Supporting Information

Di-8-ANEPPS Emission Spectra in Phospholipid / Cholesterol Membranes: A Theoretical Study

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1. Ground state geometry of di-8-ANEPPS (CASSCF(6,6) / ANO-L (C,N,O: 4*s*3*p*2*d*; H: 2*s*1*p*)

C	4.094155	-1.153976	0.000000
C	3.663248	0.192393	0.000000
C	4.675226	1.177085	0.000000
C	5.983602	0.822221	0.000000
C	5.416524	-1.445189	0.000000
C	2.288542	0.614303	0.000000
C	1.232052	-0.217260	0.000000
C	-0.172630	0.139669	0.000000
C	-1.105794	-0.880310	0.000000
C	-2.491547	-0.615911	0.000000
C	-2.946352	0.715125	0.000000
C	-1.975156	1.761717	0.000000
C	-0.638040	1.489343	0.000000
C	-3.465759	-1.661961	0.000000
C	-4.780411	-1.383422	0.000000
C	-5.246643	-0.027658	0.000000
C	-4.335040	0.987842	0.000000
N	-6.590716	0.192230	0.000000
N	6.340193	-0.470273	0.000000
H	-7.231717	-0.562059	0.000000
H	7.306998	-0.712278	0.000000
H	-6.957739	1.112231	0.000000
H	-3.136473	-2.685214	0.000000
H	-5.502214	-2.179667	0.000000
H	-4.667388	2.009920	0.000000
H	-2.311678	2.781798	0.000000
H	0.059835	2.303658	0.000000
H	-0.777274	-1.904558	0.000000
H	2.135247	1.675670	0.000000
H	1.411355	-1.277461	0.000000
H	6.779933	1.539784	0.000000
H	4.419572	2.217643	0.000000
H	3.400511	-1.967776	0.000000
H	5.785815	-2.451463	0.000000

2. 1A' excited state geometry of di-8-ANEPPS (CASSCF(6,6) / ANO-L (C,N,O: 4*s*3*p*2*d*; H: 2*s*1*p*)

c	4.165327	-1.164139	0.000000
C	3.671233	0.175879	0.000000
C	4.653605	1.203380	0.000000
C	5.969591	0.910570	0.000000
C	5.490232	-1.404996	0.000000
C	2.276713	0.516493	0.000000
C	1.239207	-0.332606	0.000000
s	-0.189187	0.054354	0.000000
C	-1.163112	-0.943127	0.000000
C	-2.538346	-0.641115	0.000000
C	-2.960369	0.713038	0.000000
C	-1.950434	1.739440	0.000000
C	-0.623635	1.416764	0.000000
C	-3.533397	-1.668613	0.000000
C	-4.848797	-1.379183	0.000000
C	-5.272589	-0.017385	0.000000
C	-4.302387	1.010850	0.000000
N	-6.568207	0.278241	0.000000
N	6.391672	-0.386987	0.000000
H	-7.258715	-0.436403	0.000000
H	7.363348	-0.589525	0.000000
H	-6.884008	1.220479	0.000000
H	-3.212858	-2.693651	0.000000
H	-5.587503	-2.158027	0.000000
H	-4.629596	2.034048	0.000000
H	-2.259311	2.767516	0.000000
H	0.096498	2.209181	0.000000
H	-0.865171	-1.974991	0.000000
H	2.084642	1.574054	0.000000
H	1.414399	-1.392010	0.000000
H	6.733513	1.661075	0.000000
H	4.359552	2.235072	0.000000
H	3.502670	-2.004645	0.000000
H	5.895663	-2.396836	0.000000

3. 2A' excited state geometry of di-8-ANEPPS (CASSCF(6,6) / ANO-L (C,N,O: 4*s*3*p*2*d*; H: 2*s*1*p*)

