Supplementary Materials for

Twisted 8-Acyl-1-dialkyl-amino-naphthalenes Emit from a Planar Intramolecular Charge Transfer Excited State.

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General Information

Electronic structure calculations were carried out using Gaussian 16 [31]. Ground state geometries were optimized using the DFT B3YLP method with the 6-311G + (2d,p) basis set. Excited states were optimized using the TD-SCF DFT B3LYP method with the 6-311G + (2d,p) basis set. Solvent effects were modeled with the IEFPCM method.

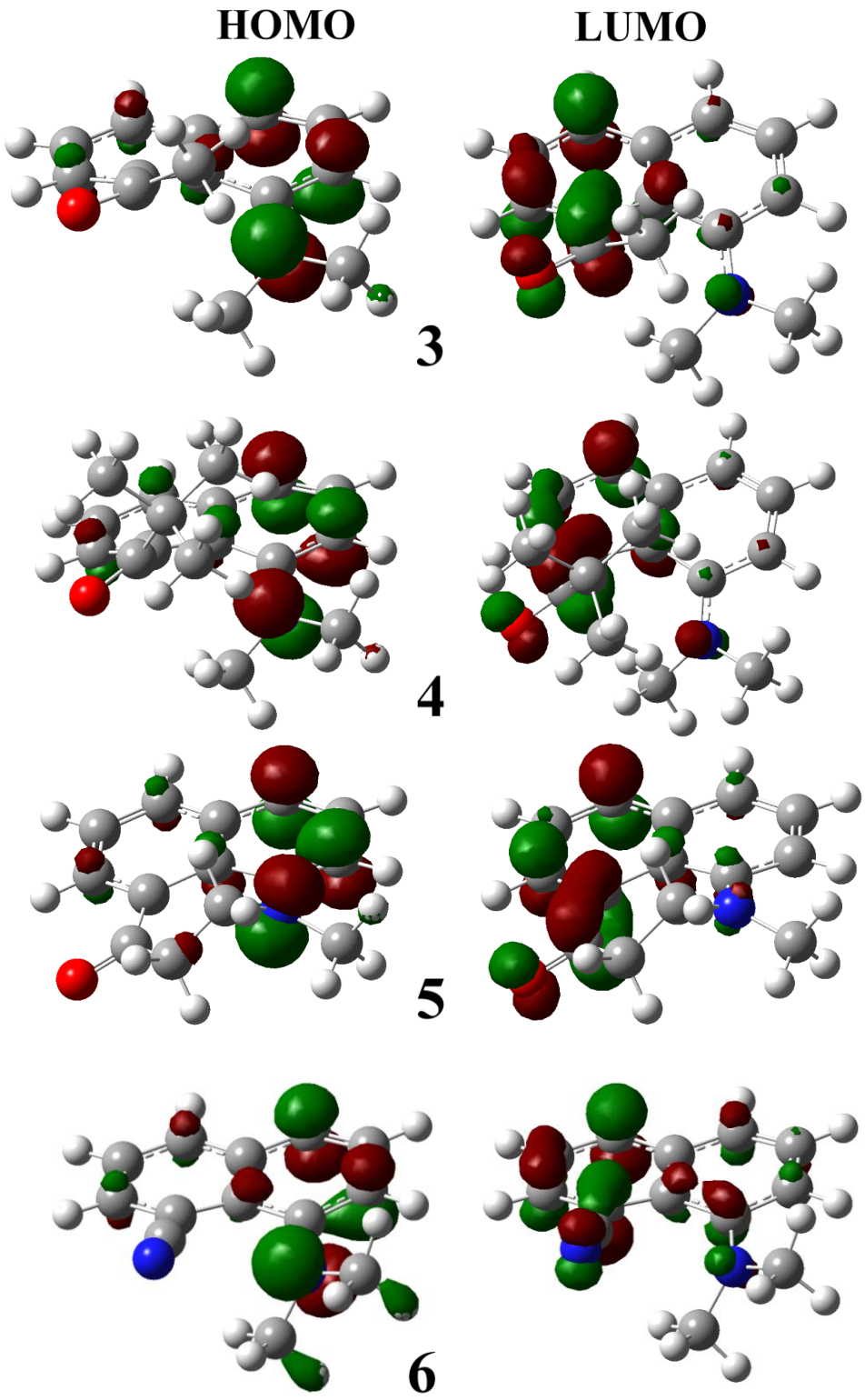

Figure S1. Frontier molecular orbitals for the relaxed first singlet excited states of **3** (top), **4** (top middle), **5** (bottom middle), and **6** (bottom) using a solvent model for acetonitrile: HOMO (left column), LUMO (right column).

