Electronic Supplementary Information (ESI) for: Predicting aromatic exciplex fluorescence emission energies

Rachel A. Krueger*and Guillaume Blanquart†

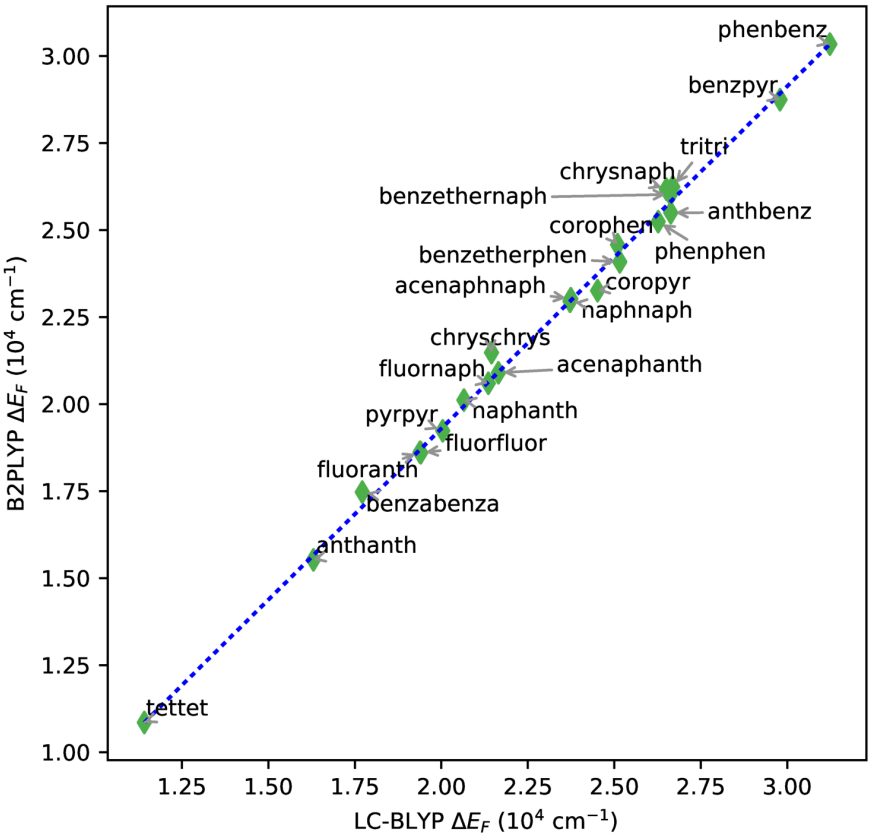

Figure 1: B2PLYP fluorescence emission energies as a function of LC-BLYP-T emission energies for a subset of noncovalent complexes. An $x = y$ curve is shown.

*1200 E. California Blvd., MC 104-44, PASADENA, CA, USA
†200 E. California Blvd., MC 104-44, PASADENA, CA, USA. Fax: 626 568 2719; Tel: 1 626 395 4306; E-mail: g.blanquart@caltech.edu

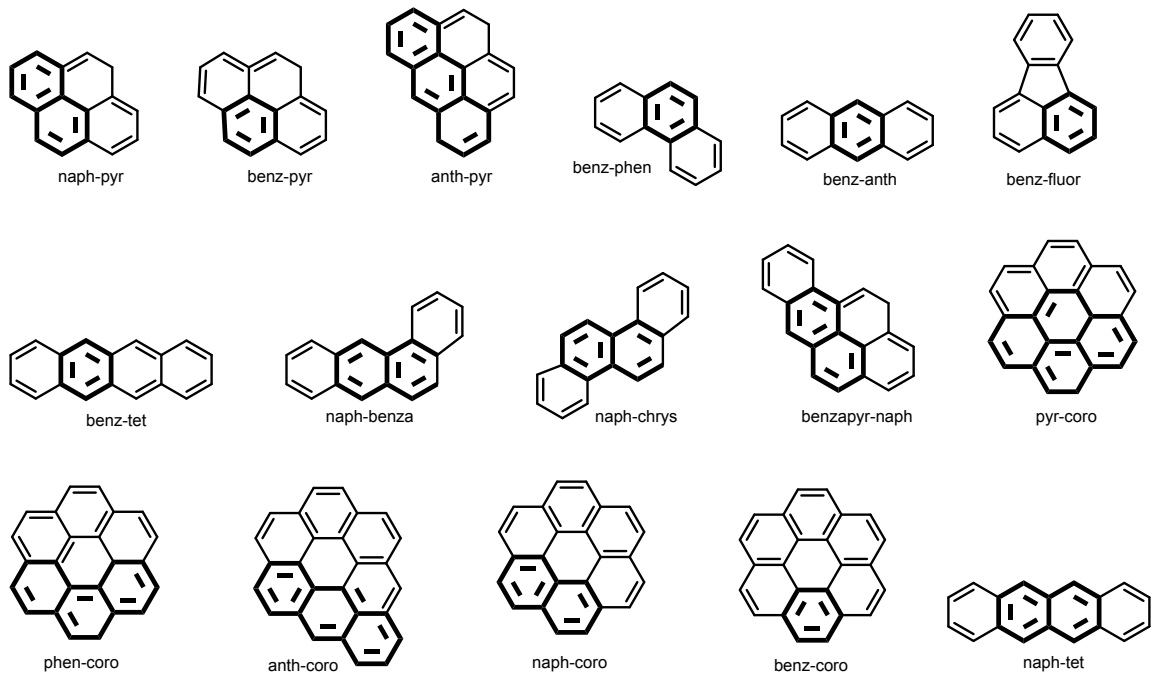

Figure 2: Global minimum configurations for exciplexes for which more than one eclipsed configurtion is possible. Complexes are shown from the top. The smaller monomer is drawn with bold lines.

Table 1: Values of the range-split parameter γ used in the tuned LC-BLYP functional for PAH monomers.

naph	0.2700
anth	0.2400
coro	0.2162
fluor	0.2300
phen	0.2349
pyr	0.2411
benz	0.3046
chrys	0.2164
tet	0.2164
benza	0.2164
tri	0.2164
benzo	0.2164
benzapyr	0.2164
benzepyr	0.2185
perl	0.2178
pentaph	0.2066
pice	0.2050
bchrys	0.2062
bnaph	0.2041
bbtri	0.2062
bgchrys	0.2041
dibenz	0.2041
dbphen	0.2082
penta	0.2041

Table 2: Values of the range-split parameter γ used in the tuned LC-BLYP functional for PAH noncovalent homodimers.

tet	0.1753
benza	0.1753
benzo	0.1795
coro	0.1774
anth	0.2000
naph	0.2185
benzepyr	0.1815
benzapyr	0.1795
pyr	0.2041
phen	0.2000
fluor	0.1959
tri	0.1758
chrys	0.1774
dibenz	0.1384
bbtri	0.1404
bnaph	0.1322
penta	0.1363
perl	0.1811
pentaph	0.1523
pice	0.1427
benz	0.2491
bgchrys	0.1445
dbphen	0.1445

Table 3: Values of the range-split parameter γ used in the tuned LC-BLYP functional for PAH noncovalent heterodimers.

coro	pyr	0.1918
benz	tet	0.2053
benza	nth	0.2200
benz	naph	0.2400
benz	phen	0.2144
coro	naph	0.1918
phen	coro	0.1856
naph	pyr	0.2103
fluor	naph	0.2041
fluor	anth	0.1979
phen	naph	0.2082
phen	anth	0.2041
phen	pyr	0.2041
chrys	naph	0.1938
benza	naph	0.1877
benzapyr	naph	0.1938
anth	naph	0.2000
benz	anth	0.2185
benz	pyr	0.2226
naph	tet	0.1925
naph	tri	0.1998
benza	anth	0.1815
anth	pyr	0.1979
fluor	benz	0.2107
coro	anth	0.1856
benz	coro	0.2071
perl	naph	0.1998

Table 4: Values of the range-split parameter γ used in the tuned LC-BLYP functional for aliphatically-linked complexes.

Complex	Linker length	Linker position	γ
anth excimer	2	α	0.1897
anth excimer	2	β	0.1897
anth excimer	2	γ	0.1897
anth excimer	3	α	0.1856
anth excimer	4	β	0.1836
anth excimer	3	γ	0.1836
anth excimer	3	β	0.1877
anth excimer	4	γ	0.1795
anth-naph exciplex	3	β	0.1961
anth-naph exciplex	4	β	0.1925
anth-naph exciplex	2	γ	0.1961
anth-naph exciplex	3	γ	0.1906
anth-naph exciplex	2	α	0.1979
anth-naph exciplex	3	α	0.1943
naph excimer	2	α	0.2103
naph excimer	3	α	0.2082
naph excimer	4	α	0.2062
naph excimer	3	β	0.2103
naph excimer	4	β	0.2082
naph excimer	2	β	0.2144
benz-naph exciplex	2	α	0.2288
benz-naph exciplex	3	α	0.2123
benz-naph exciplex	2	β	0.2217
benz-naph exciplex	3	β	0.2180
benz-naph exciplex	4	β	0.3148
benz-naph exciplex	4	α	0.2164
benz excimer	4	α	0.2205
benz excimer	2	α	0.2247
benz excimer	3	α	0.2226
anth-naph exciplex	2	β	0.1979
anth-naph exciplex	4	γ	0.1870

Table 5: Oscillator strengths for S_1-optimized monomers

coro	0.00000
pyr	0.00081
tet	0.12117
benza	0.05854
benzo	0.00005
benz	0.00000
naph	0.00001
phen	0.00163
anth	0.12785
benzepyr	0.00017
benzapyr	0.42988
fluor	0.00789
tri	0.00000
chrys	0.00416
dibenz	0.00039
bbtri	0.00242
bbchrys	0.16456
bnaph	0.10088
penta	0.11736
perl	0.59079
pentaph	0.00261
pice	0.00441

Table 6: Oscillator strengths for S_1-optimized homodimers

tet	0.00000
benza	0.00081
benzo	0.00112
coro	0.00000
anth	0.00000
naph	0.00000
benzepyr	0.00000
benzapyr	0.00234
pyr	0.00000
phen	0.00001
fluor	0.00000
tri	0.00001
chrys	0.00000
dibenz	0.00186
bbtri	0.00000
bbchrys	0.00069
bnaph	0.00009
penta	0.00000
perl	0.00000
pentaph	0.00002
pice	0.00009
benz	0.00000
bgchrys	0.00063
dbphen	0.00065

Table 7: Oscillator strengths for S_1-optimized heterodimers

coro	pyr	0.00057
tet	benz	0.09061
naph	benz	0.00013
phen	benz	0.00110
coro	naph	0.00000
coro	phen	0.00004
pyr	naph	0.02254
fluor	naph	0.02000
fluor	anth	0.00109
phen	naph	0.00469
anth	phen	0.01746
pyr	phen	0.01558
chrys	naph	0.01631
benza	naph	0.00946
benzapyr	naph	0.11103
anth	naph	0.00980
anth	benz	0.09632
pyr	benz	0.00035
tet	naph	0.03170
tri	naph	0.00358
benza	anth	0.00071
pyr	anth	0.00850
fluor	benz	0.00565
coro	anth	0.00403
coro	benz	0.00000
perl	naph	0.37630

Table 8: Oscillator strengths for S_1-optimized aliphatically-bridged complexes

Complex	Linker length	Linker position	Oscillator strength
anth dimer	2	α	0.00605
	2	β	0.01291
	2	γ	0.00813
	3	α	0.00120
	4	β	0.00273
	3	γ	0.00027
	3	β	0.00040
	4	γ	0.00317
anth-naph complex	3	β	0.01013
	4	β	0.01613
	2	γ	0.02598
	3	γ	0.01229
	2	α	0.01835
	3	α	0.00995
naph dimer	2	α	0.01292
	3	α	0.00185
	4	α	0.00017
	3	β	0.00076
	4	β	0.00413
	2	β	0.01238
benz-naph complex	2	α	0.00569
	3	α	0.01765
	2	β	0.00561
	3	β	0.01966
	4	β	0.00077
	4	α	0.01298
benz dimer	4	α	0.00019
	2	α	0.00001
	3	α	0.00003
	2	β	0.02491
	4	γ	0.01661

Table 9: Minimum-energy S1 geometry for the coro-pyr exciplex

C	0.72065245826466	1.17546165614177	3.36828019281057
C	-0.69785552590225	1.18149925315131	3.36761776626748
C	1.43805383413286	2.40341418988546	3.36550819208962
C	1.42759414917175	-0.05760531190208	3.34472736250871
C	-1.41483284412089	-0.04547992620764	3.34330000559671
C	-1.40524165749982	2.41523426562785	3.36372020935874
C	2.83981590960312	2.37165170019477	3.34649027368726
C	2.82890938062180	-0.03893390116478	3.31954954029604
C	-2.81589033042834	-0.01430567239570	3.31723298556276
C	-2.80695096605151	2.39580798722081	3.34312749183362
C	0.70228222490533	3.62698751800964	3.36630568159081
C	0.68124118952659	-1.27735626535222	3.32346477204592
C	-0.67895568556449	-1.27148922744360	3.32249043674073
C	-0.65887176932213	3.63322527919646	3.36479788448074
C	3.52416608486164	1.16469416675648	3.32792956464117
C	-3.50167932786688	1.19426689255026	3.32490550708797
H	1.25951760902696	4.56530531795762	3.35776730078897
H	1.23119893851525	-2.21910931100934	3.28616627605200
H	-1.23676523893704	-2.20863745645051	3.28444338723107
H	-1.20795264888925	4.57619840369939	3.35637245442735
H	3.38699879314836	3.31576051657846	3.34165792441517
H	3.36670741054137	-0.98731853898355	3.28443845331992
H	-3.36154689026479	-0.95837182168415	3.28145538876958
H	-3.34583563357672	3.34460859436277	3.33751770732664
H	4.61364509167203	1.16028409545782	3.30369685133641
H	-4.59106856267614	1.19813612660442	3.30081563517932
C	-2.79907398627428	-2.46908101996537	0.01163044162064
C	-3.51011626066647	-1.29341179237735	-0.00581304052232
C	-2.85405428203581	-0.03621282892342	-0.04667834997544
C	-1.42487476783971	-0.01145097540613	-0.07418457768732
C	-2.88852741054784	2.39677807941693	-0.05958283402969
C	-3.55870748133044	1.18968787891578	-0.04702485035614
C	-1.47998900228363	2.45517929891622	-0.07958517682483
C	-0.73689220239782	1.22958693989423	-0.08834787869799
C	0.61028546120542	3.70485059326788	-0.08039615379910
C	-0.76266172812956	3.68048403758523	-0.07931580086167
C	1.37201448668020	2.50837064673769	-0.07895215080786
C	0.67556797293857	1.25575465522980	-0.08630466046627
C	3.49648038545423	1.32140977996126	-0.03376483018586
C	2.78157094409059	2.50169467206906	-0.05690472316940
C	2.83738158659274	0.06888899846660	-0.02761653861940
C	1.40869449497577	0.04155525504541	-0.06534001913418
C	2.87251757692177	-2.36451603629291	0.04616023485775
C	3.53871011932072	-1.16117746107193	0.03117895801839
C	1.45941417050472	-2.42112292080577	0.00908094279225
C	0.72375704684000	-1.19857759889708	-0.05072115779287
C	-0.69461458783812	-1.22496620347443	-0.05758324661313
C	-1.38378845897121	-2.47383369828040	-0.00917732583370
C	-0.62623911058506	-3.67121710091062	0.02710780697837
C	0.74582913482131	-3.64705035419338	0.03641263133302
H	-3.32321777988213	-3.42613369261499	0.04080129925161
H	-4.60114052476156	-1.31188952623709	0.00760886461393
H	-3.45018294789631	3.33258217389182	-0.05316683500773
H	-4.64918383837965	1.16766199181815	-0.02687288586219
H	1.13956436346092	4.65948364617581	-0.07379564794489
H	-1.32642566868571	4.61490406312725	-0.07215854492613
H	4.58686335871179	1.34080155908838	-0.00945714038576
H	3.30879919540916	3.45755265634901	-0.05311773188982
H	3.43168298698119	-3.30092823273911	0.08528349588175
H	4.62954870036404	-1.13839519824589	0.05528946856981
H	-1.15869905985220	-4.62368296336746	0.05249728450943
H	1.31230712019290	-4.57919785295491	0.06903042752147

Table 10: Minimum-energy S1 geometry for the tet excimer

C	-4.881597	0.706306	3.374768
C	-4.882019	-0.703489	3.374732
C	-3.695958	-1.397072	3.311135
C	-3.695120	1.399180	3.311218
C	-2.454347	0.719144	3.257769
C	-2.454775	-0.717780	3.257747
C	-1.229286	-1.397912	3.190975
C	-1.228458	1.398551	3.191104
C	0.000209	0.723682	3.204709
C	-0.000210	-0.723783	3.204758
C	1.228479	-1.398618	3.190997
C	1.229272	1.397822	3.191007
C	2.454764	0.717713	3.257858
C	2.454365	-0.719203	3.257947
C	3.695155	-1.399201	3.311321
C	4.881620	-0.706294	3.374866
C	4.882012	0.703505	3.374740
C	3.695927	1.397048	3.311115
H	-5.827207	1.246159	3.419775
H	-5.827954	-1.242772	3.419724
H	-3.691901	-2.488520	3.305050
H	-3.690405	2.490626	3.305165
H	-1.231298	-2.490710	3.184558
H	-1.229815	2.491350	3.184739
H	1.229852	-2.491418	3.184605
H	1.231268	2.490621	3.184580
H	3.690483	-2.490646	3.305018
H	5.827253	-1.246121	3.419694
H	5.827943	1.242818	3.419456
H	3.691841	2.488495	3.304627
C	-4.881587	0.706443	-0.174780
C	-4.882015	-0.703352	-0.174815
C	-3.695957	-1.396940	-0.111229
C	-3.695111	1.399312	-0.111153
C	-2.454338	0.719273	-0.057739
C	-2.454776	-0.717652	-0.057752
C	-1.229299	-1.397794	0.008956
C	-1.228436	1.398668	0.009050
C	0.000234	0.723793	-0.004731
C	-0.000226	-0.723674	-0.004663
C	1.228431	-1.398560	0.009080
C	1.229333	1.397881	0.009044
C	2.454806	0.717723	-0.057927
C	2.454336	-0.719195	-0.057844
C	3.695090	-1.399278	-0.111122
C	4.881594	-0.706451	-0.174795
C	4.882042	0.703349	-0.174926
C	3.696001	1.396972	-0.111348
H	-5.827197	1.246296	-0.219795
H	-5.827949	-1.242635	-0.219848
H	-3.691901	-2.488389	-0.105175
H	-3.690394	2.490758	-0.105065
H	-1.231318	-2.490593	0.015358
H	-1.229787	2.491467	0.015476
H	1.229764	-2.491359	0.015546
H	1.231369	2.490679	0.015443
H	3.690353	-2.490722	-0.104634
H	5.827198	-1.246334	-0.219537
H	5.827999	1.242605	-0.219795
H	3.691981	2.488420	-0.105037

Table 11: Minimum-energy S1 geometry for the benza excimer

C	4.37367741429677	-1.35128615849466	3.29171158260318
C	4.75325536705974	-0.00650487961662	3.27596411198555
C	3.78833888953486	0.98715597298572	3.20593874538616
C	3.03039010936273	-1.69738756494671	3.24491839966195
C	2.02637740326621	-0.71089881794452	3.21036037628073
C	2.41548747958728	0.66599125564767	3.18770969903499
C	1.40461032191800	1.64157741888727	3.11302187338124
C	0.65146685235989	-1.03426194074623	3.17290908901439
C	-0.35285433350278	-0.06066289965046	3.23655577109124
C	0.04013252898731	1.31263715873516	3.20116920489813
C	-0.95391829553932	2.32741714182804	3.22915098260220
C	-2.28410032709473	2.02063962199172	3.30517418886544
C	-1.75972385350068	-0.38426743192167	3.31482942993059
C	-2.72087410854954	0.67033444600514	3.35232865604002
C	-4.09561639223725	0.35652450406138	3.43386901962014
C	-4.52430914176501	-0.94734407344165	3.47944614821553
C	-3.57997365904752	-1.99044902452558	3.44778386449585
C	-2.23466988941407	-1.71262387845576	3.37048965106322
H	5.13430813113381	-2.13061517644142	3.33091197262946
H	5.80926865261626	0.26100832851948	3.30104193474605
H	4.08059006018608	2.03847965034774	3.18365554208734
H	2.73298262268714	-2.74757726963905	3.25137122240055
H	1.68812087314553	2.69655630590440	3.08928657092766
H	0.38752841713435	-2.09207282134713	3.18179003965970
H	-0.62845434467699	3.36859265526032	3.19210548191728
H	-3.03613811758457	2.81085989423382	3.32900880216819
H	-4.81339770205294	1.17856523485307	3.45539027256049
H	-5.58801291301033	-1.17620837994469	3.53887316052793
H	-3.91678744183551	-3.02644549279093	3.48460566196478
H	-1.52634804301304	-2.53946406201298	3.34849051562770
C	4.37342926715133	-1.35158393476409	-0.09168771643412
C	4.75310492237834	-0.00682945189012	-0.07610605149716
C	3.78827272797867	0.98692373106451	-0.00616113039729
C	3.03012534635169	-1.69757130141219	-0.04459491379387
C	2.02620152133661	-0.71099361664098	-0.01000783316777
C	2.41539834336110	0.66587940920980	0.01222145891081
C	1.40459404888405	1.64156557669344	0.08673401268091
C	0.65127862112442	-1.03424254069188	0.02780244113162
C	-0.35297824392688	-0.06060811772554	-0.03624984918891
C	0.04008144284246	1.31268037367439	-0.00112237163625
C	-0.95393792447471	2.32748819906669	-0.02902434341535
C	-2.28413537298381	2.02074466590884	-0.10487781071841
C	-1.75984736726729	-0.38417188488086	-0.11468916220125
C	-2.72096096767152	0.67046353965964	-0.15219112401245
C	-4.09570179637479	0.35672091589409	-0.23394663338463
C	-4.52442817186533	-0.94712434544313	-0.27982410622034
C	-3.58012478810399	-1.99026085852049	-0.24825904141398
C	-2.23482232300593	-1.71250212164702	-0.17069453384451
H	5.13399300583092	-2.13097377491628	-0.13096123877312
H	5.80913744835618	0.26060019592181	-0.10127968001030
H	4.08060743143050	2.03822818121340	0.01596034420975
H	2.73263747912998	-2.74773866749838	-0.05086916577446
H	1.68818491234369	2.69652945318930	0.11016066905600
H	0.38724232540480	-2.09203461507234	0.01942907879442
H	-0.62843775984055	3.36865184529740	0.00805728377259
H	-3.03615539840792	2.81098935677643	-0.12853672461942
H	-4.81344988870677	1.17879224332832	-0.25543389390206
H	-5.58813030423890	-1.17594525923669	-0.33944237553063
H	-3.91696442475725	-3.02623833977628	-0.28537661367874
H	-1.52651567273077	-2.53936057412265	-0.14889594632873

Table 12: Minimum-energy S1 geometry for the benzophen excimer

C	3.20194816919721	-1.44987152984693	3.95978868908785
C	4.22045574499686	-0.57699489048077	3.57016526322489
C	3.89449060807903	0.71089217235911	3.18836283045049
C	1.87788960434050	-1.05687416156127	3.88389756304964
C	1.49604032555683	0.21695874932368	3.39822423650986
C	2.55907667328761	1.14388132353928	3.13210783261509
C	2.26706988452837	2.51723306046917	2.86825608789990
C	0.98376931503212	2.96286872418099	2.90604240132514
C	0.12545252098774	0.64743727043194	3.21172900219394
C	-0.10088006841732	2.06120929548280	3.07179357096450
C	-1.40966072302571	2.57316474584701	3.07398816890415
C	-2.50254082132437	1.74665388409638	3.13347791104230
C	-1.02836802040772	-0.23240866302312	3.17807592244110
C	-2.34573042902076	0.33596525819097	3.17618079394254
C	-3.48438308048566	-0.48641195640958	3.13245134073177
C	-3.38019977395289	-1.86861610693924	3.06184770401130
C	-2.11155930947756	-2.43102003863044	2.99574255821820
C	-0.96688724435917	-1.63776128057004	3.05190693626753
H	3.44689540426043	-2.44145664903263	4.33985182397668
H	5.26302286711430	-0.89251047396241	3.61115648045946
H	4.67884600163401	1.43104335493934	2.94795970682295
H	1.12085448449204	-1.73029894202875	4.27147256073594
H	3.10004855222210	3.20057927298487	2.69824872060186
H	0.75171099442012	4.02186041622586	2.78041774820362
H	-1.54004588778599	3.65384544332091	2.99456698564380
H	-3.51309083458631	2.15849131377608	3.12991025435441
H	-4.46404665083960	-0.00590727558756	3.14895911936405
H	-4.27127729460849	-2.49356502231693	3.02827026406935
H	-1.99874486205399	-3.51108380102108	2.89329986946084
H	-0.00894684740462	-2.12877019797690	2.94033979209740
C	2.03173177726114	-2.92610500696974	0.70726633058779
C	3.31525875971481	-2.40521500551573	0.52974905933581
C	3.45374101588516	-1.06977654555487	0.18664299104755
C	0.91383076279653	-2.13710399080155	0.50834658794173
C	1.01460121602584	-0.77565065187515	0.11080202359798
C	2.34000093573237	-0.24415712981847	-0.00175354946750
C	2.52364462146704	1.15017788798405	-0.26444594108191
C	1.46281994032266	1.99104309774259	-0.31737249809216
C	-0.11108005337902	0.09234279059997	-0.08893439827205
C	0.12935092972172	1.50829398274908	-0.18376161723916
C	-0.93792847336288	2.42000504628127	-0.11766997491240
C	-2.23438611128916	1.98313818218353	0.04109359977773
C	-1.49030042540232	-0.35751642117358	-0.21209579912698
C	-2.54113344928510	0.59962912312213	-0.05116575133618
C	-3.87778972964618	0.16032380207666	-0.03712878719453
C	-4.20640517760009	-1.16283491104971	-0.28426745603755
C	-3.19558281072015	-2.07452603737719	-0.57623499275953
C	-1.86486077228304	-1.67065697425411	-0.54836536666834
H	1.90514450191559	-3.96160420031135	1.02399772839519
H	4.19385610101727	-3.03174057510377	0.67824743423712
H	4.44604375431874	-0.62761247870233	0.08394298479210
H	-0.06114146457091	-2.56655492831849	0.70650649061534
H	3.54338575673436	1.52607906838984	-0.36242399375512
H	1.60632018802616	3.06550604672908	-0.43893790291154
H	-0.70903027577029	3.48576229057744	-0.15680211043756
H	-3.05795074779390	2.69336179518983	0.12317718020927
H	-4.66223748244705	0.89958712481660	0.13544497640324
H	-5.24985062200702	-1.47780687037285	-0.28157213857544
H	-3.44061123483554	-3.10264735219667	-0.84052037381477
H	-1.10205813294586	-2.38295145482727	-0.85027387392867

Table 13: Minimum-energy S1 geometry for the benz-tet exciplex

H	-0.95100779848245	-1.23836045523262	3.30778710811589
H	-0.95021097740821	1.23902944082725	3.30781078592524
C	-0.00578381454405	0.69499011976770	3.33458665850519
C	-0.00623103019442	-0.69492780901086	3.33457418608207
C	1.19924464353566	-1.38974179672325	3.34440741225138
C	1.20013951947427	1.38902713950108	3.34442870520951
C	2.40534825291577	0.69419409371174	3.36252133021933
C	2.40490003410219	-0.69568624358474	3.36251739809809
H	3.34948481458628	-1.23986509015910	3.35884001981464
H	3.35028393133935	1.23776214898104	3.35885809070608
H	1.19880720916112	-2.48015121516918	3.33901584554169
H	1.20040490680791	2.47943568376540	3.33906136932793
C	-4.88032603076718	0.70114255427174	0.07452424677435
C	-4.88076198675721	-0.69820263167801	0.07422640573615
C	-3.68388496257720	-1.39476648826426	0.01955813170020
C	-3.68305187511998	1.39697921445016	0.01932846897299
C	-2.45083783993052	0.71897671475387	-0.03704392279440
C	-2.45126597700397	-0.71751586297005	-0.03701381972195
C	-1.21655008274517	-1.39474115008600	-0.08641935799879
C	-1.21571512130445	1.39544586059750	-0.08654205001455
C	0.00872599696340	0.72264515530258	-0.11977926978746
C	0.00829634552740	-0.72268020451383	-0.11974993912594
C	1.23549937017593	-1.39455166624128	-0.11578143030282
C	1.23632870236057	1.39378137904011	-0.11582334637260
C	2.47008641287328	0.71713284004585	-0.09221612211864
C	2.46966131128953	-0.71863295361852	-0.09224372052721
C	3.70070499380027	-1.39668213283849	-0.03232621603855
C	4.89893951057161	-0.70089430752395	0.02767922094681
C	4.89935009863681	0.69795911601183	0.02775644463506
C	3.70152563463856	1.39445582934544	-0.03220581067666
H	-5.82369593482748	1.24464529725038	0.11696309872466
H	-5.82438988066144	-1.24113379955550	0.11821399150383
H	-3.68144090263766	-2.48606354300238	0.01778656342786
H	-3.67989249765595	2.48827610296617	0.01867302731133
H	-1.21796061259174	-2.48779064472485	-0.08231783183923
H	-1.21646324603648	2.48849655378890	-0.08252979783987
H	1.23662430656726	-2.48752072292360	-0.10194034896944
H	1.23810433406588	2.48675064531940	-0.10201343904467
H	3.69722476602037	-2.48801485255295	-0.02803084000409
H	5.84193116754002	-1.24474955705286	0.07475425558807
H	5.84265934666839	1.24125697933405	0.07491215901897
H	3.69868496162372	2.48579025839408	-0.02780766096046

Table 14: Minimum-energy S1 geometry for the naph-benz exciplex

C	-0.84573494901937	-0.00352810874016	3.12134068319164
C	0.54825452059546	-0.00349215752009	3.12133810568291
C	1.24287544923256	-1.20595081779023	3.18670933120022
C	0.54825546755298	-2.40697192082947	3.23564229891360
C	-0.84562578552867	-2.40700529792638	3.23564267913322
C	-1.54029713341605	-1.20601766156775	3.18671374679201
H	-1.38668796250759	0.94025578692582	3.06346365113023
H	1.08915785985336	0.94032043404431	3.06346013934162
H	2.33257346317003	-1.20636619937868	3.18798345802687
H	1.09171355801916	-3.35051370038992	3.27815390840067
H	-1.38903972450771	-3.35057219739134	3.27815607248684
H	-2.62999499678164	-1.20647870969652	3.18799243752618
C	-1.55370993772964	1.33454410456587	-0.03864902860354
C	-0.85618158271451	2.53396004810502	-0.03595834600820
C	0.55880059754533	2.53394139570030	-0.03596473162150
C	1.25630937275629	1.33451736200992	-0.03864928608439
C	1.25880295173552	-1.14131471211933	-0.06964948171090
C	0.55799429277988	-2.34675774018169	-0.06668286076673
C	-0.85546172643353	-2.34674739505499	-0.06668336568447
C	-1.55625475607327	-1.14129230651902	-0.06965012247555
C	-0.88428328131059	0.09504396700631	-0.05699777728752
C	0.58685780247786	0.09503176719806	-0.05699725731286
H	-2.64472604156853	1.33439640792894	-0.03385003499907
H	-1.39726567245121	3.47870157760037	-0.03031447774914
H	1.09990068237013	3.47867465836843	-0.03032574302774
H	2.34732489295242	1.33434559237248	-0.03385153395004
H	2.34936457566504	-1.14224766164191	-0.06857993035898
H	1.09966508514592	-3.29075346835285	-0.07260425706115
H	-1.39713831335789	-3.29073969743648	-0.07260249129990
H	-2.64681570845177	-1.14219934928902	-0.06858578582432

Table 15: Minimum-energy S1 geometry for the phen-benz exciplex

C	2.54906196076346	1.15855680610432	4.11869853131072
C	2.82556112220000	-0.18816930762838	3.90874847867882
C	1.81310150134292	-1.04988539705560	3.50403957107905
C	0.52488608725454	-0.56516979012683	3.30636794252988
C	0.24887602909482	0.77990288325513	3.51667905228133
C	1.26080768650312	1.64178042906250	3.92320856545637
H	3.34347563289098	1.83518853555801	4.43460321885403
H	3.83615185320536	-0.56720356561535	4.06319464503271
C	2.11022086493500	1.10850066266484	0.48484511981546
C	1.69947821747142	2.42790472931873	0.63925292696453
C	0.34828021977025	2.75805235997062	0.44794722558301
C	-0.58011667830917	1.78091518135982	0.11475352746911
C	1.20171059094894	0.09532254086892	0.14340915671174
C	-0.20460465876660	0.42535688089881	-0.04377098740149
C	0.71107758848635	-2.24636045246519	-0.33047738043107
C	1.61180793291771	-1.24290290902676	-0.00110607762487
C	-0.65680502232847	-1.97366807447389	-0.52701197568837
C	-1.13037306237135	-0.60489015570619	-0.37608419875160
C	-2.51320092879497	-0.37070641839420	-0.57083742121022
C	-3.38395685006812	-1.39734310777662	-0.91118637615381
C	-2.91642079635479	-2.71174290845475	-1.06837318649023
C	-1.56644131804628	-2.98542609402951	-0.87276469639678
H	3.15431905521641	0.83545125008279	0.64295278025617
H	2.41890654618758	3.19796831086864	0.91238869532372
H	0.02135949899758	3.79125749418481	0.56151320212881
H	-1.61852243150911	2.07336327564281	-0.02839789320163
H	1.05653838400241	-3.27515415462569	-0.44285818482033
H	2.66447867705021	-1.48258337693404	0.15441724341038
H	-2.91087145318350	0.63576653869816	-0.45724524093580
H	-4.44106997429162	-1.17739117322343	-1.05675326319877
H	-3.60588700285292	-3.51062677165939	-1.33629115284684
H	-1.18993579135076	-4.00327637131218	-0.98578608829019
H	-0.75700418903962	1.16265881632263	3.34488428099534
H	1.04557322771048	2.69906119305508	4.07820877621945
H	2.02903393576759	-2.10450212169152	3.33209663741636
H	-0.26462745544983	-1.23750673771711	2.96918254592503