C	4.207059	-1.169083	0.000000
C	3.688019	0.172078	0.000000
C	4.673435	1.212311	0.000000
C	5.984940	0.929306	0.000000
C	5.529927	-1.391050	0.000000
C	2.312028	0.489464	0.000000
C	1.267823	-0.373959	0.000000
C	-0.150021	0.008945	0.000000
C	-1.146235	-0.956944	0.000000
C	-2.553334	-0.643480	0.000000
C	-2.991005	0.716280	0.000000
C	-1.997957	1.681132	0.000000
C	-0.606484	1.341706	0.000000
C	-3.527737	-1.639404	0.000000
C	-4.848621	-1.299949	0.000000
C	-5.306421	0.058241	0.000000
C	-4.371658	1.041561	0.000000
N	-6.648066	0.285987	0.000000
N	6.426212	-0.364642	0.000000
H	-7.297357	-0.461587	0.000000
H	7.399120	-0.556655	0.000000
H	-7.009323	1.208750	0.000000
H	-3.243809	-2.674233	0.000000
H	-5.585336	-2.083315	0.000000
H	-4.658999	2.076233	0.000000
H	-2.262993	2.721884	0.000000
H	0.089128	2.156164	0.000000
H	-0.877373	-1.996667	0.000000
H	2.108985	1.546542	0.000000
H	1.442229	-1.432576	0.000000
H	6.741327	1.688014	0.000000
H	4.372086	2.242110	0.000000
H	3.554944	-2.017985	0.000000
H	5.945705	-2.378983	0.000000