Table S1. Cartesian coordinates for the optimized structures of **3** in the ground state (S_0, no solvent model), and relaxed excited states (S_1, with MeCN and toluene)

	S_0	gas phase			S_1	MeCN			S_1	Toluene	
Symbol	X	Y	Z		X	Y	Z		X	Y	Z
C	-2.02979	0.332672	0.009503		1.672195	1.081103	-0.03251		-1.76822	0.924006	0.033231
C	-0.62544	0.065708	-0.00262		0.501576	0.271512	-0.02598		-0.53017	0.226754	0.033597
C	-2.48211	1.667579	0.157683		1.554528	2.465863	-0.33159		-1.77454	2.316141	0.3273
C	0.283585	1.170808	-0.00202		-0.76578	0.969748	0.014826		0.668236	1.038491	-0.01675
C	-2.94047	-0.7457	-0.11322		2.944088	0.511096	0.227867		-2.98137	0.236643	-0.22211
C	-1.58516	2.695729	0.269585		0.325575	3.064572	-0.55001		-0.60648	3.02874	0.535156
H	-3.54864	1.85867	0.187549		2.461097	3.05467	-0.40866		-2.73165	2.8177	0.412625
C	-1.10816	-2.30559	-0.17228		1.913943	-1.66404	0.4242		-1.74717	-1.83165	-0.42006
C	-0.20039	2.450106	0.167479		-0.83594	2.335592	-0.35999		0.617631	2.408701	0.344056
N	1.664743	0.886408	-0.2063		-1.89811	0.401553	0.529524		1.845637	0.567213	-0.53143
C	-2.4894	-2.03355	-0.23124		3.022677	-0.84431	0.542532		-2.92816	-1.11999	-0.53789
H	-1.93467	3.713344	0.398375		0.265212	4.11675	-0.79594		-0.64394	4.083458	0.775896
H	-0.76114	-3.33144	-0.21044		2.002102	-2.73069	0.582556		-1.72776	-2.90132	-0.58236
C	2.613405	1.766235	0.462903		-3.2291	0.934751	0.248719		3.123355	1.215664	-0.25905
C	2.019889	0.680544	-1.61563		-1.87371	-0.57714	1.613542		1.906762	-0.42783	-1.60013
H	-3.19088	-2.85197	-0.34071		3.973658	-1.27475	0.836872		-3.83312	-1.63927	-0.83362
H	3.012288	0.230725	-1.6738		-2.30747	-1.52457	1.290427		2.414709	-1.332	-1.26235
H	2.022309	1.62887	-2.17362		-2.48474	-0.18133	2.428581		2.481742	0.006381	-2.42309
H	0.484312	3.288168	0.186099		-1.78807	2.843122	-0.37781		1.519215	3.002335	0.348521
H	1.316702	-0.00241	-2.08706		-0.86191	-0.73943	1.964162		0.91263	-0.6835	-1.94531
C	-0.18734	-1.29098	-0.02821		0.655212	-1.17016	-0.03254		-0.54488	-1.22168	0.04254
C	1.766845	-1.56181	1.627421		-1.36243	-1.72483	-1.55522		1.502539	-1.58728	1.584859
H	3.604676	1.310286	0.419031		-3.94165	0.114646	0.327872		3.904921	0.458963	-0.32241
H	2.686789	2.762853	0.000714		-3.50894	1.700966	0.977143		3.342331	1.992986	-0.99832
H	2.855623	-1.52775	1.618302		-2.36994	-1.81129	-1.13411		2.523267	-1.57858	1.186464
H	1.455926	-2.44879	2.19096		-1.31142	-2.43386	-2.38544		1.49983	-2.30559	2.408031
H	-4.00329	-0.53156	-0.11629		3.82225	1.143422	0.221854		-3.9161	0.781678	-0.21511
C	1.244931	-1.71361	0.212242		-0.29514	-2.1268	-0.55275		0.499765	-2.08588	0.554207
O	1.871376	-2.32186	-0.6308		-0.18908	-3.35923	-0.28855		0.53771	-3.30507	0.256068
H	1.358595	-0.68764	2.132132		-1.23984	-0.71956	-1.95621		1.273762	-0.6014	1.989455
H	2.334845	1.889844	1.509725		-3.27714	1.343173	-0.75616		3.135234	1.643209	0.739401