Table 16: Minimum-energy S1 geometry for the coro excimer

C	-2.80081112595841	-2.47589366003179	-0.05916857829019
C	-3.50572209094001	-1.29793999707749	-0.05979667790583
C	-2.84367833597201	-0.04447652907667	-0.06493159403054
C	-1.41983927498853	-0.02220818089535	-0.07336808749618
C	-2.87686586025045	2.38709119128517	-0.05881592781136
C	-3.54459280434649	1.18767078406130	-0.05954525399581
C	-1.46035228010240	2.44041592779815	-0.06409708223181
C	-0.72916439264993	1.21851414032492	-0.07310933623163
C	0.62879164056598	3.68499001864094	-0.05951271752342
C	-0.74373992460010	3.66352408389373	-0.05938217725250
C	1.38331139276619	2.48488836547212	-0.06433245822879
C	0.69068754681759	1.24072480569479	-0.07323082765248
C	3.50571065760767	1.29794165144603	-0.05985477930824
C	2.80080230753042	2.47589657631901	-0.05923168570852
C	2.84366652942902	0.04447880886211	-0.06495742359327
C	1.41982836467550	0.02220817034308	-0.07340943736833
C	2.87685636028210	-2.38708979066712	-0.05892998613077
C	3.54458338827079	-1.18766976283182	-0.05964942971859
C	1.46034294367591	-2.44041424986848	-0.06414565982372
C	0.72915259661148	-1.21851507941033	-0.07312587937626
C	-0.69069825845182	-1.24072585118988	-0.07319435073551
C	-1.38332155963085	-2.48489126149866	-0.06429192156097
C	-0.62880230272488	-3.68499383013280	-0.05954601062049
C	0.74372931458424	-3.66352130733621	-0.05944584266760
H	-3.32710064755486	-3.43188011037703	-0.05217277752764
H	-4.59693661905055	-1.30991031527634	-0.05291206247720
H	-3.43280915960136	3.32614071550997	-0.05160976653298
H	-4.63564736871600	1.16549455354881	-0.05257078909044
H	1.16407850710568	4.63597369275960	-0.05290232040113
H	-1.30850837378272	4.59729932400230	-0.05263721501245
H	4.59692546653187	1.30991678193419	-0.05298260892246
H	3.32708603505006	3.43188616674467	-0.05223483427079
H	3.43279377781497	-3.32614392588979	-0.05183402365358
H	4.63563829581806	-1.16549529815141	-0.05270718668079
H	-1.16408783265511	-4.63597847169837	-0.05291812340999
H	1.30850076695056	-4.59729594201585	-0.05276896914747
C	-2.80080695107317	-2.47588524885186	3.33913993648215
C	-3.50571743456204	-1.29793053909077	3.33980109626853
C	-2.84367292932938	-0.04446829084822	3.34496617276924
C	-1.41983220174999	-0.02219829429698	3.35340726931717
C	-2.87685380404421	2.38709897730204	3.33879787553461
C	-3.54458465940143	1.18768129082873	3.33956242912604
C	-1.46034198610949	2.44042093524143	3.34410384233231
C	-0.72915518169631	1.21852140522171	3.35314013817918
C	0.62880599764656	3.68499296376118	3.33950405160091
C	-0.74372479461292	3.66352560760530	3.33936080821988
C	1.38332537036872	2.48489145767502	3.34433073479715
C	0.69069646446606	1.24072974524194	3.35325994373300
C	3.50572406373777	1.29794325794414	3.33986049759118
C	2.80081593400419	2.47589847324126	3.33920310027852
C	2.84367551427244	0.04448340052510	3.34503255023768
C	1.41983775797925	0.02221360949060	3.35349400294048
C	2.87686101583228	-2.38708543499871	3.33897330262253
C	3.54458902549444	-1.18766669293577	3.33970215463475
C	1.46034796787867	-2.44040662266414	3.34419387602002
C	0.72916003961698	-1.21850881427364	3.35317478790858
C	-0.69069375688775	-1.24071688519223	3.35318938227104
C	-1.38331770839506	-2.48488194891671	3.34426807182381
C	-0.62879792656517	-3.68498465523728	3.33948550193001
C	0.74373325801627	-3.66351297946350	3.33941736598859
H	-3.32709683624361	-3.43187121510769	3.33213515922366
H	-4.59693208848768	-1.30990198467732	3.33292425168186
H	-3.43278726211970	3.32615502391378	3.33161893040578
H	-4.63563949542099	1.16550466638699	3.33256641262024
H	1.16408991701760	4.63597863666913	3.33286151796325
H	-1.30849743031614	4.59729907237788	3.33263883491449
H	4.59693839178480	1.30991330649675	3.33295709218938
H	3.32710071613820	3.43188661332748	3.33215457788886
H	3.43279716720974	-3.32613971001039	3.33185095878842
H	4.63564383657511	-1.16549515247402	3.33273183141388
H	-1.16408290917069	-4.63596916821520	3.33281088397561
H	1.30850323803497	-4.59728800121152	3.33270845871691

Table 17: Minimum-energy S1 geometry for the anth excimer

C	1.39442021578748	2.46590758175380	0.01418286822409
C	0.69996675976468	3.65941063137036	-0.05434692967056
C	-0.69999721506153	3.65941143376201	-0.05435222741290
C	-1.39445882857080	2.46591085588150	0.01415219723644
C	-1.39444612195224	-2.46592423333625	0.01414330314565
C	-0.69997219840788	-3.65941841543127	-0.05436282906186
C	0.69999058318428	-3.65940540541535	-0.05434446323594
C	1.39443324669348	-2.46589659198518	0.01419189334198
C	1.39425329777237	0.00000699813315	0.12660630401973
C	-1.39430398594806	-0.00000675462275	0.12654411434318
C	0.71677984911173	1.22978702771949	0.05596185121357
C	-0.71683178738471	1.22978399102872	0.05593549366993
C	-0.71682379478021	-1.22979377853763	0.05592711479912
C	0.71679073888657	-1.22977986948442	0.05596903058501
H	2.48585880860591	2.46383651325784	0.02075887706428
H	1.24336588245152	4.60302843633457	-0.09721279705865
H	-1.24339262730961	4.60303143902904	-0.09720926138249
H	-2.48589738945599	2.46385073359292	0.02070779323277
H	-2.48588424508984	-2.46387015035408	0.02068661719765
H	-1.24335529348533	-4.60304539011868	-0.09723239367296
H	1.24339767004597	-4.60301848870349	-0.09720927023467
H	2.48587221955507	-2.46382327379746	0.02077931218553
H	2.48700135655312	0.00001601615670	0.13389008617685
H	-2.48705169005071	-0.00001241507417	0.13376754263531
C	1.39446278450735	2.46591446875870	3.28580913274347
C	0.70000056006670	3.65941515547121	3.35432694661466
C	-0.69996358857516	3.65941188324703	3.35434635019403
C	-1.39441482278468	2.46590779830432	3.28584231887920
C	-1.39443648094501	-2.46589967015884	3.28580060837566
C	-0.69999053275677	-3.65940693155100	3.35432278449596
C	0.69997221613682	-3.65941726487470	3.35435396973995
C	1.39444153638089	-2.46592021495429	3.28585409919034
C	1.39430030570319	-0.00000312819540	3.17343039940532
C	-1.39425856536804	0.00000549319423	3.17348769095543
C	0.71683182250296	1.22978752176678	3.24407130622707
C	-0.71677964336786	1.22978484528929	3.24405111048192
C	-0.71679150221177	-1.22977998189662	3.24405719462444
C	0.71682273050782	-1.22979095615848	3.24406448586095
H	2.48590093761107	2.46385032018688	3.27923892284666
H	1.24339385956761	4.60303712323802	3.39717122275150
H	-1.24336584744819	4.60302759809727	3.39721297787414
H	-2.48585375761407	2.46383980434850	3.27928165548291
H	-2.48587506728863	-2.46382307333667	3.27921990381466
H	-1.24339366631537	-4.60302353117452	3.39717017200869
H	1.24335984605602	-4.60304108150745	3.39722395364013
H	2.48588012263440	-2.46386855014283	3.27930663797604
H	2.48704799677810	-0.00000498364808	3.16617869376236
H	-2.48700669469266	0.00001046453729	3.16624323471344

Table 18: Minimum-energy S1 geometry for the naph excimer

C	-1.28848368273397	-0.03554927847211	0.06747051092804
C	-0.58981788602004	-1.24344936686092	0.00533298435179
C	0.79520562460266	-1.24345752054682	0.00533838433176
C	1.49388601969571	-0.03556573607447	0.06747940760824
C	1.49389776179011	2.43555162690132	0.06749234769765
C	0.79523059665328	3.64345249397303	0.00535616992873
C	-0.58979264364758	3.64345775817656	0.00535781839428
C	-1.28847020755333	2.43556489748324	0.06749328570464
C	-0.61169624650684	1.20000424847566	0.04070168395604
C	0.81711233228201	1.19999492784116	0.04070261195660
H	-2.37960651267523	-0.03430329370809	0.07229872755587
H	-1.13773218188338	-2.18479403780573	-0.02071303222988
H	1.34310889575899	-2.18480867287369	-0.02070167048874
H	2.58500849305560	-0.03433058274893	0.07231273831912
H	2.58502030577869	2.43430656078691	0.07232758063742
H	1.34314388357994	4.58479778656411	-0.02068074978010
H	-1.13769843023770	4.58480768643899	-0.02067703782110
H	-2.37959301826093	2.43432847060292	0.07232581618513
C	-1.28848185309513	-0.03556590186297	3.13255795920323
C	-0.58980167972543	-1.24345853425295	3.19468448653519
C	0.79522191850877	-1.24345073169794	3.19464608600053
C	1.49388774160957	-0.03555111925924	3.13249564908522
C	1.49387466988873	2.43556465671444	3.13251583933613
C	0.79519690382359	3.64345772569179	3.19465153768190
C	-0.58982634841308	3.64345150650522	3.19463416584016
C	-1.28849295767536	2.43555026608565	3.13249827742710
C	-0.61170620801566	1.19999360509100	3.15930691270409
C	0.81710237891944	1.20000338206848	3.15929824806345
H	-2.37960430969785	-0.03432973720820	3.12774738931887
H	-1.13770450663669	-2.18480926335485	3.22074399881769
H	1.34313686485250	-2.18479581059978	3.22066918414423
H	2.58501052828382	-0.03430624803786	3.12763901350154
H	2.58499761738381	2.43432962858582	3.12768655265182
H	1.34310199845305	4.58480783351309	3.22069314741364
H	-1.13774052759360	4.58479672442336	3.22066031102276
H	-2.37961533454844	2.43430404944177	3.12765366401698

Table 19: Minimum-energy S1 geometry for the benzepyr excimer

C	4.06409705167020	-0.58822325572432	-0.21927660782013
C	4.02500515583066	0.81369613228301	-0.21966984829091
C	2.81409213380200	1.46330971213373	-0.18567196879718
C	2.89126347244012	-1.30428963834791	-0.18498715957033
C	1.63283332805163	-0.66697722483615	-0.14055679671219
C	1.59313818416853	0.75688510538460	-0.14077157047851
C	-3.32429585410164	0.59686889529121	-0.03481368708482
C	-3.28589493840970	-0.78110783526940	-0.03492035075944
C	0.40158218396499	-1.42703651432858	-0.09981349021827
C	-0.83574641623126	-0.73941394156032	-0.10069915471848
C	-2.05909678073209	-1.47586409446200	-0.06165709426019
C	-2.01466966690470	-2.89094909047989	-0.01791160108065
C	-0.80262114683849	-3.55143283631645	-0.02915671824848
C	0.38974551750648	-2.83965517772474	-0.04170645936887
C	-0.87563817563633	0.69168539055809	-0.10079182124076
C	-2.17254611707472	2.77423205634889	-0.01790122210215
C	-2.13808560960881	1.35887436558958	-0.06162783701633
C	-0.99916365822777	3.50120398443248	-0.02924295519982
C	0.23098194491957	2.85692104240093	-0.04187820402303
C	0.32147145930611	1.44716622415666	-0.10002486061502
H	5.02059752286950	-1.10992917047640	-0.24574701176533
H	4.95092641086476	1.38790757747277	-0.24655142590129
H	2.80444236434714	2.55131896094158	-0.19057234058485
H	2.94226383001966	-2.39114667344789	-0.18923437107499
H	-4.28034491795360	1.12202428466698	-0.00793395921570
H	-4.21119457484798	-1.35872311597607	-0.00811539027034
H	-2.95391853518846	-3.44535464827253	-0.00077124629566
H	-0.77607741589325	-4.64061661753133	0.00929768383081
H	1.32656879344249	-3.39176120528796	-0.03903995448265
H	-3.14125431333446	3.27538997897933	-0.00060535237785
H	-1.03329368528355	4.59017555523491	0.00923099082592
H	1.13561465371606	3.46032487046916	-0.03921654062083
C	4.06413584654592	-0.58818375631280	3.41930955711216
C	4.02503605358867	0.81373487142868	3.41979399128335
C	2.81411991127054	1.46334228152399	3.38579915715135
C	2.89130611927912	-1.30425590799972	3.38500057084472
C	1.63287326048293	-0.66694895029579	3.34060840242784
C	1.59317189879027	0.75691272258668	3.34086635414713
C	-3.32426136077979	0.59687873794450	3.23477181345148
C	-3.28585676274377	-0.78110110400899	3.23487215176381
C	0.40162531439558	-1.42700845652130	3.29975891467520
C	-0.83570990557983	-0.73939422994784	3.30068540614121
C	-2.05905568429395	-1.47585144429432	3.26166948046016
C	-2.01462116627717	-2.89093764315204	3.21791572097035
C	-0.80256715950632	-3.55141185933321	3.22911799160543
C	0.38979571768635	-2.83962667517404	3.24165584200249
C	-0.87560613766974	0.69170233302712	3.30077279832248
C	-2.17251610732045	2.77424720422940	3.21794484678628
C	-2.13805461093030	1.35888847944181	3.26165345432239
C	-0.99913252330647	3.50121951077974	3.22920265435552
C	0.23101527390936	2.85693915731039	3.24179583039715
C	0.32150538997331	1.44718386533477	3.29997448786700
H	5.02064022637260	-1.10988581575989	3.44571896577728
H	4.95095548125139	1.38794918795746	3.44667763558218
H	2.80446131638543	2.55135131553957	3.39075501127603
H	2.94231749325382	-2.39111270909738	3.38915406269180
H	-4.28031159412409	1.12203098358219	3.20787222864837
H	-4.21115307466709	-1.35871973423883	3.20803641600596
H	-2.95386602431421	-3.44535065210474	3.20080779940854
H	-0.77601475228144	-4.64059550581903	3.19066391062355
H	1.32662220059811	-3.39172727538938	3.23897943542306
H	-3.14122424948465	3.27540691982581	3.20070606166998
H	-1.03326551654182	4.59019102387700	3.19073030128907
H	1.13564792538456	3.46034302875822	3.23906807105503

Table 20: Minimum-energy S1 geometry for the benzapyr excimer

C	4.39498186565850	-1.17950254811699	3.43003978742701
C	4.79404951385667	0.15738767539062	3.33296867872257
C	3.84180069259523	1.14730378738237	3.22133121357211
C	3.04837588796787	-1.50740296544956	3.42947666570459
C	2.05341649708284	-0.52453540697821	3.32821732004343
C	2.46136931585451	0.83942359601313	3.22652097767730
C	1.48991627018802	1.85510291598362	3.11726136022351
C	0.12076780936695	1.58373716185744	3.22055393960069
C	-0.85154458187863	2.61738691949991	3.20894040476073
C	-2.19308951493183	2.33917409159510	3.25544793737695
C	-2.66052107834191	1.00089428249707	3.29272057914109
C	-4.03562675074295	0.68643913312324	3.27693495265704
C	-4.46447163569893	-0.63003854994475	3.27720736786774
C	-3.54336371627489	-1.67142123242111	3.27176095973655
C	0.63383968540112	-0.83375928205907	3.31821510983417
C	-0.31408419351814	0.22264893478774	3.29893506334662
C	-1.70759060794541	-0.06074808799824	3.31402342998301
C	-2.16140557909114	-1.40795480370762	3.30941466787692
C	-1.19110741988680	-2.44276145645440	3.30736922810723
C	0.15110164543096	-2.16068606734696	3.32850391147629
H	5.14283689865071	-1.96752107020041	3.51451087275280
H	5.85353442070537	0.41290223808344	3.33040702748634
H	4.13801609403714	2.19471598216317	3.14146267481858
H	2.76624837225431	-2.55573493567039	3.51552001348420
H	1.82103635665247	2.89415694634787	3.05418283542303
H	-0.50468087119589	3.65076909392333	3.15559000518282
H	-2.92600810643600	3.14748181628581	3.24263175122946
H	-4.75908026777746	1.50322196009863	3.26863433430393
H	-5.53152950866003	-0.85168533570013	3.25412049278709
H	-3.88126142483525	-2.70875225291297	3.26475755724687
H	-1.53340507829047	-3.47893120045382	3.29644106447535
H	0.85890069494333	-2.98823951772346	3.32281060937451
C	4.39502280367997	-1.17950203871750	-0.23002454425548
C	4.79408614400354	0.15739068670315	-0.13296291864770
C	3.84183055303220	1.14730046904245	-0.02133148348381
C	3.04841979907259	-1.50741506584944	-0.22945515353816
C	2.05345433282002	-0.52455508995419	-0.12820479660301
C	2.46140038306273	0.83940917595812	-0.02653176376755
C	1.48994843578854	1.85508325573910	0.08268302822420
C	0.12080469753320	1.58371363662182	-0.02054726759972
C	-0.85149792396264	2.61737428331332	-0.00897855357094
C	-2.19304587102972	2.33917095961632	-0.05543238622218
C	-2.66048837999898	1.00089182821347	-0.09264421758240
C	-4.03559487231303	0.68644605571445	-0.07683068993012
C	-4.46444751770078	-0.63003048375476	-0.07713222899260
C	-3.54334653931783	-1.67141970134170	-0.07174487036384
C	0.63387356591635	-0.83377803907645	-0.11817401316732
C	-0.31406005169565	0.22262998515991	-0.09893674092124
C	-1.70756552374256	-0.06075665654027	-0.11399489490927
C	-2.16138581359736	-1.40796054888855	-0.10939284019817
C	-1.19108953209158	-2.44276780193943	-0.10743623320934
C	0.15112226493381	-2.16070111398230	-0.12853775934742
H	5.14288244360142	-1.96751501755697	-0.31450482648252
H	5.85356966445419	0.41291065404400	-0.13039760862152
H	4.13803905172394	2.19471478657361	0.05853490637190
H	2.76630196845078	-2.55575124793819	-0.31548214047597
H	1.82106597921173	2.89414286649497	0.14570093114876
H	-0.50462453677815	3.65075722230404	0.04429652510723
H	-2.92595545172269	3.14748675172178	-0.04263249995212
H	-4.75904201706683	1.50323416857031	-0.06849223424554
H	-5.53150659621013	-0.85166989211280	-0.05403325872279
H	-3.88125249389552	-2.70874780517856	-0.06478452379816
H	-1.53339326511516	-3.47893601647203	-0.09658648052854
H	0.85891361381335	-2.98826208838207	-0.12292825541516

Table 21: Minimum-energy S1 geometry for the naph-coro exciplex

C	-3.09131831539391	-2.47215495850383	-0.37915385139235
C	-3.79162403770109	-1.28866947990272	-0.46914227288163
C	-3.13492054674191	-0.03777212568058	-0.38853682673702
C	-1.71314335507226	-0.01728402921693	-0.20472525592231
C	-3.15965389741547	2.39686507748758	-0.39595627003157
C	-3.82638434934079	1.19371208590892	-0.47839207361101
C	-1.75722970462528	2.44898619170700	-0.21609881524096
C	-1.02977799321206	1.21806247064061	-0.11359496125770
C	0.31636600817249	3.68856870577790	0.08650705507542
C	-1.04756777405417	3.66853820522341	-0.11323631022277
C	1.05978899751011	2.49027620990513	0.20169067159205
C	0.37064521404533	1.23813778924209	0.08477947710472
C	3.15347217845443	1.29477132972610	0.54582061695746
C	2.45705334454939	2.47891416020932	0.42517115552443
C	2.50068530841467	0.04373414264894	0.43665826839378
C	1.08656249711622	0.02316933652461	0.19704326388632
C	2.52568258234689	-2.39170898664745	0.43820645853298
C	3.18837747615488	-1.18776980575034	0.55302928760322
C	1.12946446244608	-2.44363137693184	0.21416662935774
C	0.40515470159541	-1.21209097703395	0.09152032207470
C	-0.99534063731672	-1.23245679932838	-0.10624582066066
C	-1.68779686254208	-2.48395859775717	-0.20119543246856
C	-0.94403660925954	-3.68249289748785	-0.09186101808138
C	0.42003642660026	-3.66306164732912	0.10633521076799
H	-3.61595347570344	-3.42668736845641	-0.44328431590778
H	-4.87390925469348	-1.30066518592993	-0.60725109644394
H	-3.71070806389954	3.33592003755777	-0.46669962581731
H	-4.90850072617198	1.17440664270141	-0.61699092012394
H	0.84545690604568	4.63959808885772	0.16586881080098
H	-1.60408815621943	4.60367324512852	-0.19294345543893
H	4.22972579165643	1.30718827840332	0.72466007411944
H	2.97954303420313	3.43310304693468	0.50871782314980
H	3.07482922272071	-3.33032618745896	0.52701144219026
H	4.26447571276661	-1.16887332907776	0.73224185856801
H	-1.47421308066887	-4.63329638122030	-0.16552643203738
H	0.97581405504112	-4.59833724673635	0.19034368837752
C	-2.15633889890788	-2.47365903583307	3.24164767484675
C	-2.87017656639785	-1.30357248141272	3.22330191533567
C	-2.20916531145335	-0.05110055503631	3.25071782176942
C	-0.78636435067026	-0.02465984496338	3.30247743541172
C	-2.24606478870150	2.37140797035828	3.21496614465927
C	-2.91614200924386	1.17546899451844	3.20881290965715
C	-0.83551375173087	2.39802447346204	3.26485889717009
C	-0.12365158140291	1.22743195591690	3.30608978930282
C	-0.07770949653437	-1.25119269257737	3.31824143733996
C	-0.74558202641689	-2.44772857277691	3.28894173432515
H	-2.67633338493734	-3.43128038310337	3.20848832443560
H	-3.96048269189717	-1.31803843462438	3.17549867972378
H	-2.80082159844366	3.30879589186347	3.16992758329190
H	-4.00617762061066	1.14882098715778	3.16016288255110
H	-0.31341401207271	3.35454879635181	3.24576983286207
H	0.96833242460947	1.24063877385023	3.31908025195141
H	1.01405240756044	-1.22382762857047	3.32827798758222
H	-0.18863782255646	-3.38449287871611	3.27857133798431

Table 22: Minimum-energy S1 geometry for the pyr excimer

C	0.37606982765502	0.60188861600298	-0.03433896502836
C	-0.37607404811202	-0.60188620072711	-0.03433564736585
C	-0.29173626374350	1.85755703865412	-0.00797801373310
C	1.79741631979598	0.55212791843569	-0.00942738719410
C	0.29173237912178	-1.85755446589478	-0.00798075311082
C	-1.79742051375075	-0.55212549923605	-0.00941767981150
C	0.48079511338355	3.04264967478113	0.04404467416571
C	2.52402691208338	1.76606109189709	0.03968563355076
C	-0.48079923196102	-3.04264726407776	0.04404379336499
C	-2.52403080137742	-1.76605842172783	0.03969652372118
C	-1.70566015835682	1.87624676468546	-0.00219510533085
C	2.43406761514302	-0.71040868985793	-0.00374274488679
C	1.70565665990109	-1.87624388227343	-0.00221662150887
C	-2.43407227798097	0.71041079775720	-0.00371769287311
C	1.86522551831194	2.98472418849948	0.03813048789806
C	-1.86522965027305	-2.98472154289756	0.03813350021480
H	-2.21386164399095	2.84173302786478	0.01572577507639
H	3.52464329854251	-0.74385944096626	0.01311929811828
H	2.21385829587170	-2.84173017846295	0.01568936427829
H	-3.52464778912782	0.74386219704644	0.01316233635473
H	-0.03291280038009	4.00482416339957	0.05142193324299
H	3.61404988477655	1.72607785490689	0.04307105232713
H	0.03290808492184	-4.00482189369481	0.05141751590072
H	-3.61405382947923	-1.72607472424932	0.04308570160268
H	2.44273337312130	3.90886314967987	0.07061753314132
H	-2.44273771845116	-3.90886031461725	0.07062016984340
C	0.37607473178446	0.60188575051291	3.33434095768609
C	-0.37607147553486	-0.60188763910436	3.33433624836987
C	-0.29173032289052	1.85755329535257	3.30799572649075
C	1.79742221415568	0.55212588991246	3.30942538633929
C	0.29173357540027	-1.85755457882338	3.30798739851760
C	-1.79741952564496	-0.55212802945006	3.30942697754897
C	0.48080261681280	3.04264443017095	3.25598706282712
C	2.52403567796812	1.76605848750876	3.26031115489419
C	-0.48079820434908	-3.04264576914074	3.25597960577386
C	-2.52403223024436	-1.76606187728550	3.26030924858722
C	-1.70565420728476	1.87624293793398	3.30217303593513
C	2.43407236647541	-0.71041150892274	3.30373058735663
C	1.70565837036948	-1.87624519097193	3.30221473426723
C	-2.43406887787234	0.71040842247947	3.30368485834562
C	1.86523272407571	2.98472138550795	3.26188829895551
C	-1.86522778472475	-2.98472433045089	3.26188427822827
H	-2.21385427475679	2.84172927857182	3.28422697855460
H	3.52464784483634	-0.74386412008261	3.28684865347523
H	2.21385877515393	-2.84173205897770	3.28429520033815
H	-3.52464375808113	0.74386095006682	3.28677443260893
H	-0.03290538134750	4.00481895117302	3.24862425642969
H	3.61405863908483	1.72607436873771	3.25691061508537
H	0.03291107481641	-4.00481976766703	3.24861639806326
H	-3.61405503942426	-1.72607965623077	3.25691002445596
H	2.44273903934652	3.90886124906329	3.22940318847415
H	-2.44273312376952	-3.90886483481168	3.22940001043328

Table 23: Minimum-energy S1 geometry for the coro-phen exciplex

C	-2.80977317326619	-2.48711109090771	-0.11911501044355
C	-3.51817533159622	-1.30386184862782	-0.11937423641131
C	-2.85924735756782	-0.05151677696208	-0.13302584224334
C	-1.42369115395930	-0.02970113556561	-0.13084339679184
C	-2.88691855520506	2.38294892090832	-0.10424202909770
C	-3.55696987726215	1.17713298922225	-0.12134235665446
C	-1.47317338349481	2.43626399353315	-0.08837586141306
C	-0.73700442261511	1.20769593791559	-0.09930802997642
C	0.61820354744143	3.67807819324159	0.01564143533277
C	-0.75767161928262	3.65658309189213	-0.03252086774158
C	1.37273706540515	2.47912859130596	0.01073370703459
C	0.67783530507552	1.23022603635568	-0.05049274453856
C	3.49506776058938	1.28806682531079	0.06662816574953
C	2.78812596610542	2.46908955528386	0.06683094188549
C	2.83519240447231	0.03581327109268	0.00912026721017
C	1.40601653715533	0.01363502711953	-0.05088966991729
C	2.86624403183988	-2.39807966189106	-0.03874922559274
C	3.53539992967541	-1.19563856270838	0.01154188622274
C	1.45260745295030	-2.45175205309413	-0.08970619683670
C	0.71763085436094	-1.22251631685027	-0.10080518681255
C	-0.69746545005061	-1.24295753959091	-0.13116163108597
C	-1.39487721394085	-2.49773156322978	-0.13319780254593
C	-0.64155076024753	-3.69327282665206	-0.13045736370220
C	0.73756770494542	-3.67255284968488	-0.11547614828876
H	-3.33731357530089	-3.44201308204793	-0.09976462096665
H	-4.60900290792868	-1.31799341235982	-0.09952246884319
H	-3.44439931534037	3.32053529968181	-0.08685789232341
H	-4.64790606943498	1.15633097324527	-0.11510289837426
H	1.15179788387860	4.62891537363016	0.05855949328383
H	-1.32173245546128	4.59068680910786	-0.02513619303119
H	4.58524950638546	1.30061449091984	0.11061555555631
H	3.31425105384457	3.42397703088059	0.11112325151096
H	3.42290282797333	-3.33662629593784	-0.03419598346927
H	4.62557866897901	-1.17476145658884	0.05320979967116
H	-1.17529218556869	-4.64498511642972	-0.13017680027796
H	1.30061135794257	-4.60694180057368	-0.10517249866989
C	-2.76332675724772	-2.44147864367269	3.41030041818953
C	-3.45984066651448	-1.27778523587723	3.40938619833812
C	-2.78940295261908	-0.01513024704314	3.39627411233242
C	-1.37060636235817	0.02844990650774	3.37102378588196
C	-2.88428109400954	2.40782784870713	3.35989446530802
C	-3.52208989699698	1.18910594167535	3.39359760139376
C	-1.48289156502567	2.45596953005736	3.32228315920041
C	-0.74571935318778	1.29071250256913	3.32978246064981
C	1.46158835503331	-2.46325439805748	3.32667710227608
C	0.78286386326174	-1.26301732927358	3.33186686338710
C	-0.62491152551619	-1.21737562781407	3.37167952306773
C	-1.33369245654978	-2.44719720760829	3.39819228535313
C	-0.61850040509329	-3.66192785348209	3.39745032331827
C	0.75702530560112	-3.67560347574599	3.36516089241065
H	-3.28246780130276	-3.40151431746739	3.41555334398514
H	-4.55125882092877	-1.28166458366010	3.41375596659689
H	-3.46319134517975	3.33126273097078	3.35234424287057
H	-4.61212121926405	1.13388084172412	3.41132558636438
H	-1.18221701468386	-4.59646593596590	3.41647753431678
H	1.29743329216042	-4.62207416756574	3.36024565739642
H	-0.97096072236112	3.41698806223789	3.27484768438409
H	2.55051916000056	-2.46608435760752	3.28096925124021
H	0.34056911898785	1.35589000118739	3.28668099910185
H	1.35344581229711	-0.33636200574021	3.28837899522889

Table 24: Minimum-energy S1 geometry for the naph-pyr exciplex

C	-0.60792026775970	-0.50671674679051	3.22360106104673
C	0.01152916250477	-1.75106627036563	3.13400167062908
C	1.39687505896073	-1.84174708004613	3.06117060737191
C	2.16971000828892	-0.68627894897126	3.05306200150374
C	2.33400060610060	1.77178077419559	3.11047464380718
C	1.71435703983025	3.01185860441621	3.20783049866857
C	0.33041537883948	3.10364658558758	3.30422533530574
C	-0.44665146845179	1.94915194972584	3.31212993553833
C	0.15454824307724	0.67786552958133	3.25251649290006
C	1.57300043428192	0.58478393497085	3.15336989337783
H	-1.69439361343796	-0.43678986952016	3.27112379268683
H	-0.59802509212307	-2.65208202204056	3.08699405284040
H	1.87440071833556	-2.81585366478994	2.97133674455592
H	3.25494114368695	-0.75154482570778	2.97181511501170
H	3.41854392877187	1.70196085825713	3.03149274751953
H	2.31731067367950	3.91846421958263	3.17852398892229
H	-0.14799980460946	4.08024361429873	3.36046509859649
H	-1.53300476465469	2.01337633834011	3.36791997871023
C	0.53412927459992	0.55358593842541	0.06486597224163
C	-0.19590247052639	-0.66516893533026	0.08319112120418
C	-0.15131921357439	1.80028893682787	0.16770272532431
C	1.95852770670282	0.52931507931185	-0.01809541523471
C	0.48963595581918	-1.91893611330125	-0.03070093022317
C	-1.61947614030267	-0.64695794130941	0.23682480391783
C	0.59524754541195	3.00977206383099	0.09024764800418
C	2.66163884210621	1.75291034317767	0.00901240621664
C	-0.26657928282808	-3.11674246057212	-0.02105286920536
C	-2.32190204903255	-1.86435684367019	0.23093379459603
C	-1.55792213578632	1.78512100082657	0.34641726731785
C	2.60751625327071	-0.72495334964378	-0.08350089380048
C	1.89527971553980	-1.90852787712084	-0.11348637793748
C	-2.26498936680150	0.61139841799388	0.38654980968399
C	1.97070186731386	2.96858065906895	0.00944370217972
C	-1.64294761752681	-3.07416065682937	0.10015909924694
H	-2.07675836037255	2.74207993572831	0.43256360558797
H	3.69740839448269	-0.74261223653461	-0.14920865224268
H	2.42145013772636	-2.86125222062301	-0.19618737141236
H	-3.34977481249167	0.62377411774313	0.50690943540232
H	0.06158005042232	3.96044803822021	0.09641794628278
H	3.75012535585695	1.73843134385943	-0.06418982460591
H	0.25527095951820	-4.06939527775687	-0.11860315519267
H	-3.40813200879673	-1.84838189431506	0.32736219993500
H	2.53655115729245	3.90037709667883	-0.04039953831759
H	-2.21099114334491	-4.00569214541039	0.09477283203848

Table 25: Minimum-energy S1 geometry for the fluor-naph exciplex

C	-2.66502048082200	-1.20724875230637	3.16515595425544
C	-1.97039875817562	-2.41177267465964	3.18213951183191
C	-0.58160541337300	-2.41787869142253	3.15274694681457
C	0.12492515203647	-1.21761836616216	3.11087970052265
C	0.13615405091422	1.24281670966575	3.10907700065774
C	-0.55872880441288	2.44977006117502	3.15078639528733
C	-1.94746785018451	2.45623804618982	3.18018435813935
C	-2.65333939719563	1.25815451649885	3.16329416178622
C	-1.97644113128125	0.02215218892316	3.17756482856808
C	-0.55272449346547	0.01563013049397	3.15465835954660
H	-3.75518322765976	-1.20052103208799	3.17041734478192
H	-2.51927481719886	-3.35230976337120	3.18420719219946
H	-0.04070598944991	-3.36306080067788	3.13684480403905
H	1.21350262155061	-1.21847069007746	3.05144470031470
H	1.22466345453823	1.23309653729361	3.04878499681444
H	-0.00916136560807	3.38989299760500	3.13487711018499
H	-2.48781274716488	3.40172911961852	3.18206241790386
H	-3.74353115503021	1.26177531693173	3.16866252332265
C	1.12550978996421	0.70626898189504	0.17012606980432
C	1.10849743346161	-0.72811666928062	0.16933175793478
C	2.30636435403755	-1.43624354216080	0.25997939923567
C	3.50325822586165	-0.74068595018126	0.36525202839157
C	3.51990764524763	0.66227759202487	0.36669463613395
C	2.33980281968056	1.38594134565823	0.26259074454381
C	-0.27474774293867	-1.16369732932280	0.06947036942861
C	-3.09144170116930	-1.23397715289882	0.00599406451381
C	-2.32618375446697	-2.40938000480315	-0.04116950340088
C	-0.93336514099909	-2.40242425993245	-0.00601782227935
C	-1.05522260811245	0.01444697822916	0.02907537013265
C	-0.24642625821850	1.17441911981874	0.07122307491850
C	-0.87548093481865	2.42872173926644	-0.00480334816299
C	-2.26730230336414	2.46876879750750	-0.03995826471846
C	-3.06032338644729	1.31121614119773	0.00780822139723
C	-2.45685427157536	0.03124964319871	-0.00217434375373
H	2.30546110535482	-2.52814664989303	0.24984118740908
H	4.44305372259778	-1.28827961538139	0.43651040653702
H	4.47235677954866	1.18734888288305	0.43927860147975
H	2.36448320967120	2.47759601400222	0.25454686510365
H	-4.18071750754928	-1.29645912582286	-0.02093487861265
H	-2.84723554245655	-3.36664487469714	-0.08967982867954
H	-0.38049414412090	-3.34212218073124	-0.03413921801869
H	-0.30018586098635	3.35483131956905	-0.03411172966428
H	-2.76579502201698	3.43789402389966	-0.08949025804834
H	-4.14781955420267	1.39996092232496	-0.01903490859644

