	3.144	3.078	3.063
2,7-Ph		3.168	3.112	3.085
2,7-F	3.041	3.165	3.106	3.086
2,7-Br	3.045	3.196	3.107	3.101
2,7-CN	3.089	3.237	3.167	3.149
2,7-NO_2	3.093	3.248	3.173	3.162
2-NH_2	3.013	3.115	3.058	3.040
2-OH	3.034	3.177	3.080	3.063
2-OCH_3	3.031	3.144	3.087	3.067
2-CH_3	3.036	3.159	3.092	3.075
2-F	3.051	3.169	3.104	3.089
2-CN	3.076	3.215	3.138	3.120
2-NO_2	3.081	3.216	3.145	3.128
3,6-$N(CH_3)_2$	2.980	3.112	3.014	3.023
3,6-NH_2	2.988	3.140	3.047	3.043
3,6-OH	3.027	3.181	3.081	3.073
3,6-OCH_3	3.022	3.166	3.093	3.067
3,6-$N(Ph)_2$	3.056	3.186	3.112	3.066
3,6-t-Bu	3.074	3.231	3.118	3.094
3,6-CH_3	3.020	3.162	3.085	3.074
3,6-Ph	3.056	3.193	3.126	3.093
3,6-F	3.054	3.195	3.118	3.100
3,6-Br	3.048	3.196	3.140	3.121
3,6-CN	3.085	3.234	3.164	3.149
3,6-NO_2	3.087	3.239	3.158	3.150
3-NH_2	3.034	3.157	3.080	3.063
3-OH	3.047	3.192	3.098	3.086
3-OCH_3	3.046	3.167	3.097	3.073
3-CH_3	3.047	3.171	3.103	3.079
3-F	3.057	3.191	3.113	3.092
3-CN	3.077	3.203	3.141	3.120
3-NO_2	3.075	3.212	3.141	3.123

Table S7, Change in donor bond lengths (Å) upon complexation with F_4-TCNQ using M06-2X/6-31G(d).

R	2	2,7	3	3,6
N_9-C_{10}				
NMe_2		0.001		-0.002
NH_2	-0.004	-0.001	0.006	-0.001
OH	-0.005	-0.002	0.006	-0.002
OCH_3	-0.004	0.001	0.005	-0.001
$N(Ph)_2$		0.000		-0.004
CH_3		-0.004		-0.002
Ph	-0.001	-0.001	0.001	-0.001
H		-0.001		-0.002
F	0.000	0.000	0.000	0.000
Br	-0.007	-0.001	0.003	-0.001
CN		-0.002		-0.001
NO_2	-0.003	-0.001	-0.001	-0.001
C_{11}-C_{12}				
NMe_2		0.021		0.007
NH_2	0.014	0.024	0.007	0.008
OH	0.011	0.015	0.008	0.010
OCH_3	0.010	0.012	0.006	0.006
$N(Ph)_2$		0.014		0.003
CH_3		0.010		0.009
Ph	0.009	0.010	0.007	0.006
H		0.007		0.005
F	0.007	0.007	0.007	0.007
Br	0.008	0.008	0.006	0.005
CN		0.009		0.004
NO_2	0.005	0.004	0.005	0.004

Table S8. Mulliken charges on F_4-TCNQ for LC-ωPBE, ωB97X-D, M06, and M06-2X for a series of carbazoles.