4. CHARMM topology entry for di-8-ANEPPS

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RESI DIA          0.00  !  Di-8-ANEPPS
GROUP                   ! Naphthalene group
ATOM CE3  CA     -0.27  !
ATOM CZ3  CBD     0.09
ATOM CH2  CA     -0.10
ATOM CZ2  CA     -0.27
ATOM CE2  CBN     0.16
ATOM CD2  CBN     0.18
ATOM CZ1  CA     -0.44
ATOM CD3  CBD     0.39
ATOM CE4  CA     -0.31
ATOM CD4  CA     -0.19
ATOM HC7  HP      0.14
ATOM HC8  HP      0.20
ATOM HC9  HP      0.22
ATOM HC10 HP      0.15
ATOM HC11 HP      0.13
ATOM HC12 HP      0.17
GROUP                   !Ethylene group
ATOM CC1  CC2    -0.15
ATOM CC2  CC2    -0.15
ATOM HC5  HE2     0.15
ATOM HC6  HE2     0.15
GROUP                   !Pyridinium group
ATOM CP1  CAP    -0.115
ATOM CP2  CAP    -0.115
ATOM CP3  CAP     0.170
ATOM NP   NR2     0.170
ATOM CP4  CAP     0.170
ATOM CP5  CAP    -0.115
ATOM HC1  HP      0.115
ATOM HC2  HP      0.150
ATOM HC3  HP      0.115
ATOM HC4  HP      0.115
GROUP                   !Alkyl group before SO3-
ATOM CA1  CT2     0.03
ATOM CA2  CT1     0.25
ATOM CA3  CT1    -0.15
ATOM HC13 HA      0.01
ATOM HC14 HA      0.07
ATOM HC15 HA     -0.03
ATOM HC16 HA     -0.07
ATOM HC17 HA      0.03
ATOM HC18 HA      0.04
GROUP                   !SO3- group
ATOM S    S       0.95
ATOM OS1  OSD    -0.65
ATOM OS2  OSD    -0.65
ATOM OS3  OSD    -0.65
GROUP
ATOM NA1  N      -0.49  !Amine Nitrogen
GROUP
ATOM CB1  CT1     0.33
ATOM CB2  CT1     0.06
ATOM CB3  CT1     0.01
ATOM CB4  CT1     0.16
ATOM HD16 HA     -0.07
ATOM HD17 HA     -0.03
ATOM HD18 HA     -0.03
ATOM HD19 HA     -0.05
ATOM HD20 HA     -0.03
ATOM HE1  HA     -0.03
ATOM HE2  HA     -0.05
ATOM HE3  HA     -0.04
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GROUP
ATOM CB5  CT1     0.01
ATOM CB6  CT1     0.07
ATOM CB7  CT1     0.23
ATOM CB8  CT1    -0.16
ATOM HE4  HA     -0.03
ATOM HE5  HA     -0.02
ATOM HE6  HA     -0.03
ATOM HE7  HA     -0.05
ATOM HE8  HA     -0.06
ATOM HE9  HA     -0.06
ATOM HE10 HA      0.02
ATOM HE11 HA      0.02
ATOM HE12 HA      0.03
GROUP
ATOM CF1  CT1     0.41
ATOM CF2  CT1     0.02
ATOM CF3  CT1     0.01
ATOM CF4  CT1     0.14
ATOM HC19 HA     -0.08
ATOM HC20 HA     -0.06
ATOM HD1  HA     -0.03
ATOM HD2  HA     -0.04
ATOM HD3  HA     -0.04
ATOM HD4  HA     -0.02
ATOM HD5  HA     -0.04
ATOM HD6  HA     -0.03
GROUP
ATOM CF5  CT1     0.00
ATOM CF6  CT1     0.06
ATOM CF7  CT1     0.19
ATOM CF8  CT1    -0.07
ATOM HD7  HA     -0.02
ATOM HD8  HA     -0.03
ATOM HD9  HA     -0.03
ATOM HD10 HA     -0.03
ATOM HD11 HA     -0.06
ATOM HD12 HA     -0.05
ATOM HD13 HA      0.00
ATOM HD14 HA      0.00
ATOM HD15 HA      0.00
BOND CZ3 CC1   CC2 CP1   NP CA1
BOND CA1 CA2   CA2 CA3   CA3 S
BOND CD3 NA1   NA1 CB1   CB1 CB2
BOND CB2 CB3   CB3 CB4   CB4 CB5
BOND CB5 CB6   CB6 CB7   CB7 CB8
BOND NA1 CF1   CF1 CF2   CF2 CF3
BOND CF3 CF4   CF4 CF5   CF5 CF6
BOND CF6 CF7   CF7 CF8   CP3 HC1
BOND CP2 HC2   CP5 HC3   CP4 HC4
BOND CC2 HC5   CC1 HC6   CD4 HC7
BOND CE4 HC8   CZ1 HC9   CZ2 HC10
BOND CH2 HC11  CE3 HC12  CA1 HC13
BOND CA1 HC14  CA2 HC15  CA2 HC16
BOND CA3 HC17  CA3 HC18  CB1 HD16
BOND CB1 HD17  CB2 HD18  CB2 HD19
BOND CB3 HD20  CB3 HE1   CB4 HE2
BOND CB4 HE3   CB5 HE4   CB5 HE5
BOND CB6 HE6   CB6 HE7   CB7 HE8
BOND CB7 HE9   CB8 HE10  CB8 HE11
BOND CB8 HE12  CF1 HC19  CF1 HC20
BOND CF2 HD1   CF2 HD2   CF3 HD3
BOND CF3 HD4   CF4 HD5   CF4 HD6
BOND CF5 HD7   CF5 HD8   CF6 HD9
BOND CF6 HD10  CF7 HD11  CF7 HD12
BOND CF8 HD13  CF8 HD14  CF8 HD15
BOND CZ3 CH2   CZ2 CE2   CD2 CE3
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BOND CE2 CZ1   CD3 CE4   CD4 CD2
BOND CP2 CP3   NP CP4    CP5 CP1
DOUBLE CE3 CZ3  CH2 CZ2  CE2 CD2
DOUBLE CZ1 CD3  CE4 CD4  CC1 CC2
DOUBLE CP1 CP2  CP3 NP  CP4 CP5
DOUBLE S   OS1  S   OS2  S  OS3
ACCEPTOR OS1
ACCEPTOR OS2
ACCEPTOR OS3
IC CE3  CH2  CZ3  CE3   2.4220  30.40      0.00   117.88    1.3865
IC CZ3  CZ2  CH2  CZ3   2.4370  30.59      0.00   120.60    1.4406
IC CH2  CE2  CZ2  CH2   2.4374  28.34      0.00   122.01    1.3646
IC CZ2  CZ3  CH2  CZ2   2.4370  28.81      0.00   120.60    1.3646
IC CE2  CZ1  CZ3  CH2   1.4144   0.55     17.17    58.97    1.4406
IC CD2  CD3  CZ1  CZ3   2.8624  59.30     -0.13   121.31    4.2662
IC CZ1  CE4  CD3  CZ1   2.4269  30.62      0.00   117.66    1.3955
IC CD3  CD4  CE4  CD3   2.4500  30.28      0.00   120.95    1.4406
IC CE4  CC1  CD4  CE4   6.1742   6.15      0.00   151.26    1.3747
IC CD4  CC2  CC1  CD4   6.2158  17.05      0.00   158.32    4.9333
IC CC1  CP1  CC2  CC1   2.4945  26.26      0.00   125.65    1.3583
IC CC2  CC1  CC2  CP1   1.3583   0.00      0.00   125.65    1.4455
IC CP1  CP3  CC1  CC2   2.4296   2.87    177.61    25.30    1.3583
IC CP2  NP   CP3  CC1   2.3817  29.38      0.03    93.98    4.9181
IC CP3  CP4  NP   CP3   2.3587  29.85      0.00   120.15    1.3579
IC NP   CP4  CP5  CC2   1.3636 120.01      1.40   149.86    2.5331
IC CP4  CA1  CP4  CP5   2.4834   0.00      0.00   151.12    1.3767
IC CP5  CA2  CA1  CP4   4.5404  50.39     10.89   110.31    2.4834