Table 26: Minimum-energy S1 geometry for the fluor-anth exciplex

C	0.41315044143629	3.46761582535802	3.13978300152010
C	-0.19027010948218	4.70976116701078	3.11505317483885
C	-1.58862279096624	4.81942390747680	3.08698894419357
C	-2.37271300317583	3.68410920918524	3.08236926999603
C	-2.74762477520613	-1.22210184678360	3.13201206103917
C	-2.13861457600195	-2.46532658540650	3.18190569283792
C	-0.74613296462883	-2.57256014802597	3.21863255074313
C	0.04065019848015	-1.43152685643917	3.20087052542557
C	0.22744697611716	1.01185805927022	3.14662951580736
C	-2.56249624381570	1.22813365328279	3.10597509501082
C	-0.36380783146618	2.29440412418895	3.15012797603126
C	-1.78680597281806	2.40348592330486	3.12401623782357
C	-1.97588053956879	-0.04097827719917	3.15443553399074
C	-0.54689366799390	-0.15074943343135	3.18727930489894
H	1.49991118832522	3.37517401465709	3.14537701807596
H	0.42200726850651	5.61116885713537	3.11051353638976
H	-2.05381481225239	5.80410142899509	3.05834871459209
H	-3.45998545633289	3.76059974550268	3.04084454995049
H	-3.83359592853283	-1.14044581614844	3.08522215153362
H	-2.75016397759984	-3.36645871052855	3.16404407734960
H	-0.27838745469454	-3.55580284845370	3.23641339799580
H	1.12844226288341	-1.50587038116147	3.18698349755712
H	1.31576603357207	0.92852194786663	3.13146427689817
H	-3.64995839598602	1.31135978616859	3.07161251240931
C	0.90532968865913	0.91504424157632	0.26554558052231
C	1.02175249940000	-0.51710615012618	0.25099588724877
C	2.27480591846325	-1.11034524743656	0.41473164831389
C	3.39426745510754	-0.30828062327083	0.58488580207697
C	3.28162998128703	1.09245488202594	0.57719017642281
C	2.04854325306053	1.70490754996364	0.40860166566890
C	-0.30499883602199	-1.07644910450976	0.09165943509723
C	-3.10006775796277	-1.39710502840282	-0.09381436396445
C	-2.23187278028978	-2.49663092727905	-0.09924577989418
C	-0.84510367687666	-2.36426799253006	-0.00367609126503
C	-1.19325121876902	0.03111694403668	0.02653055950876
C	-0.49904742896173	1.25881369417165	0.10315489782620
C	-1.23100869505554	2.44738270342606	0.01010971577038
C	-2.62572710764409	2.36050496151955	-0.07889094867508
C	-3.30911556948595	1.14436227265958	-0.07054634244904
C	-2.58844867111735	-0.08065411195568	-0.06232561092478
H	2.37557353924302	-2.19772477151324	0.40650519002358
H	4.37526606272091	-0.76660674299992	0.71022162567396
H	4.17816465278854	1.70181719597128	0.69415825773051
H	1.97040679876967	2.79394974730722	0.39570146952720
H	-4.17690633692413	-1.55907719094274	-0.17048646373201
H	-2.65999770863848	-3.49786742520358	-0.16698544069489
H	-0.21136523427871	-3.25215595546690	-0.00111636159724
H	-0.74535592209986	3.42401380621857	0.02342300636650
H	-3.20361349771824	3.28460515434720	-0.13333436547041
H	-4.39824727645384	1.13081137258845	-0.13989276601982

Table 27: Minimum-energy S1 geometry for the naph-phen exciplex

C	-0.55606399184784	-0.46695679715661	3.15452354639151
C	0.16249183273680	-1.66013298473899	3.19691189209408
C	1.54891819088982	-1.63518993425556	3.19995766061328
C	2.22577055179767	-0.40988987195785	3.16778259211227
C	2.18267510764944	2.06090731237992	3.19075598708793
C	1.45949299755957	3.25255732467693	3.25701325876241
C	0.07372456997995	3.22637496011658	3.24922126269975
C	-0.60260890939844	2.00327187102830	3.19005669582318
C	0.09839614156039	0.78452609359456	3.20341545009010
C	1.52745205498068	0.80970805343214	3.20774824037107
H	-1.64623421829442	-0.48804427473888	3.11951687563916
H	-0.37001417578993	-2.61042890686435	3.19150764667386
H	2.11449152853590	-2.56617959843474	3.21322062487310
H	3.31680521105277	-0.38882794903474	3.16485532945672
H	3.27353871745199	2.08132861579438	3.19256963020184
H	1.98787066710249	4.20497869671026	3.28647847062522
H	-0.49114660071660	4.15734649124635	3.28047449347308
H	-1.69343477370245	1.97950195292344	3.18154045006144
C	2.16817191992574	2.04935159273893	0.14095031957264
C	1.49491679830910	3.26860172958825	0.05701182827534
C	0.11497638232603	3.28470607055863	0.01636007217211
C	-0.60317187131853	2.07830157948362	0.04778862131674
C	1.46836840735527	0.82370232163747	0.09791662879159
C	0.04540577915357	0.83852111201374	0.05832561223282
C	1.47833252972815	-1.61998117104252	0.08061970590700
C	2.15504406230917	-0.41381551512859	0.14052273613374
C	0.07593430004560	-1.65183837405797	0.05419601589330
C	-0.66424844670402	-0.42348018041224	0.08457087208821
C	-2.07518018966007	-0.50061198510511	0.09103464422865
C	-2.73003635273543	-1.70635592141994	0.08497743839214
C	-1.99810155098737	-2.91585128765992	0.06030739589656
C	-0.63137203185240	-2.88202836520797	0.04161617929431
H	3.25861433201449	2.02490179527256	0.16895813084997
H	2.05779657734730	4.20170182582312	0.04895994510933
H	-0.42430614641171	4.22985796590411	-0.03688570845966
H	-1.69012986672106	2.12109232851935	0.00731971247459
H	2.02702056927863	-2.56249212888122	0.06959412490734
H	3.24592061125625	-0.39920934150183	0.15930265666643
H	-2.66216746113247	0.41651234973759	0.11069355900533
H	-3.81945165506610	-1.73375523135660	0.09431524125266
H	-2.52571167048756	-3.86942158824609	0.05117652413180
H	-0.05294392752037	-3.80760663597850	0.02281963681705

Table 28: Minimum-energy S1 geometry for the anth-phen exciplex

C	2.20585608586031	2.07745690302237	3.25501742284528
C	1.50501345244757	3.28318480972708	3.31181129210599
C	0.11504691123991	3.28331216806027	3.30864434487061
C	-0.58223365561911	2.07569468315546	3.25692859241541
C	-0.58788932335917	-2.85089025332466	3.32469619232099
C	0.10284078660126	-4.05215703499905	3.34817639421607
C	1.49983809080150	-4.05706299616859	3.30539139962332
C	2.19921622832250	-2.85956755702000	3.24752189706309
C	2.20579429971184	-0.38704793986121	3.18073415011389
C	-0.58036390263486	-0.38528747047889	3.21242213778219
C	1.53313704233116	0.84131770313066	3.24204185689544
C	0.09491033883344	0.84187495651115	3.24820010477073
C	0.09558732482573	-1.62323208272358	3.26378710229203
C	1.52619328269782	-1.62614770987436	3.23722669500026
H	3.29713175113481	2.07995764739862	3.24784130574828
H	2.05146836736576	4.22531286599866	3.34174569777494
H	-0.43195959566863	4.22503531537862	3.33620314609710
H	-1.67348296223228	2.07208437970772	3.25358769715583
H	-1.67877806886707	-2.84061708398334	3.34237827528417
H	-0.44331835030245	-4.99393160167623	3.39557904290193
H	2.04188419633064	-5.00230323720679	3.32304944339312
H	3.29043972431865	-2.86177317722805	3.21977215682075
H	3.29852165984708	-0.38997749702794	3.16183687269203
H	-1.67288307258308	-0.38773020447072	3.19110939152471
C	2.14941396650920	2.05480522199510	0.06689289065138
C	1.46852752488482	3.26051483679122	0.00620860726679
C	0.07866596866512	3.26377160905696	-0.01438495531241
C	-0.62345226184635	2.06532503788034	0.02226160232267
C	1.45915268136430	0.82859391570140	0.06583200174921
C	0.04080493058219	0.82708259364165	0.04397131165783
C	1.50582901009861	-1.60695878598326	0.02436450752705
C	2.16529007815357	-0.40937772636172	0.10769626006313
C	0.09310881437122	-1.65464316554672	-0.00421633565692
C	-0.65788673410269	-0.44124949262640	0.06262711521296
C	-2.06871691442730	-0.53496536603822	0.09179061690007
C	-2.70450862545890	-1.75081962725473	0.05260003935603
C	-1.95793709288084	-2.94554290933093	-0.03690601089492
C	-0.59087222889815	-2.89165648521936	-0.06314978112510
H	3.24040810193943	2.03756076779922	0.08339374329110
H	2.02032506674965	4.20003938702464	-0.01267896933040
H	-0.46636560391448	4.20667266199106	-0.05117956692732
H	-1.71151427023508	2.09536382987310	-0.00211155530775
H	2.05744744926734	-2.54783173876456	0.02005655483889
H	3.25575243242360	-0.37928298655859	0.13428291156572
H	-2.66717776175527	0.37291004407765	0.15119344265769
H	-3.79342197487492	-1.79387902369598	0.07646234712701
H	-2.47242135731967	-3.90554767617976	-0.07534348835171
H	0.00182458930127	-3.80676690831933	-0.10536590098917

Table 29: Minimum-energy S1 geometry for the phen excimer

C	2.82861266189291	-0.87824447111339	-0.05779823635100
C	3.55490240442033	0.29951045105080	-0.06651407085163
C	2.87359037014950	1.52415835787275	-0.06070458301658
C	1.49055752010641	1.56666384317353	-0.04827874450832
C	1.42295294727442	-0.86622124052804	-0.05057661008756
C	0.71959067286953	0.38400015349131	-0.04597527323761
C	-0.68913409229919	-2.07287650816499	-0.03967188822344
C	0.68151627835096	-2.07539742082576	-0.03972335164921
C	-1.42612561399311	-0.86098603832208	-0.05044819355765
C	-0.71817230975948	0.38664558197010	-0.04598826336552
C	-1.48478380696032	1.57213750501463	-0.04839701089428
C	-2.86795920548447	1.53472508202521	-0.06084963525693
C	-3.55376767306396	0.31258486716598	-0.06652092417043
C	-2.83181826523077	-0.86783241396641	-0.05771307297282
H	3.33834205718559	-1.84335203018069	-0.05756523869157
H	4.64370532492027	0.27716571361695	-0.07526854975627
H	3.43787898864403	2.45687546264473	-0.06293713267011
H	0.99529024344135	2.53591918178104	-0.04686887924105
H	-1.24102776066060	-3.01451079917797	-0.03758188901946
H	1.22993240621470	-3.01906098384882	-0.03768234992488
H	-0.98593173322987	2.53955317942454	-0.04704701304586
H	-3.42884309802724	2.46949296313352	-0.06320570650079
H	-4.64264615088922	0.29425567476810	-0.07522794616718
H	-3.34511451787061	-1.83104802263845	-0.05742538454727
C	2.82860243938319	-0.87825962407984	3.25777545230801
C	3.55489828887509	0.29949216087833	3.26648697454396
C	2.87359168384946	1.52414298197577	3.26071148525148
C	1.49055935841072	1.56665586240650	3.24831021061356
C	1.42294311128752	-0.86622925296565	3.25058241562417
C	0.71958821604334	0.38399575992229	3.24598431211347
C	-0.68914868838818	-2.07287263790647	3.23968558681364
C	0.68150105821965	-2.07540105678896	3.23973441328654
C	-1.42613311089800	-0.86097784536701	3.25045277019050
C	-0.71817299953155	0.38665153426492	3.24600268859388
C	-1.48477839073659	1.57214893554219	3.24838947909580
C	-2.86795428696350	1.53474067032111	3.26083776015087
C	-3.55376639653988	0.31260363539611	3.26651843694233
C	-2.83182464460912	-0.86781656893382	3.25771900679399
H	3.33832629346118	-1.84337010392895	3.25752696509536
H	4.64370129570002	0.27714245857402	3.27522061893001
H	3.43788423352344	2.45685770565065	3.26295469200085
H	0.99529560114321	2.53591297798083	3.24693154904134
H	-1.24104773475452	-3.01450380070928	3.23759415828357
H	1.22991126021344	-3.01906803643469	3.23769650348832
H	-0.98592358237093	2.53956316214130	3.24702033443181
H	-3.42883586789434	2.46951007792010	3.26317954965936
H	-4.64264513064482	0.29427914439116	3.27522242887972
H	-3.34512638197998	-1.83102934561721	3.25743215557487

Table 30: Minimum-energy S1 geometry for the fluor excimer

C	1.28479701639484	0.70995605555908	-0.03047128191448
C	1.26456292704904	-0.74189078258855	-0.03040494586977
C	2.46753065303207	-1.45296447674019	-0.06898196504737
C	3.65840252909814	-0.75579218174991	-0.08418573891202
C	3.67809474053143	0.65709669572040	-0.08413692239449
C	2.50711505753185	1.38720736453850	-0.06895152738004
C	-0.10704492700012	-1.17550990751698	-0.03784078536271
C	-2.92613903052022	-1.23184079751803	-0.07646902802999
C	-2.16826744721341	-2.39835789210016	-0.08898274753499
C	-0.76530934767064	-2.39936791143018	-0.07031677738273
C	-0.89167546356145	0.01421580744658	-0.03576574107245
C	-0.07421913583562	1.18162408364938	-0.03779023711064
C	-0.69815998147895	2.42331925928521	-0.07070609102358
C	-2.10060657811138	2.46135182635713	-0.08940089513569
C	-2.89068965263458	1.31640793275406	-0.07676872401033
C	-2.29461777398161	0.03374198346419	-0.06694901192372
H	2.46410611216806	-2.54361128799445	-0.07695085595382
H	4.60321804947460	-1.29878854761611	-0.10552867348920
H	4.63767997376808	1.17354746524666	-0.10540559217816
H	2.53412367684884	2.47752454172775	-0.07690061667678
H	-4.01524356446070	-1.29182369384050	-0.08869248895956
H	-2.68858600272615	-3.35667095142730	-0.10286743828634
H	-0.22122815026684	-3.34403446750193	-0.08144372460847
H	-0.12800037568258	3.35247510227913	-0.08205712848286
H	-2.59403596393194	3.43378178274750	-0.10346903146782
H	-3.97769134583081	1.40669323741132	-0.08970601069414
C	1.28480084613218	0.70995710881768	3.23046793397082
C	1.26456793552796	-0.74188880752004	3.23040489889105
C	2.46753563660433	-1.45296164060297	3.26898353558210
C	3.65840725199323	-0.75578824968584	3.28419586788098
C	3.67809851928675	0.65709989814332	3.28414667674726
C	2.50711790211480	1.38720906780102	3.26894989610231
C	-0.10704108271715	-1.17550895744970	3.23783168915601
C	-2.92613418790208	-1.23184220224669	3.27646207396578
C	-2.16826192982355	-2.39835819690979	3.28897621468901
C	-0.76530302084072	-2.39936676529010	3.27031584690433
C	-0.89167153254534	0.01421584316183	3.23574697280762
C	-0.07421625293011	1.18162499110007	3.23777343054737
C	-0.69815705860602	2.42331933675846	3.27070267018086
C	-2.10060379289908	2.46135024519016	3.28940126228986
C	-2.89068593208107	1.31640613777413	3.27676917085767
C	-2.29461350721013	0.03374135569753	3.26694904792642
H	2.46411176333025	-2.54360851262490	3.27694975925091
H	4.60322252325465	-1.29878485863689	3.30554346627467
H	4.63768330665569	1.17355118678986	3.30542095410372
H	2.53412684721084	2.47752637098700	3.27689448798899
H	-4.01523858063963	-1.29182537120159	3.28869302198785
H	-2.68857874923615	-3.35667222673500	3.30286181118748
H	-0.22122093708373	-3.34403272308029	3.28144989567126
H	-0.12799729163106	3.35247496388638	3.28205771647074
H	-2.59403312014277	3.43378015164451	3.30347619383948
H	-3.97768755081202	1.40669061406923	3.28972048562763

Table 31: Minimum-energy S1 geometry for the phen-pyr exciplex

C	2.84123455853229	-1.21297404603364	3.23609943689073
C	3.55769472599219	-0.03998461019633	3.28971931481942
C	2.88301304097404	1.18180257480700	3.32007437974649
C	1.49092646655112	1.21350025146119	3.34588602440476
C	1.42118355730918	-1.20585130841587	3.25617648976935
C	0.73269142022766	0.04475001215205	3.31584332075867
C	-0.69519021120534	-2.40371686210100	3.18093512441063
C	0.69109537376201	-2.40538175255677	3.18110374015070
C	-1.42242984854788	-1.20243627644694	3.25574281969124
C	-0.73095601314392	0.04651467499415	3.31575636341842
C	-1.48637270150663	1.21708789130966	3.34576414503653
C	-2.87853999145081	1.18868110619178	3.31972150357332
C	-3.55613494424138	-0.03147942006126	3.28921801050325
C	-2.84249851643941	-1.20618617661515	3.23559417956726
H	3.35242848021020	-2.17629720460287	3.20099337426764
H	4.64725729231411	-0.06270974718938	3.27313791615710
H	3.44307015463029	2.11582393424216	3.35098603199277
H	0.99288256179951	2.18169610315049	3.37076274382390
H	-1.24426829849853	-3.34527700457911	3.13611340975234
H	1.23791722401796	-3.34825207953877	3.13622864275836
H	-0.98604535498745	2.18409688036220	3.37081493929574
H	-3.43640406017252	2.12401962323310	3.35053853221199
H	-4.64574784006817	-0.05156454745664	3.27254712301359
H	-3.35598388841928	-2.16827168835873	3.20012955658021
C	0.71038500390058	-0.00574915278137	-0.01321182601939
C	-0.71108861890343	-0.00490788913551	-0.01331043093990
C	1.42059723679920	1.22005440359742	-0.02709324130140
C	1.42399048329430	-1.24271238864190	0.03733517653372
C	-1.42613776143703	-1.24103328257152	0.03713583865274
C	-1.41986112579833	1.22173211938223	-0.02727938459688
C	2.83644177310167	1.20025318237063	-0.00678848421334
C	2.83822003903175	-1.20833761953724	0.05835469834065
C	-2.84033167124965	-1.20499737033967	0.05790546554874
C	-2.83572499069589	1.20359948554882	-0.00712325417629
C	0.68488734534650	2.43378900073483	-0.03115653024736
C	0.69290038793270	-2.44435333385651	0.10734048108520
C	-0.69646860564366	-2.44352830517996	0.10721588846588
C	-0.68271748478160	2.43459955364296	-0.03125424304032
C	3.52184843640032	-0.00176223032527	0.01033039394821
C	-3.52253848801569	0.00237380772583	0.00981953851070
H	1.23675653002444	3.37550624939371	-0.03467160002127
H	1.23870083463057	-3.38813416278914	0.14794611046382
H	-1.24339107055322	-3.38666516259709	0.14771634846064
H	-1.23346650694423	3.37697094951867	-0.03483241603928
H	3.37630852731795	2.14768959836915	-0.03126989918192
H	3.38521232593174	-2.15191173978992	0.08607217642729
H	-3.38844238233782	-2.14793022440765	0.08544108616199
H	-3.37447965564975	2.15166740115917	-0.03158681737140
H	4.61206004476789	-0.00115164196448	0.02388147869787
H	-4.61275179410854	0.00425042472250	0.02319332325689

Table 32: Minimum-energy S1 geometry for the tri excimer

C	-1.170137	0.837477	3.281047
C	0.133124	1.432768	3.281371
C	0.224574	2.841018	3.290594
C	-0.895584	3.647237	3.299187
C	-2.170134	3.065107	3.298076
C	-2.294340	1.690617	3.290058
C	-0.140318	-1.432057	3.281293
C	-1.307397	-0.601022	3.281367
C	-2.572679	-1.226128	3.291414
C	-2.710708	-2.599211	3.301589
C	-1.569262	-3.411945	3.301571
C	-0.316909	-2.832180	3.290741
C	1.310296	0.594552	3.282214
C	1.174181	-0.831690	3.281840
C	2.348075	-1.614995	3.291500
C	3.606293	-1.047999	3.298346
C	3.739420	0.346857	3.299398
C	2.611195	1.141640	3.292632
H	1.203276	3.315939	3.290654
H	-0.785743	4.731239	3.307083
H	-3.061328	3.691929	3.305563
H	-3.294171	1.261948	3.289389
H	-3.473376	-0.616073	3.291042
H	-3.704381	-3.046115	3.310814
H	-1.666458	-4.497145	3.310400
H	0.554293	-3.483655	3.289849
H	2.270059	-2.700042	3.291529
H	4.490173	-1.685102	3.305322
H	4.727863	0.805244	3.307062
H	2.739853	2.221851	3.293696
C	-1.170121	0.837470	-0.081026
C	0.133140	1.432759	-0.081400
C	0.224585	2.841010	-0.090657
C	-0.895575	3.647227	-0.099202
C	-2.170126	3.065099	-0.098003
C	-2.294327	1.690608	-0.089956
C	-0.140296	-1.432061	-0.081301
C	-1.307378	-0.601029	-0.081340
C	-2.572660	-1.226137	-0.091401
C	-2.710688	-2.599220	-0.101628
C	-1.569240	-3.411950	-0.101613
C	-0.316887	-2.832184	-0.090747
C	1.310317	0.594548	-0.082256
C	1.174206	-0.831693	-0.081869
C	2.348100	-1.614996	-0.091495
C	3.606319	-1.047999	-0.098310
C	3.739441	0.346859	-0.099396
C	2.611213	1.141640	-0.092693
H	1.203284	3.315934	-0.090779
H	-0.785735	4.731230	-0.107135
H	-3.061321	3.691920	-0.105445
H	-3.294157	1.261937	-0.089232
H	-3.473357	-0.616082	-0.091015
H	-3.704360	-3.046125	-0.110876
H	-1.666434	-4.497151	-0.110456
H	0.554315	-3.483659	-0.089839
H	2.270083	-2.700044	-0.091519
H	4.490200	-1.685100	-0.105233
H	4.727882	0.805250	-0.107037
H	2.739867	2.221850	-0.093779

Table 33: Minimum-energy S1 geometry for the chrys excimer

C	-3.463016	-2.609618	-0.176184
C	-2.724173	-3.792417	-0.124320
C	-1.347195	-3.730048	-0.034811
C	-2.818759	-1.379751	-0.151204
C	-1.423382	-1.283219	-0.066846
C	-0.673291	-2.491420	-0.013906
C	0.739776	-2.424575	0.086042
C	1.403510	-1.212846	0.034957
C	-0.717569	-0.006471	-0.020941
C	0.717626	0.006397	-0.021211
C	-0.739747	2.424480	0.086456
C	-1.403493	1.212741	0.035309
C	0.673304	2.491313	-0.013951
C	1.423412	1.283133	-0.067042
C	2.818787	1.379735	-0.151386
C	3.463010	2.609615	-0.176499
C	2.724147	3.792392	-0.124444
C	1.347193	3.729945	-0.034522
H	-4.550123	-2.647082	-0.242412
H	-3.230809	-4.757111	-0.140222
H	-0.753356	-4.644804	0.009464
H	-3.422988	-0.475318	-0.204067
H	1.304801	-3.356789	0.126489
H	2.491449	-1.215719	0.080190
H	-1.304781	3.356707	0.126462
H	-2.491441	1.215600	0.080213
H	3.423050	0.475289	-0.203684
H	4.550115	2.647125	-0.242730
H	3.230754	4.757103	-0.140145
H	0.753327	4.644655	0.010362
C	-3.463059	-2.609564	3.426089
C	-2.724197	-3.792355	3.374309
C	-1.347220	-3.729964	3.284814
C	-2.818820	-1.379685	3.401101
C	-1.423439	-1.283131	3.316848
C	-0.673338	-2.491325	3.263871
C	0.739730	-2.424481	3.163940
C	1.403461	-1.212754	3.214995
C	-0.717624	-0.006380	3.270978
C	0.717575	0.006488	3.271162
C	-0.739773	2.424580	3.163709
C	-1.403534	1.212844	3.214821
C	0.673282	2.491402	3.264048
C	1.423380	1.283213	3.317031
C	2.818762	1.379783	3.401301
C	3.463006	2.609650	3.426419
C	2.724154	3.792438	3.374455
C	1.347193	3.730021	3.284639
H	-4.550169	-2.647042	3.492270
H	-3.230815	-4.757059	3.390254
H	-0.753358	-4.644706	3.240564
H	-3.423070	-0.475263	3.453908
H	1.304755	-3.356694	3.123464
H	2.491396	-1.215628	3.169696
H	-1.304802	3.356816	3.123816
H	-2.491486	1.215722	3.170023
H	3.423012	0.475325	3.453518
H	4.550117	2.647141	3.492569
H	3.230780	4.757141	3.390140
H	0.753346	4.644747	3.239835

Table 34: Minimum-energy S1 geometry for the chrys-naph exciplex

C	-1.40118143895995	-1.23026627050334	3.20598280533669
C	-0.71174122596996	-2.42893661718402	3.20711238766978
C	0.69179782283883	-2.43341424655858	3.21082463721901
C	1.39043976073691	-1.24176250458091	3.21286781955388
C	1.40131622230163	1.23041528561286	3.20580880673315
C	0.71187297828028	2.42908453542155	3.20694138907717
C	-0.69166045543149	2.43357764071267	3.21079406216855
C	-1.39032662947013	1.24193482528217	3.21295908720297
C	-0.71400502581559	0.00270411681524	3.22205334007006
C	0.71410537028604	-0.00254385115416	3.22186076479040
H	-2.49168550638402	-1.22596013257500	3.18009886745717
H	-1.26069277674174	-3.36906499291785	3.18476693758097
H	1.23103939903337	-3.37984054366384	3.20088111610929
H	2.48163367836950	-1.24152982857629	3.20326096875186
H	2.49181427029542	1.22606603151867	3.17979271405947
H	1.26083608825101	3.36920475091930	3.18447549475898
H	-1.23091129227302	3.37999889071532	3.20085759591226
H	-2.48152102045688	1.24174480018698	3.20346291907301
C	-3.46199367726401	-2.60966527116009	0.13070622396889
C	-2.71946083743245	-3.79617947316991	0.15836464232756
C	-1.33798892736761	-3.72863908139919	0.11235083670403
C	-2.82746956819801	-1.38119481558772	0.06420673960307
C	-1.41912602593121	-1.27346402361038	0.01462316254649
C	-0.66546591435710	-2.49547818850406	0.02921147551890
C	0.75071898319490	-2.42880057535990	-0.01644757715090
C	1.40899802425936	-1.21556650254068	-0.04493731232087
C	-0.72308072162237	-0.01229052780948	-0.02678123119902
C	0.72297027766196	0.01225635236414	-0.02713111252665
C	-0.75079527320609	2.42871944411320	-0.01635052000372
C	-1.40914238497253	1.21551403841378	-0.04476132912602
C	0.66538684049454	2.49545243162262	0.02901467203570
C	1.41901548259389	1.27343781526617	0.01461011030193
C	2.82735737519379	1.38107785537259	0.06457995277833
C	3.46192074355002	2.60954562667842	0.13101749060957
C	2.71940923372936	3.79607388178715	0.15837197087931
C	1.33794018450217	3.72858631128433	0.11219364770033
H	-4.55108835916333	-2.64901471741757	0.16183121827733
H	-3.22387431173044	-4.76027452793671	0.21272815173384
H	-0.73926386864543	-4.64156759602518	0.12757805693926
H	-3.43844343999445	-0.48004650163618	0.05221103015826
H	1.31734244586847	-3.36080814111716	-0.02932593201954
H	2.49783663111813	-1.22223279931724	-0.07519268378637
H	-1.31740911502787	3.36073821400377	-0.02926434373466
H	-2.49798906313267	1.22222143965765	-0.07456066554698
H	3.43823503493364	0.47986361649610	0.05296353285364
H	4.55100652236738	2.64883522769087	0.16251122926333
H	3.22385377692378	4.76014635275592	0.21288464758053
H	0.73919431276400	4.64149144561396	0.12799220210975

Table 35: Minimum-energy S1 geometry for the benza-naph exciplex

C	4.39556195845606	-1.32608741292517	3.21136974546354
C	4.77238787293002	0.01957896896459	3.17695096000662
C	3.80291528398663	1.01119211042316	3.15543512268979
C	3.05100044160384	-1.67015382431064	3.22364785852493
C	2.04865875564210	-0.68518877921184	3.21122113938963
C	2.43376359596886	0.68809370883814	3.17702660362952
C	1.41241871936846	1.66715286164364	3.12706501238962
C	0.66454605330188	-1.01031205898870	3.19613926553816
C	-0.33965205474294	-0.04046450705514	3.24165264881711
C	0.05277536912731	1.33817577678401	3.21429719797116
C	-0.94562422648060	2.34492231182721	3.22231533872276
C	-2.28703199208348	2.03579392870739	3.27506791354925
C	-1.74374015006103	-0.36190158231543	3.25465451432790
C	-2.71666687182311	0.69362707953825	3.28255815314801
C	-4.09408826466074	0.36707189554639	3.28757952508965
C	-4.51705372013891	-0.93686085389282	3.26754969436091
C	-3.56353665469146	-1.97936040234021	3.25106593240094
C	-2.21993408211395	-1.69557570855093	3.25002057755461
H	5.15724626858368	-2.10532715550252	3.22907725984735
H	5.82821230184687	0.28966245335481	3.16771299758282
H	4.09260878242960	2.06345731866316	3.12694097204976
H	2.75328296515042	-2.72036229290371	3.24906799786685
H	1.69652293493194	2.72226561125943	3.10398724060412
H	0.40559287793542	-2.06906018910523	3.22186892895500
H	-0.62401247538219	3.38797859701739	3.20648329835940
H	-3.03781337709523	2.82720447212660	3.29203085347194
H	-4.81676088645636	1.18522339142018	3.30584180062796
H	-5.58103679910104	-1.17212854469577	3.27205065790223
H	-3.89791702509916	-3.01685166784959	3.24565871564595
H	-1.50755085246277	-2.51923923750633	3.24030333067907
H	3.42411874441732	0.82788534704569	0.04803191101231
H	2.71425199182178	-1.54301220896683	0.07622019163254
C	1.96470548104597	-0.75293942405775	0.06763395840706
C	2.36383243755398	0.57924593236951	0.05039498400007
C	1.41018481779359	1.59364357186611	0.09639220816287
C	0.61014758293047	-1.07592134999051	0.13134233106731
C	-0.38134198200017	-0.07029763370589	0.08058192224150
C	0.02738907611452	1.29646780626700	0.05745683605215
C	-0.96009558182618	2.30021097021612	0.04370691574670
C	-2.31021058077322	1.97584248531935	0.02196184768600
C	-1.75911408732160	-0.36871033808542	0.09923384105541
C	-2.71033760679386	0.63976810019639	0.05172814264496
H	-3.76956055024566	0.38567266971853	0.06451527638855
H	-2.07095090492975	-1.41309157955632	0.14706792419231
H	1.72101339600129	2.63945482521656	0.09138498188834
H	0.29503538356012	-2.12014550716057	0.15593556764298
H	-0.64600965141493	3.34528030885477	0.03295354085015
H	-3.05862271480379	2.76749975549294	0.00101636216222

Table 36: Minimum-energy S1 geometry for the benzapyr-naph exciplex

C	4.58147401084035	-0.49887568835891	-0.29887647763928
C	4.73219219105974	0.86616659608023	-0.05511314132429
C	3.61262964528683	1.65264032149050	0.15266736271755
C	3.31187415000473	-1.06516915791599	-0.31563432679531
C	2.16274883760988	-0.29701759790452	-0.09494489990968
C	2.31522485945105	1.10290088513972	0.12319269303434
C	1.16970071680818	1.90708596689058	0.33720741784877
C	-0.12879306746931	1.39884161838937	0.21542557903345
C	-1.27421108678174	2.22171213961439	0.33945218947511
C	-2.54955449118945	1.70446452625709	0.24522224172350
C	-2.76255159789212	0.32293473837479	0.05950932478269
C	-4.06022910650981	-0.23953420992803	-0.01064485769375
C	-4.23179794286999	-1.60012067408527	-0.14336420877828
C	-3.12330648369488	-2.45527240478761	-0.19967929449125
C	0.82207799949617	-0.86618690214665	-0.06308657378111
C	-0.31071426103467	-0.00769561673222	0.02295291631105
C	-1.62354763460564	-0.53968268049133	-0.02688552963577
C	-1.82464669436016	-1.94734432047770	-0.13678999369716
C	-0.66967263326604	-2.78638809570147	-0.14431772257530
C	0.59396200406795	-2.25938149537199	-0.12510383037137
H	5.45557713940730	-1.12385069953716	-0.47977902194555
H	5.72595603182275	1.31359417867452	-0.03787041139125
H	3.71803744551954	2.72412149876949	0.33364415613995
H	3.21773929999891	-2.13155574346052	-0.51738143386890
H	1.30583410832482	2.97948779283512	0.49639102131599
H	-1.12760554354275	3.29221145951931	0.49529244528927
H	-3.41619874671131	2.36329444097760	0.32347467316272
H	-4.92252131612905	0.42680507060173	0.04571264370137
H	-5.23712903453112	-2.01809228712096	-0.19944116226853
H	-3.26583697208317	-3.53341376883019	-0.28783161224181
H	-0.81304080587984	-3.86720501609920	-0.19418373296193
H	1.44549350669299	-2.93878704541295	-0.14694937494966
C	1.38651388126951	-1.29704497088306	3.03929570716310
C	2.54104816941669	-0.52707096057381	3.10704483612800
C	2.44931114711788	0.85525371894776	3.26535096085216
C	1.20686967663539	1.46956115320925	3.32629058971473
H	1.13225547237467	2.55174050615113	3.44116590973759
H	-1.32734719857041	2.37950856496154	3.51366359664648
H	-3.38628542026186	0.99942948618293	3.40240166177002
C	0.11102853714651	-0.71081122037275	3.16870931121904
C	0.01522754032718	0.70364867322606	3.31814989975196
C	-1.25833711784426	1.29641522815887	3.40329215403208
C	-2.40761736670916	0.52412840144911	3.34726671967532
C	-2.31533829776340	-0.86221288793313	3.19066107788889
C	-1.07736727480507	-1.47359841324401	3.10422735931968
H	3.35632733144718	1.45801325578621	3.28743845520809
H	-3.22302437807645	-1.46034857346436	3.11232364976774
H	-1.00134589125707	-2.55376352282756	2.97321569248752
H	1.45136595532767	-2.37592261894636	2.89027252317227
H	3.51777970638486	-0.99877364907956	3.00783883724978