	Mulliken charge on F_4-TCNQ			
R	LC-ωPBE	ωB97X-D	M06	M06-2X
H	-0.072	-0.125	-0.193	-0.145
2,7-$N(CH_3)_2$	-0.210	-0.410	-0.550	-0.439
2,7-NH_2	-0.230	-0.398	-0.541	-0.422
2,7-OH	-0.111	-0.209	-0.332	-0.239
2,7-OCH_3	-0.109	-0.211	-0.336	-0.240
2,7-$N(Ph)_2$	-0.163	-0.361	-0.525	-0.384
2,7-t-Bu		-0.118		-0.143
2,7-CH_3	-0.085	-0.158	-0.251	-0.180
2,7-Ph	-0.060	-0.132	-0.246	-0.160
2,7-F	-0.069	-0.125	-0.204	-0.150
2,7-Br	-0.057	-0.103	-0.178	-0.131
2,7-CN	-0.033	-0.063	-0.103	-0.080
2,7-NO_2	-0.030	-0.057	-0.090	-0.074
2-NH_2	-0.124	-0.228	-0.348	-0.256
2-OH	-0.087	-0.157	-0.256	-0.184
2-OCH_3	-0.086	-0.162	-0.260	-0.188
2-CH_3	-0.078	-0.138	-0.220	-0.160
2-F	-0.070	-0.124	-0.197	-0.147
2-CN	-0.049	-0.089	-0.142	-0.107
2-NO_2		-0.083	-0.132	-0.103
3,6-$N(CH_3)_2$	-0.111	-0.224	-0.356	-0.246
3,6-NH_2	-0.129	-0.234	-0.358	-0.257
3,6-OH	-0.091	-0.165	-0.264	-0.191
3,6-OCH_3	-0.076	-0.140	-0.226	-0.163
3,6-$N(Ph)_2$	-0.038	-0.167	-0.332	-0.184
3,6-t-Bu	-0.041	-0.103	-0.185	-0.120
3,6-CH_3	-0.072	-0.141	-0.219	-0.161
3,6-Ph	-0.049	-0.109	-0.202	-0.132
3,6-F	-0.062	-0.108	-0.173	-0.132
3,6-Br	-0.052	-0.096	-0.165	-0.119
3,6-CN	-0.020	-0.064	-0.096	-0.080
3,6-NO_2	-0.020	-0.059	-0.096	-0.075
3-NH_2		-0.183	-0.304	-0.206
3-OH	-0.078	-0.137	-0.225	-0.162
3-OCH_3	-0.074	-0.132	-0.218	-0.155
3-CH_3	-0.071	-0.132		-0.152
3-F	-0.066	-0.115	-0.183	-0.139
3-CN	-0.047	-0.089	-0.136	-0.108
3-NO_2	-0.047	-0.087	-0.136	-0.104

Table S9. Mulliken charges on F_4-TCNQ for LC-ωPBE, ωB97X-D, M06, and M06-2X for a series of diphenylamines.

	Mulliken charge on F_4-TCNQ			
R	LC-ωPBE	ωB97X-D	M06	M06-2X
H	-0.034	-0.159	-0.258	-0.187
4,4'-$N(CH_3)_2$	-0.195	-0.426		-0.449
4,4'-NH_2	-0.188	-0.418	-0.576	-0.461
4,4'-OH	-0.101	-0.274	-0.425	-0.320
4,4'-OCH_3	-0.045	-0.271		-0.303
4,4'-$N(Ph)_2$	-0.031	-0.351	-0.561	-0.397
4,4'-t-Bu	-0.074	-0.193	-0.307	-0.218
4,4'-CH_3	-0.051	-0.204	-0.319	-0.234
4,4'-Ph	-0.030	-0.171	-0.312	-0.210
4,4'-F	-0.026	-0.158	-0.266	-0.192
4,4'-Br	-0.027	-0.124	-0.236	-0.164
4,4'-CN	0.003	-0.075	-0.141	-0.106
4,4'-NO_2	0.005	-0.061	-0.114	-0.091
4-NH_2	-0.138	-0.311	-0.445	-0.347
4-OH	-0.084	-0.220	-0.348	-0.249
4-OCH_3	-0.063	-0.205	-0.333	-0.237
4-CH_3	-0.041	-0.190	-0.297	-0.219
4-F	-0.032	-0.163	-0.268	-0.192
4-CN	-0.009	-0.096	-0.192	-0.138
4-NO_2	-0.007	-0.075	-0.168	-0.111

Table S10. The Mulliken charge using M06-2X/6-31G(d) for all the acceptors for a series of carbazoles.