Table S2. Cartesian coordinates for the optimized structures of **4** in the ground state (S_0, no solvent model), and relaxed excited states (S_1, with MeCN and toluene)

	S_0	gas phase			S_1	MeCN			S_1	Toluene	
Symbol	X	Y	Z		X	Y	Z		X	Y	Z
C	-2.23989	-0.88756	0.261143		-2.2418	-0.88814	0.263394		2.300969	-0.97341	-0.12825
C	-0.99807	-0.28013	-0.08765		-1.00134	-0.28067	-0.07999		1.081159	-0.267	0.125211
C	-3.22919	-0.10661	0.920899		-3.23104	-0.10428	0.922531		3.435079	-0.26943	-0.60526
C	-0.97339	1.16786	-0.10635		-0.97842	1.167404	-0.10382		1.089548	1.16222	0.009934
C	-2.47679	-2.25118	-0.0242		-2.47474	-2.25214	-0.02185		2.35778	-2.37198	0.08512
C	-3.05925	1.249594	1.140605		-3.06606	1.253065	1.136451		3.377786	1.081651	-0.80683
H	-4.128	-0.60115	1.270184		-4.12608	-0.60065	1.279506		4.343284	-0.82318	-0.81338
C	-0.25238	-2.42397	-0.95015		-0.25224	-2.41303	-0.9589		0.036665	-2.3799	0.70404
C	-1.95748	1.899199	0.610822		-1.96421	1.903525	0.605285		2.210395	1.799475	-0.47764
N	-0.1123	1.875936	-0.89409		-0.11334	1.869454	-0.89437		-0.06863	1.878576	0.43351
C	-1.50364	-2.96864	-0.723		-1.50155	-2.961	-0.72991		1.256839	-3.05767	0.521423
H	-3.82047	1.819353	1.657622		-3.82932	1.82209	1.651865		4.240634	1.616526	-1.18587
H	0.521851	-3.01788	-1.41796		0.521931	-2.99558	-1.44123		-0.83861	-2.94044	1.008923
C	0.11076	3.308563	-0.70152		0.120732	3.29747	-0.70134		-0.30949	3.153817	-0.23276
C	0.386801	1.379605	-2.17668		0.389393	1.365517	-2.1738		-0.14319	2.03655	1.89383
H	-1.70812	-3.98351	-1.04569		-1.70532	-3.97315	-1.06109		1.308775	-4.12441	0.70368
H	1.471802	1.276419	-2.15877		1.473702	1.258921	-2.15357		-1.14225	2.378451	2.167666
H	0.118682	2.114478	-2.93961		0.119742	2.094947	-2.94282		0.597469	2.766904	2.252171
H	-1.91387	2.976399	0.646401		-1.92371	2.981507	0.631517		2.21547	2.876315	-0.58062
H	-0.06017	0.423397	-2.41959		-0.05309	0.405787	-2.41045		0.028786	1.085256	2.389891
C	0.110522	-1.13196	-0.4638		0.109365	-1.12735	-0.45952		-0.0765	-1.02312	0.4821
C	2.222646	-0.17417	0.847848		2.224576	-0.17894	0.855828		-2.35551	-0.34548	-0.67849
H	1.086952	3.554763	-1.11644		1.104142	3.535299	-1.10512		-1.31061	3.501148	0.028653
H	-0.64238	3.900574	-1.22918		-0.62103	3.900614	-1.23487		0.39935	3.941298	0.065962
H	-3.423	-2.69871	0.251014		-3.41796	-2.70476	0.254791		3.293341	-2.88796	-0.0987
C	1.534959	-0.83506	-0.38574		1.534493	-0.82103	-0.38804		-1.48508	-0.4687	0.59978
O	2.310323	-1.32987	-1.25167		2.302706	-1.28121	-1.26877		-1.99265	-0.34457	1.695062
H	0.107526	3.564437	0.354039		0.110395	3.55401	0.35447		-0.25607	3.031806	-1.3147
C	3.141354	-1.27685	1.434618		3.127618	-1.30034	1.429851		-3.11913	-1.68938	-0.78571
H	3.699545	-0.88144	2.287655		3.702615	-0.9206	2.279392		-3.7946	-1.65491	-1.64434
H	2.553301	-2.13071	1.782612		2.526453	-2.14448	1.778218		-2.43833	-2.53055	-0.93402
H	3.848734	-1.6313	0.686191		3.81718	-1.66423	0.669491		-3.7117	-1.87365	0.111844
C	3.113039	1.00229	0.402274		3.131443	0.9866	0.416736		-3.37263	0.789741	-0.49111
H	3.728794	1.350458	1.236709		3.755222	1.322033	1.25069		-4.07138	0.805287	-1.33149
H	3.776678	0.695636	-0.40739		3.785769	0.671501	-0.39697		-3.93882	0.656511	0.430226
H	2.519969	1.851538	0.057987		2.549049	1.846943	0.078435		-2.87303	1.758332	-0.44714
C	1.294859	0.282893	1.984526		1.299414	0.28191	1.992275		-1.5469	-0.13344	-1.96528
H	0.706675	1.163061	1.729995		0.721705	1.170781	1.740209		-0.99228	0.804237	-1.94433
H	0.60825	-0.50942	2.289388		0.601656	-0.50328	2.289532		-0.83705	-0.94374	-2.14009
H	1.901589	0.54782	2.854962		1.904871	0.534409	2.867626		-2.22764	-0.10041	-2.82005