Table 37: Minimum-energy S1 geometry for the naph-anth exciplex

C	-1.39189438131376	-0.02798382757289	3.10601487900843
C	-0.69549715449216	-1.23179177670646	3.15838772804938
C	0.69553768304482	-1.23180019290166	3.15841393760279
C	1.39195612410754	-0.02800571054606	3.10606537089079
C	1.39271276473550	2.44547353843215	3.17040548575766
C	0.69746581174318	3.64373628438387	3.22536683110619
C	-0.69734835230261	3.64375045156791	3.22535307736129
C	-1.39261457550050	2.44549930081001	3.17037319462649
C	-0.71289755923098	1.21076710199770	3.15920095406574
C	0.71297472943683	1.21075327076560	3.15920256029917
H	-2.48306567993825	-0.02542899826044	3.09332100360305
H	-1.23878654309411	-2.17584268611776	3.15145982178882
H	1.23881429312889	-2.17585901939494	3.15150211438972
H	2.48312777849816	-0.02546213354970	3.09339902312010
H	2.48403532257124	2.44242168120655	3.16133667334169
H	1.24237815519135	4.58699582902105	3.25160899830179
H	-1.24224189535120	4.58702090552413	3.25158029848927
H	-2.48393684881454	2.44246847167577	3.16128909078317
C	1.39297822732363	2.46901533368169	-0.02387498136124
C	0.69588134784782	3.67315595129641	-0.08734107128023
C	-0.69600048983063	3.67314123094836	-0.08735415584807
C	-1.39307072636912	2.46898714914127	-0.02392099096575
C	-1.39334209326313	-2.46813727819749	0.00833888665663
C	-0.69983523498851	-3.66633168331775	-0.01285468918700
C	0.69982168913724	-3.66632557025660	-0.01283757207723
C	1.39331817362481	-2.46812519735243	0.00839923764825
C	1.39354657076431	0.00486103269061	0.06294683076217
C	-1.39359731538895	0.00483905590633	0.06276372068119
C	0.71890215163718	1.23215079663543	-0.00353765565879
C	-0.71896960901223	1.23213538851211	-0.00357833590194
C	-0.71514032919836	-1.23451225768394	0.01783231678856
C	0.71510846886754	-1.23450701155387	0.01788219673686
H	2.48446198143449	2.46910322437081	-0.01717029601776
H	1.24380155977975	4.61432385193296	-0.12322916322874
H	-1.24394362373689	4.61429593556367	-0.12324356390225
H	-2.48455517472208	2.46904628690661	-0.01724288374634
H	-2.48503435502809	-2.46502277496497	0.01120049577714
H	-1.24473898268744	-4.61002379340633	-0.02836786890062
H	1.24473431594291	-4.61001239044400	-0.02835120112728
H	2.48501015623624	-2.46500208015700	0.01130884923990
H	2.48654525015732	0.00313504425127	0.06911900319370
H	-2.48659763094721	0.00309726516201	0.06883184913326

Table 38: Minimum-energy S1 geometry for the anth-benz exciplex

C	-1.15142101306816	0.04327704466125	3.77329379955929
C	0.20726271254653	-0.01390288704746	3.49058070367235
C	0.88311830211618	1.13607792665795	3.09666225243049
C	0.20332035515179	2.34524891395422	2.99649271580013
C	-1.15546925588536	2.40132653847056	3.27858485510544
C	-1.83450301725952	1.24956332212668	3.66228399039818
H	-1.68392551428156	-0.86045443089847	4.07055658897651
H	0.73835520710649	-0.96408281522775	3.55438541868934
H	1.94588369601853	1.08769313504782	2.85885811904598
H	0.73078472786903	3.24367114208703	2.67486075560127
H	-1.69134382356141	3.34642164261570	3.18696502140376
H	-2.90189028561231	1.29309387079727	3.88131047356937
C	1.61298312901335	2.89415905613783	-0.87594710020425
C	0.95309987781520	4.12516999714802	-0.95923213914458
C	-0.39940607600637	4.20980932846051	-0.65929569532046
C	-1.10492351720423	3.06313508225739	-0.27803757100756
C	-1.18012905508597	-1.75006659161736	0.76404819893289
C	-0.50629166475710	-2.96622045047805	0.92120963056074
C	0.85323944517127	-3.04578203959340	0.65352887894718
C	1.54913992348964	-1.91192474552519	0.21914226715846
C	1.56651307074588	0.48029964487941	-0.37677481295066
C	-1.14841763458359	0.64643204711054	0.19877069144390
C	0.93040029148667	1.73028718084624	-0.49080573835569
C	-0.47208108615590	1.81426233861083	-0.19874868620818
C	-0.50810636747370	-0.59817382129379	0.32982856498910
C	0.89655740112035	-0.68178497972157	0.04784636741378
H	2.67749861211257	2.82754812424188	-1.10601003746454
H	1.50480196906166	5.01522701466967	-1.25943515424446
H	-0.91446138189510	5.16782878890829	-0.71911680549546
H	-2.16666913508586	3.12852091883900	-0.03598664676393
H	-2.24570785367158	-1.68146539274661	0.98731291300415
H	-1.05063244622584	-3.84787578404146	1.25738191454066
H	1.38191871766070	-3.99032664016081	0.77635948278540
H	2.61739747870103	-1.97437952186749	0.00579313268951
H	2.63391734171987	0.41503509515550	-0.60478705826283
H	-2.21278313109319	0.71425994653582	0.43624370870475

Table 39: Minimum-energy S1 geometry for the benz-pyr exciplex

C	-1.32162352953850	-0.39404739105814	3.42206931743572
C	0.06734854579784	-0.43906678039979	3.42992796255226
C	0.80055724776343	0.73999274377972	3.38124442487443
C	0.14634871485755	1.96462770656091	3.32593565615873
C	-1.24225691308877	2.00948944196891	3.31910411311056
C	-1.97618156707539	0.83087914720133	3.36582657217886
H	-1.89674257549206	-1.31959486670962	3.44947099350650
H	0.58207879123446	-1.39942213124052	3.45978076135304
H	1.88982475835040	0.70485549521481	3.36765552995906
H	0.72354118768284	2.88722939095495	3.26499334867357
H	-1.75552491618761	2.96997177689400	3.26648883584458
H	-3.06552213404521	0.86674585448376	3.35411158830015
C	0.17919804642547	0.57502159691507	0.00502670299493
C	-0.53460931919785	-0.60920253097974	-0.08397250366062
C	-0.49331276768812	1.84668214100999	-0.11355187072568
C	1.60853591095244	0.55589210282659	0.20611059711481
C	0.13601922700185	-1.88094145652543	0.04820579857264
C	-1.96549808178693	-0.58979662955108	-0.27567820092078
C	0.25300244750871	3.02742243745041	-0.00836040729902
C	2.30200508155039	1.76916958777692	0.30550322983251
C	-0.60943095860387	-3.06247638007851	-0.06021170418182
C	-2.65900559703195	-1.80345758787192	-0.37343762530500
C	-1.90169313918258	1.84337339543612	-0.30023102202215
C	2.25027964467164	-0.70597695480150	0.32614702212619
C	1.54235819113701	-1.87736473356207	0.25204395429437
C	-2.60938629016746	0.67268324809887	-0.37844268266564
C	1.63611437416602	2.99444029936423	0.19763062014525
C	-1.99244755261746	-3.02926744172438	-0.27032589117961
H	-2.41609690043392	2.80212095575521	-0.38120073632656
H	3.33005189812418	-0.72657794860797	0.48207597724379
H	2.05549272765709	-2.83566055667394	0.34682297212176
H	-3.69053796820483	0.69307292327773	-0.52396566670289
H	-0.26536576217803	3.98364684025213	-0.09097489891888
H	3.38100684971790	1.74574997085071	0.46455613322020
H	-0.09335645473968	-4.01954519560024	0.02661185698449
H	-3.73836999702747	-1.77969436622692	-0.52918666180090
H	2.19627561970284	3.92517907097095	0.27140405600837
H	-2.55192684001438	-3.95992617543154	-0.34921015289722

Table 40: Minimum-energy S1 geometry for the naph-tet exciplex

H	-3.37974194196650	-1.23919444699630	3.22109613665620
H	-3.37897434511819	1.24128919195766	3.22109526247917
C	-2.43294048525779	0.70081336725202	3.23303035622927
C	-2.43337433794262	-0.69930402676999	3.23302941286219
C	-1.23870522591681	-1.39369274341343	3.20511913691721
C	-1.23784591617553	1.39446636027786	3.20512502649324
C	0.00021245971011	0.71285486892504	3.22273621616980
C	-0.00022474341698	-0.71284365552314	3.22274935615578
C	1.23783932628615	-1.39444092069968	3.20519875709082
C	1.23869195880540	1.39369849216827	3.20519543059149
C	2.43336407735592	0.69933417948770	3.23291158443814
C	2.43293436519309	-0.70080615111317	3.23291694993194
H	3.37900529143959	-1.24121547354518	3.22106111154000
H	3.37976386777749	1.23916747439623	3.22105121461807
H	-1.23478443573338	-2.48516479014755	3.19742736946471
H	-1.23325170182906	2.48593649977899	3.19742435822501
H	1.23325446206478	-2.48591367606671	3.19758247315033
H	1.23477206615800	2.48517435027474	3.19756905582121
C	-4.89268208624947	0.70360845373483	-0.00827398702957
C	-4.89309871446392	-0.70069549551196	-0.00827202770008
C	-3.69848789083875	-1.39473700600937	-0.01416778300590
C	-3.69765978427544	1.39694270852669	-0.01415870652810
C	-2.46156964014495	0.71786984027100	-0.02396581041118
C	-2.46199559327986	-0.71639591350830	-0.02397523395951
C	-1.22768004506337	-1.39557064595250	-0.00133252159918
C	-1.22684507981198	1.39630460640974	-0.00124559932429
C	0.00022812706752	0.72346678128768	-0.02345779639634
C	-0.00020721083409	-0.72346398146508	-0.02345585741056
C	1.22685752887618	-1.39630475980919	-0.00130966728400
C	1.22770209922530	1.39555863841026	-0.00122600685789
C	2.46203014963583	0.71639116756280	-0.02369513244973
C	2.46159504907715	-0.71788587619139	-0.02370287055979
C	3.69768559363894	-1.39697423799583	-0.01414580494997
C	4.89270035158803	-0.70364144078264	-0.00822299415122
C	4.89312795321441	0.70066308017979	-0.00819714180115
C	3.69853443558400	1.39472488167602	-0.01409174845852
H	-5.83816368710645	1.24549185467338	-0.00456151535549
H	-5.83890123848413	-1.24201880700219	-0.00455360749290
H	-3.69403039288010	-2.48632585580566	-0.01145741501133
H	-3.69256057385512	2.48852835947274	-0.01144674751554
H	-1.22990341622362	-2.48854698991307	0.00595603744573
H	-1.22841765652403	2.48928190489519	0.00607923510581
H	1.22842059968268	-2.48928268893049	0.00612577711857
H	1.22993342298707	2.48853497973902	0.00624810420502
H	3.69257679641473	-2.48856048693816	-0.01181175826831
H	5.83818148853698	-1.24552800308025	-0.00466604751557
H	5.83893934851049	1.24197240132805	-0.00460980266283
H	3.69409532456228	2.48631363048555	-0.01172477901080

Table 41: Minimum-energy S1 geometry for the naph-tri exciplex

C	-1.32470216481352	0.83036389016420	3.22394133248341
C	-0.07112803510328	1.41224132859881	3.18604773506551
H	0.02849634000867	2.49813098170568	3.15375544611939
H	-2.21257646498617	1.46059083805584	3.23041842275111
C	-0.32815028839556	-1.36925508962411	3.19157462204398
C	-1.45373653242642	-0.56743551558454	3.22696824586142
H	-2.44215996086005	-1.02421124739189	3.23548182897328
H	-0.42910975962245	-2.45520463614852	3.16487339062174
C	1.09640263039746	0.61966022078730	3.16961776037867
C	0.96493826492492	-0.80429719671807	3.17287707874816
C	2.13218511010624	-1.59619677480998	3.13449887824873
C	3.38547472210868	-1.01619732711946	3.10150935301971
C	3.51465556119871	0.38360236098029	3.09803241080348
C	2.38918190367722	1.18393582782393	3.12757990333810
H	2.02648315997632	-2.68231509587929	3.12418709195489
H	4.27514250065325	-1.64332675778418	3.07052145878877
H	4.50413560247978	0.83705149536329	3.06363660118490
H	2.48447830984814	2.27094686989902	3.11157860617479
C	-1.05066765016162	0.82891602772173	0.07043838936804
C	0.25569511601299	1.41859984309056	0.00716291194036
C	0.34057588667531	2.83498930157897	0.02062718387925
C	-0.77945859823381	3.63353542923057	0.09515982274551
C	-2.05251319685512	3.05601965420731	0.16598989248426
C	-2.16833254336471	1.67746840302626	0.15707545038037
C	-0.02225552508196	-1.44828345809057	0.00478976062086
C	-1.19069465229172	-0.61864209375612	0.06486847999165
C	-2.45170348385503	-1.23736978239800	0.13371604177826
C	-2.60259613451641	-2.61197376691165	0.13427300370318
C	-1.46375644708415	-3.42340703489493	0.07101369499534
C	-0.21090864500934	-2.85414602885583	0.01050767649646
C	1.41874543739619	0.58604655049777	-0.04879605590231
C	1.28027676820826	-0.85436439727059	-0.04341981706482
C	2.45810936680611	-1.63311949580978	-0.07914669218107
C	3.72226586677393	-1.07038406596463	-0.10750799535195
C	3.85684213550349	0.32979846574051	-0.12006066955900
C	2.72451583187525	1.12457600782507	-0.09639110283270
H	1.31568986668907	3.31417764811002	-0.03578683733430
H	-0.66987091038722	4.71841111317634	0.09504264383181
H	-2.94259565422601	3.68112018090160	0.22293931778693
H	-3.16551570307327	1.24492795219116	0.20924759725443
H	-3.34791602914193	-0.62167392564280	0.17641431966902
H	-3.59680555086684	-3.05468480596897	0.17777765146810
H	-1.56468509497248	-4.50906085503827	0.06428387533764
H	0.65446280097250	-3.51120750639190	-0.04510020115215
H	2.38107242921409	-2.71895570584647	-0.08151851753111
H	4.60276191529690	-1.71108047229979	-0.13869651785475
H	4.84347882210877	0.78989671484012	-0.16198230318805
H	2.85673267641681	2.20483593068398	-0.11714117033929

Table 42: Minimum-energy S1 geometry for the benza-anth exciplex

C	4.40972105269774	-1.31879562165897	3.29478759267194
C	4.78511021684808	0.02768914782871	3.27727416491278
C	3.81856858807611	1.01894804589707	3.21792977880655
C	3.06815716254154	-1.66704596536813	3.25217165254015
C	2.06210478490000	-0.68245036123603	3.22036623464816
C	2.44628744282441	0.69527286010189	3.20544963349848
C	1.43144185863578	1.66954024024552	3.14988292924662
C	0.68869462731877	-1.00874880249426	3.16828208967129
C	-0.31888185010039	-0.03772375625608	3.23684658818727
C	0.07000316271356	1.33671855686995	3.23397632488221
C	-0.93005274289366	2.34761950930165	3.28150978629625
C	-2.25830936479528	2.03473586521044	3.33546657136409
C	-1.72456193258837	-0.36664604957376	3.26211284576800
C	-2.69000487516798	0.68167162189499	3.31687367539705
C	-4.06487652201758	0.35958005425394	3.32482711580618
C	-4.49046732081191	-0.94593942104769	3.27689905803185
C	-3.54128538593189	-1.98480139912542	3.22847121346470
C	-2.19559909777425	-1.69897834082520	3.22687693973283
H	5.17266578646129	-2.09600050724312	3.33208034295373
H	5.84061808088536	0.29812298196398	3.29917330780388
H	4.10846591375245	2.07109731600421	3.19919030193891
H	2.77203776118191	-2.71768892731804	3.25900579952320
H	1.71331869628769	2.72530391063754	3.13880808179619
H	0.42815043107286	-2.06732698557951	3.16910274568202
H	-0.60773562235960	3.39047074235043	3.28083412818052
H	-3.01390130720804	2.82086227373284	3.37493515168830
H	-4.78687133663857	1.17740336357741	3.36489093307950
H	-5.55491234276637	-1.17941671165581	3.28176297717514
H	-3.87483004626292	-3.02210394876701	3.19780473916439
H	-1.48262971907930	-2.52143024338619	3.19105229068630
C	4.31191287054631	-1.40341298780032	-0.08271432681248
C	4.70126243306828	-0.05956089835266	-0.10532666510796
C	3.74714402711437	0.94209142218305	-0.04433887270052
C	2.97012196319367	-1.73826912688545	0.00025719612502
C	1.97153773793414	-0.74351755045695	0.03237446956677
C	2.37081763599032	0.63550157965620	0.00883131336749
C	1.37975521957691	1.62928649541693	0.07058641606095
C	0.60152461114496	-1.05111899702005	0.12195310166942
C	-0.39272285547364	-0.05738550937072	0.05596664860334
C	0.00696915067666	1.31958823520029	0.02741421203578
C	-0.99032862190877	2.31527168892695	-0.01323128267193
C	-2.33271738947531	1.98095155462920	-0.04466157655147
C	-1.76978695578026	-0.36383668134228	0.05121675209130
C	-2.72407613757730	0.63628610851022	-0.00967379286460
H	-3.78204901621686	0.37591334946233	-0.01211766386727
H	-2.07490036571195	-1.41033159515567	0.09808807267191
H	5.06684966627378	-2.18839844306534	-0.11680673982219
H	5.75855048292313	0.19890718467081	-0.15639289469406
H	4.04820451665361	1.99103764457755	-0.05317977547736
H	2.66500586449327	-2.78576745584636	0.02848367034943
H	1.68316827535885	2.67899634192307	0.05835132034558
H	0.29700384021441	-2.10019884981973	0.14886354344444
H	-0.68191019620606	3.36214695436305	-0.02677077956382
H	-3.08820085661396	2.76541108726052	-0.08161534079627

Table 43: Minimum-energy S1 geometry for the dibenzanth excimer

C	5.02224990332702	-1.75804962011260	3.51998023642613
C	4.96028173227057	-0.38568722282851	3.47596017992852
C	2.60657572663805	-1.88040645533392	3.42853611142419
C	3.82957490237628	-2.50996863198536	3.49462375095113
C	2.50346371367434	-0.47092696437948	3.37530968936361
C	3.71913246483585	0.28891263348871	3.40120899044558
C	3.66239630545035	1.70458140478326	3.34930913958218
C	2.45924864521144	2.35872931865246	3.27119892253597
C	1.23736090743034	0.22019312769536	3.31042759631383
C	1.23018901054706	1.64563882908760	3.25821931713618
C	-0.00329426201434	2.31822573038784	3.17536588734996
C	0.00063938492171	-0.45197980795039	3.28464510001136
C	-1.23797981710585	0.21668237083900	3.31061226438199
C	-1.23486123868555	1.64213757561386	3.25828908360668
C	-2.46594480629279	2.35172149599513	3.27103744156837
C	-3.66724015922718	1.69415957083346	3.34907264670723
C	-2.50211389372268	-0.47803208990759	3.37554266149704
C	-3.71994234697125	0.27834660160581	3.40123409291477
C	-4.95918023173890	-0.39978289921469	3.47577687804042
C	-5.01725511322252	-1.77231363754237	3.51991549423519
C	-3.82243332400024	-2.52082991118926	3.49479767229649
C	-2.60122092478486	-1.88779145402342	3.42880884474295
H	5.98487441443826	-2.26513320345186	3.57388385294454
H	5.87271824389178	0.21270232567276	3.49204967552945
H	1.70346115351266	-2.48830047168679	3.40951755543877
H	3.87601913163018	-3.59810935998326	3.52942828955148
H	4.59878340319203	2.26390623418510	3.36533410693909
H	2.42470016083818	3.44851461514199	3.22739679167277
H	-0.00484806708662	3.41005687545957	3.14109491417890
H	0.00218858906465	-1.53854064293718	3.31931952016042
H	-2.43449992602145	3.44158711804438	3.22689003491854
H	-4.60521383444044	2.25082409959875	3.36492237761140
H	-5.87332251365098	0.19600791395139	3.49154357492259
H	-5.97844202486131	-2.28213273462584	3.57366259254464
H	-3.86578122162456	-3.60909767637231	3.52962663520281
H	-1.69637684980508	-2.49311306002847	3.40998028429132
C	5.02224858579245	-1.75779811886295	-0.21988952326155
C	4.96028558364672	-0.38543857568305	-0.17576395554797
C	2.60656768320410	-1.88016016292923	-0.12851961364796
C	3.82956550309326	-2.50971247147762	-0.19470451569701
C	2.50346748935257	-0.47069208935046	-0.07506374187621
C	3.71913477403602	0.28915446152075	-0.10099881890977
C	3.66237106131955	1.70483154346151	-0.04938387470843
C	2.45920649100407	2.35898565618090	0.02842467540354
C	1.23736636138831	0.22040689192845	-0.01015440625541
C	1.23015675965606	1.64587033747390	0.04160198050251
C	-0.00333555987460	2.31843402118958	0.12433490308582
C	0.00065999493962	-0.45180188435285	0.01602691450228
C	-1.23797175703574	0.21683111083484	-0.01031093078934
C	-1.23488072358338	1.64230646180505	0.04154764372881
C	-2.46598547815590	2.35184934832209	0.02861154963762
C	-3.66726690496115	1.69423096148480	-0.04915162914925
C	-2.50208041744860	-0.47792052988519	-0.07526061571213
C	-3.71993833793999	0.27840932716707	-0.10103911289027
C	-4.95914605767447	-0.39976656918832	-0.17560049976357
C	-5.01715605539389	-1.77229658399140	-0.21981380237438
C	-3.82229685178456	-2.52075727178893	-0.19480425689173
C	-2.60111590035865	-1.88767387414144	-0.12870387396996
H	5.98486945166367	-2.26487865971032	-0.27387948110305
H	5.87271868462594	0.21295699043505	-0.19187761740531
H	1.70343268094019	-2.48803526981125	-0.10998765229631
H	3.87600009208218	-3.59784402276947	-0.22979024423771
H	4.59875025238970	2.26417077886395	-0.06546640955153
H	2.42464779703538	3.44878228525882	0.07196248635150
H	-0.00490804507212	3.41027721596185	0.15830349150536
H	0.00223484391781	-1.53840095043169	-0.01735993707423
H	-2.43457850247455	3.44172973877060	0.07246099263972
H	-4.60525537999526	2.25087144109728	-0.06507321819132
H	-5.87331242933704	0.19598718951332	-0.19141042067191
H	-5.97831759144345	-2.28215407394876	-0.27364258511425
H	-3.86558886900644	-3.60901933507373	-0.22985884679358
H	-1.69622746654197	-2.49294031535630	-0.11028526083953

Table 44: Minimum-energy S1 geometry for the benzobtri excimer

C	-5.14201652753142	0.68684643636516	3.31586074584349
C	-5.13888277374754	-0.70973580339198	3.31588918275677
C	-3.93417953725798	-1.40492610547227	3.26095187114759
C	-3.94043990445565	1.38742677774983	3.26090922803369
C	-2.70465230224511	0.70870145129726	3.24860248787524
C	-2.70144455573524	-0.72067598263094	3.24856168653095
C	-1.45970554108012	-1.38703915510507	3.21079027967937
C	-1.46590072098828	1.38061452893003	3.21092434079068
C	-0.23215245162254	0.71071290737704	3.30689664923915
C	-0.22896264441430	-0.71166009676268	3.30681042108010
C	1.02288923752536	1.43808098303190	3.38866220609466
C	2.25749038606437	0.73314660399643	3.43640207573066
C	3.45459077777299	1.47383720119654	3.49572290833289
C	3.45590385147299	2.85358456231389	3.51594885589951
C	2.24011416521294	3.54867746761281	3.48676339706579
C	1.05352964856616	2.85047643802740	3.42504261624073
C	2.26074419292915	-0.72301683183184	3.43646747561182
C	1.02930241874217	-1.43344125992703	3.38859620006400
C	1.06624171268628	-2.84568957475388	3.42489724674040
C	2.25592958085561	-3.53858900818086	3.48660634800606
C	3.46860295720579	-2.83808274945897	3.51606081598052
C	3.46113092702267	-1.45835212080394	3.49596500230734
H	-6.08611849106883	1.22942483479145	3.34689837051139
H	-6.08053888631365	-1.25654739951905	3.34694950917388
H	-3.92907125869831	-2.49614986194800	3.25559277243707
H	-3.94021148363697	2.47866205212477	3.25553676239368
H	-1.48287879806013	-2.47555188588462	3.19276262685902
H	-1.49394792305121	2.46901066712117	3.19293111065700
H	4.40913529154282	0.95304324592300	3.52398198116535
H	4.39918437002556	3.39695246355233	3.55888577783759
H	2.22999814265482	4.63801813486701	3.50902243162689
H	0.12101855092102	3.40988668672414	3.40652194443440
H	0.13624137563124	-3.40926057711059	3.40616523507160
H	2.25067813378267	-4.62796786511026	3.50867463731826
H	4.41429173149593	-3.37724203134709	3.55906148593662
H	4.41333375770725	-0.93329795037672	3.52439273111832
C	-5.14196496877930	0.68666876182053	-0.01592612448382
C	-5.13882870792809	-0.70991292512616	-0.01582981940300
C	-3.93411941161941	-1.40508754526233	0.03920094289379
C	-3.94039717553513	1.38726642896709	0.03898687599212
C	-2.70459984979716	0.70856224326896	0.05141887662184
C	-2.70139607473724	-0.72081564234504	0.05152606885626
C	-1.45963688940016	-1.38714680694259	0.08939434004631
C	-1.46586512448759	1.38049916735433	0.08914447943266
C	-0.23210553132154	0.71064655484663	-0.00683363317161
C	-0.22890794622422	-0.71172565338771	-0.00678511564993
C	1.02292343079989	1.43804825244542	-0.08867070916872
C	2.25753390677795	0.73314178365137	-0.13640894110189
C	3.45462661803314	1.47384350268066	-0.19574123849795
C	3.45592486689621	2.85359096798493	-0.21593054050268
C	2.24012417126888	3.54866396832836	-0.18668664871572
C	1.05354926440518	2.85044280968429	-0.12499577325555
C	2.26079412893855	-0.72302173889905	-0.13645120159542
C	1.02936037150601	-1.43347458683236	-0.08860679477409
C	1.06631087796518	-2.84571953383983	-0.12505858913330
C	2.25600809392024	-3.53859785567508	-0.18682785017402
C	3.46867271288917	-2.83807323281459	-0.21615837712113
C	3.46118904445974	-1.45834367074799	-0.19596603679351
H	-6.08606785360633	1.22924221952088	-0.04703349908918
H	-6.08048291005056	-1.25672894048589	-0.04686678827795
H	-3.92898887066369	-2.49631042372747	0.04464625524595
H	-3.94019181591092	2.47850232298403	0.04428736542100
H	-1.48278912238992	-2.47565522101194	0.10759299949768
H	-1.49392771192989	2.46889916261082	0.10704276564659
H	4.40917482966161	0.95305755604852	-0.22402213988300
H	4.39919709146096	3.39697432645844	-0.25884402945103
H	2.22999132476959	4.63800588000230	-0.20885492742578
H	0.12103260616849	3.40984497713805	-0.10637633517806
H	0.13631186660530	-3.40929482662423	-0.10649859552821
H	2.25077383233231	-4.62797399637107	-0.20905798225180
H	4.41436865471172	-3.37721805039202	-0.25919857700811
H	4.41338986090054	-0.93328241869659	-0.22432411961128

Table 45: Minimum-energy S1 geometry for the benzobchrys excimer

C	5.49413117379660	-1.33883551508507	3.37316176887031
C	5.86897331134953	0.01173470097175	3.35763501734938
C	4.90137435134908	1.00165780598100	3.29556767486660
C	4.15335567691061	-1.69087897891479	3.33410565607465
C	3.14320810691221	-0.70675179824280	3.29865667044062
C	3.52737166862145	0.67430427981801	3.27550889527537
C	2.51137030848968	1.64539634486587	3.20881110166075
C	1.76955391696408	-1.03819422303020	3.26802647989772
C	0.75718766952908	-0.07205103221392	3.30641649782425
C	1.14946916997944	1.30837006695751	3.27053732524501
C	0.14517471718508	2.30518556645861	3.27040651157867
C	-1.19106241087457	1.98271216663672	3.33497589161428
C	-0.64951818230508	-0.39992055743802	3.35592360566872
C	-1.62680169448940	0.63978934248178	3.38084928469248
C	-2.41401189675019	-2.07547539126812	3.44573722442447
C	-1.09151454982849	-1.75232553560494	3.39755062635440
C	-3.42319340716767	-1.06756274827699	3.47479590638159
C	-3.03622388422244	0.30087540386134	3.44967725483491
C	-4.05823428464483	1.27356530764194	3.48778546675244
C	-5.39101185947684	0.91594115851767	3.54175117829043
C	-5.76545258196171	-0.43650760046034	3.55856389833655
C	-4.78998859924649	-1.41016695167212	3.52694079657779
H	6.25876053468038	-2.11398615973626	3.41001046998132
H	6.92395386205970	0.28256520494489	3.38134681216956
H	5.18877888113798	2.05410637130784	3.27538384056085
H	3.85983822895774	-2.74193508426593	3.34206427339802
H	2.78892512162374	2.70178664294678	3.18318844797134
H	1.51778192141884	-2.09853001210831	3.27792875612824
H	0.45323573176573	3.35127244324748	3.23232306380502
H	-1.92322945342249	2.78750413438974	3.33921912899464
H	-2.72605995185588	-3.12073945666621	3.47039424069612
H	-0.35610418568078	-2.55435932305032	3.38111416751280
H	-3.80163039680154	2.33124881192240	3.47473908119633
H	-6.15636309797602	1.69117291678455	3.56796507321980
H	-6.81872375144219	-0.71220631073210	3.59607489109533
H	-5.06009970369220	-2.46740335266581	3.53932884442434
C	5.49430037447686	-1.33841001240551	-0.07362813237184
C	5.86902130422792	0.01218849529448	-0.05758627933210
C	4.90133788370502	1.00200817592548	0.00479917402291
C	4.15355323029138	-1.69057976055728	-0.03479020023100
C	3.14332237644774	-0.70654910163956	0.00100962702897
C	3.52736400772789	0.67452985801970	0.02467511197070
C	2.51125486134092	1.64549928761023	0.09174333051664
C	1.76970910707875	-1.03813654080886	0.03141920536496
C	0.75724988731030	-0.07208894696130	-0.00650979549099
C	1.14938477874676	1.30836528753394	0.02971593349769
C	0.14498081130971	2.30507230230045	0.02993993443603
C	-1.19121545054056	1.98246261438748	-0.03486047180645
C	-0.64942153273407	-0.40011073292420	-0.05595916336650
C	-1.62681070580319	0.63949684842064	-0.08087835574340
C	-2.41374379889605	-2.07586206772891	-0.14538570705114
C	-1.09127659954719	-1.75256767873987	-0.09736119457044
C	-3.42302297674402	-1.06805614273589	-0.17464505220892
C	-3.03619333685773	0.30042616586079	-0.14977475125623
C	-4.05829690008180	1.27300588219047	-0.18816752886789
C	-5.39103702773639	0.91523594663785	-0.24208601493184
C	-5.76534423243133	-0.43725405661672	-0.25854474199948
C	-4.78978499782454	-1.41080996576571	-0.22669894334180
H	6.25899991238919	-2.11348025457782	-0.11071479349349
H	6.92398020428962	0.28311706573689	-0.08113854327373
H	5.18865604008443	2.05447209777701	0.02538231891558
H	3.86012263997938	-2.74165743500695	-0.04315334797102
H	2.78870764321711	2.70190688189856	0.11772718365012
H	1.51805205403876	-2.09849476537213	0.02102174395613
H	0.45291612221513	3.35118777049207	0.06822517535443
H	-1.92347071149143	2.78717512817350	-0.03900329304935
H	-2.72569125646455	-3.12116282793687	-0.16975542862032
H	-0.35579251790459	-2.55452891579875	-0.08069849338593
H	-3.80178778851335	2.33071612840450	-0.17543896728964
H	-6.15646501853692	1.69038386715115	-0.26853063145859
H	-6.81858854340393	-0.71306591871971	-0.29598285638117
H	-5.05979030425737	-2.46807631782275	-0.23884287538602