	Acceptor			
R	PCHL	TCNQ	F_4-TCNQ	F_2-HCNQ
H	-0.103	-0.123	-0.145	-0.188
2,7-$N(CH_3)_2$	-0.254	-0.318	-0.439	-0.585
2,7-NH_2	-0.225	-0.317	-0.422	-0.548
2,7-OH	-0.153	-0.187	-0.239	-0.313
2,7-OCH_3	-0.160	-0.185	-0.240	-0.318
2,7-$N(Ph)_2$	-0.173	-0.271	-0.384	-0.534
2,7-t-Bu	-0.113	-0.113	-0.143	-0.195
2,7-CH_3	-0.125	-0.147	-0.180	-0.237
2,7-Ph	-0.107	-0.125	-0.160	-0.224
2,7-F	-0.105	-0.123	-0.150	-0.197
2,7-Br	-0.087	-0.102	-0.131	-0.171
2,7-CN	-0.060	-0.065	-0.080	-0.107
2,7-NO_2	-0.051	-0.060	-0.074	-0.098
2-NH_2	-0.152	-0.199	-0.256	-0.340
2-OH	-0.124	-0.140	-0.184	-0.240
2-OCH_3	-0.127	-0.153	-0.188	-0.251
2-CH_3	-0.112	-0.134	-0.160	-0.212
2-F	-0.104	-0.124	-0.147	-0.192
2-CN	-0.079	-0.089	-0.107	-0.142
2-NO_2	-0.073	-0.087	-0.103	-0.136
3,6-$N(CH_3)_2$	-0.133	-0.206	-0.246	-0.344
3,6-NH_2	-0.145	-0.206	-0.257	-0.335
3,6-OH	-0.109	-0.148	-0.191	-0.247
3,6-OCH_3	-0.112	-0.137	-0.163	-0.216
3,6-$N(Ph)_2$	-0.081	-0.135	-0.184	-0.288
3,6-t-Bu	-0.099	-0.090	-0.120	-0.170
3,6-CH_3	-0.115	-0.134	-0.161	-0.211
3,6-Ph	-0.092	-0.114	-0.132	-0.186
3,6-F	-0.089	-0.113	-0.132	-0.174
3,6-Br	-0.079	-0.102	-0.119	-0.157
3,6-CN	-0.059	-0.069	-0.080	-0.107
3,6-NO_2	-0.057	-0.062	-0.075	-0.099
3-NH_2	-0.120	-0.166	-0.206	-0.271
3-OH	-0.105	-0.125	-0.162	-0.221
3-OCH_3	-0.106	-0.132	-0.155	-0.210
3-CH_3	-0.107	-0.128	-0.152	-0.197
3-F	-0.095	-0.116	-0.139	-0.180
3-CN	-0.078	-0.093	-0.108	-0.142
3-NO_2	-0.077	-0.088	-0.104	-0.137

Table S11. The Mulliken charge using M06-2X/6-31G(d) for all the acceptors for a series of diphenylamines.

	Acceptor			
R	PCHL	TCNQ	F_4-TCNQ	F_2-HCNQ
H	-0.112	-0.150	-0.187	-0.246
4,4'-$N(CH_3)_2$	-0.211	-0.334	-0.449	-0.630
4,4'-NH_2	-0.200	-0.340	-0.461	-0.606
4,4'-OH	-0.155	-0.236	-0.320	-0.407
4,4'-OCH_3	-0.159	-0.221	-0.303	-0.402
4,4'-$N(Ph)_2$	-0.161	-0.249	-0.397	-0.568
4,4'-t-Bu	-0.127	-0.165	-0.218	-0.291
4,4'-CH_3	-0.128	-0.182	-0.234	-0.303
4,4'-Ph	-0.112	-0.158	-0.210	-0.293
4,4'-F	-0.113	-0.149	-0.192	-0.254
4,4'-Br	-0.092	-0.123	-0.164	-0.207
4,4'-CN	-0.063	-0.077	-0.106	-0.131
4,4'-NO_2	-0.053	-0.067	-0.091	-0.109
4-NH_2	-0.173	-0.261	-0.347	-0.455
4-OH	-0.139	-0.202	-0.249	-0.331
4-OCH_3	-0.144	-0.182	-0.237	-0.312
4-CH_3	-0.121	-0.170	-0.219	-0.282
4-F	-0.113	-0.152	-0.192	-0.253
4-CN	-0.078	-0.099	-0.138	-0.177
4-NO_2	-0.072	-0.088	-0.111	-0.156

Table S12. Charges on F_4-TCNQ for a series of carbazoles using the NBO and ChelpG methodology using M06-2X/6-31G(d).