Table S3. Cartesian coordinates for the optimized structures of **5** in the ground state (S_0, no solvent model), and relaxed excited states (S_1, with MeCN and toluene)

	S_0	gas phase			S_1	MeCN			S_1	Toluene	
Symbol	X	Y	Z		X	Y	Z		X	Y	Z
C	1.905706	-0.57289	0.101458		1.914873	-0.54035	0.104495		-1.99012	0.328932	0.087263
C	0.546819	-0.13002	0.060812		0.551527	-0.12053	0.060719		-0.57863	0.076465	0.017789
C	2.22165	-1.95275	-0.00945		2.252394	-1.9163	-0.00287		-2.49341	1.650043	-0.01
C	-0.44839	-1.18967	-0.03116		-0.42477	-1.20006	-0.02891		0.297468	1.218281	-0.07594
C	2.99304	0.340675	0.181949		2.988708	0.391015	0.179583		-2.89556	-0.75161	0.209171
C	1.255618	-2.91966	-0.209		1.306026	-2.90251	-0.19718		-1.63611	2.699729	-0.18265
H	3.266217	-2.23763	0.031351		3.302381	-2.18152	0.035241		-3.56478	1.805047	0.03282
C	1.440015	2.161889	0.015226		1.403571	2.184026	-0.00038		-1.09174	-2.31015	0.023995
C	-0.07014	-2.54122	-0.23542		-0.02674	-2.54631	-0.22495		-0.24736	2.485163	-0.20298
N	-1.77858	-0.96005	0.142968		-1.76146	-0.99172	0.140422		1.683176	1.025783	-0.04079
C	2.735069	1.701355	0.138965		2.70587	1.745426	0.122368		-2.4582	-2.04866	0.192941
H	1.526898	-3.96198	-0.31261		1.597046	-3.94006	-0.29709		-2.01577	3.710196	-0.27779
H	1.248287	3.222687	-0.05337		1.190256	3.239458	-0.08648		-0.74475	-3.33106	-0.06579
C	-2.25448	0.167879	0.934812		-2.26215	0.130164	0.927965		2.178113	0.160747	1.039815
C	-2.81064	-1.8799	-0.32905		-2.77353	-1.92352	-0.34387		2.554365	2.132542	-0.39489
H	3.552943	2.412356	0.185918		3.511274	2.471156	0.155238		-3.15895	-2.87024	0.278738
H	-3.70009	-1.29511	-0.55822		-3.6716	-1.35293	-0.57722		3.570485	1.754707	-0.51259
H	-3.06845	-2.60809	0.4447		-3.02845	-2.66493	0.419958		2.573189	2.935238	0.35836
H	-0.83419	-3.29868	-0.31195		-0.7791	-3.31653	-0.29497		0.404688	3.342762	-0.28588
H	-2.49109	-2.39379	-1.23008		-2.43957	-2.42653	-1.2466		2.246907	2.560833	-1.34913
C	0.294766	1.306502	-0.02216		0.272734	1.310704	-0.02317		-0.15431	-1.29441	-0.0488
C	-2.31263	1.433215	0.103177		-2.34129	1.392939	0.095052		2.417697	-1.2448	0.525218
H	-3.23994	-0.09848	1.313444		-3.24296	-0.15789	1.30619		3.104508	0.582457	1.434623
H	-1.58793	0.300322	1.787929		-1.59958	0.277397	1.781871		1.460585	0.154901	1.865771
H	-2.90089	1.266998	-0.80723		-2.91136	1.212948	-0.82444		3.296681	-1.28705	-0.12131
H	-2.84842	2.197336	0.674908		-2.89946	2.148179	0.655534		2.598048	-1.94119	1.353743
H	4.002281	-0.04624	0.227776		4.00435	0.021564	0.224672		-3.95303	-0.52793	0.294834
C	-0.95787	2.008613	-0.24027		-0.99209	2.000604	-0.23078		1.250685	-1.79896	-0.27136
O	-0.96335	3.207056	-0.64408		-1.01922	3.197492	-0.60793		1.435327	-2.73613	-1.0223