Table 46: Minimum-energy S1 geometry for the dbphen excimer

C	-3.50919938782388	-2.19603773723140	3.42191369685571
C	-2.21199447330160	-2.23986856701520	2.87864164084895
C	-1.34452818036459	-1.18422351612291	3.05851170857675
C	-3.92724801103089	-1.05972188716423	4.07918526352781
C	-3.06616294454403	0.05046392808139	4.23922609195506
C	-1.71953890548216	-0.03158096487054	3.78325025297712
C	-2.78514508337312	2.39987498508696	4.73022217920382
C	-3.55896828724766	1.28096835843829	4.76956790346313
C	-1.42957037883764	2.34737740210139	4.28203778722839
C	-0.83640965645811	1.10289405378172	3.95455099985942
C	0.57156359758260	3.52057189957047	3.60534907929089
C	-0.69157571880681	3.55145464282710	4.12192949124593
C	1.23816137224956	2.28047213640590	3.40516282863750
C	0.58154132419425	1.06495023328618	3.71481879045258
C	3.27896536691921	1.10285256139159	2.81377982681847
C	2.57829127139956	2.26525964363095	2.91398936488845
C	2.73662700075334	-0.10660450007322	3.34130622266492
C	1.40517146473234	-0.12113912103583	3.84781297233747
C	0.99570594817932	-1.25997332712294	4.57855182971950
C	1.81170685864420	-2.36329093169467	4.70940726557348
C	3.08413766664606	-2.38398754172076	4.11015874005406
C	3.53839142662012	-1.26494826403981	3.44934092380673
H	-4.18595588007873	-3.03990948741408	3.29268052083185
H	-1.89478637828738	-3.10305977079474	2.29335828554497
H	0.01961037839578	-1.25822407747270	5.06137039296003
H	-4.94507938425755	-0.98161146403632	4.46457623385128
H	-3.18133466347646	3.36646573854774	5.04523583471765
H	-4.58587867351067	1.31848244486234	5.13564091827941
H	1.11504755534651	4.44116160515749	3.38848203547272
H	-1.18019782646404	4.49665169003727	4.36275243491599
H	4.28845039748900	1.08701022022896	2.40107719254596
H	3.02125892133123	3.21417942893016	2.60901604822021
H	-0.35229936533941	-1.22881365624102	2.61240346117268
H	1.46943695467093	-3.21930984956843	5.29029792070140
H	3.71648189373461	-3.26697589819915	4.19735317418450
H	4.54053507766359	-1.24050041248792	3.01905914842318
C	-2.91415536132307	-3.08151007917337	-1.12565958554428
C	-1.60188150691161	-2.97816039743257	-1.60937096358965
C	-0.84596943330132	-1.84209725204568	-1.36696326358618
C	-3.47166920570997	-2.01296404561819	-0.43962617243900
C	-2.74008753546812	-0.83509934623762	-0.20639266877483
C	-1.36500294243770	-0.75500904241151	-0.62533355567276
C	-2.68320379459337	1.50402719297324	0.46060860100890
C	-3.34912209669106	0.29824227745118	0.39695248968515
C	-1.34761731551846	1.63135318202289	0.01995380756804
C	-0.61227199061991	0.43829232113652	-0.35046714293057
C	0.54907892289156	3.01461835267658	-0.61921029957838
C	-0.74224712332432	2.89976702417032	-0.12113245436888
C	1.34601446302877	1.86636995990954	-0.81674342961985
C	0.80698440205404	0.55750586300787	-0.50709535053071
C	3.50087934090521	0.86250062296855	-1.35108399660152
C	2.67560097053645	1.96564934663410	-1.28893247149792
C	3.07356387085603	-0.39447992518888	-0.83785635675817
C	1.72785268311961	-0.52757920376643	-0.34859537671575
C	1.38972885977792	-1.72261911824334	0.32355491240080
C	2.28610741597696	-2.77438144833052	0.42256077957926
C	3.56658114455204	-2.67706424568527	-0.14506509376288
C	3.95196721941091	-1.49064089310114	-0.75502403516279
H	-3.49748021472082	-3.98280865424414	-1.30857562424787
H	-1.16948996982089	-3.79419792188342	-2.18767508181298
H	0.41088171297913	-1.80722099363061	0.79500835704913
H	-4.50286554485248	-2.05836328777793	-0.08578149830584
H	-3.18521485320318	2.39139066813707	0.84887320259266
H	-4.37706316172861	0.21332881616413	0.75138678715117
H	0.98654795830026	3.99322224020820	-0.81947908506100
H	-1.32996468175019	3.78500389712225	0.11944037348047
H	4.51776006551436	0.94960692467670	-1.73610774218251
H	3.03684451921007	2.94559368398043	-1.60531496053650
H	0.16170778911959	-1.77437310774754	-1.77267259663927
H	1.99395998536083	-3.67755315949656	0.95760670699707
H	4.26054994783043	-3.51399342669381	-0.08098098722407
H	4.95754918268338	-1.37908882259104	-1.16405868617648

Table 47: Minimum-energy S1 geometry for the benzoanaph excimer

C	5.73143414412983	-1.25001906123887	3.41183685553487
C	5.97852303604089	0.13613417994807	3.40613776644717
C	4.92731657207636	1.02940621666596	3.34810541173682
C	4.43606209498333	-1.72570039646975	3.36093157283994
C	3.33385771475180	-0.83943105951537	3.31664968215513
C	3.58641110930324	0.57786467967196	3.30954009580071
C	2.49452353043649	1.46218845826240	3.24691006056314
C	2.00301554186950	-1.29369206499517	3.26374681942577
C	0.91225870500544	-0.41285581717751	3.28362504174167
C	1.16651643846688	1.00938735453695	3.27426024655967
C	0.06448456412467	1.87986767478636	3.26743908927705
C	-0.42156196917268	-0.86549879960748	3.28993702845393
C	-1.51472668114218	0.00554738535705	3.35327636271464
C	-1.25657749809087	1.41711944711076	3.33713511406450
C	-2.35096510709602	2.33275292665541	3.37793695361908
C	-3.63957528940756	1.89556278466013	3.43776598754399
C	-2.88833083628786	-0.45645580134080	3.42145710484286
C	-3.94570359683669	0.50023610662801	3.46218891225215
C	-5.28329921931573	0.05649175157459	3.52633529904187
C	-5.58758127230267	-1.28769424260006	3.55291490648086
C	-4.54935350089669	-2.23404857918132	3.51909032136083
C	-3.23267632474929	-1.82463065247960	3.45545644639656
H	6.56680815056447	-1.94818744060299	3.45012181469563
H	7.00374913838506	0.50293717919806	3.43958732475573
H	5.11568511268790	2.10409792971457	3.33704779286514
H	4.24173006232773	-2.79938529596010	3.35956520372116
H	2.68622935667045	2.53767219676238	3.23373645001545
H	1.81363333346246	-2.36978020010566	3.26200378884977
H	0.24260312806448	2.95760851370532	3.25181371027789
H	-0.58304144545949	-1.94366874261565	3.28730160215990
H	-2.12768773632120	3.40059173314193	3.35644089505024
H	-4.46719850877861	2.60569725914955	3.46642336058259
H	-6.07688231194712	0.80504213860147	3.55058707016776
H	-6.62504413113115	-1.61645755675653	3.60004223552958
H	-4.78419805679381	-3.29779524767082	3.54092773741809
H	-2.44789162874364	-2.57895311328582	3.42980956690689
C	5.73147996123589	-1.24983546101768	-0.11199635669386
C	5.97857507739660	0.13631490401792	-0.10604324560626
C	4.92737480344609	1.02959331412467	-0.04788616159842
C	4.43610478624440	-1.72550823282174	-0.06124018808860
C	3.33391982547808	-0.83922786330419	-0.01675516602593
C	3.58645533704205	0.57807023310699	-0.00951213268269
C	2.49453293510311	1.46235098376935	0.05339683941518
C	2.00309858429120	-1.29354599993738	0.03586401678021
C	0.91233417206128	-0.41273000307564	0.01630268617409
C	1.16652856993790	1.00952464861226	0.02575971139136
C	0.06440745081536	1.87989186623153	0.03282982913029
C	-0.42143596045272	-0.86550429552360	0.00971467363161
C	-1.51466976405222	0.00545425230500	-0.05340087804576
C	-1.25662059750741	1.41704327851133	-0.03709357652632
C	-2.35108083609367	2.33258427367057	-0.07802657672888
C	-3.63965287966876	1.89527859376059	-0.13793726475839
C	-2.88823807199937	-0.45667402236486	-0.12139143007621
C	-3.94568698166086	0.49992742765873	-0.16224711909664
C	-5.28324697586482	0.05606369270194	-0.22638751527425
C	-5.58741310505449	-1.28815381172313	-0.25281101014215
C	-4.54911174080479	-2.23441923342095	-0.21878170205924
C	-3.23246830142977	-1.82488716199657	-0.15516766188122
H	6.56684676558629	-1.94800909860893	-0.15035842352813
H	7.00380688870527	0.50310925293178	-0.13940070247941
H	5.11577742246792	2.10427698405883	-0.03667778149300
H	4.24174412521751	-2.79918852696518	-0.06003654900788
H	2.68622443958934	2.53783504642341	0.06676847315298
H	1.81373638170578	-2.36963689900843	0.03739652563308
H	0.24240768655700	2.95765010374013	0.04862613208767
H	-0.58279450958374	-1.94369132635974	0.01216639537679
H	-2.12790880048749	3.40044461855338	-0.05658267941409
H	-4.46732723877525	2.60534857610341	-0.16670781571528
H	-6.07689371499520	0.80454085481545	-0.25077803103082
H	-6.62484553342724	-1.61701400625629	-0.29994468324091
H	-4.78387100225355	-3.29818939173996	-0.24044077067937
H	-2.44763281764743	-2.57914741550043	-0.12930849634862

Table 48: Minimum-energy S1 geometry for the penta excimer

C	6.11159245783251	-0.70932453214504	3.47467516867355
C	6.11188925609734	0.70670325237323	3.47467624855176
C	4.92784240505154	1.40064322911498	3.42837502809622
C	4.92725712285667	-1.40277416452595	3.42838246966988
C	3.68127073134741	-0.72184639553646	3.38227812583022
C	3.68157513713669	0.72022648684239	3.38225663383235
C	2.45890719080252	1.40096775502162	3.32147117304957
C	2.45832458418373	-1.40209338922183	3.32151851671466
C	1.22986302822904	-0.72645057726699	3.30120042973915
C	1.23016612650646	0.72582630421034	3.30120997951361
C	0.00027778670118	1.40234330799728	3.25865537590257
C	-0.00030484438037	-1.40247895779136	3.25867817111828
C	-1.23018800217830	-0.72595234822578	3.30130120531960
C	-1.22987955535794	0.72632271551620	3.30122312302414
C	-2.45834477302589	1.40196416388975	3.32138903100011
C	-2.45895035388959	-1.40106573841820	3.32139783693545
C	-3.68161382133932	-0.72032238565196	3.38231984446960
C	-3.68129776555789	0.72175314774806	3.38225314812175
C	-4.92727114100451	1.40270578021436	3.42833906940909
C	-6.11161781933878	0.70927518039267	3.47461326765976
C	-6.11193117630795	-0.70675225262677	3.47464502974913
C	-4.92789153179916	-1.40071477612738	3.42840676160833
H	7.05834389148138	-1.24758474585331	3.50591533192911
H	7.05886447460560	1.24456931586943	3.50592867851291
H	4.92439842581157	2.49178437082416	3.42212172564278
H	4.92336113742866	-2.49391341416948	3.42214276368671
H	2.46155988395624	2.49349850340462	3.31396983679756
H	2.46052640350609	-2.49462432979597	3.31403364704518
H	0.00049517572770	2.49480455704597	3.25001120927340
H	-0.00053012360970	-2.49493926282508	3.25006975738095
H	-2.46054187491303	2.49449430518037	3.31348648483469
H	-2.46161921197661	-2.49359444723717	3.31354469795798
H	-4.92335055267262	2.49384584245167	3.42215751082137
H	-7.05835980092371	1.24755192327562	3.50586084665045
H	-7.05891332702243	-1.24460464329217	3.50591167979308
H	-4.92446031570981	-2.49185620955496	3.42229163616882
C	6.11158802665260	-0.70936354547980	-0.17467859039384
C	6.11190389918319	0.70666377295357	-0.17475673282845
C	4.92786862500347	1.40062878725099	-0.12850902643099
C	4.92724194070306	-1.40278945520040	-0.12832928420161
C	3.68126990388815	-0.72183143918149	-0.08224066145584
C	3.68158898025556	0.72024174095193	-0.08234979550078
C	2.45893821395020	1.40102106048431	-0.02160590402341
C	2.45830890946816	-1.40203791914702	-0.02135779622986
C	1.22985947048147	-0.72636552273532	-0.00116482673354
C	1.23018529767171	0.72591064839727	-0.00124611932121
C	0.00031009449708	1.40246691390256	0.04135249865581
C	-0.00032268728765	-1.40234503914540	0.04150499666660
C	-1.23018910408155	-0.72579837546535	-0.00121849991396
C	-1.22986643621551	0.72647639345090	-0.00126980162575
C	-2.45833163846928	1.40212970485881	-0.02141437571668
C	-2.45894617447842	-1.40090448589997	-0.02138966484904
C	-3.68160233454868	-0.72015919927766	-0.08228748516417
C	-3.68129027147405	0.72191645879012	-0.08230138443559
C	-4.92727189637086	1.40285334816837	-0.12837657042963
C	-6.11161351129816	0.70940890879278	-0.17464695776641
C	-6.11191672833035	-0.70661857169605	-0.17466829147212
C	-4.92787162756997	-1.40056584399129	-0.12840190576590
H	7.05833053816533	-1.24764109091445	-0.20590030577396
H	7.05888851757878	1.24451168216031	-0.20603051650997
H	4.92444433205230	2.49176983002831	-0.12233011242551
H	4.92332542725241	-2.49392872081420	-0.12201247019578
H	2.46161475785199	2.49355120710000	-0.01416705983660
H	2.46049020893188	-2.49456905954008	-0.01374428708417
H	0.00055612900444	2.49492752897230	0.04996188316350
H	-0.00057600256410	-2.49480548896436	0.05024666038370
H	-2.46052389580264	2.49465918020290	-0.01355454766955
H	-2.46162027760059	-2.49343337238766	-0.01348035580300
H	-4.92336542547690	2.49399306066266	-0.12222451569793
H	-7.05836137772826	1.24767410792101	-0.20590494878977
H	-7.05889236099051	-1.24448194055376	-0.20595131010068
H	-4.92442775055902	-2.49170783576173	-0.12226537920766

Table 49: Minimum-energy S1 geometry for the bgchrys excimer

C	-0.06622810019074	-3.99554959998550	3.99910328723463
C	0.56646280207695	-2.77207478940246	3.90790334170983
C	-2.15761434019907	-2.93682003462291	3.47040712310213
C	-1.43623256463982	-4.09009456266160	3.73632944073207
C	-1.54490821821119	-1.67881084443374	3.39267179270185
C	-0.13008631118271	-1.59465977960339	3.54362506417296
C	-0.24804888474144	0.86925989441064	3.53874374109130
C	0.53381967052664	-0.32565994941667	3.42235565290595
C	1.80029415572998	2.17028425129272	3.76828868560572
C	0.41670375689308	2.08626724920297	3.74827390053614
C	2.60538106319679	1.02836790929843	3.52726880683758
C	1.96359607775681	-0.22239704499513	3.27877625233899
C	2.77176739771237	-1.28479721502106	2.83052114662354
C	4.16193471886729	-1.18286795290833	2.76926027999670
C	4.78967199560278	0.00836772849203	3.12494878895404
C	4.01182730900554	1.11278571204813	3.46529468246770
C	-2.33309602289936	-0.45458799034930	3.24146304584373
C	-1.69871201971640	0.80156278761604	3.41393210218023
C	-2.50168164859699	1.96133804775981	3.39463949809034
C	-3.86477027814692	1.89853555551312	3.18024126284578
C	-4.47934882978816	0.66251512209399	2.96287422703757
C	-3.71654671024903	-0.49039276342732	2.99532312742796
H	0.50102860087801	-4.87715789662405	4.29606460344536
H	1.61814649563066	-2.69860478246149	4.18284966521114
H	-3.23581334739044	-3.01508923923508	3.34898803414544
H	-1.94656690963250	-5.05072219891810	3.79453065292679
H	2.28995020158621	3.12615336926131	3.96005127554683
H	-0.15924477392232	2.99648005524039	3.89713831921479
H	2.27459097792565	-2.19413076982343	2.49167297060582
H	4.74863701181080	-2.03606193237232	2.43153505293747
H	5.87542266897381	0.09017951231323	3.09464006014734
H	4.48097298638786	2.07047952218005	3.69742664689549
H	-2.04285572896797	2.93876262824965	3.52563512820375
H	-4.45309451148907	2.81526094622324	3.16170513374958
H	-5.54804109940830	0.60524274752908	2.76085026345476
H	-4.20626168973675	-1.44526401383352	2.81458312458455
C	-0.48944157395256	-3.24241755460131	0.36465927629318
C	0.29423126227504	-2.10601573780949	0.33748837383372
C	-2.42767858607559	-1.89696432285909	-0.11083906364898
C	-1.86168190032432	-3.14459419858239	0.11719887684608
C	-1.65952342474457	-0.72623659042348	-0.13360227028513
C	-0.24835943636760	-0.82620435008417	0.05448631985377
C	-0.06588084421475	1.63134502676231	0.19670087801896
C	0.56862454040556	0.35429263722852	0.05249090897188
C	2.09167727809900	2.64196186920717	0.68830668243428
C	0.71247408781814	2.73546544729665	0.56926902189515
C	2.76997377836410	1.46644974651683	0.27942937049695
C	2.00754990201686	0.31760501532553	-0.09825677603311
C	2.69938918489352	-0.75858172786535	-0.68131340385170
C	4.08957238436533	-0.75936003394168	-0.79968857385148
C	4.83427621250104	0.32539774151621	-0.34232766975108
C	4.17637799290533	1.42738806455411	0.19180804903549
C	-2.26886832915528	0.59223616941641	-0.31654476346775
C	-1.49171572938562	1.75388079645893	-0.08366078498868
C	-2.10839169545144	3.01407370808022	-0.20601160698345
C	-3.44096604275522	3.13746942340342	-0.55457873293519
C	-4.20061143448642	1.99233223552791	-0.80289504423113
C	-3.61555881846578	0.74279073122907	-0.68666737708147
H	-0.04159060490000	-4.20370132227213	0.61643357733668
H	1.35203158201419	-2.16222766223396	0.59948394551901
H	-3.50628566267607	-1.83097674941417	-0.24375005422137
H	-2.49122170023084	-4.03310695457791	0.13490700516018
H	2.67973663557731	3.51170076231976	0.98153424944155
H	0.22806215366214	3.68578069594927	0.78529399595984
H	2.13666842459480	-1.58998933673762	-1.10611090068921
H	4.58637498121862	-1.61063209922956	-1.26375045516829
H	5.92153348926537	0.31700464045988	-0.41415711943642
H	4.73843300069098	2.30362431779079	0.51770228717897
H	-1.51968591857230	3.91694330546148	-0.05561197073753
H	-3.88837328123985	4.12621733621170	-0.65148395723792
H	-5.24555233343039	2.07846359022192	-1.09922439861341
H	-4.21605447569075	-0.13923029893519	-0.90191071656830

Table 50: Minimum-energy S1 geometry for the anth-pyr exciplex

C	-0.60884373436720	-0.28915880648384	3.45798386040159
C	-0.09682564480872	-1.58286914802462	3.30158129634871
C	1.30862053435203	-1.75347894553033	3.06522075103046
C	2.13115049800294	-0.61202963469683	2.99927034736375
C	2.44365663629136	1.82889401768515	3.09876097207766
C	1.90931803297704	3.09472101021591	3.26982651971792
C	0.53966320204569	3.25987692012261	3.49235521320060
C	-0.29419428286414	2.15179687957874	3.56058744827852
C	0.21646069950522	0.85122384732316	3.41017549664625
C	1.62226653754390	0.68031741500046	3.17490948845351
H	-1.67772364547304	-0.15954372230232	3.63996579191695
H	3.20144077603917	-0.74209853701389	2.82657308806314
H	3.51170341027779	1.69837657453565	2.92175221878230
H	2.55725778259724	3.96890500715843	3.20990271791982
H	0.12633649729894	4.26024722156506	3.61749844141371
H	-1.36502543779255	2.27657394809372	3.72886201237973
C	0.61863929211225	0.42825016789894	0.05932893907964
C	0.01492209718864	-0.85738678333752	0.06832494561601
C	-0.17810974602025	1.59770178477753	0.24295522802372
C	2.02444593583720	0.55113714952458	-0.11538034467231
C	0.80464754269531	-2.02362128047507	-0.15807849449685
C	-1.37831313863470	-0.98569471145237	0.32356538608262
C	0.43894767351337	2.87016250852269	0.16468093217435
C	2.59764841069795	1.83002559152784	-0.12246537014576
C	0.16761817158651	-3.28772476133725	-0.20462521157962
C	-1.95236896183625	-2.26410368011278	0.32690266667191
C	-1.55788357978211	1.43907324619116	0.51654677605077
C	2.79672558776640	-0.63882307792402	-0.25156235409371
C	2.20441830046982	-1.87343835212773	-0.30715274473603
C	-2.12959408891842	0.19546217834872	0.59050232301228
C	1.79865196683596	2.97427006076221	-0.02359228000330
C	-1.18496934841634	-3.39481272246627	0.02622111452675
H	-2.16001583196813	2.33348934716064	0.68593313112041
H	3.87859125963154	-0.54232633038126	-0.36224924087868
H	2.81074311901716	-2.76968359954806	-0.45042801562987
H	-3.19474994800711	0.09169784569555	0.80637932458625
H	-0.17937688678765	3.76222230780695	0.26990518829077
H	3.67636807092143	1.92458588150408	-0.25773328350548
H	0.76953974408587	-4.17325558880268	-0.41148983524893
H	-3.02176480588971	-2.36292158802750	0.52011592428315
H	2.26586729407964	3.95845153474565	-0.06901567178704
H	-1.66254287529347	-4.37477828827863	0.00304378502870
C	-0.92408903352012	-2.72863388163105	3.33562213204736
C	1.81403425789379	-3.05182587639825	2.88163544333813
C	-0.38891392104416	-3.99563062320605	3.17128832325251
H	-1.99188875560052	-2.59861639987632	3.51509763306397
C	0.97832781286662	-4.15945563662213	2.93524621295560
H	2.88099642221677	-3.17441378254759	2.68894459140671
H	1.39047489338420	-5.15862754780019	2.79767781044169
H	-1.04129679270715	-4.86786013934086	3.20598937172965

Table 51: Minimum-energy S1 geometry for the fluor-benz exciplex

H	-2.97156367189179	-1.27766072301280	3.86185068218536
H	-0.54383489229028	-1.35863528303045	3.35881803227492
C	-0.38189630230199	0.76831741761989	3.06639475951050
C	-1.05171563762810	1.98753156343318	3.05680766415103
C	-2.41209240207695	2.03200529155919	3.33265591828716
C	-3.10092289837695	0.85926556011594	3.62461776291259
C	-2.42923925576184	-0.35830921948925	3.64182638598232
C	-1.06893105162040	-0.40395154529188	3.36568687610292
H	0.68172771556234	0.73033678396402	2.82846446586561
H	-0.51387000541845	2.90204922209756	2.80876317619422
H	-2.94216298991007	2.98423295600406	3.31212407029509
H	-4.16958189165169	0.89424232406222	3.83762877080503
C	1.39432537593063	0.86945057552951	-0.15837936714426
C	1.33455848757693	-0.59211748498366	0.05887798656829
C	2.53700140351540	-1.32955501056959	0.13314576592044
C	3.73069164997022	-0.67120481360146	0.01574938888493
C	3.78870653652287	0.74204422903403	-0.19033789372212
C	2.65301233437102	1.49987398922644	-0.27782471780806
C	-0.01252790638453	-0.97815428147469	0.15430754167230
C	-2.84085446956123	-0.93631363722326	0.22198272181536
C	-2.10655920204704	-2.12605742331271	0.36302778321314
C	-0.71922423850666	-2.18471041515872	0.33906066577439
C	-0.77206267984823	0.23431294956752	0.01061467556026
C	0.08437973288491	1.37428980273027	-0.18347261084937
C	-0.52083028905293	2.63749977663246	-0.34762563003862
C	-1.90750857984284	2.69999056241584	-0.31751124905200
C	-2.73642525576951	1.57966165732793	-0.13293814666808
C	-2.18780918172782	0.29584774246255	0.03510206342038
H	2.50769086019759	-2.40838689308017	0.28771610903699
H	4.66549237138829	-1.22825576745098	0.07613116493286
H	4.76579654455851	1.21653346366601	-0.27918274117471
H	2.71204519631929	2.57676560140794	-0.43730499724927
H	-3.93000365031770	-0.96947024421838	0.25597318351289
H	-2.66296734846550	-3.05406237250277	0.50233618877525
H	-0.20379819216804	-3.13763027289962	0.45253287945781
H	0.07023822094727	3.53883220912671	-0.50498496831116
H	-2.38641487619485	3.67151300922929	-0.44741790711370
H	-3.81887956092988	1.70922870008786	-0.12144645398069

Table 52: Minimum-energy S1 geometry for the anth-coro exciplex

C	-0.29549294044831	3.39410905641369	3.14553336524868
C	-0.97645238627696	4.59525663959297	2.99303387415871
C	-2.36637302013684	4.60958739777702	2.83453828457254
C	-3.07731254300308	3.42012338835185	2.83160422140650
C	-3.14536110563272	-1.49579513447416	3.18308016520711
C	-2.46487858206885	-2.69849350316508	3.29451794667922
C	-1.06668303021422	-2.71495419712389	3.38384973686934
C	-0.35572121928175	-1.53028201945140	3.37286290704133
C	-0.32590819726315	0.93216802159809	3.25815173535095
C	-3.11282094672776	0.96380534198974	3.01217992064992
C	-0.99108585281557	2.16899796960828	3.15101854593892
C	-2.42121063985665	2.18044661439604	3.00849751959836
C	-2.45139871129826	-0.27101514576400	3.16632019132924
C	-1.01983258923301	-0.28429599268430	3.27539511924180
H	0.78991673623304	3.38183077773279	3.25140987663759
H	-0.42188809869692	5.53350650574736	2.98980371361178
H	-2.88779634359980	5.55783946888440	2.70691052471630
H	-4.16108849258653	3.42162391601548	2.70885653386189
H	-4.23275581904974	-1.48278498029560	3.10012453915381
H	-3.01938169651973	-3.63668607346482	3.30210307860282
H	-0.53807370938932	-3.66501620489302	3.44826786297155
H	0.73444613803340	-1.53856400994886	3.42293032185772
H	0.76405725783926	0.92347658559311	3.33577017421372
H	-4.20054743211460	0.97095619554427	2.91590204922512
C	-3.08481898529837	-2.26347462796953	-0.00864409314993
C	-3.79095108019317	-1.08873992714916	-0.06475705474893
C	-3.12967559019116	0.16709142950565	-0.06922838397282
C	-1.70507734605788	0.18217366310282	-0.00627018662299
C	-3.15906910351879	2.59630232282214	-0.19657610726803
C	-3.82813504137509	1.39732725705551	-0.15198078546878
C	-1.74202299329929	2.64440967666674	-0.12405288155544
C	-1.01529734910170	1.42268154247560	-0.00243596111534
C	0.34545453748753	3.87772650195503	-0.00337324758800
C	-1.02219767813850	3.86280373446270	-0.15418873093663
C	1.08779048264598	2.68669536626933	0.15726013026735
C	0.40188282421511	1.44587432018816	0.12956689207636
C	3.20082694211407	1.51590526462715	0.43098389772371
C	2.50404752129533	2.68272072986814	0.31993812421991
C	2.53897185667188	0.25175441393396	0.37813251923013
C	1.12798862875246	0.22817030036230	0.23083588190347
C	2.57296606982414	-2.17625836185094	0.40114510470434
C	3.23583309597049	-0.97336948423239	0.46203747028500
C	1.16557863950798	-2.22990949762065	0.26574983346578
C	0.43936292281124	-1.01516174072844	0.18230903313651
C	-0.97949466382072	-1.03706330776798	0.07433820070205
C	-1.66835626050470	-2.27851797676246	0.05742180078970
C	-0.91886044729674	-3.47640763754540	0.13299841696891
C	0.44750967699535	-3.45817155298835	0.23141706740935
H	-3.61216732345014	-3.21966738727036	-0.01384102742755
H	-4.88097987526345	-1.10394596097929	-0.11641379062434
H	-3.70577261277385	3.53531628107625	-0.29004927154397
H	-4.91790430057214	1.36982392295667	-0.20788854372122
H	0.88383273799337	4.82787434925536	-0.00510685009051
H	-1.57559017626465	4.79538302690452	-0.26724471390445
H	4.28563682032168	1.52832374089140	0.54930662042491
H	3.02556572939144	3.64150858735770	0.34598224736271
H	3.12715094846955	-3.11427300640336	0.46243382406664
H	4.32163702413200	-0.94926001335436	0.57053095681736
H	-1.45575711452664	-4.42711138616610	0.11826614758698
H	1.00898370715547	-4.39198618092831	0.28960725245282

Table 53: Minimum-energy S1 geometry for the perl excimer

C	0.72980319418909	-1.23923939632727	3.35195367790290
C	1.47580705697416	-2.42763654241789	3.33791835713384
C	2.86616647761539	-2.41385090418057	3.33215893048794
C	3.55252603926962	-1.21631011250103	3.31394914030110
C	-0.72977949105440	1.23923585372322	3.35186290337655
C	-1.47577974310451	2.42764320920207	3.33800031749583
C	-2.86613953953895	2.41385290871279	3.33219076969137
C	-3.55249902547094	1.21631356381811	3.31388507326784
C	-0.72125191806585	-1.24422255235750	3.35200003028244
C	-1.42501021945295	-0.00489747620371	3.35575356566292
C	-2.85405665910115	-0.00979429536043	3.33481237345424
C	-3.54410875358578	-1.24065354152303	3.31389943354553
C	-2.84951802918194	-2.43344317682105	3.33217408722552
C	-1.45909565596990	-2.43770164871460	3.33795671950367
C	1.42502739574993	0.00489396513703	3.35564282127783
C	2.85407677049298	0.00979668424146	3.33480363418974
C	3.54413271143005	1.24065744999982	3.31389770839112
C	2.84953763021814	2.43344790071740	3.33211694490590
C	1.45911623418091	2.43769777246080	3.33789551654385
C	0.72127598202162	1.24422052433492	3.35201577340932
H	0.96532151367699	-3.38818850942728	3.34279931038708
H	3.41342774356058	-3.35653630848809	3.32183113452328
H	4.64325861250162	-1.19837220380108	3.30224344027350
H	-0.96530061549909	3.38819561253719	3.34325605077332
H	-3.41340635988884	3.35653652751883	3.32193750462970
H	-4.64323076449623	1.19837939031402	3.30206471374365
H	-4.63493971240882	-1.23023717197436	3.30249564912311
H	-3.39029003883987	-3.37986909826479	3.32193606790019
H	-0.94205261337349	-3.39473885744775	3.34305374452523
H	4.63496354798473	1.23024247128063	3.30256785943872
H	3.39029979767462	3.37987822623747	3.32181954937863
H	0.94206374894604	3.39473014486962	3.34284708523420
C	0.72980467760009	-1.23923277769455	-0.05207297949614
C	1.47582464002159	-2.42761805917116	-0.03813469802475
C	2.86618369678711	-2.41380892953349	-0.03230302400828
C	3.55252328492810	-1.21625848133121	-0.01392068844862
C	-0.72981505331448	1.23922368546239	-0.05198366328391
C	-1.47583099475439	2.42761816659813	-0.03816087877934
C	-2.86618819684946	2.41380814707734	-0.03231721006283
C	-3.55252925297854	1.21625880849545	-0.01394510572619
C	-0.72124912370413	-1.24423162762031	-0.05195498317854
C	-1.42502614817055	-0.00491746048194	-0.05579279330530
C	-2.85407017481556	-0.00984058418216	-0.03486796878310
C	-3.54410439210440	-1.24070816339574	-0.01386077060897
C	-2.84949598846290	-2.43348886453595	-0.03201979415822
C	-1.45907495543425	-2.43772043125330	-0.03781003423262
C	1.42500742985805	0.00491130761376	-0.05565205069085
C	2.85405518402196	0.00984017231436	-0.03471064376460
C	3.54409118186549	1.24070947409167	-0.01378318070839
C	2.84948125644728	2.43348973153251	-0.03198561972608
C	1.45905849965225	2.43772565055695	-0.03778227428421
C	0.72123803589998	1.24423245657072	-0.05194496054141
H	0.96535734892549	-3.38817879082961	-0.04324120531505
H	3.41346279901063	-3.35648492800351	-0.02203709410005
H	4.64325473452187	-1.19830644890187	-0.00212356489888
H	-0.96536224761480	3.38817632235376	-0.04342797850258
H	-3.41346553960870	3.35648528146670	-0.02206409281486
H	-4.64325985963521	1.19830978537952	-0.00208810099986
H	-4.63493482812037	-1.23030512558017	-0.00245948290457
H	-3.39024817839544	-3.37992472925411	-0.02170263075869
H	-0.94201231539059	-3.39474864356150	-0.04272151101707
H	4.63492228531951	1.23030815550978	-0.00243349812377
H	3.39023480829971	3.37992529071988	-0.02168392598176
H	0.94199659874092	3.39475281029272	-0.04275288075055

Table 54: Minimum-energy S1 geometry for the pentaph excimer

C	5.04222680628868	-2.04067920118055	3.40185710657721
C	5.72138420181212	-0.80442847008011	3.40477825712205
C	5.00413476485099	0.37063225372000	3.38486914031897
C	3.66587828354883	-2.08645166440733	3.37863520947834
C	2.89661764321909	-0.89783706811331	3.36064024075274
C	3.58949011272013	0.35853905850532	3.36537995976234
C	2.82207384601399	1.53740617982439	3.33653840033541
C	1.48653812350857	-0.91441462436380	3.32823380778700
C	0.72462993038917	0.25369523556505	3.33375577533113
C	1.42912951915832	1.50943473129005	3.33529727663451
C	0.68626039620069	2.72749511181774	3.32316790281832
C	-0.67887844599737	2.72930557124738	3.32314504011208
C	-0.72392665627337	0.25563515687440	3.33383931464836
C	-1.42504390098597	1.51326009335168	3.33527172793715
C	-2.81790538190433	1.54502425404336	3.33655126770589
C	-1.48897816325374	-0.91041793363753	3.32819438893722
C	-2.89901319629785	-0.89002677076235	3.36043040881123
C	-3.58849459252933	0.36821676546785	3.36512564302724
C	-5.00309828491507	0.38413176735976	3.38487140397071
C	-5.72352095015793	-0.78898688778881	3.40479019671696
C	-5.04770283344222	-2.02706455150200	3.40185575890272
C	-3.67148286314075	-2.07655860853553	3.37861167795763
H	5.61473061599076	-2.96827299665118	3.40920991595572
H	6.81041964976197	-0.78385396852541	3.41330610480631
H	5.51699948575919	1.33411953883641	3.37715257177938
H	3.14518279765320	-3.04541042619964	3.36589590413424
H	3.33110818075787	2.50429038690147	3.33023643154601
H	0.99656901907090	-1.88826561546935	3.32157260088792
H	1.23895233903879	3.66863964622538	3.31591257400124
H	-1.22907013378234	3.67191475747661	3.31560393877615
H	-3.32432334494807	2.51327948503978	3.33029091473404
H	-1.00165217902635	-1.88559283006207	3.32133680270069
H	-5.51335554332196	1.34900542196134	3.37755954699038
H	-6.81249619306781	-0.76547238186607	3.41338638988736
H	-5.62270892272804	-2.95310901133271	3.40928320278955
H	-3.15338086917309	-3.03692640475260	3.36630387173807
C	5.04220103641030	-2.04071307248391	-0.10193612820075
C	5.72136508481086	-0.80446569980849	-0.10494175319549
C	5.00412094530916	0.37059748418649	-0.08500142277955
C	3.66585429020329	-2.08647860369519	-0.07859426890685
C	2.89659975693463	-0.89785976145141	-0.06056261448937
C	3.58947833372030	0.35851255140894	-0.06540660323357
C	2.82207397343982	1.53738514119063	-0.03653485415880
C	1.48652114938354	-0.91442843947582	-0.02802414431753
C	0.72461791360387	0.25369016094715	-0.03358484383248
C	1.42913220683128	1.50942374146656	-0.03520364858822
C	0.68626900334902	2.72748994373829	-0.02306706656891
C	-0.67886975474691	2.72931302215743	-0.02306157789801
C	-0.72393638410749	0.25564168045332	-0.03372240264678
C	-1.42504167524186	1.51327178293038	-0.03520341918893
C	-2.81790311523823	1.54504357325627	-0.03654616992394
C	-1.48899583054740	-0.91040521172825	-0.02805428670412
C	-2.89902755574936	-0.89000572569609	-0.06036950286608
C	-3.58850096945493	0.36824236621816	-0.06516400511576
C	-5.00310338371328	0.38415887654676	-0.08501046558910
C	-5.72352604721717	-0.78895936128429	-0.10495808173946
C	-5.04771439129978	-2.02704022869149	-0.10194189995497
C	-3.67149729871531	-2.07653668818733	-0.07858332024847
H	5.61469875999062	-2.96831034695916	-0.10931696398335
H	6.81039987015956	-0.78389618323802	-0.11356175447549
H	5.51699025744845	1.33408324164936	-0.07735107867601
H	3.14515538247234	-3.04543443683009	-0.06578356338404
H	3.33111682984940	2.50426550915875	-0.03029237887431
H	0.99654605809677	-1.88827590205936	-0.02128921734913
H	1.23896703300227	3.66863148002269	-0.01582307406040
H	-1.22905272525274	3.67192732292744	-0.01553298584109
H	-3.32431263479664	2.51330395715592	-0.03032454619319
H	-1.00167723203174	-1.88558335031928	-0.02112750596660
H	-5.51336091609577	1.34903298260188	-0.07776145510907
H	-6.81250065508482	-0.76544099076106	-0.11364076032614
H	-5.62272219110305	-2.95308318339666	-0.10939809191621
H	-3.15339538541665	-3.03690363222813	-0.06621282007010