	Atomic Charge Method		
R	Mulliken	NBO	ChelpG
H	-0.145	-0.120	-0.239
2,7-$N(CH_3)_2$	-0.439	-0.456	-0.629
2,7-NH_2	-0.422	-0.419	-0.597
2,7-OH	-0.239	-0.219	-0.351
2,7-OCH_3	-0.240	-0.233	-0.365
2,7-$N(Ph)_2$	-0.384	-0.400	-0.587
2,7-t-Bu	-0.143	-0.129	-0.263
2,7-CH_3	-0.180	-0.165	-0.302
2,7-Ph	-0.160	-0.146	-0.311
2,7-F	-0.150	-0.130	-0.234
2,7-Br	-0.131	-0.118	
2,7-CN	-0.080	-0.066	-0.148
2,7-NO_2	-0.074	-0.063	-0.128
2-NH_2	-0.256	-0.238	-0.394
2-OH	-0.184	-0.161	-0.287
2-OCH_3	-0.188	-0.171	-0.301
2-CH_3	-0.160	-0.140	-0.272
2-F	-0.147	-0.124	-0.238
2-CN	-0.107	-0.088	-0.191
2-NO_2	-0.103	-0.085	-0.178
3,6-$N(CH_3)_2$	-0.246	-0.244	-0.419
3,6-NH_2	-0.257	-0.232	-0.410
3,6-OH	-0.191	-0.174	-0.301
3,6-OCH_3	-0.163	-0.146	-0.272
3,6-$N(Ph)_2$	-0.184	-0.199	-0.366
3,6-t-Bu	-0.120	-0.118	-0.252
3,6-CH_3	-0.161	-0.142	-0.277
3,6-Ph	-0.132	-0.115	-0.275
3,6-F	-0.132	-0.108	-0.212
3,6-Br	-0.119	-0.106	
3,6-CN	-0.080	-0.066	-0.148
3,6-NO_2	-0.075	-0.065	-0.127
3-NH_2	-0.206	-0.182	-0.333
3-OH	-0.162	-0.142	-0.272
3-OCH_3	-0.155	-0.134	-0.264
3-CH_3	-0.152	-0.130	-0.258
3-F	-0.139	-0.114	-0.227
3-CN	-0.108	-0.088	-0.189
3-NO_2	-0.104	-0.086	-0.178

Table S13. the charges on F_4-TCNQ for a series of diphenylamines using the NBO and ChelpG methodology using M06-2X/6-31G(d).

	Atomic Charge Method		
R	Mulliken	NBO	ChelpG
H	-0.187	-0.172	-0.284
4,4'-$N(CH_3)_2$	-0.449	-0.465	
4,4'-NH_2	-0.461	-0.465	-0.642
4,4'-OH	-0.320	-0.317	-0.430
4,4'-OCH_3	-0.303	-0.306	-0.430
4,4'-$N(Ph)_2$	-0.397	-0.425	-0.612
4,4'-t-Bu	-0.218	-0.221	-0.337
4,4'-CH_3	-0.234	-0.229	-0.350
4,4'-Ph	-0.210	-0.203	-0.354
4,4'-F	-0.192	-0.182	-0.278
4,4'-Br	-0.164	-0.158	
4,4'-CN	-0.106	-0.099	-0.160
4,4'-NO_2	-0.091	-0.084	-0.125
4-NH_2	-0.347	-0.346	-0.493
4-OH	-0.249	-0.245	-0.365
4-OCH_3	-0.237	-0.232	-0.344
4-CH_3	-0.219	-0.211	-0.327
4-F	-0.192	-0.180	-0.283
4-CN	-0.138	-0.128	-0.212
4-NO_2	-0.111	-0.102	-0.187

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