Table S4. Cartesian coordinates for the optimized structures of **6** in the ground state (S_0, no solvent model), and relaxed excited states (S_1, with MeCN and toluene)

	S_o	gas phase			S_1	MeCN			S_1	Toluene	
Symbol	X	Y	Z		X	Y	Z		X	Y	Z
C	1.682134	0.822991	0.040026		1.626183	0.884635	0.036619		1.771264	0.651562	0.000293
C	0.462826	0.073864	-0.01504		0.453029	0.082422	-0.01473		0.47242	0.019825	0.000776
C	1.645411	2.238302	-0.01616		1.500512	2.295806	-0.07962		1.851707	2.066447	-0.0014
C	-0.7802	0.792481	-0.0325		-0.80889	0.758929	-0.04202		-0.63563	0.889444	0.001051
C	2.923119	0.145941	0.1149		2.913132	0.295096	0.152823		2.937627	-0.14804	0.001342
C	0.450255	2.893131	-0.12973		0.276441	2.916695	-0.25846		0.723776	2.868404	-0.00297
H	2.579584	2.786312	0.014963		2.405418	2.892265	-0.06018		2.836084	2.520003	-0.00175
C	1.811235	-1.97101	-0.03713		1.930203	-1.91212	0.085102		1.63997	-2.17997	0.000334
C	-0.75732	2.170612	-0.12494		-0.88083	2.156111	-0.25183		-0.537	2.287465	-0.00177
N	-1.98969	0.067155	0.02178		-1.99971	0.105401	0.222947		-1.98155	0.364555	0.000148
C	2.989379	-1.22238	0.094755		3.03261	-1.10078	0.220171		2.859365	-1.54562	0.001143
H	0.42188	3.974483	-0.19292		0.216478	3.991823	-0.36672		0.816729	3.947424	-0.00442
H	1.859893	-3.04965	-0.11116		2.039883	-2.98931	0.097691		1.577958	-3.26031	-0.00043
C	-3.1401	0.63145	-0.66495		-3.25757	0.535245	-0.36908		-2.68298	0.219093	-1.25035
C	-2.34502	-0.46285	1.33909		-2.13991	-0.77443	1.376713		-2.68429	0.229533	1.250969
H	3.94382	-1.73057	0.151578		4.008743	-1.55144	0.359004		3.768521	-2.13537	0.001331
H	-3.05599	-1.28223	1.221783		-2.69419	-1.6697	1.099262		-3.5776	-0.375	1.126071
H	-2.79461	0.314197	1.976955		-2.70083	-0.23599	2.148766		-2.95462	1.233344	1.600309
H	-1.692	2.71432	-0.163		-1.84492	2.640955	-0.29828		-1.43234	2.895819	-0.00368
H	-1.46446	-0.85049	1.847731		-1.16799	-1.04873	1.770686		-2.01613	-0.20795	1.989153
C	0.572181	-1.35258	-0.10026		0.617182	-1.36054	-0.11184		0.425415	-1.42713	0.000248
H	-3.89209	-0.15179	-0.78039		-3.85999	-0.35388	-0.56292		-3.52356	-0.45947	-1.13844
H	-3.60972	1.467662	-0.12206		-3.81859	1.178997	0.31579		-3.0436	1.209485	-1.55575
H	3.8294	0.737548	0.177695		3.785404	0.933728	0.18849		3.901029	0.346107	0.002062
C	-0.53739	-2.23827	-0.31452		-0.39652	-2.22393	-0.53409		-0.78451	-2.13669	-0.00019
H	-2.85058	0.976587	-1.65736		-3.08167	1.052836	-1.30666		-1.99136	-0.1345	-2.01023
N	-1.31519	-3.07238	-0.49107		-1.21189	-2.98546	-0.88631		-1.80474	-2.69964	-0.00031