Table 55: Minimum-energy S1 geometry for the pice excimer

C	5.03213635678597	-1.61656575022442	3.39507792740836
C	5.71650630420630	-0.39187219821999	3.39864062277471
C	4.99348302045685	0.78635214374920	3.38928677221061
C	3.65029624177154	-1.65619638858688	3.37709674768488
C	2.88101360336854	-0.46935461605469	3.36524919445126
C	3.58625342212581	0.77327171915145	3.37511533728972
C	2.83703177039258	1.98272502736567	3.35508858678419
C	1.46853526369751	1.98173772525468	3.34563292372757
C	1.43947943063836	-0.46319395105017	3.33346630836602
C	0.71898133362006	0.77460403649709	3.33816996843766
C	-0.68817709467968	-1.66222258403517	3.29951070140229
C	0.68940269371074	-1.66171650177554	3.29959730089033
C	-1.43913612537265	-0.46424336775618	3.33327236239843
C	-0.71953708034312	0.77407935413923	3.33802926219451
C	-1.46995602825096	1.98068232829202	3.34572762969101
C	-2.83844870766961	1.98067534889741	3.35515533050758
C	-2.88066073014173	-0.47144236518719	3.36499872756744
C	-3.58679312521093	0.77067370004822	3.37495469406618
C	-4.99403054999666	0.78274341457396	3.38935742027481
C	-5.71619829911820	-0.39600448337061	3.39876419419725
C	-5.03094762227880	-1.62020560061793	3.39513855522142
C	-3.64908350127102	-1.65883886171035	3.37700790146170
H	5.59484874041352	-2.55005350966558	3.39561350291871
H	6.80539036805329	-0.37223467439926	3.40171038164781
H	5.50349090038837	1.75118754332933	3.38301398044388
H	3.15495283443927	-2.62528038183735	3.36778196045620
H	3.38181123831452	2.92841417303673	3.35250355133945
H	0.95051705941736	2.93845004072617	3.33527063436341
H	-1.20403504817139	-2.62036937928957	3.28034653019245
H	1.20596812074412	-2.61947681555603	3.28018773270690
H	-0.95261567533443	2.93776212026432	3.33551172752005
H	-3.38392737042294	2.92596142352591	3.35240731027284
H	-5.50473354667505	1.74721231719987	3.38341302751786
H	-6.80509630775064	-0.37715387384818	3.40192617480117
H	-5.59298935983435	-2.55409705873203	3.39574100083413
H	-3.15302841720724	-2.62756088882861	3.36791270450739
C	5.03213367435613	-1.61655956833149	-0.09505287436443
C	5.71650014845006	-0.39186327614197	-0.09860971708464
C	4.99347257638217	0.78635909193757	-0.08923607438631
C	3.65029364964173	-1.65619314538844	-0.07707687782325
C	2.88100737620680	-0.46935525077321	-0.06522509517177
C	3.58624345671399	0.77327346534985	-0.07506310567742
C	2.83701322207328	1.98272363992674	-0.05500621313998
C	1.46851466736761	1.98172925204252	-0.04560245658941
C	1.43947352840640	-0.46320218618280	-0.03351791098029
C	0.71896791635065	0.77459202174142	-0.03819697253454
C	-0.68818261394528	-1.66223794244648	0.00036536647654
C	0.68939724348884	-1.66172809201879	0.00031514435393
C	-1.43914744852590	-0.46426529014171	-0.03338277145452
C	-0.71955503415530	0.77405828162989	-0.03813052676833
C	-1.46998024261347	1.98065672876771	-0.04579773322306
C	-2.83847389135170	1.98064284273723	-0.05519499237800
C	-2.88067646030696	-0.47147266850603	-0.06505094189958
C	-3.58681460280750	0.77063937991276	-0.07498799542560
C	-4.99405364013599	0.78270468216360	-0.08934013002645
C	-5.71621911448635	-0.39604488778148	-0.09870554488362
C	-5.03096376283516	-1.62024417639226	-0.09508223993421
C	-3.64909783420369	-1.65887096199250	-0.07700814160748
H	5.59484807472320	-2.55004609560225	-0.09559620269601
H	6.80538393664161	-0.37222412724200	-0.10168600023766
H	5.50347757409725	1.75119579359907	-0.08295313086259
H	3.15495334898272	-2.62527920006469	-0.06777882412628
H	3.38178617449769	2.92841612948406	-0.05237815573023
H	0.95049113302953	2.93843854850397	-0.03521698695428
H	-1.20403821747676	-2.62038661096839	0.01951554404631
H	1.20596385740864	-2.61948787015809	0.01972524323149
H	-0.95264399460501	2.93773827075575	-0.03556339811495
H	-3.38395611208628	2.92592663039439	-0.05240978750787
H	-5.50475928093796	1.74717198155696	-0.08338393226367
H	-6.80511726506141	-0.37719809254777	-0.10182546876437
H	-5.59300136137492	-2.55413819609872	-0.09563882709475
H	-3.15304079472394	-2.62759226702993	-0.06790095693289

Table 56: Minimum-energy S1 geometry for the benz excimer

C	-0.84933199571921	0.05410047055174	3.03190850284418
C	0.55189063235907	0.05410814287123	3.03190713410494
C	1.25247235231358	-1.15946117792513	3.04222228210479
C	0.55191724520604	-2.37298944270035	3.03189145915092
C	-0.84933185710117	-2.37299369165007	3.03189271782074
C	-1.54990043912727	-1.15947547730263	3.04222594019229
H	-1.39332949015539	0.99684120575125	3.05040523186685
H	1.09587656811894	0.99685537496736	3.05040167437389
H	2.34078156532180	-1.15942801074422	3.06764722641731
H	1.09596855697338	-3.31569990493389	3.05040098834572
H	-1.39337420705955	-3.31570987294943	3.05040522904752
H	-2.63820971294555	-1.15945256088864	3.06765374185394
C	-0.84932695193219	0.05410140626418	0.06809428456396
C	0.55189565949901	0.05410900305161	0.06808934112551
C	1.25247710711627	-1.15945971244998	0.05777038247633
C	0.55192341173244	-2.37298791140572	0.06810621021339
C	-0.84932568659326	-2.37299355056887	0.06811159749613
C	-1.54989544374467	-1.15947528303944	0.05778022320442
H	-1.39332422247748	0.99684218306174	0.04959861447053
H	1.09588209843175	0.99685600112691	0.04959243374807
H	2.34078638661023	-1.15942613819081	0.03234174392928
H	1.09597594557429	-3.31569772789879	0.04959567739805
H	-1.39336688146331	-3.31571035846225	0.04960173000051
H	-2.63820464093774	-1.15945296653580	0.03235563325075

Table 57: Minimum-energy S1 geometry for the coro-benz exciplex

C	-1.36446226389711	1.81426632164755	3.26513851869663
C	-0.66075024143349	0.61747498370400	3.18275285108960
C	0.72960660954733	0.62652600741556	3.18990669397464
C	1.41681177529372	1.83229096141069	3.28071696979922
H	1.25187057414531	3.97376590720904	3.43312322785075
H	-1.22910067091919	3.95778242413834	3.41752661383560
C	-0.67756726437626	3.01939141599316	3.35722785336775
C	0.71332063545212	3.02834096257228	3.36551980194116
H	-2.45461306604975	1.80737800105603	3.24185858989155
H	-1.19936489184101	-0.32654531799690	3.09154554978113
H	1.28134772260972	-0.31045083965116	3.10394637709880
H	2.50709029450220	1.83956400987942	3.27043171425767
C	-2.80625541653111	-2.20627447093200	0.32620614047687
C	-3.51420244227072	-1.03326516360782	0.18243662939343
C	-2.85459380633424	0.20682692522705	0.01266103697055
C	-1.42193194484440	0.22695805593340	-0.01432030035096
C	-2.88444483092944	2.62370349958234	-0.27297897795196
C	-3.55403683879571	1.42899923260919	-0.12222681164609
C	-1.47153005874913	2.67604567684447	-0.29206302229178
C	-0.73522306430877	1.45374960065430	-0.16282270194472
C	0.61946948511785	3.91083588524983	-0.43783711237244
C	-0.75733341454551	3.88789999059043	-0.43932480335647
C	1.37334013258190	2.72350742986505	-0.28861842378818
C	0.67791951021609	1.47726547139544	-0.16166785111340
C	3.49572326745038	1.54687372465895	-0.11151350220635
C	2.78710728118943	2.71836321852980	-0.26565796068459
C	2.83714654863507	0.30200907060322	0.02086623296908
C	1.40478285934427	0.27402526734673	-0.01166512242781
C	2.86856031760378	-2.11098129178843	0.33754929065003
C	3.53726937603780	-0.91485580994364	0.19620571344677
C	1.45517060449896	-2.17002464546382	0.31136927128457
C	0.71845083938822	-0.95351410121812	0.13358224387831
C	-0.69535956561782	-0.97708052697451	0.13207538143030
C	-1.39156416876180	-2.21776180581228	0.30626010466058
C	-0.63711703082703	-3.40210138782330	0.47859518604227
C	0.74023592103868	-3.37901293079051	0.48110284920544
H	-3.33321607870804	-3.15204984456272	0.46037778291995
H	-4.60493513994313	-1.04496753629316	0.20265783592977
H	-3.44208309507300	3.55576463029638	-0.37587724957204
H	-4.64478848413196	1.40966506370571	-0.10617571964280
H	1.15295989342832	4.85675078633285	-0.54236838735736
H	-1.32177715197010	4.81548447795749	-0.54560135026614
H	4.58644534188209	1.56412553715863	-0.09109399035939
H	3.31359099684937	3.66856256374280	-0.36675100923554
H	3.42640745075441	-3.03834893817754	0.47532252745109
H	4.62767014958992	-0.88980080298697	0.22176007468987
H	-1.17012037240885	-4.34453029675236	0.61240587475578
H	1.30403271611062	-4.30300739253495	0.61724335882887

Table 58: Minimum-energy S1 geometry for the naph-perl exciplex

H	1.32357629431802	-1.22708192275597	-0.33100621823942
C	0.23588653536726	1.23935634324237	-0.16868423398396
C	-0.44599642342024	2.42496823276941	-0.02556387683915
C	-1.83105889009920	2.42039182217072	0.22450933527640
C	-2.51177026446327	1.23029679724092	0.33011688214646
C	0.24417773218901	-1.23572110109466	-0.16882890270329
C	-0.43723866738838	-0.00046985446378	-0.06996014958658
C	-1.83827181763057	-0.00525042624275	0.18712938209212
C	-2.50361257536863	-1.24527253051582	0.32981714342224
C	-1.81486528637496	-2.43070408866396	0.22410023846849
C	-0.42980100567568	-2.42588924290655	-0.02590200046002
H	1.31511571488001	1.23760666287303	-0.33217750092122
H	0.09029653641660	3.37135911371534	-0.09194287163322
H	-2.36281434087721	3.36390032803507	0.34573452981380
H	-3.58061684829705	1.22110404786466	0.55127605807526
H	-3.57245497459423	-1.24307522553598	0.55114082428337
H	-2.33998129249597	-3.37789941181194	0.34555541421848
H	0.11294498103787	-3.36860686562670	-0.09211120720018
C	0.15388066816918	-1.23714897722259	3.15384630404541
C	0.88415802442601	-2.43739325694264	3.00307528766351
C	2.23306294018644	-2.42103633646740	2.68106922335621
C	2.89667326947863	-1.21903967231292	2.50240043000487
C	-1.26786381535240	1.23425402602178	3.44014992415496
C	-2.00417578132562	2.43443772817303	3.55778861806245
C	-3.37177602067046	2.41767241144933	3.78874582272740
C	-4.04927963445165	1.21559962978781	3.90175684935049
C	-1.25887000900365	-1.24249328473448	3.44026589875500
C	-1.95026941765729	-0.00661220238809	3.57320635239889
C	-3.36116119401086	-0.01164370154258	3.79869764921000
C	-4.04040911949588	-1.24385769623337	3.90141019343391
C	-3.35429825960539	-2.44099258194560	3.78809292469373
C	-1.98654032270183	-2.44793460166817	3.55759356675431
C	0.83121418283003	0.00346882150006	2.99778585625817
C	2.22026708540899	0.00848843355425	2.66351130595924
C	2.88791989309715	1.24084996655532	2.50288202048367
C	2.21570068201212	2.43801030625920	2.68186588608785
C	0.86668216078738	2.44463256055782	3.00372663640625
C	0.14496314294214	1.23917748025601	3.15405412203213
H	0.38869049819754	-3.39487714495258	3.14509174612859
H	2.77209163892055	-3.36213020952467	2.57068083479281
H	3.95840295642734	-1.20246727464169	2.25140448453942
H	-1.49991881092141	3.39202442372122	3.45259718472227
H	-3.91557206582926	3.35871967341379	3.87337874556727
H	-5.12621292528813	1.19884410192986	4.07642044980272
H	-5.11749915666354	-1.23499563794290	4.07570660996104
H	-3.89154321054902	-3.38592401339413	3.87131286130514
H	-1.47568744529235	-3.40175749588295	3.45007265386658
H	3.94980470266859	1.23195138597313	2.25215920247765
H	2.74792651331387	3.38299218277801	2.57168497206333
H	0.36428142242938	3.39854027757272	3.14548553670514

Table 59: Minimum-energy S1 geometry for the anth excimer with C2 linker in the α position.

C	1.38770028544281	2.51657623369352	-0.10490868685596
C	0.66483360544544	3.68526325884019	0.06822559107804
C	-0.71753203568408	3.65025673945549	0.30879448542048
C	-1.36749552477065	2.42377487468746	0.25756388293558
C	-1.24143706868322	-2.50074674974770	0.08076885391465
C	-0.51924181764661	-3.67702904922172	-0.00277589380128
C	0.87863070357935	-3.63527741972082	-0.09815287567153
C	1.54177632653240	-2.42398813625341	-0.11089681541537
C	1.47416105070528	0.04516471943344	-0.07065964338011
C	-1.30739315817849	-0.03388783804251	0.15774946457535
C	0.76034551552498	1.25386245800075	-0.05377120691778
C	-0.66858465400756	1.20930636177887	0.08239373136564
C	-0.59841926347318	-1.24752903869055	0.05191987531416
C	0.83124450863201	-1.20348073175323	-0.05309364978348
H	2.46925759021682	2.55768053890743	-0.24522275252868
H	1.18262562981647	4.64593921557527	0.08340228598222
H	-2.44797587252185	2.38190825178760	0.41397823774033
H	-2.32895122425918	-2.52686936501753	0.16774530315967
H	-1.03473947949111	-4.63665516895660	0.01597028926807
H	1.44554687571098	-4.56461887250630	-0.15306080793924
H	2.63042040501130	-2.39154091946425	-0.18251253124645
H	2.56383745539378	0.07587744032825	-0.14987761871032
H	-2.39498474210973	-0.06600161525674	0.25659920754016
C	1.38296247853473	2.41667217883101	3.27243874095796
C	0.72243410566412	3.62514267882215	3.13699527143378
C	-0.67197369999392	3.67418817591404	2.99075576525355
C	-1.39473101929974	2.49355443125327	3.11461224014024
C	-1.54080525640817	-2.43357700841264	3.36812023303994
C	-0.88000159878075	-3.64868505958713	3.38317774810896
C	0.51987767096640	-3.69110693146216	3.33047930071095
C	1.24733443992278	-2.51866635466417	3.27222944948607
C	1.31823269288021	-0.05065106184948	3.24187094597660
C	-1.47202348704873	0.03402318800939	3.26137124167726
C	0.67585251102929	1.19661025774817	3.28090872128103
C	-0.76022556722063	1.23970086824803	3.26390010874589
C	-0.82840227294221	-1.21840883032498	3.32109357965823
C	0.60492548129600	-1.26009761926067	3.28420280495769
H	2.47265980433605	2.39022656822104	3.32700951333416
H	1.29474524736608	4.55156828603485	3.06572857337859
H	-2.48445765069671	2.51763690138343	3.03357490179190
H	-2.63147817589573	-2.39916054007001	3.39815484303729
H	-1.44962458897270	-4.57683088885947	3.42698878480951
H	1.03385593817507	-4.65199000934987	3.32666746105653
H	2.33743343449731	-2.54674792627968	3.22937292381470
H	2.41044430374724	-0.08211377584586	3.22682939909241
H	-2.56462800902277	0.06379700208059	3.25369436554063
C	-1.32264103326082	4.91207834029259	2.43983403590824
C	-1.43832717973866	4.84692221780145	0.86482332754450
H	-2.49924976262930	4.79824504735223	0.58351634845390
H	-1.03254318839200	5.77303476932472	0.43587300873485
H	-0.73056880384785	5.79298116825720	2.72171418947972
H	-2.32592092545056	5.04579073853504	2.86786944655078

Table 60: Minimum-energy S1 geometry for the anth excimer with C2 linker in the β position.

C	1.37528008901676	2.50270568484094	0.30097057201672
C	0.64806703827115	3.67071476858804	0.10093382489987
C	-0.72836105913033	3.64236843426082	-0.14729918230060
C	-1.39862698845058	2.43765161861448	-0.16897824675309
C	-1.32989946519540	-2.48791463488057	-0.07585212836078
C	-0.61529320510197	-3.67039600628158	-0.10384131321817
C	0.78446935340587	-3.64832776525715	-0.05502367718758
C	1.45753570638459	-2.44294386616989	0.04453979884682
C	1.41187768092584	0.01835900293238	0.23850929232189
C	-1.35991485107497	-0.01731004164797	-0.03159679803699
C	0.72909079460021	1.24843512250460	0.14517792133251
C	-0.69594941793739	1.21907269676438	-0.03560957427974
C	-0.67053782891469	-1.24037278153847	-0.01529744037830
C	0.75933340203358	-1.21965440278088	0.07116426911476
H	1.16112489785329	4.63021362840952	0.18535232322795
H	-1.27409321499447	4.57596580769682	-0.28204468938081
H	-2.47968820723916	2.40437430822503	-0.31287656054914
H	-2.42023739497153	-2.50029538685511	-0.12163356903278
H	-1.14125536414336	-4.62305100545727	-0.16193808854649
H	1.34360463676555	-4.58336995497183	-0.08047187596898
H	2.54754958773424	-2.42443494372787	0.10106832554621
H	2.49919598238273	0.01161355234758	0.32344195796992
H	-2.44931617072624	-0.02704885990644	-0.11751403540661
C	1.39696885072223	2.47799852806088	2.98157731786836
C	0.70774258560839	3.66513904677410	3.20349232459380
C	-0.66399916884759	3.67586854113459	3.47706266330935
C	-1.36878917922049	2.49113252994823	3.50673868682289
C	-1.44698360310854	-2.43310376469039	3.41530982598000
C	-0.76621314096502	-3.63557054496667	3.41992557732051
C	0.63125847249046	-3.65572999208252	3.32506139927144
C	1.33541510335454	-2.47002627923135	3.20723651602950
C	1.35910947616086	-0.00816084341913	3.02881009252964
C	-1.40509388074575	0.03719818209191	3.36765967263548
C	0.71623613905780	1.24190121690271	3.14158180874803
C	-0.70487846434492	1.25350581847597	3.35459063350465
C	-0.75346190882727	-1.20536621670464	3.33371422671822
C	0.67297673549993	-1.22692641117910	3.20562391810301
H	1.24733419879332	4.60986401796725	3.11648623568871
H	-1.17910666554912	4.62429539841736	3.62765466925019
H	-2.44698541764186	2.48867910950823	3.67389215799263
H	-2.53523706416252	-2.41404705761185	3.49584726853603
H	-1.31811943448462	-4.57238272951213	3.49435766062292
H	1.16266862725864	-4.60694699369773	3.32924505662663
H	2.42292637164505	-2.48294260872346	3.11546662899076
H	2.44335956102954	-0.04905926121014	2.92339165501344
H	-2.49182870324556	0.06010433746933	3.48082750886903
C	2.77627219456353	2.59787205422911	0.84374290046836
C	2.79204325209966	2.53883858722685	2.41759376660035
H	3.21191656228097	3.55268261091031	0.52111073736240
H	3.42114544496856	1.80894393470574	0.43558837195600
H	3.39721299850562	1.68760702854609	2.75322509582532
H	3.28812705561043	3.44104878495093	2.79932351688579

Table 61: Minimum-energy S1 geometry for the anth excimer with C2 linker in the γ position.

C	1.39526309253570	2.48212877068225	0.11198184031317
C	0.69368184022102	3.66555778987971	-0.04671340737824
C	-0.70119908046176	3.65344042762125	-0.14484361545296
C	-1.37864047145392	2.45113346417291	-0.10773758441536
C	-1.38070441183815	-2.44997360882222	-0.10840685794314
C	-0.70436464950818	-3.65288582801566	-0.14567394956709
C	0.69050981628283	-3.66624790611825	-0.04739326633795
C	1.39313819296610	-2.48348640529794	0.11155915348339
C	1.41960199908177	-0.00063782004318	0.36054239311857
C	-1.37092919057758	0.00053400460228	0.03095280683899
C	0.74160522553788	1.23075007167105	0.13726112623636
C	-0.68827632798351	1.22457330640418	0.00346275108178
C	-0.68919673519618	-1.22410347471316	0.00320063464965
C	0.74059516535459	-1.23153963265046	0.13709922784757
H	2.47932006374055	2.52542186286039	0.20081108291140
H	1.23343967601752	4.61173232478865	-0.07793127538962
H	-1.25058236846513	4.58914425477311	-0.24517325597002
H	-2.46722605365030	2.42652628983031	-0.18114301033606
H	-2.46925930767888	-2.42432050150293	-0.18191682321096
H	-1.25451162968336	-4.58811097452197	-0.24628325317415
H	1.22941116857812	-4.61290547708967	-0.07873821751591
H	2.47713853481368	-2.52791852775445	0.20036947121886
H	-2.46126083152092	0.00080242873071	-0.03975142275850
C	1.39265671428329	2.48367364749191	3.18890453581973
C	0.68979628723993	3.66633805858500	3.34757093814869
C	-0.70511186380815	3.65272948551755	3.44515802078030
C	-1.38127761637141	2.44972868001364	3.40756631087546
C	-1.37820027317770	-2.45140972995014	3.40749118611270
C	-0.70055060897999	-3.65359256071563	3.44499158227293
C	0.69438234498099	-3.66540394719782	3.34738913126778
C	1.39579835132083	-2.48186961300903	3.18879032604316
C	1.41965911091274	0.00092229764235	2.93987808945647
C	-1.37097470380258	-0.00083059478522	3.26840082758818
C	0.74033590777556	1.23160740801431	3.16304990188634
C	-0.68958786281236	1.22390265672276	3.29640176216203
C	-0.68798317582643	-1.22477773109599	3.29636537955682
C	0.74185899538357	-1.23066403089442	3.16304779818064
H	2.47669745399368	2.52816148119788	3.10060435670221
H	1.22856089277093	4.61306118140140	3.37923270177760
H	-1.25552010395018	4.58783516452087	3.54546570016078
H	-2.46986376415926	2.42396817076925	3.48057058096171
H	-2.46681599157726	-2.42696191770415	3.48048421417857
H	-1.24970645910709	-4.58943299865953	3.54526440810413
H	1.23430714648851	-4.61147498673687	3.37894270936357
H	2.47989804213377	-2.52504820651602	3.10040305012666
H	-2.46133473311794	-0.00169044526264	3.33864550319180
C	2.84328421629583	0.00164088929676	2.43352829449781
C	2.84323297561211	-0.00106996043012	0.86691462219553
H	3.39066810616153	0.87093986762795	0.49159992324774
H	3.38893505244909	-0.87556177746874	0.49498079038036
H	3.38890497886022	0.87605820483607	2.80577122478372
H	3.39082686291586	-0.87045453269833	2.80847058192679

Table 62: Minimum-energy S1 geometry for the anth excimer with C3 linker in the α position.

C	1.35173088187104	2.41842510496301	0.05268828387700
C	0.68164331558140	3.62538673411423	0.07160591504174
C	-0.72174641958786	3.67249591330393	0.12570806133024
C	-1.42858633142838	2.47847715269833	0.07787538052081
C	-1.54094733588836	-2.45493395106905	-0.07774297005323
C	-0.87103760434115	-3.66492116116870	-0.10073446865138
C	0.52762002249255	-3.69777774037183	-0.02753880500903
C	1.24572619289265	-2.51911555978659	0.05712629407554
C	1.30056589408867	-0.05007263246324	0.11883066733688
C	-1.48894336127474	0.01230579471739	0.04183606782453
C	0.65204831725682	1.19081649183623	0.05168445810281
C	-0.78260728530952	1.22523676290692	0.02763238369862
C	-0.83730400557704	-1.23415735321751	-0.00986830881566
C	0.59545486737478	-1.26686042443953	0.05030084357702
H	2.44297579765783	2.39616024508262	0.04880479240757
H	1.24839101741997	4.55801413266613	0.09120871579707
H	-2.52111381558225	2.50086265847623	0.10574624217114
H	-2.63124664764621	-2.42746753457571	-0.12420569698216
H	-1.43321021197898	-4.59653002232925	-0.16361647853995
H	1.04932593615415	-4.65444485172388	-0.02944336602154
H	2.33512291068925	-2.54050486244144	0.11811120602207
H	2.39230100527909	-0.07540528768199	0.15723475772999
H	-2.58156194818991	0.03675705556379	0.02230024702842
C	1.42117465009212	2.51400700782284	3.39401866369284
C	0.69794903376257	3.68792237739397	3.31279245944377
C	-0.69548440193367	3.67070952280205	3.12678144690944
C	-1.34203981966726	2.44324325518411	3.08969803298298
C	-1.24011865453564	-2.48837602686430	3.18541517669719
C	-0.52614027662620	-3.66803685360077	3.29309961540711
C	0.87000883577342	-3.63436207136128	3.40463512668603
C	1.54105186621389	-2.42531148027259	3.40904564675624
C	1.49160243278485	0.04375037261713	3.33176907414111
C	-1.28945363045407	-0.02110002104493	3.09321338323598
C	0.78516176612100	1.25415659272849	3.32171465574016
C	-0.64347449117272	1.22169528087217	3.18951491651070
C	-0.58936964238068	-1.23742931987713	3.20965862283317
C	0.83984489542372	-1.20335474362001	3.32682326021304
H	2.50564830176946	2.54474710992882	3.51405507992649
H	1.21757467373242	4.64695472252175	3.36008849839116
H	-2.42628124633900	2.41260587280541	2.95679271367444
H	-2.32682156480266	-2.50881865956864	3.08780164744597
H	-1.04757829897145	-4.62456952320179	3.27859451031868
H	1.43035311441413	-4.56626751487136	3.47947165263084
H	2.62910467180894	-2.39884294279518	3.49196775269776
H	2.58127033722186	0.06771521866886	3.41409400103260
H	-2.37761393818919	-0.04589095937463	2.99944189572226
C	-1.45211327130576	4.95334509793211	2.90670466144280
C	-1.05777908467443	5.70302848084119	1.62551004819444
H	-1.28479128369303	5.62764335259396	3.76178115163507
H	-2.53196646889523	4.73734772133721	2.88304678793739
C	-1.42811023221299	4.98685840685165	0.31860899626475
H	0.02701266064004	5.89330831708960	1.63981527114921
H	-1.54387412057350	6.69043690576649	1.63257125831441
H	-2.51653426459854	4.82052628013773	0.29094264874476
H	-1.19114774068618	5.66140155549697	-0.51990687924128

Table 63: Minimum-energy S1 geometry for the anth excimer with C4 linker in the β position.

C	1.49025310524775	2.41990002972012	-0.04966324326827
C	0.80627655744384	3.62774414771910	-0.08946252569828
C	-0.59085735441079	3.68424429139670	-0.04847244397871
C	-1.32707559366696	2.51652077740487	0.02461311442863
C	-1.53361454805594	-2.40607260075671	-0.02584755107153
C	-0.88832957127785	-3.62876469513085	-0.08023843659750
C	0.51127892370769	-3.68996621361201	-0.05398029546003
C	1.25433708100827	-2.52562241565211	0.01337238038253
C	1.36270222987585	-0.06020592590376	0.07650491483938
C	-1.41972857530573	0.06097712608925	0.10284490033827
C	0.74891812420396	1.20414557148435	0.02173436152824
C	-0.68712339825064	1.26052523842592	0.04226536160552
C	-0.80323185705938	-1.20002891394808	0.02547897331228
C	0.62845740445696	-1.26047976978603	0.03456163430542
H	1.38020636732430	4.55300463579982	-0.16797952555406
H	-1.09550029575097	4.64972265526174	-0.07608634887880
H	-2.41770210139327	2.54846028850034	0.04580859670023
H	-2.62413248019922	-2.35710386121332	-0.03636212458639
H	-1.47072646030206	-4.54867321483407	-0.13142045754150
H	1.01347522427850	-4.65661739803215	-0.08085999972135
H	2.34477067813457	-2.56796599729374	0.03437499034656
H	2.45081656470546	-0.13392099666142	0.06697704412777
H	-2.51141042521757	0.11475335046048	0.10723209334627
C	1.39733300742976	2.57785400964390	3.42530843187461
C	0.60269974864005	3.71940714997187	3.41655956043331
C	-0.78496593080279	3.65453085516483	3.29089347069545
C	-1.40687942043525	2.42528864772243	3.17330715756628
C	-1.20453628682085	-2.48664011384510	3.17741472278407
C	-0.47100990547068	-3.65500425301403	3.28254041450361
C	0.92544910281442	-3.59886240346646	3.38200033597207
C	1.57758512178684	-2.37950541276493	3.38036277205329
C	1.49088282274155	0.08637142808233	3.31055169532731
C	-1.28249788796539	-0.01941563673192	3.08212303378093
C	0.77761010849859	1.30054651940761	3.31872463019469
C	-0.65622692385175	1.23429406883514	3.19978465678811
C	-0.57152132787760	-1.22696947272896	3.19423651382497
C	0.85573096351548	-1.16829938429571	3.30359882764349
H	1.08782731999768	4.69255262524797	3.51724726237196
H	-1.37439789792834	4.57104753744267	3.28245692838729
H	-2.49148801200852	2.35762606679011	3.07565984745678
H	-2.29150230257025	-2.52366762053185	3.08933778300551
H	-0.97710853577089	-4.61975669938658	3.27453152267023
H	1.50104520870753	-4.52169967628958	3.45255520547259
H	2.66574899001980	-2.33614992089096	3.45481624997658
H	2.57800221677967	0.09788374143283	3.39635631397345
H	-2.37131471305056	-0.05362950811939	3.00088661854560
C	2.88497117676462	2.77036478065469	3.56691701340062
C	2.99226425422327	2.39757936648576	-0.12319564154726
C	3.68602606067499	2.08332364724451	1.20988465782755
H	3.34500802777064	3.37585615480833	-0.48458659914748
H	3.30831027548948	1.65630502321280	-0.87408488651478
C	3.56942912065436	3.19968883829192	2.26156506158812
H	3.37164874661461	1.86445064891888	3.95443018330345
H	3.05069845846728	3.55423927983754	4.32176145991069
H	4.57012399233353	3.58524574210781	2.50554980892396
H	3.00591940997168	4.04848084407049	1.84144481215594
H	4.74700887935789	1.87803246498753	1.00542691138250
H	3.26685453180239	1.15128455226508	1.61488185050982

Table 64: Minimum-energy S1 geometry for the anth excimer with C3 linker in the γ position.

C	1.47125083929510	2.35744134285202	-0.02255562491384
C	0.78932878968580	3.55551693694163	-0.14463060807577
C	-0.60963274009853	3.58044764106521	-0.12074662090325
C	-1.31066573935375	2.39705625891572	-0.00300987979889
C	-1.43142102114292	-2.49606019950082	0.03367924268759
C	-0.79735313345051	-3.72100710669839	-0.02566721018979
C	0.59909571635948	-3.77514495418769	0.02131807536564
C	1.34454132620836	-2.61422883492816	0.13316488052278
C	1.46565971923166	-0.11830077623130	0.29636527084358
C	-1.34984984084628	-0.05187823031248	0.17457227122295
C	0.79042806733969	1.12714125639829	0.11389654438338
C	-0.64238935166525	1.15710602943892	0.08647877029247
C	-0.69831853489852	-1.29269875871363	0.11042012295201
C	0.73760146190660	-1.33759957126501	0.16969992732244
H	2.55942345541445	2.36811510928042	-0.05703260473455
H	1.34805380395305	4.48437107691261	-0.25754875504171
H	-1.14148994844399	4.52842474382196	-0.19717007775323
H	-2.40207800288697	2.39783924738817	0.00166319677935
H	-2.52080027006447	-2.43491492707356	0.00593604559294
H	-1.38005615014953	-4.63889560525747	-0.09794688795428
H	1.10816495603299	-4.73789964667850	-0.01955226111201
H	2.42829688774435	-2.70119732759478	0.17112294680117
H	-2.44207685293506	-0.02787637309882	0.15518278965077
C	1.37257022753779	2.38428137289169	3.46819185841628
C	0.68646662026125	3.58465786612246	3.52871232714335
C	-0.70831425599287	3.61025762439809	3.41812239263483
C	-1.40284404622113	2.42554615480564	3.27710032826575
C	-1.52893321281378	-2.46753069117920	3.31782515537212
C	-0.90138289235214	-3.69149486960397	3.43714189602479
C	0.49527946042390	-3.74703698628372	3.47553309572073
C	1.24783527697622	-2.58861842079804	3.38801685012870
C	1.38219389512089	-0.09612296556160	3.18789939945915
C	-1.43519162958044	-0.02614203569968	3.13851993626675
C	0.69926822374133	1.15243824386638	3.31037577858473
C	-0.73251088215661	1.18380032615423	3.24975281418559
C	-0.79074830772459	-1.26601293789912	3.26434667693656
C	0.64605712894585	-1.31265465247354	3.29249404083881
H	2.45659019147956	2.39472935301069	3.56943832464213
H	1.23878417507112	4.51482541921001	3.66076647161609
H	-1.24217113608044	4.55978172868420	3.44570462942003
H	-2.49188234905320	2.42704565236971	3.20511348826799
H	-1.48873806263947	-4.60772142864973	3.49036381560053
H	0.99953703685850	-4.70909381506402	3.56434980201497
H	2.33178971981117	-2.67666217181340	3.41722175294670
H	-2.52651321291883	-0.00121596595113	3.09061910877600
C	2.95489528574881	-0.11635734803913	0.49438765495894
C	2.88025661217643	-0.09832567810806	3.07531624856696
C	3.42821395070177	0.55145298242118	1.79501878653012
H	3.27098817300340	-1.12011418218977	3.13919280636356
H	3.31217672840503	0.44172501868991	3.93522319015376
H	3.43447845094418	0.41294657199950	-0.34667592068908
H	3.34972381708728	-1.13816136302630	0.46648139094939
H	4.52794229653615	0.51592451513662	1.82715753070109
H	3.14777379040556	1.61141804255635	1.77957688338439
H	-2.61790351093841	-2.40547269145059	3.27853793187857

Table 65: Minimum-energy S1 geometry for the anth excimer with C3 linker in the β position.