IC CA1  CA3  CA2  CA1   2.5945  32.70      0.00   115.08    1.5474
IC CA2  S    CA3  CA2   2.8098  30.08      0.00   112.80    1.5275
IC CA3  OS1  S    CA3   2.6369  42.73      0.00   103.39    1.8394
IC S    NA1  OS1  S    14.7672   5.85      0.00    95.04    1.5109
IC OS1  CB1  NA1  OS1  15.4462  50.20      0.00   125.39   14.5576
IC NA1  CB2  CB1  NA1   2.5149  31.85      0.00   114.23    1.4554
IC CB1  CE2  CZ2  CH2   4.2949 121.60   -178.24   122.01    1.3646
IC CB2  CB4  CE2  CZ2   2.5564  32.96    163.72    95.93    1.4219
IC CB3  CB5  CB4  CE2   2.5623  33.47     52.95   136.08    6.7373
IC CB4  CB6  CB5  CB4   2.5664  33.38      0.00   113.18    1.5360
IC CB5  CB7  CB6  CB5   2.5718  33.22      0.00   113.66    1.5383
IC CB6  CB7  CB6  CB5   1.5341   0.00      0.00   113.66    1.5383
IC CB7  CB7  CB6  CB5   0.0000   0.00      0.00   113.66    1.5383
IC CB8  CA1  CP4  CP5  20.2127  46.57     20.65   151.12    1.3767
IC CF1  CF3  CA1  CP4   2.5605  46.12    124.60    11.02    2.4834
IC CF2  CF4  CF3  CA1   2.5625  33.29    -42.95   111.82   17.2122
IC CF3  CF5  CF4  CF3   2.5640  33.25      0.00   113.64    1.5345
IC CF4  CF6  CF5  CF4   2.5638  33.21      0.00   113.31    1.5291
IC CF5  CF7  CF6  CF5   2.5690  33.33      0.00   113.55    1.5399
IC CF6  CF8  CF7  CF6   2.5593  33.32      0.00   113.34    1.5310
IC CF7  OS2  CF8  CF7  18.9345   4.18      0.00    64.29    1.5320
IC CF8  OS3  OS2  CF8  20.8763  55.31      0.00   118.59   19.5488
IC OS2  CZ2  CH2  CZ3   9.7377  21.54    -41.27   120.60    1.4406
IC OS3  CH2  CZ3  CZ1  10.8761  38.07   -157.75    58.97    4.2662
IC HC1  CE3  CZ3  CZ1   8.3215  29.17    179.99    58.91    4.2662
IC HC2  CD2  CE2  CZ2   7.5136  85.53     -0.32   118.10    1.4219
IC HC3  CZ1  CD3  CE4   8.3533 112.63     -0.65   117.66    1.4406
IC HC4  CD3  CE4  CD4  11.4605  58.84     -0.75   120.95    1.3747
IC HC5  CP3  CC1  CD4   3.9856  24.71   -177.70   176.38    4.9333
IC HC6  NP   CP4  CP5   5.0787  37.18     -1.03   120.01    1.3767
IC HC7  CP5  CC2  CP1   7.4879  55.04   -179.12    26.94    1.4455
IC HC8  CP1  CP2  CE4   9.5346 149.45      0.34    29.88    9.8775
IC HC9  CP2  CE4  CD4   9.3696  20.27    179.84    27.22    1.3747
IC HC10 CD4  CE4  CP2   4.6047  92.83     -0.56    27.22    9.8775
IC HC11 CB4  CE2  CZ2   8.6878  21.07     -7.33    95.93    1.4219
IC HC12 CB4  CE2  CZ2   9.9527   8.29   -121.75    95.93    1.4219
IC HC13 CB5  CB4  CE2  17.8816  54.34    -27.82   136.08    6.7373
IC HC14 CB5  CB4  CE2  18.2070  48.92    -26.25   136.08    6.7373
IC HC15 CB6  CB5  CB4  18.6837  56.18     60.93   113.18    1.5360
IC HC16 CB6  CB5  CB4  19.8239  60.01     62.22   113.18    1.5360
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IC HC17 CA2  CA1  CP4   2.1562 143.48    -79.85   110.31    2.4834
IC HC18 CA2  CA1  CP4   2.1871 100.27   -106.86   110.31    2.4834
IC HC19 CA3  CA2  CA1  16.4205  68.18     65.29   115.08    1.5474
IC HC20 CA3  CA2  CA1  17.6929  64.89     67.84   115.08    1.5474
IC HD1  S    CA3  CA2  16.2401 127.64     22.08   112.80    1.5275
IC HD2  S    CA3  CA2  14.8523 131.56     21.39   112.80    1.5275
IC HD3  OS1  S    CA3  16.2226  96.61    135.75   103.39    1.8394
IC HD4  OS1  S    CA3  17.5206  95.13    132.01   103.39    1.8394
IC HD5  NA1  OS1  S     5.2058 117.41     59.81    95.04    1.5109
IC HD6  NA1  OS1  S     5.2143  99.92     68.79    95.04    1.5109
IC HD7  CB1  NA1  OS1   7.4628  48.16    158.51   125.39   14.5576
IC HD8  CB1  NA1  OS1   7.1466  61.80    158.88   125.39   14.5576
IC HD9  CB2  CB1  NA1   9.4149  38.26    -76.29   114.23    1.4554
IC HD10 CB2  CB1  NA1   9.7303  36.43    -59.40   114.23    1.4554
IC HD11 CB3  CB2  CB1  11.8537  45.76     55.28   113.27    1.5389
IC HD12 CB3  CB2  CB1  11.3828  54.05     56.75   113.27    1.5389
IC HD13 CB3  CB2  CB1  12.7478  56.96     44.94   113.27    1.5389
IC HD14 CF3  CA1  CP4   6.6754 119.50    -62.76    11.02    2.4834
IC HD15 CF3  CA1  CP4   7.3089 132.35    -57.12    11.02    2.4834
IC HD16 CF4  CF3  CA1   6.3984  44.65    -60.64   111.82   17.2122
IC HD17 CF4  CF3  CA1   5.2730  41.04    -79.32   111.82   17.2122
IC HD18 CF5  CF4  CF3   7.7079  43.70     19.49   113.64    1.5345
IC HD19 CF5  CF4  CF3   8.7851  35.37     11.71   113.64    1.5345
IC HD20 CF6  CF5  CF4  10.8587  37.55    -28.16   113.31    1.5291
IC HE1  CF6  CF5  CF4   9.8795  36.25    -41.41   113.31    1.5291
IC HE2  CF7  CF6  CF5  12.2407  45.95     23.84   113.55    1.5399
IC HE3  CF7  CF6  CF5  13.2138  40.20     19.09   113.55    1.5399
IC HE4  CF8  CF7  CF6  15.4056  34.72    -33.31   113.34    1.5310
IC HE5  CF8  CF7  CF6  14.5028  34.05    -43.50   113.34    1.5310
IC HE6  OS2  CF8  CF7  19.2041  48.22    -29.18    64.29    1.5320
IC HE7  OS2  CF8  CF7  18.0936  52.35    -30.16    64.29    1.5320
IC HE8  OS3  OS2  CF8  21.7506  14.03    -57.42   118.59   19.5488
IC HE9  OS3  OS2  CF8  22.7518  16.40    -46.48   118.59   19.5488
patc firs none last none

BONDS
!atom type Kb          b0
CT2  CT1   222.500     1.5380 ! ALLOW   ALI
CT1  CT1   222.500     1.5000 ! ALLOW   ALI
HA   CT1   309.000     1.1110 ! ALLOW   ALI
HA   CT2   309.000     1.1110 ! ALLOW   ALI
HP   CA    340.000     1.0800 ! ALLOW   ARO
CA   CA    305.000     1.3750 ! ALLOW   ARO
!
OT   HT    450.000     0.9572 ! ALLOW   WAT
HT   HT      0.000     1.5139 ! ALLOW WAT
OC   CD    314.500     1.2940 ! carbonate
C3   C3    240.000     1.5010 ! cyclopropane
C3   HB    340.000     1.0830 ! cyclopropane
CA   CC2   250.000     1.4481 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CC2  CAP   250.000     1.4478 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
NR2  CT2   250.000     1.4902 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CT1  S     350.000     1.7996 !
CA   N     450.000     1.3795 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
N    CT1   200.000     1.4635 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CAP  HP    340.000     1.0831 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CC2  HE2   365.000     1.0888 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CAP  CAP   305.000     1.3811 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CC2  CC2   510.000     1.3588 !
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                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CAP  NR2   420.000     1.3050 ! pyridine, adm jr., 7/94
CA   CBN   280.000     1.4260 !
CBN  CBN   198.000     1.4355 !
CA   CBD   310.000     1.4075 !
S    OSD   500.000     1.4725 !
CBD  N     300.000     1.4078 !
CBD  CC2   300.000     1.4000 !