C	1.38973332614399	2.45655588636247	-0.00605394730205
C	0.70444494942631	3.65704241654587	-0.03469609421546
C	-0.68794093489495	3.66535738082834	0.06120569436476
C	-1.42427477285825	2.48925690506430	0.16700790767564
C	-1.40636934796400	-2.46208896814838	-0.04124716044145
C	-0.71269823337974	-3.65686084872131	-0.08841693450411
C	0.68897214213247	-3.65862840595836	-0.07053191648770
C	1.38411232768273	-2.46651577131398	-0.00552755146808
C	1.37572850718966	0.00386804045548	0.07890034280889
C	-1.40933472775624	0.00382133121436	0.08519079408047
C	0.69471328640452	1.23091875449908	0.04086677560651
C	-0.74438064134628	1.23826064042768	0.08391993194606
C	-0.72693040020108	-1.22755880531339	0.01025295822696
C	0.70468771386524	-1.22944921487606	0.02317376823690
H	2.48010002215319	2.43797484073050	-0.04459170955378
H	1.24967411342345	4.59836502221191	-0.09876464318759
H	-1.21944485676174	4.61817422068337	0.08834302452193
H	-2.49795798536623	-2.45803716888222	-0.04659275633856
H	-1.25595418154973	-4.60052874267315	-0.13216639852357
H	1.23048751938174	-4.60395707874237	-0.09819423756041
H	2.47543832241532	-2.46361568787246	0.01172682051858
H	2.46846250535360	0.01084539899544	0.06956558733016
H	-2.49932874750354	-0.02263430998189	0.06550084165583
C	1.40391474324743	2.46530606067329	3.28168202196471
C	0.71779319585190	3.66527175528280	3.31101289972341
C	-0.67538919136145	3.67188507397028	3.22693155029463
C	-1.41150782310725	2.49476318359586	3.13201826048512
C	-1.38692646446053	-2.45584032571325	3.35747845134186
C	-0.69178502932621	-3.64974112330658	3.40519503895963
C	0.70974228109485	-3.65009184197368	3.37833319451096
C	1.40326862128393	-2.45762577388261	3.30345541503554
C	1.39164810304198	0.01234801091053	3.20759874517543
C	-1.39337176287265	0.00956168453522	3.22178792583630
C	0.70967384991890	1.23885025386868	3.24557736401863
C	-0.72973675929449	1.24466147279028	3.21383544103689
C	-0.70912206325484	-1.22086797579884	3.29646808512104
C	0.72237163069964	-1.22137623952053	3.27373323318144
H	2.49457865865067	2.44785849653365	3.31135019591904
H	1.26261877001500	4.60736165304337	3.36664723941261
H	-1.20804786014165	4.62409250426433	3.20092855935740
H	-2.47845958032146	-2.45284932730761	3.36984011112558
H	-1.23375427979727	-4.59375883642377	3.45646903661522
H	1.25243289964627	-4.59473617638002	3.40675239931634
H	2.49445555715212	-2.45373240343383	3.27900171995156
H	2.48441853136314	0.02055034964430	3.20849247126764
H	-2.48317848096050	-0.01806027671171	3.24911121038719
C	-2.91537433512002	2.57268414413330	0.35412013223303
C	-2.90437989902507	2.57603050647254	2.95841512874474
C	-3.47002308846732	1.98142193245493	1.65939130014246
H	-3.19674672542428	3.63563623705431	3.02226334292869
H	-3.40428584123454	2.06808360168503	3.80063015758714
H	-4.55987194952875	2.13443156459075	1.66353901007989
H	-3.31434793858507	0.89649812628194	1.66030550688152
H	-3.42414772812290	2.06398446411449	-0.48233135433944
H	-3.20677094754998	3.63262338901734	0.29109210831382

Table 66: Minimum-energy S1 geometry for the anth excimer with C4 linker in the γ position.

C	1.69027138463407	2.28038624264132	-0.06035803415492
C	1.17571002992975	3.55345924014599	-0.21208515275523
C	-0.21015886405512	3.73985717542611	-0.23748927134688
C	-1.06427887304052	2.65873741463429	-0.10290455961871
C	-1.66210959870121	-2.27467370982615	-0.16594739278101
C	-1.08322862957473	-3.52999159731562	-0.21363457170877
C	0.29866880316774	-3.68678984254593	-0.05553861358798
C	1.08999757295352	-2.56566068832502	0.09587972991269
C	1.35948358778550	-0.13717109562666	0.20218656220343
C	-1.44611391474621	0.20481950785494	0.17448470043661
C	0.84280651282453	1.15702428543756	0.04077655830026
C	-0.57815315972343	1.33688378358161	0.03575792237360
C	-0.89396867117029	-1.10319772610294	0.03873472951187
C	0.53391148655108	-1.26975050499182	0.10795702331410
H	2.76954332842980	2.11830232228180	-0.03626480263787
H	1.84588190143712	4.40789445268289	-0.30593315299102
H	-0.62338761398063	4.74062824860738	-0.36010547132284
H	-2.13556461357459	2.84103134841435	-0.13452624530351
H	-2.73358551434722	-2.18916644265061	-0.31884963272834
H	-1.71406888367212	-4.40383165316775	-0.37703034252837
H	0.74532536851021	-4.68023955255029	-0.07077857626844
H	2.17338066210594	-2.66060838520665	0.18461503925918
H	2.44232836719000	-0.27645161498845	0.24371047953997
C	1.03692123450022	2.54527206376019	3.08872025911577
C	0.26243424175368	3.68957557004604	3.15232235235501
C	-1.12787505456908	3.57016289923606	3.23004620060212
C	-1.73403029040395	2.32399282798395	3.24646592370876
C	-1.21217529887782	-2.61827931802759	3.61114727801842
C	-0.37876316581752	-3.71904471953319	3.68810328544351
C	1.00310752433106	-3.57445420904401	3.51453648060920
C	1.53448147902065	-2.32012211244317	3.29174867042307
C	1.25087204156926	0.10648061604723	3.04254382412440
C	-1.55146972704956	-0.17123276621990	3.24166910013873
C	0.45565043981225	1.26209116278770	3.12587120895215
C	-0.97495223164680	1.12720381101007	3.21324271873856
C	-0.70901391779807	-1.31931958648208	3.36163643342983
C	0.71037579900189	-1.17567724903679	3.23717549921421
H	2.12340809976847	2.61661277940201	3.02032368724754
H	0.72934387372736	4.67342402380874	3.13181641941978
H	-1.74764182673606	4.46588698341009	3.27526201067563
H	-2.81815065968473	2.27690546265407	3.32818705923116
H	-2.27944856343536	-2.76170977589120	3.76756675631144
H	-0.80218644709797	-4.70293283397867	3.88837783409182
H	1.65528377130662	-4.44629463784268	3.56168781357425
H	2.61160682766122	-2.18788125611213	3.17341296296760
H	2.33497189899447	0.21803840965472	2.96947811162090
C	-2.90552837282418	0.54513146919704	0.35433456275285
C	-3.04253021135433	-0.38132526232245	3.30321592501978
H	-3.57642564688335	0.57498044915740	3.35952484968168
H	-3.27274915201690	-0.89910546571914	4.24925560710440
C	-3.62177220078089	-1.21570304391625	2.14510785226919
C	-3.95815195914678	-0.43933261211919	0.87532857564298
H	-3.28992743049028	0.97209101024104	-0.59029971483805
H	-2.91002404360084	1.40103724207231	1.05352904260301
H	-4.54554904568622	-1.70314717267954	2.49350219445267
H	-2.92166243365876	-2.02379983288365	1.90197356946128
H	-4.25855807671448	-1.15186436700224	0.09360670909016
H	-4.85823414410639	0.16835423237489	1.06589201162835

Table 67: Minimum-energy S1 geometry for the anth-naph exciplex with C3 linker in the β position.

C	1.38159854347114	2.49255807352968	0.04925296049584
C	0.69213490678535	3.70133311124514	0.01768237604575
C	-0.69354607702116	3.70480078771642	0.09605650829848
C	-1.42775742109647	2.51404851653904	0.18907478608272
C	-1.39775345267073	-2.43703138654692	-0.04759300376035
C	-0.70336874365929	-3.63347149422158	-0.06344568722065
C	0.69750145680478	-3.63161656971582	-0.02740226913433
C	1.38827840803125	-2.43482238439243	0.02034595653185
C	1.37674686327361	0.04026837298007	0.07952810236644
C	-1.40915817111946	0.03453381800282	0.04563057897496
C	0.69444589514772	1.26199445060876	0.05512558134211
C	-0.74807184229819	1.26448808834531	0.07851360006301
C	-0.72115751288222	-1.20292045214073	-0.00428126038117
C	0.70674466608367	-1.20118198303594	0.02632159672798
H	2.47240409709534	2.47979100511547	0.01717923596590
H	1.23953977698062	4.64199341390444	-0.03365704522798
H	-1.23398991173923	4.65257241254721	0.11908006040366
H	-2.48932738758312	-2.43395949267655	-0.07169973618699
H	-1.24537909065164	-4.57814040456223	-0.10276152981559
H	1.24267917874333	-4.57532116552026	-0.03888728464218
H	2.47965507487481	-2.42897096848978	0.04693755531511
H	2.46953705629185	0.04815696882631	0.08324017692468
H	-2.49852482975429	0.00424226543439	0.00475055196677
C	1.40712504546655	2.41553677801808	3.22759052687004
C	0.72966276200955	3.62400846112159	3.25994242526847
C	-0.65843786885932	3.64016442024585	3.19274398970950
C	-1.40367489310539	2.46279330231036	3.10533731111670
C	1.37862709175825	-0.04409715259029	3.20980803074601
C	-1.40134396483827	-0.02960668448435	3.22840947093899
C	0.70176982761703	1.19449361440036	3.22650153800896
C	-0.72733042590936	1.20904080760764	3.20236710105159
C	-0.70714870513524	-1.23440794418226	3.28581762330726
C	0.68366665288781	-1.24473511618577	3.26465800876949
H	2.49773607244172	2.39014038883236	3.24838647869550
H	1.28352000897773	4.56147906413174	3.30042814989906
H	-1.18695523233862	4.59449187671199	3.17029389811577
H	2.46977511046450	-0.03862779602660	3.20409353880250
H	-2.48999217641498	-0.04601379022729	3.25251667060237
C	-2.91706433696643	2.58843705673442	0.36260796977784
C	-2.89594709706874	2.55184849643398	2.95418874348088
C	-3.47122995774989	1.96967963109070	1.65507315881624
H	-3.18627189777678	3.61090996660142	3.03153932659242
H	-3.38570398501512	2.03438585935225	3.79640790738885
H	-4.56205509170066	2.11315777960531	1.66689316297654
H	-3.30222021417077	0.88683775643276	1.63713604438423
H	-3.41625266083641	2.08525591136877	-0.48360233401796
H	-3.21767897663850	3.64648971864657	0.31441683795281
H	1.22282936619900	-2.19117287121568	3.26395421790969
H	-1.25761593640533	-2.17413451822673	3.31488839170028

Table 68: Minimum-energy S1 geometry for the anth-naph exciplex with C4 linker in the β position.

C	1.51306126218367	2.39484224650005	-0.03315709458626
C	0.81204873708687	3.59561857559696	-0.05727561192439
C	-0.58058769797305	3.63245677932219	-0.00335669623491
C	-1.29967397847255	2.45113185883659	0.07487202113935
C	1.42094030479531	-0.09465731597469	0.05418376053103
C	-1.35720539286757	-0.01062475314004	0.13342386055689
C	0.78729546194504	1.16946407652958	0.02450348500363
C	-0.63960218038251	1.20609412856672	0.06636527662493
C	-0.70404414790065	-1.23578863883712	0.07876235101889
C	0.68631879943088	-1.27573187738271	0.04872559420516
H	1.37370147352562	4.52872914606921	-0.12996973743978
H	-1.09997044379281	4.59025189352267	-0.01662034717592
H	-2.39016731707732	2.46671072043485	0.10723171503440
H	2.50852674181795	-0.14879899169145	0.03044351721623
H	-2.44733626975355	0.03106947950985	0.16046067767045
C	1.37722796647017	2.60184641480974	3.38725428033416
C	0.58587004460309	3.75718412798622	3.35326141375119
C	-0.79403060815141	3.69409765598332	3.22856535812961
C	-1.42149273957177	2.45412829632073	3.13600670033829
C	-1.22888132807190	-2.46383218747807	3.18142264400506
C	-0.49335600675707	-3.63639571284282	3.24769754414878
C	0.90299631964183	-3.58199828010945	3.33144330330580
C	1.55137027613483	-2.35848800315408	3.35375815454466
C	1.46531761328710	0.11219430725967	3.31522537887940
C	-1.30954937646494	0.00930416198468	3.11228642781808
C	0.75645099414563	1.32458621823426	3.30990801379116
C	-0.68082162410149	1.25974258571907	3.19888848977892
C	-0.59696698086946	-1.20671388461647	3.20915745276296
C	0.82833936534949	-1.14988060367622	3.30166084523809
H	1.07872516693028	4.72772175533389	3.43794435796208
H	-1.38495663804376	4.60924091543485	3.20199194674926
H	-2.50742304960023	2.39101921508746	3.04886897317854
H	-2.31773928370777	-2.50003617676679	3.11031182649623
H	-1.00103411666278	-4.60053658459455	3.23219631788143
H	1.48105286016999	-4.50468729543713	3.38035293322899
H	2.64018122410909	-2.31398085332845	3.41947534527143
H	2.55293580139314	0.12050756271246	3.39540145946986
H	-2.39955837324929	-0.02490464317370	3.04397060147234
C	2.85986443387232	2.79051289579383	3.55770610407727
C	3.01377664520526	2.39421914248940	-0.11279221060723
C	3.71071677958855	2.09179510410013	1.22078528731797
H	3.35221842592140	3.37696103484674	-0.47528917901822
H	3.33910037183031	1.65685956718673	-0.86300489241638
C	3.58162347722493	3.20949739114213	2.26947187784500
H	3.33298647304691	1.88499098055688	3.96203078025050
H	3.01104240691752	3.57955840196073	4.31111253247731
H	4.58148670921171	3.57866010680998	2.54069541028399
H	3.04453309825548	4.06801036804197	1.83471670772770
H	4.77393270942283	1.90099779923423	1.01496326226168
H	3.30460222360673	1.15494307719136	1.62892576722673
H	-1.27538205254877	-2.16278952398842	0.10517415718847
H	1.20281543889671	-2.23511266491694	0.05189185520915

Table 69: Minimum-energy S1 geometry for the anth-naph exciplex with C2 linker in the γ position.

C	1.27200544503219	2.58970008192294	0.09788778517853
C	0.50544016756746	3.74603508874426	-0.04309855723408
C	-0.87955007026448	3.65819036230073	-0.13691100997194
C	-1.49395206948728	2.41161973579401	-0.12027695971276
C	-1.22921286000334	-2.49455110016581	-0.13022691012310
C	-0.48083568244197	-3.65967922283268	-0.12608268269466
C	0.90954460587788	-3.59003025911902	-0.00776947046928
C	1.53930651419783	-2.36115486848736	0.13222746664143
C	1.41441193875206	0.11546761246138	0.36117223086751
C	-1.35691022165898	-0.03621229521066	-0.03519946188230
C	0.68744519871440	1.30704606030112	0.11128064925252
C	-0.74245685561041	1.22230495923387	-0.03609167868518
C	-0.61354080469469	-1.23140356609721	-0.02828391724748
C	0.80685344762706	-1.15826032576690	0.13329682761082
H	2.35371560367054	2.68930456811245	0.16202566177222
H	0.99647490741570	4.71825970050888	-0.06529681974722
H	-1.48335436372009	4.56154308298280	-0.21929673607631
H	-2.58049861586301	2.33328056324831	-0.18618751657322
H	-2.31582277104643	-2.53640934158811	-0.22366298057785
H	-0.97405158404556	-4.62696314829168	-0.21807645784344
H	1.50355844920474	-4.50376674214007	-0.01644978339541
H	2.62410497929591	-2.32715337726176	0.23119714963508
H	-2.44379148180097	-0.09266755599259	-0.13355837804471
C	1.51613622470488	2.31832101534276	3.13887049541669
C	0.93113192515874	3.56813300269189	3.28093699688015
C	-0.45448847591426	3.69090970140983	3.39356639699641
C	-1.24652212945799	2.55672757576394	3.39511122653193
C	1.29115052551322	-0.15381421539482	2.93676108631570
C	-1.47321898705165	0.10160561183887	3.33765072989511
C	0.73672194074309	1.14285931692940	3.14674244751226
C	-0.67696386306863	1.26949182908243	3.30609666842692
C	-0.88795679984124	-1.15340277257785	3.31708940188088
C	0.48459527550054	-1.27851002594879	3.12146601963218
H	2.59965285813231	2.23917784918811	3.04727030356690
H	1.55796814913224	4.45980005974713	3.28659638715418
H	-0.91000386351677	4.67698941230843	3.47844125503488
H	-2.33037988360141	2.63996629721528	3.49078611869632
H	-2.55377733372040	0.20803339428367	3.44543544766781
C	2.70593473912077	-0.33137645061624	2.43759501916077
C	2.79551249792681	0.16317883488844	0.96567361319466
H	3.18126340328218	1.18655110948762	0.94688359301510
H	3.51576517620873	-0.44765092860438	0.40088475681540
H	3.43986313765473	0.19549103338466	3.06580105653126
H	2.95374328444454	-1.39960383343330	2.48851466215052
H	0.92708540213988	-2.26935950086856	3.01578865047576
H	-1.50615708020886	-2.04755832877540	3.39299921636903

Table 70: Minimum-energy S1 geometry for the anth-naph exciplex with C3 linker in the γ position.

C	-1.56759331838787	-2.36415938421373	-0.04242985637360
C	-1.00754041084694	-3.62820412207135	-0.07918879472251
C	0.37480634610451	-3.77666427517556	0.03043545264156
C	1.18617833336089	-2.66270469890008	0.18422966648993
C	1.45179857232271	-0.18179534775605	0.37893689700377
C	-1.33496902332006	0.07919267576160	0.09776985707639
C	0.84380230119925	1.07507499940365	0.24349313591687
C	-0.52908772826700	1.21231497253710	0.11073632958472
C	-0.76320735788205	-1.21215002816857	0.07176825237627
C	0.65365845158395	-1.35770564210825	0.20125897791035
H	-2.64853563833874	-2.23660886856612	-0.12286198200554
H	-1.64590495899037	-4.50556768260330	-0.18158123421908
H	0.82074778535608	-4.77046379032399	0.01001095953029
H	2.26032093584498	-2.81020326625525	0.27414368579438
H	-2.41905180012593	0.17166083229116	0.01591184133019
C	1.33013764405455	2.41889865303689	3.47987791782872
C	0.60077933145150	3.59715485271656	3.52748373129088
C	-0.79334498771095	3.56784426522392	3.42368994672007
C	-1.44306295085684	2.35443708781882	3.29370714548797
C	-1.38477865667738	-2.54712536059238	3.23174394373095
C	-0.71232695959383	-3.75685269709612	3.33676152193523
C	0.67732462973617	-3.75894651158654	3.41951886639455
C	1.39042835856426	-2.56301349473658	3.38780410220692
C	1.43125110667632	-0.06616128002265	3.23976945276518
C	-1.38105334902703	-0.10030071868293	3.13778514988590
C	0.70112542750743	1.16334671030352	3.34252853570764
C	-0.72702838018886	1.14046305275990	3.26727290681895
C	-0.69524642354294	-1.31734528046698	3.24236617139438
C	0.74454527799208	-1.31065706956628	3.31085667010527
H	2.41396486302618	2.47069781435084	3.57312148195264
H	1.11914266163798	4.54857064415087	3.64542753698810
H	-1.36446045021157	4.49560402697115	3.45216566929297
H	-2.53150289887926	2.31522188198415	3.22000628311780
H	-1.26645211074094	-4.69483332693522	3.34408429355951
H	1.21849227387973	-4.70164140653881	3.50047932863796
H	2.47570756292444	-2.61078717523533	3.45438006822550
H	-2.47202594945750	-0.11477425686736	3.07391678858910
C	2.93922270278303	-0.24255420171098	0.58913945594397
C	2.92467501226852	0.00141352549281	3.13516660907670
C	3.42627091594846	0.56695714039386	1.79328907263588
H	3.37159442765917	-0.98929424713283	3.27773586734247
H	3.32771858406679	0.63424599058725	3.94323697100136
H	3.43970761754310	0.14632471291795	-0.31396767352653
H	3.27805747003417	-1.27985731163838	0.70240085416268
H	4.52648470148562	0.57996151523901	1.79904983325075
H	3.09998726714111	1.61161153293779	1.69136510487388
H	-2.47362497254207	-2.52610413944964	3.16145152633510
H	1.46437055522247	1.97020641170512	0.30040478282414
H	-0.97442279178733	2.20532228581734	0.06806689510945

Table 71: Minimum-energy S1 geometry for the anth-naph exciplex with C2 linker in the α position.

C	1.38457665059295	2.44610563663545	-0.02047101134489
C	0.70754648968430	3.65627086320505	0.12258303098123
C	-0.67515747509235	3.68534439265113	0.29649024028138
C	-1.38668128313692	2.48244997740825	0.20019481222720
C	-1.46980628092875	-2.44607387472473	-0.00530274625066
C	-0.79569350394125	-3.65589937269335	0.00125864353729
C	0.60438538806866	-3.67840603099082	0.01638294466756
C	1.31711702521438	-2.49267118762548	0.01586305383216
C	1.35701789737158	-0.02007308083875	-0.00565632207330
C	-1.43258356289981	0.02727345444098	0.03957180310184
C	0.69841971125274	1.21647722134263	-0.02169061903530
C	-0.74042637523657	1.23793682551347	0.02738057439480
C	-0.77178308140991	-1.22485500292353	-0.00707979128323
C	0.65895872686369	-1.24587342164868	-0.00761197164196
H	2.47346341491064	2.43696026304208	-0.09436737311940
H	1.27205374098114	4.58756281450527	0.18845594780187
H	-2.47604856678861	2.49543162046765	0.28760622949745
H	-2.56127007933832	-2.42450750644288	-0.00966738553316
H	-1.35507194206020	-4.59117840420187	-0.00210090399062
H	1.13286799985431	-4.63145889898804	0.02747591502534
H	2.40860183840005	-2.50615737742723	0.02647198913972
H	2.44960556445126	-0.03737274700990	-0.02097364121806
H	-2.52514967133042	0.04049739288865	0.07398411709038
C	1.41324377795780	2.57484853291888	3.33715247555816
C	0.63692787905156	3.71298409111832	3.17730715423543
C	-0.74124184100019	3.61581115898466	2.95620511478908
C	-1.33393381609810	2.35736747146497	2.99980250011928
C	1.60651033986649	0.10313312313650	3.35242177508285
C	-1.16414611387263	-0.10290479964103	3.13070972337035
C	0.83709525513372	1.28719863904689	3.31379934045396
C	-0.57861901849534	1.17711907374128	3.18603455140833
C	-0.38574935133355	-1.25187635568150	3.21899902996952
C	1.00056250391414	-1.14381229576283	3.32402966359975
H	2.49379708944428	2.66241962745374	3.46275660599949
H	1.11245454526201	4.69495120080555	3.15294065738569
H	-2.41398895918754	2.26806054115847	2.86371558202785
H	2.69199680564924	0.18567042905611	3.43017162070470
H	-2.24807456639814	-0.17973624631902	3.03218122440729
C	-1.52535473464923	4.78084194884029	2.41776351322459
C	-1.33938886998810	4.90967107101829	0.85804449186145
H	-2.32065215451959	5.07701944554368	0.39095175407473
H	-0.72065327704181	5.78933535925550	0.63642513290366
H	-1.21157033982165	5.71729314181477	2.89828416177230
H	-2.59004879254076	4.63974361751469	2.64896920725434
H	-0.85317723411449	-2.23438122971667	3.16606972243361
H	1.61145824729929	-2.04564110233689	3.35445746127592

Table 72: Minimum-energy S1 geometry for the anth-naph exciplex with C3 linker in the α position.

C	1.40639542914793	2.47000440848822	-0.01926899063239
C	0.72143341798503	3.67804741647106	0.02186008763970
C	-0.67171805054197	3.70644816333760	0.13148849781823
C	-1.36685842838948	2.49288916290288	0.12529725119543
C	-1.42977681111391	-2.44182768629072	0.02415349979890
C	-0.75071912670439	-3.64870842651583	0.00122595625347
C	0.64925334573599	-3.66314450118213	-0.01401986428657
C	1.35686342113157	-2.47333393042874	-0.00956769239661
C	1.38767319996660	0.00128124004938	0.02298674507263
C	-1.40218687076991	0.03126636283328	0.07988359546327
C	0.72612438490348	1.23262832569485	-0.00365827222122
C	-0.71157446071196	1.24797403509701	0.03905338909841
C	-0.73760910004025	-1.21628511154835	0.02120134485133
C	0.69304466655138	-1.23076029231615	0.00154552500753
H	2.49665932398140	2.46289639608008	-0.07330386454874
H	1.27929773206762	4.61612494959691	0.01409476794716
H	-2.45801824637557	2.50483389590283	0.18662570485933
H	-2.52131343285386	-2.42481487199472	0.04109842703386
H	-1.30531118143181	-4.58679666776382	-0.00317387145018
H	1.18299526703064	-4.61332218204645	-0.03014296407501
H	2.44843231421179	-2.48223297281861	-0.02020842135949
H	2.48049942582286	-0.01377421579550	0.00767219212669
H	-2.49475964406555	0.04277941092594	0.10615042710407
C	1.35024399907122	2.41285862312349	3.26824366242223
C	0.66886771837331	3.61499944215207	3.22130998051190
C	-0.72553322222424	3.64811323332101	3.09438421822697
C	-1.41963447655551	2.44079088775946	3.08144126826722
C	1.32597556049869	-0.06412373682446	3.23613384634322
C	-1.45779488193710	-0.03095334147168	3.12431289572978
C	0.66160623132026	1.17889281322618	3.24414583719040
C	-0.76222188161263	1.19714805937777	3.17594458004193
C	-0.77923231634552	-1.24309872305224	3.19926708557677
C	0.61208022965873	-1.25861176155249	3.24484820880874
H	2.43954147263674	2.40173155660834	3.33494301749203
H	1.22658850317490	4.55303273276168	3.23825467170838
H	-2.50922677366665	2.45100968100004	2.99917296408317
H	2.41674862229169	-0.07611439359434	3.26629195406811
H	-2.54762445883944	-0.01305304367318	3.07159104328932
C	-1.44648696525579	4.95593368278695	2.91020016605218
C	-1.04192377389031	5.71924426078327	1.64202003578584
H	-1.25216665134598	5.60540600559419	3.77859263548289
H	-2.53200685196763	4.77113601873281	2.89244368674138
C	-1.39956581573829	5.00675040512061	0.33023205049694
H	0.04230644621319	5.91041850748466	1.66434398580274
H	-1.53048633168707	6.70530612208326	1.65403249004309
H	-2.48531358202052	4.82438895265127	0.30030613538953
H	-1.17098400291651	5.68912867214898	-0.50395800533866
H	1.14329720434723	-2.20972110984981	3.25339267495859
H	-1.33221057712040	-2.18102645537689	3.17364544052549

Table 73: Minimum-energy S1 geometry for the naph excimer with C2 linker in the α position.

C	-1.22221764751213	-0.01803651685187	-0.06423476788875
C	-0.52417608566099	-1.22243426912385	0.06001030963721
C	0.84630012231314	-1.22665081363245	0.28452095509530
C	1.53365243765399	-0.00261291215981	0.28171396393613
C	1.54433995174735	2.45985987628122	0.09365362769072
C	0.85060402511153	3.66811303440685	-0.00935842155863
C	-0.53509760655905	3.66120260235680	-0.10071313759496
C	-1.23259185191883	2.45742472782648	-0.10461740755763
C	-0.55364133066832	1.22246371918358	-0.05321318787473
C	0.86977899014946	1.23153680635439	0.06914259386729
H	-2.30681059075669	-0.02637262751636	-0.18371310120472
H	-1.07065408243708	-2.16642701565676	0.07533423930495
H	2.61999629152339	0.00071252049714	0.39472634783828
H	2.63194485830654	2.45957234669917	0.18473788227074
H	1.39552111844956	4.61125636133292	-0.00280762171553
H	-1.08198003344057	4.60217487516465	-0.15823700940074
H	-2.32123209071763	2.45445449146207	-0.18024007603168
C	-1.32750784692846	-0.05605535788083	3.15888705053125
C	-0.62066983064832	-1.25693129100929	3.05138725788313
C	0.76064087299298	-1.25531765914170	2.90797452025126
C	1.44400501131074	-0.03093472553580	2.97792986300847
C	1.43817066713259	2.42695400506238	3.21945996189283
C	0.73697219444321	3.63216318847783	3.30656830855899
C	-0.65169935789295	3.62209043232416	3.31447740001314
C	-1.34566138113193	2.41794974341764	3.25076563139890
C	-0.66224214831982	1.18501101539796	3.21316718985667
C	0.76594374159354	1.19782668786368	3.17698962764324
H	-2.41729186712027	-0.06803275480927	3.21324838922978
H	-1.16341793417210	-2.20083889921942	2.98443136792036
H	2.53510812607149	-0.02423262385993	2.93043867288755
H	2.52925209520219	2.42953193594864	3.19378027388085
H	1.27923496395031	4.57570013515165	3.35292534714748
H	-1.20311900839837	4.56112712405951	3.35912126062570
H	-2.43688772461014	2.41253575570240	3.26072233795787
C	1.53282045528448	-2.45065426868733	0.81726001644376
C	1.48148779619840	-2.46754635272361	2.39394972176952
H	1.04377108588375	-3.35292495259880	0.42773867621790
H	2.57933410684414	-2.47704235177204	0.48241250261808
H	0.96934944224737	-3.37783126720581	2.73171917038357
H	2.50414006448359	-2.50125472558617	2.79534026306640

Table 74: Minimum-energy S1 geometry for the naph excimer with C3 linker in the α position.

C	-0.00231671048836	1.41841148162624	3.14360386446437
C	1.19583406592371	0.68566923742447	3.01891768004511
C	1.21597988099869	-0.72114003179801	3.04058374914785
C	0.00820826362034	-1.40064637170063	3.14248446533532
C	-1.19998966978940	-0.71025423472587	3.16831853351395
C	-1.23843553751511	0.70317457011049	3.19371667578384
H	2.13859131552411	1.23577135573843	2.97077642461407
H	0.01062370292795	-2.49162809211344	3.14125690034461
H	-2.14248261021813	-1.25812844779283	3.21663783710852
C	0.00321047053831	1.41076178947392	0.03389696258669
C	1.20102342230211	0.67875037388047	0.16589495078921
C	1.22129923347146	-0.72816358643779	0.15162541164674
C	0.01386863904880	-1.40827337163430	0.04992266195916
C	-1.19429450516691	-0.71809604939496	0.01723075156421
C	-1.23272900094412	0.69517954875891	-0.01579861149905
H	2.14363681193032	1.22913787911051	0.21379924982205
H	0.01634864229374	-2.49922946587927	0.05683880554809
H	-2.13662402771518	-1.26627128237945	-0.03081927882371
C	2.52087783556534	-1.46209478124664	0.31499553660423
C	2.51602844241869	-1.45601102418537	2.88525646617479
C	3.27661019595239	-1.10472776998116	1.60073394136355
H	2.32086681843805	-2.53920695336507	2.91035609193995
H	3.17180464724268	-1.23091513733358	3.74281745807169
H	4.24330726257605	-1.62901044136060	1.60379359042850
H	3.51119763888591	-0.02924478743654	1.59863005564455
H	3.17980469663611	-1.24080645560714	-0.54113172207237
H	2.32599398716110	-2.54542886987834	0.29418121398418
C	-2.43979450282493	1.43181707579858	3.21658270045307
C	-0.03114831238340	2.82620888267005	3.13625894399302
C	-2.43618510865108	2.82601626261493	3.25373411509233
H	-3.38444144594458	0.88587499493282	3.23981579336129
C	-1.23590735717041	3.52274602022878	3.22089581475426
H	0.91496657779037	3.36889426118469	3.09885707622073
H	-1.23463169500571	4.61204802878928	3.23763318003763
H	-3.38062571620125	3.36803730248874	3.29723501859908
C	-2.43407754147907	1.42359436506949	-0.04569551426589
C	-0.02573830586840	2.81857446984037	0.03337314804283
C	-2.43046839589246	2.81756606266221	-0.09041422096203
H	-3.37861755181055	0.87745886172949	-0.06854162590754
C	-1.23031207233844	3.51454436768141	-0.05831214845349
H	0.92024199536728	3.36152923214904	0.07039514353193
H	-1.22905360464021	4.60373977986033	-0.08107243990020
H	-3.37481987456578	3.35926695042734	-0.13941565068710

Table 75: Minimum-energy S1 geometry for the naph excimer with C4 linker in the α position.

C	0.021257	1.458853	3.313670
C	1.280921	0.827630	3.273448
C	1.331333	-0.599222	3.244339
C	0.116454	-1.314340	3.233243
C	-1.107272	-0.658328	3.363870
C	-1.170208	0.730752	3.417526
H	-0.015311	2.550364	3.353409
H	0.151725	-2.404618	3.204833
H	-2.028987	-1.239585	3.426874
C	-0.021528	1.418886	0.160992
C	1.229905	0.777218	0.146433
C	1.267027	-0.652162	0.159419
C	0.047298	-1.353818	0.210968
C	-1.177716	-0.683920	0.130104
C	-1.227096	0.702897	0.092004
H	-0.047383	2.511550	0.134153
H	0.071513	-2.444698	0.230203
H	-2.107029	-1.254390	0.092917
C	-2.523425	1.448925	-0.046534
C	-2.492906	1.421451	3.601856
C	-2.934869	2.244728	1.196687
H	-3.326753	0.740954	-0.301728
H	-2.434584	2.144493	-0.896211
C	-3.407695	1.377599	2.374031
H	-3.735301	2.940088	0.906862
H	-2.086588	2.872233	1.514433
H	-3.507128	0.330728	2.045128
H	-4.412235	1.697113	2.686816
H	-2.321688	2.471433	3.884845
H	-3.016638	0.949997	4.447843
C	2.490857	1.550263	3.228966
C	2.588508	-1.232034	3.182463
C	3.771883	-0.490189	3.232217
H	2.626389	-2.322289	3.162262
C	3.723765	0.894744	3.253763
H	2.449584	2.640668	3.244010
H	4.732721	-1.004125	3.230835
H	4.646059	1.474570	3.267284
C	2.447991	1.488877	0.146518
C	2.520793	-1.295184	0.167086
C	3.708145	-0.562830	0.075533
H	2.550664	-2.385968	0.177229
C	3.673079	0.822883	0.066780
H	2.415536	2.579608	0.140140
H	4.599643	1.393943	0.019532
H	4.663200	-1.085950	0.033438

Table 76: Minimum-energy S1 geometry for the naph excimer with C3 linker in the β position.

C	-1.312561	-0.068808	0.183603
C	-0.570414	-1.259462	0.088447
C	0.810032	-1.249127	0.041354
C	1.494281	-0.033641	0.098718
C	1.474358	2.425598	0.015043
C	0.780078	3.627612	-0.081192
C	-0.606070	3.621095	-0.118902
C	-1.304653	2.415326	-0.040260
C	-0.634248	1.183570	0.044661
C	0.796487	1.192181	0.039505
H	-1.107944	-2.208996	0.095643
H	1.363858	-2.186533	0.003380
H	2.584998	-0.014143	0.083561
H	2.565365	2.420405	0.031365
H	1.325546	4.570241	-0.117788
H	-1.156156	4.558195	-0.199722
H	-2.392789	2.432510	-0.083423
C	-1.310731	-0.068076	3.021893
C	-0.568358	-1.258617	3.116716
C	0.812156	-1.248152	3.161703
C	1.496227	-0.032647	3.102468
C	1.476224	2.426654	3.184517
C	0.781991	3.628673	3.281113
C	-0.604092	3.622043	3.321129
C	-1.302693	2.416166	3.244352
C	-0.632314	1.184425	3.159074
C	0.798425	1.193158	3.161994
H	-1.105833	-2.208191	3.110914
H	1.366107	-2.185493	3.199458
H	2.586964	-0.013052	3.115911
H	2.567203	2.421546	3.166415
H	1.327425	4.571379	3.316180
H	-1.154137	4.559141	3.402289
H	-2.390761	2.433267	3.289278
C	-2.802808	-0.143635	0.318374
C	-3.372646	0.470976	1.603969
H	-3.105478	-1.200540	0.262032
H	-3.282073	0.364698	-0.536374
C	-2.801135	-0.143077	2.889084
H	-3.279404	0.365498	3.744245
H	-3.103615	-1.200000	2.946170
H	-4.465293	0.342786	1.604734
H	-3.183938	1.551197	1.603599

Table 77: Minimum-energy S1 geometry for the naph excimer with C4 linker in the β position.

C	-1.35460561508529	-0.03209763538448	-0.03548398210035
C	-0.64990971754333	-1.24285619091311	-0.01926684685288
C	0.73145378024658	-1.27729670242411	0.06430207993967
C	1.45059476726430	-0.08277377408401	0.13941371724976
C	1.50842629616997	2.37718588034757	0.08223948398970
C	0.85225066942618	3.60429901838485	-0.02785137208454
C	-0.53085589621887	3.64134975998368	-0.09140223793415
C	-1.26806978897457	2.45578270854129	-0.05816525884158
C	-0.63366493962954	1.19534769670626	-0.01879981526435
C	0.79472151147171	1.16191702894900	0.05340390067503
H	-1.21334830120570	-2.17538441478645	-0.08355809143551
H	1.25513551547727	-2.23252398060928	0.08272008160502
H	2.54056121817886	-0.09805436021931	0.18370528639313
H	2.59805238539656	2.33979932443177	0.12729404989942
H	1.42813700577402	4.52931836994784	-0.04298114712519
H	-1.05022487958229	4.59693775647164	-0.15867886506459
H	-2.35415716284583	2.50782882996278	-0.11860081881197
C	-1.31692663022457	-0.11791225245350	3.28976545509892
C	-0.53261406354469	-1.28192217292056	3.28460786091977
C	0.84287350241357	-1.23027190217378	3.17503325642060
C	1.48145734860857	0.00637499254027	3.06398841318277
C	1.39071451634542	2.45801427839981	3.06258023802541
C	0.66709930200476	3.65000021867527	3.13596165331264
C	-0.71512677066153	3.60398603608371	3.20309262121380
C	-1.38402982374120	2.37882059053459	3.21594003074586
C	-0.68200892642573	1.15255047770849	3.22363974175765
C	0.74793428274935	1.20660124894091	3.13219976969186
H	-1.03416311841359	-2.24717103283402	3.37679390846372
H	1.42800368189993	-2.14937996786404	3.16538160958340
H	2.56880656884102	0.06100787768509	2.99633555202577
H	2.48009693469878	2.47916436034009	3.01046038723368
H	1.18650531887661	4.60721767465190	3.11606640169495
H	-1.29180099866889	4.52822550094571	3.23367467064451
H	-2.47121637549650	2.37687903473647	3.27354575330861
C	-2.84863970141109	-0.03682554876065	-0.17931345449006
C	-2.79941822606787	-0.29093340139493	3.46947520782175
C	-3.53303424937141	-0.74775165938482	2.20358022288576
H	-3.26418963390782	0.63173247885471	3.84256166664739
H	-2.95382505000884	-1.05085772523423	4.25202010974430
C	-3.61715448745223	0.31839224458940	1.09983460157340
H	-3.17101628826858	-1.03439349204518	-0.51563074380557
H	-3.13746143684796	0.66846931584752	-0.97499448539675
H	-4.66963042537190	0.48292965301358	0.82699190707539
H	-3.24630531667618	1.27928195069287	1.48598145357501
H	-4.54640533450431	-1.06177467994987	2.49335614999221
H	-3.03234144769314	-1.64824341453075	1.81258187681668

Table 78: Minimum-energy S1 geometry for the naph excimer with C2 linker in the β position.

C	-1.28214125103142	-0.05359691301459	0.30696477502155
C	-0.57025242636830	-1.25013032673608	0.11178530835881
C	0.79779162672459	-1.24410713673772	-0.10359792834837
C	1.48643406591063	-0.03787927937876	-0.12448444060324
C	1.47615094634288	2.42366138282226	-0.10290221460054
C	0.78305539402439	3.63370104910604	-0.08838043322795
C	-0.59475006644642	3.63710102250488	0.03892714400978
C	-1.28980174284723	2.43086433091172	0.18982108225258
C	-0.62429865657780	1.18653299801319	0.11541169898624
C	0.79683099827024	1.19112396040269	-0.05683819804224
H	-1.10917067878343	-2.19675823535372	0.17339345290383
H	1.33728224861877	-2.18372390052162	-0.21841672328580
H	2.56919275602862	-0.02225618639284	-0.25764458830827
H	2.56293496838864	2.41480867734270	-0.19908681797563
H	1.32880920111547	4.57348263111853	-0.16732887261653
H	-1.14193872220392	4.57909598871992	0.05278694646978
H	-2.37444278240300	2.45418169813235	0.27930902165544
C	-1.28157285291282	-0.05378982113772	2.89304516239760
C	-0.56889517574988	-1.24982241053291	3.08807849691873
C	0.79919659312191	-1.24282146631285	3.30319231252151
C	1.48704360298920	-0.03617568980614	3.32399053720186
C	1.47521530566828	2.42534872549304	3.30256636584299
C	0.78135573754006	3.63496027901541	3.28819801665739
C	-0.59645187466624	3.63744558686635	3.16100701905263
C	-1.29077550623019	2.43079005627917	3.01009107503553
C	-0.62449646603388	1.18684720549312	3.08442761195540
C	0.79665310081411	1.19240844443609	3.25649625545261
H	-1.10716990465427	-2.19681257609280	3.02652680298185
H	1.33936812501358	-2.18206854570855	3.41788259333733
H	2.56981932498994	-0.01988517596050	3.45694805578418
H	2.56200758389282	2.41716673631987	3.39871311743508
H	1.32650457555590	4.57508841327465	3.36717491832045
H	-1.14424540676711	4.57909495752062	3.14721834824524
H	-2.37542787277591	2.45344310036585	2.92056134775885
C	-2.69777323994672	-0.12971812372231	2.38287014152745
C	-2.69820173398999	-0.12893613292758	0.81768025927627
H	-3.31149692232514	0.69342129604114	2.76980626555940
H	-3.15767493469970	-1.05793011768827	2.74791591475432
H	-3.15875633529270	-1.05647276174220	0.45172702114430
H	-3.31171160230393	0.69500625958757	0.43215314818959

Table 79: Minimum-energy S1 geometry for the benz-naph exciplex with C2 linker in the α position.

C	-0.57307674065769	1.66641664185543	3.71715621124530
C	0.55274715154059	1.21588020169103	3.00504469258048
C	0.85016554725153	-0.14366785593620	2.85725179273255
C	-0.04527044835669	-1.11243882071632	3.39498951468353
C	-1.16494518672742	-0.70590732321936	4.11880603264296
C	-1.46363855916462	0.65490949289427	4.31160321579274
H	1.22930868595324	1.95501628567570	2.57097145710833
H	0.17262724668578	-2.17274271656700	3.27508147473833
H	-1.82992310813751	-1.45066858555026	4.55880030606874
C	1.56373667645360	0.11594568853952	-2.35557465156024
C	2.11763123469287	-0.50638847402674	-1.24431036967422
C	1.31783568954479	-0.91955271293721	-0.18203826452656
C	-0.05525027197218	-0.68966850845953	-0.25240728500750
C	-0.61351941073756	-0.06807934210908	-1.36090325307862
C	0.19443010825454	0.33600389109527	-2.41666585966175
H	2.20545285190686	0.42611075854506	-3.18029174009032
H	3.19414566867915	-0.68427938627000	-1.20068177928778
H	-0.69218624351507	-1.00613735067815	0.57604321960690
H	-1.68959466424435	0.10008791951937	-1.40234011309362
H	-0.24454665557616	0.81964934280004	-3.28891006434120
C	-2.55912915529310	1.10460444036612	5.07334464890354
C	-0.87604143588053	3.02897928334057	3.89351944597325
C	-2.81123619815481	2.46404286686046	5.24427080154282
H	-3.21616435258942	0.36587299911377	5.53424560941582
C	-1.96887301774232	3.43753214107234	4.65620552913812
H	-0.22067208867242	3.77050154461005	3.43441235758376
H	-2.17833850522423	4.49587524663983	4.79614178491686
H	-3.66359820042593	2.78093004519748	5.84390494591477
C	2.11628217438933	-0.58469549794869	2.19995210854670
C	1.93196384721422	-1.56410874842031	1.02777061206304
H	2.91613736278357	-1.97419493480624	0.76140057024717
H	1.31336484296679	-2.41147075627379	1.35667208689325
H	2.74193404030232	-1.08586537915725	2.95993881424902
H	2.67844111445283	0.29405760325981	1.85270614773386

Table 80: Minimum-energy S1 geometry for the benz-naph exciplex with C3 linker in the α position.

C	-0.09851457421135	1.28735248798438	3.00702156153054
C	1.11826290853803	0.58747615746020	2.92935379104311
C	1.16856554958905	-0.82257417302603	3.02680890160900
C	-0.01085361756422	-1.53707916397413	3.29268450135230
C	-1.21890277917736	-0.86883096426693	3.43201849006699
C	-1.30281833638597	0.54257279460732	3.29024787088380
H	2.03998358810554	1.15033503601304	2.77615415179158
H	0.03750961348205	-2.62266263427712	3.38496682587103
H	-2.13290858450222	-1.42114458808771	3.65567561726404
C	0.28802108822034	1.62489326395810	-0.08198571009122
C	1.40657656112321	0.81373125483540	-0.01717697048441
C	1.27571449241765	-0.57869635763328	0.17235377876343
C	-0.00349378934014	-1.13608860031964	0.26301725918891
C	-1.12796745860016	-0.31875594583414	0.26061655726065
C	-0.98065055831768	1.06245435207033	0.10212717748421
H	0.38630125559214	2.69799519281442	-0.23658791718952
H	2.40536984085914	1.24084799369203	-0.12288214711278
H	-0.10336109487118	-2.21468253714719	0.38159846145090
H	-2.12065737711085	-0.74874135315471	0.38186936420847
H	-1.85759932193047	1.70901900218584	0.12928706321701
C	2.49611418233641	-1.43136968452305	0.31153309288088
C	2.47298843314007	-1.53510758951001	2.86572459824259
C	3.26602519563265	-1.15315136846513	1.61192845039314
H	2.29393940498923	-2.62096423917188	2.87290604681739
H	3.11048583983308	-1.31226516671636	3.74110155331302
H	4.21105671222753	-1.71446203902204	1.60056329264086
H	3.53526891781677	-0.08721967579005	1.64872633982461
H	3.17434563595326	-1.23969687711381	-0.53534208774419
H	2.21267284231506	-2.49364781849668	0.27350385652717
C	-2.50797400399860	1.25387008229553	3.41498517710158
C	-0.18891708869054	2.67850123469038	2.78365867500083
C	-2.55476514950726	2.63686169825340	3.22153307874158
H	-3.41957826682673	0.70584200661102	3.65780532499223
C	-1.40596550315129	3.35605344978625	2.90343567281205
H	0.72782611587182	3.22623934561488	2.55879753841242
H	-1.45430061847001	4.43310378016851	2.75146918488238
H	-3.50718005538700	3.15749164348886	3.32755157705339

Table 81: Minimum-energy S1 geometry for the benz-naph exciplex with C2 linker in the β position.

C	-1.68976507581247	-1.41253199399279	5.28514849370661
C	-0.56236534890743	-0.60191642300444	5.29705465027967
C	0.39644172827460	-0.74609831968712	4.30159354230461
C	0.22830822784295	-1.69585973062689	3.30326075248646
C	-0.89854664141057	-2.51746918169281	3.28156163027186
C	-1.85382761797125	-2.36116062894985	4.28291949439397
H	-2.44451226937541	-1.31026567937600	6.06493579008773
H	-0.42807221006530	0.13987001366546	6.08404187462939
H	1.28525339213827	-0.11508729623608	4.30342169340034
H	0.98318625306116	-1.80596977788309	2.52237522634597
H	-2.73774860706827	-3.00244341480319	4.28149308179868
C	-0.95748549768422	1.72584556270184	-0.72767319275468
C	-0.12603157995919	2.70487287858211	-1.26980820090233
C	1.20956035363153	2.37670338782577	-1.60483352829667
C	1.70080223029586	1.08810811693176	-1.40375085692956
C	1.32861460530455	-1.25161353527449	-0.67897371469895
C	0.49469942933235	-2.22912071856837	-0.13813444380758
C	-0.83468731448372	-1.89887705166514	0.25364268803669
C	-1.30288611530326	-0.59593181373031	0.05111953168202
C	-0.50004308624820	0.41313570411921	-0.51006023303936
C	0.88336157566969	0.06785818803093	-0.87996700994182
H	-1.98577806738341	1.96884063251727	-0.45598424380805
H	-0.49673626856643	3.71463070809478	-1.43277552876431
H	1.86440223342652	3.14138301056256	-2.02077151258654
H	2.73309466908274	0.85166845404348	-1.66535198284671
H	2.35166264756044	-1.50290503026303	-0.96328237400491
H	0.85936733372379	-3.24632217256926	-0.00061336605764
H	-2.32207029256338	-0.34787708542022	0.35506682527734
C	-1.09191112761734	-3.52964430796231	2.18653170908279
C	-1.69798491519119	-2.92970785107123	0.90206863754450
H	-1.75574046339909	-4.33162249451526	2.53942709352611
H	-0.12801443135381	-3.99899104718078	1.94284807298392
H	-2.68113070517745	-2.49487709273244	1.13267505129582
H	-1.86816704380305	-3.75913400987006	0.19321434930466

Table 82: Minimum-energy S1 geometry for the benz-naph exciplex with C3 linker in the β position.

C	-0.799249	0.037763	3.101277
C	0.566958	0.100058	3.225574
C	1.321858	-1.088312	3.197059
C	0.665882	-2.329127	3.228240
C	-0.699916	-2.390514	3.108358
C	-1.458845	-1.205301	2.941515
H	-1.386834	0.955374	3.056140
H	1.067445	1.065224	3.283437
H	2.407122	-1.045252	3.279725
H	1.249006	-3.246297	3.309250
H	-1.206897	-3.356054	3.107741
C	-1.501434	1.179321	-0.013571
C	-0.830193	2.405818	-0.046316
C	0.551662	2.448737	0.025213
C	1.270405	1.255634	0.121282
C	1.353579	-1.200922	0.256976
C	0.711385	-2.444664	0.127286
C	-0.659769	-2.500660	0.095060
C	-1.445026	-1.317082	0.196448
C	-0.806206	-0.036183	0.081829
C	0.624879	0.012577	0.136713
H	-2.588535	1.181270	-0.070122
H	-1.404261	3.328922	-0.125639
H	1.076433	3.403366	0.006855
H	2.360146	1.276134	0.180167
H	2.442998	-1.148958	0.280766
H	1.302820	-3.358876	0.083652
H	-1.172454	-3.461085	0.017615
C	-2.943397	-1.274836	2.787130
C	-2.925057	-1.481045	0.265369
C	-3.389268	-2.113349	1.587398
H	-3.254295	-2.142616	-0.555720
H	-3.445826	-0.525667	0.129633
H	-2.971389	-3.127696	1.673185
H	-4.483889	-2.219980	1.585700
H	-3.351491	-0.256459	2.699485
H	-3.384867	-1.716354	3.697810

Table 83: Minimum-energy S1 geometry for the benz-naph exciplex with C4 linker in the β position.

C	-0.348609	-0.668884	4.328443
C	0.696343	-0.855530	5.213841
C	0.698045	-1.948572	6.065105
C	-0.351038	-2.848722	6.020227
C	-1.395401	-2.655772	5.130423
C	-1.409837	-1.564956	4.274472
H	-0.348633	0.195856	3.664510
H	1.514927	-0.138940	5.244527
H	1.516677	-2.094840	6.766620
H	-0.360598	-3.708093	6.687894
H	-2.223279	-3.363990	5.104842
C	-1.904560	1.265558	-0.735396
C	-1.413954	2.562425	-0.673460
C	-0.046020	2.820755	-0.909809
C	0.806711	1.776806	-1.236041
C	1.189491	-0.607871	-1.683856
C	0.711803	-1.908943	-1.741788
C	-0.625820	-2.183836	-1.393335
C	-1.512260	-1.172907	-1.020143
C	-1.069676	0.169377	-1.014566
C	0.350404	0.453025	-1.319521
H	-2.966189	1.097583	-0.577912
H	-2.088408	3.383555	-0.444952
H	0.332787	3.837688	-0.852920
H	1.858161	1.974982	-1.438781
H	2.228761	-0.392936	-1.927119
H	1.372218	-2.721801	-2.031979
H	-0.981778	-3.211845	-1.409280
C	-2.899640	-1.544542	-0.590545
C	-2.526760	-1.347959	3.295888
C	-2.155516	-1.705668	1.861345
H	-2.823180	-0.289643	3.322348
H	-3.407985	-1.926125	3.604806
C	-3.218573	-1.250738	0.879532
H	-1.986410	-2.789127	1.778536
H	-1.198525	-1.229056	1.609543
H	-3.367414	-0.172968	1.021094
H	-4.179361	-1.723990	1.125996
H	-3.034001	-2.617314	-0.776979
H	-3.639686	-1.028613	-1.220080

Table 84: Minimum-energy S1 geometry for the benz-naph exciplex with C4 linker in the α position.

C	-0.01971122062598	1.34045220881994	3.19640896451447
C	1.21053947169992	0.65793861772393	3.16333004483490
C	1.20112100162781	-0.77525035384812	3.39982916935571
C	-0.04152834310319	-1.43615868570675	3.55769338590339
C	-1.24139840016272	-0.73320635447945	3.55735299047511
C	-1.23446221504378	0.66961474845136	3.41221869208074
H	-0.02469038371984	2.42674496323257	3.08818150700476
H	-0.03383549008088	-2.51484695192102	3.72322057772627
H	-2.18747385944142	-1.24671648180094	3.73036873841468
C	-0.01674726274791	1.61502020220201	-0.01876547744849
C	1.25184875782658	1.07579344402759	0.09156197967002
C	1.40052524307127	-0.28388943490982	0.38966503029716
C	0.27651323237839	-1.10143725000903	0.52460102031311
C	-0.99561851244352	-0.55932260413146	0.37309031609884
C	-1.15744934658784	0.80202946774935	0.11239721592119
H	-0.14720844671301	2.67501476698697	-0.24456963186064
H	2.13538796141222	1.70011671504759	-0.03185589808170
H	2.39799193427236	-0.69771231275033	0.53563089608875
H	0.40046126179712	-2.16213955322431	0.73629552423990
H	-1.87776119759616	-1.19517153136057	0.45144443081341
C	-2.51827241275114	1.40131975540831	-0.07871179135774
C	-2.51573524730809	1.43185691597939	3.54493179897459
C	-3.03900391838868	2.20011359513318	1.12233203271349
H	-3.24015744699146	0.60510978594602	-0.31527137363631
H	-2.48308682806700	2.07082998422327	-0.95167632345604
C	-3.46054113682965	1.35921157115192	2.33615776779876
H	-3.90221485214778	2.78515873230186	0.77508830838625
H	-2.27463330703493	2.93381186940707	1.42505481826720
H	-3.58290101764484	0.30565057046832	2.03865847619019
H	-4.44921185775596	1.69756399841365	2.67700245955933
H	-2.29581575209098	2.48962614007884	3.75566970417265
H	-3.05370385553257	1.03608807734383	4.42075212171160
C	2.43840071912847	1.30543878968669	2.90876164739542
C	2.44163512978381	-1.43833584566792	3.47380372463094
C	3.63798988449146	-0.75503444562206	3.25254921971924
H	2.45563364804640	-2.50574869965933	3.69831634794980
C	3.65030722471683	0.61048138059242	2.95313363767208
H	2.42358542069553	2.37949959535961	2.71649942397319
H	4.58036931892986	-1.30043474114273	3.31513805755300
H	4.59187410093131	1.12636935049814	2.77509146542078

Table 85: Minimum-energy S1 geometry for the benz excimer with C4 linker in the α position.

C	0.03558698776110	1.40281189331993	3.29418888337006
C	1.22993441349433	0.67506720373243	3.21819238638184
C	1.18718503626369	-0.72679279736313	3.18033423335792
C	-0.04401837679885	-1.39695202713556	3.20179351628644
C	-1.23541672703408	-0.66266140269160	3.25409523847168
C	-1.20541236122556	0.74484755019959	3.32017749892372
H	0.05962235783653	2.49026979069386	3.36891770904145
H	2.18834679611649	1.19128750186528	3.22729963119437
H	2.11482917689630	-1.29755322927017	3.16197832519344
H	-0.07101849833413	-2.48530938065847	3.19700832669503
H	-2.19474275900576	-1.17856764309924	3.30740633862069
C	-0.04226337934786	1.40138093928930	0.23080855929348
C	1.18859374489467	0.73694283241853	0.29726471742411
C	1.22415639026439	-0.66447992120069	0.31555726805697
C	0.03153804195892	-1.40268059851617	0.28123374083332
C	-1.19703197149334	-0.73181847289984	0.22571617450672
C	-1.24687580861860	0.67150313176148	0.17887625974397
H	-0.07468681381304	2.48958403813128	0.16691900091110
H	2.11779906299754	1.30428373726928	0.30112860948779
H	2.18253176510365	-1.18211024788350	0.33090642311117
H	0.06345936534844	-2.49079361688460	0.27271159462436
H	-2.12765133022174	-1.29647459177248	0.16400280803023
C	-2.54751396234834	1.38458860136857	-0.03429051615304
C	-2.47405176084390	1.51300214755547	3.53480248976511
C	-3.02288515759902	2.26152601974111	1.12789218234069
H	-3.33106961887882	0.64609952633466	-0.26249706446371
H	-2.44549742338651	2.02204584200931	-0.92819719218463
C	-3.47125932387897	1.48590956465102	2.37263878676950
H	-3.85981184502480	2.87113028126522	0.75837544414337
H	-2.22406601675633	2.96967190928789	1.40097731394547
H	-3.68589905946432	0.44020659416893	2.09964848858275
H	-4.41757356577807	1.90643012310130	2.74172824274293
H	-2.22715434473987	2.56091906580841	3.76343017452213
H	-2.97456403434412	1.10503463540261	4.42864440642956

Table 86: Minimum-energy S1 geometry for the benz excimer with C2 linker in the α position.

C	-0.007180	1.437151	3.159417
C	1.184647	0.722069	2.986941
C	1.162570	-0.680642	2.868466
C	-0.059259	-1.364579	3.020352
C	-1.254310	-0.651437	3.183428
C	-1.225896	0.748649	3.223274
H	0.010813	2.522986	3.234507
H	2.139533	1.244737	2.930181
H	-2.201258	-1.180966	3.271814
H	-2.154691	1.304888	3.345795
C	-0.038630	1.379791	-0.013818
C	1.153018	0.663389	0.155947
C	1.125193	-0.734739	0.322468
C	-0.103516	-1.414938	0.219936
C	-1.297872	-0.700160	0.060215
C	-1.262452	0.697876	-0.024631
H	-0.016407	2.462435	-0.125191
H	2.111880	1.181528	0.173243
H	-0.115622	-2.502674	0.288668
H	-2.249585	-1.226238	0.010834
H	-2.190702	1.255776	-0.143797
C	2.347071	-1.460880	0.813007
C	2.378644	-1.413747	2.374187
H	3.252736	-0.996080	0.399005
H	2.327785	-2.502361	0.462937
H	-0.065508	-2.454122	2.989767
H	3.288646	-0.905613	2.722069
H	2.397609	-2.432388	2.786287

Table 87: Minimum-energy S1 geometry for the benz excimer with C3 linker in the α position.

C	-0.004156	1.401213	3.130486
C	1.207543	0.705096	3.056070
C	1.215019	-0.703139	3.001381
C	-0.007889	-1.396667	3.057834
C	-1.223449	-0.702738	3.118690
C	-1.215902	0.696874	3.141323
H	-0.008849	2.488961	3.179825
H	2.153666	1.246486	3.060041
H	0.004496	-2.486820	3.051045
H	-2.165282	-1.246670	3.159920
H	-2.156927	1.243554	3.195730
C	-0.003191	1.401167	0.069489
C	1.208394	0.704793	0.143274
C	1.215581	-0.703423	0.198004
C	-0.007464	-1.396719	0.141894
C	-1.222904	-0.702547	0.081595
C	-1.215086	0.697071	0.059137
H	-0.007686	2.488922	0.020266
H	2.154623	1.245996	0.139162
H	0.004707	-2.486873	0.148868
H	-2.164869	-1.246287	0.040810
H	-2.156023	1.243953	0.005231
C	2.508652	-1.445372	0.326565
C	2.508289	-1.444919	2.873288
C	3.286568	-1.096228	1.599958
H	2.311747	-2.527571	2.896569
H	3.148797	-1.214533	3.741410
H	4.246935	-1.631923	1.600191
H	3.525155	-0.022373	1.599797
H	3.149392	-1.215435	-0.541500
H	2.311941	-2.528006	0.303709

Table 88: Minimum-energy S1 geometry for the anth-naph exciplex with C2 linker in the β position.

C	1.39614470624040	2.36341445890957	0.35954016607417
C	0.79836496304323	3.60172564223411	0.12828940151107
C	-0.55939166244136	3.71443365101734	-0.16783112621249
C	-1.34558233567317	2.58104888110009	-0.22304866714102
C	1.17162604287963	-0.12126440653397	0.31340676745883
C	-1.56266344064272	0.13097535403643	-0.12492109292450
C	0.62917190152450	1.18204688883976	0.17801793658619
C	-0.77255490313007	1.30027405444797	-0.07259261879656
C	-0.99223711811605	-1.12957228701147	-0.03088827064047
C	0.37802719509291	-1.25729019945054	0.16921759674105
H	1.40612253669915	4.50328046843942	0.22552953591875
H	-1.00258646896247	4.69825992276684	-0.31900994928012
H	-2.41697065075121	2.65575875760406	-0.41521123071160
H	2.24332770682941	-0.24627307463327	0.44980174423435
H	-2.63757481516996	0.23886999748488	-0.27908309510898
C	1.35110763368255	2.54756761095156	3.00367096262061
C	0.60074642631600	3.71640462204392	3.18588887796837
C	-0.76885982504831	3.66337348100140	3.42252935778329
C	-1.41587987567881	2.43618217510299	3.45864810560561
C	-1.25361106448883	-2.49146787915827	3.33316527071805
C	-0.51995378040382	-3.66666940472682	3.32154978137883
C	0.87753413560058	-3.61791354351149	3.28181922170177
C	1.52984196151111	-2.39526104077328	3.23381989543323
C	1.44283694660007	0.07405582428956	3.10583623244454
C	-1.33078503785776	-0.01820608769538	3.35130698721937
C	0.73558298587036	1.28510503657366	3.18485026368386
C	-0.69315025715785	1.22935604966068	3.35250705237217
C	-0.61716953822208	-1.23468856523604	3.31419712341502
C	0.81024867826550	-1.18701924920361	3.23763844101186
H	1.10208199644854	4.68130549281604	3.09780595144969
H	-1.33833581361913	4.58472397140974	3.54140715796776
H	-2.49692079206135	2.38603448865174	3.59864984639723
H	-2.34395229853003	-2.52357401623810	3.37478605708276
H	-1.03096506464518	-4.62875844358725	3.34834106161258
H	1.45470545014312	-4.54244009273611	3.28277632602809
H	2.62004851860721	-2.35557416986910	3.18853461041930
H	2.53155677295576	0.09112711452885	3.02626225787753
H	-2.42040713893344	-0.05082199840715	3.42798815297198
C	2.78964533161765	2.32635885399344	0.93618472848280
C	2.75283382490447	2.65813462014059	2.46549258301063
H	3.42205932317395	3.06278495265003	0.42130728342849
H	3.25802442766093	1.34981973101584	0.77414429274942
H	3.45408032227006	2.00678338152910	3.00691786485273
H	3.09961373802239	3.68858612937629	2.62008355011895
H	0.82703631377581	-2.24533318494458	0.26202417885778
H	-1.61837795820170	-2.01910396889949	-0.09240057437297

Table 89: Minimum-energy S1 geometry for the anth-naph exciplex with C4 linker in the γ position.

C	1.74427780316109	2.17430820017258	-0.12470462009408
C	1.27934425980997	3.47074359395306	-0.25009962296255
C	-0.09449552077656	3.72726783138234	-0.23771025248153
C	-0.99054781911515	2.68348259217648	-0.08368569403866
C	1.30873408294014	-0.24460405723941	0.10591356278227
C	-1.45900834428130	0.25574903816873	0.21060895807989
C	0.85164096715703	1.08997656305295	-0.00812779511047
C	-0.54902977591499	1.35028788048760	0.03350693275819
C	-0.95927148621422	-1.04691481236025	0.16790959850498
C	0.40876436384204	-1.30288487609460	0.11495050391011
H	2.81649762330386	1.96959576917409	-0.13476123088924
H	1.98678036157824	4.29363026312519	-0.35425330149028
H	-0.46042868099995	4.74858855225247	-0.33586014767700
H	-2.05698562246934	2.89946047516826	-0.06370217788795
H	2.38360241769322	-0.43243196920744	0.09541516061836
C	0.98098749534136	2.60329941465766	3.04387780864920
C	0.19204629423331	3.74733371793508	3.09264034840049
C	-1.19027530703655	3.61569029157660	3.17904196154748
C	-1.78665346153979	2.35478096293257	3.21886020180614
C	-1.21146095551632	-2.56448043727398	3.72367751096268
C	-0.36311279015649	-3.65548593769553	3.84598067340610
C	1.01287077999086	-3.50310736632493	3.65337072979416
C	1.52873347242424	-2.25036158219558	3.37317540522362
C	1.21583329529783	0.16720600966044	3.04676968343834
C	-1.57839007045429	-0.13842284741873	3.24448277366502
C	0.41313916344562	1.31619503267296	3.10663644321715
C	-1.01872582894325	1.16824165298635	3.20229408476473
C	-0.72315136842492	-1.27516599047213	3.41594969197920
C	0.69237943753371	-1.12017465306865	3.27797006143400
H	2.06653721563299	2.68452005905717	2.97386635023143
H	0.65062473956829	4.73460306247943	3.05555480463387
H	-1.82135499526478	4.50382837534697	3.21756222280901
H	-2.86894626765606	2.29924892469168	3.32255882600086
H	-2.27603856146074	-2.70984152753467	3.89894222039850
H	-0.77474393433877	-4.63359764497072	4.09384431102887
H	1.67670923478382	-4.36342236933600	3.73632472856234
H	2.60350607530791	-2.11184988115116	3.24148334788502
H	2.29847216875253	0.28648516063099	2.95834401749605
C	-2.91293942513813	0.56976001707511	0.37876985809454
C	-3.06423959360711	-0.37823646313354	3.24037582292916
H	-3.61974676515723	0.56724542979089	3.22289760149810
H	-3.33954751638983	-0.86254826520907	4.19285407183824
C	-3.55988935453316	-1.27911733148208	2.08743436054091
C	-3.85774990009185	-0.56303749152213	0.76534598886574
H	-3.28956533296218	1.03753292812381	-0.54771820635706
H	-2.98344953722798	1.37100475174254	1.13833510790471
H	-4.47914242097257	-1.79164248290613	2.40896679125062
H	-2.81686085057909	-2.06910341151150	1.92710516899685
H	-3.89848193349993	-1.31231734685817	-0.04137793730772
H	-4.86749407507864	-0.12703710424455	0.81647293961269
H	-1.65265332047942	-1.88525665088618	0.22044680443385
H	0.76887956448247	-2.33031405037690	0.14147354634307