ANGLES
!atom types     Ktheta    Theta0   Kub     S0
! di-8-anepps specific
HP   CA   CA    30.000    120.00   22.00   2.15250 ! ALLOW   ARO
HA   CT1  CT1   34.500    110.10   22.53   2.17900 ! ALLOW   ALI
HA   CT1  CT2   34.500    110.10   22.53   2.17900 ! ALLOW   ALI
HA   CT2  CT1   33.430    110.10   22.53   2.17900 ! ALLOW   ALI
HA   CT1  HA    35.500    109.00    5.40   1.80200 ! TEST for test cpd
CT1  CT1  CT1   53.350    111.00    8.00   2.56100 ! ALLOW ALI
HA   CT2  HA    35.500    109.00    5.40   1.80200 ! ALLOW   ALI
CT2  CT1  CT1   53.350    111.00    8.00   2.56100 ! ALLOW   ALI
!
HT   OT   HT     55.000   104.5200 ! ALLOW WAT
CC2  CC2  CC2   50.000      0.00 !
CAP  CT2  CAP   80.000     57.00 !
OC   CD   OC    40.000    120.00    99.5   2.24127 ! carbonate
C3   C3   C3    77.350    111.00    8.00   2.56100 ! cyclopropane
C3   C3   HB    23.000    117.10   22.53   2.17900 ! cyclopropane
HB   C3   HB    23.000    117.00    5.40   1.80200 ! cyclopropane
CA   CBD  CC2    80.000   121.0000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CA   CPT  CA     60.000   122.0000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CA   CBD  N      85.000   111.1680 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
N    CA   HA     51.500   120.0000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CBD  CC2  CC2    80.000   127.3600 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CBD  CC2  HE2    60.000   115.0000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CC2  CC2  HE2    55.500   119.2860 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CC2  CC2  CAP    70.000   125.7170 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CAP  CC2  HE2    40.000   115.0000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CC2  CAP  CAP    60.000   124.9300 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CAP  CAP  CAP    40.000   120.0000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
HP   CAP  CAP   30.00    119.00   22.00   2.15250 ! pyridine
CAP  CAP  NC    120.000   120.3500 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
NC   CAP  HP     32.000   116.0160 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CAP  NC   CAP    60.000   120.0000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
CAP  NR2  CT2    60.000   119.3000 !
                ! di-8-anepps B3LYP 6-31G* geom, guess freqs
NR2  CT2  CT1    67.700   112.6000 !
NR2  CT2  HA     51.500   105.8000 !
CT1  CT1  SL     34.000   112.8500 !
S    CT1  HA     46.100   107.1000 !
CBD  N    CT1    70.000   121.3000 !
CT1  N    CT1    70.000   116.2550 !
N    CT1  CT1    70.000   114.2560 !
N    CT1  HA     51.500   109.5710 !
```

```
  CAP  CAP  NR2   10.00    129.00  ! pyridine
  CAP  NR2  CAP   10.00     96.00   55.00   2.28000 ! pyridine
  HP   CAP  NR2   30.00    112.00   35.00   2.05000 ! pyridine
  CA   CBN  CA    40.00    122.58   35.00   2.41020 !
  CA   CBN  CBN   40.00    118.71   35.00   2.51600 !
  CBD  CA   CBN   35.00    120.55   20.00   2.40630 !
  CBD  CA   CA    35.00    120.55   20.00   2.40630 !
  CA   CBD  CA    36.00    118.94   31.00   2.41730 !
  CBN  CA   CA    40.00    120.74   35.00   3.43620 !
  S    CT1  CT1   20.00    119.56 !
  OSD  S    CT1   75.00    105.38 !
  OSD  CT1  OSD   85.00    113.18 !
  OSD  S    OSD   75.00    113.18 !
  CBD  CA   HP    29.000    120.00   25.00   2.15250 !
  CBN  CA   HP    29.000    120.00   25.00   2.15250 !

  DIHEDRALS
  !atom types             Kchi    n   delta
  ! di-8-anepps specific
  HP   CA   CA   HP       2.4000  2   180.00 ! ALLOW   ARO

  CA   CBD  CA   CA       3.1000  2   180.00 !
  C3   C3   C3   HB       0.1000  6     0.00 ! hf/6-31g* cyclopropane
  HB   C3   C3   HB       0.2000  5   180.00 ! hf/6-31g* cyclopropane
  HP   CA   CA   HA       2.5000  2     0.00 !
                 ! di-8-anepps B3LYP 6-31G* geom, guess freqs
  CA    CA    CC2   CC2      15.1000  2      0.00 ! THIS ONE (orig. 1.3 2 0.0), then
(5.1, 2,   0.0)
  CA   CA   CC2  HE2      5.2000  2     0.00 !
  CA   CPT  CA   CA       3.1000  2     0.00 !
  CA   CPT  CA   HP       0.8000  2     0.00 !
  !CA   CA   CPT  CA       3.1000  2     0.00 !
  CA   CC2  CC2  CAP       3.1000  2   180.00 ! THIS ONE (orig. 1.3, 2, 0.0), then
(3.1,2,180.0)
  !CA   CC2  CC2  HE2      0.0300  2     0.00 !
  CA   CC2  CC2  HE2      4.0300  2   180.00 ! THIS ONE (modified from one above)
  CA   CA   CA   CC2      3.1000  2     0.00 !
  CPT  CA   CA   CC2      3.0000  2     0.00 !
  CA   N    CT1  CT1      3.0000  2     0.00 !
  CA   N    CT1  HA       2.5000  2     0.00 !
  CC2  CA   CA   HP       4.0000  2     0.00 !
  CAP   CAP   CC2   CC2       3.1000  2    180.00 ! THIS ONE (modified version of one
below)
  !CC2  CC2  CAP  CAP      3.1000  2   180.00 ! THIS ONE
  CC2  CAP  CAP  CAP      3.1000  2   180.00 !
  CC2  CAP  CAP  HP       4.0000  2   180.00 !
  CAP  CC2  CC2  HE2      4.0000  2   180.00 !
  CAP  CAP  CAP  NC       2.8000  2     0.00 !
  CAP  CAP  CAP  HP       4.20  2   180.00 ! pyridines
  CAP  CAP  CC2  HE2      4.0000  2   180.00 !
  !   CAP  CAP  CAP  CAP      3.1000  2     0.00 !
  CAP  CAP  CAP  CAP      1.20  2   180.00 ! pyridines
  CAP  CAP  NC   CAP      2.8000  2     0.00 !
  CAP  CAP  NR2  CT2      0.2000  2     0.00 !
  CAP  NC   CAP  HP       2.0000  2     0.00 !
  CAP  NR2  CT2  CT1      0.2000  2     0.00 !
  CAP  NR2  CT2  HA       2.5000  2     0.00 !
  NC   CAP  CAP  HP       0.8000  2     0.00 !
  CT2  NC   CAP  HP       1.0000  2     0.00 !
  CT1  N    CT1  CT1      0.0000  2     0.00 !
  CT1  N    CT1  HA       0.0000  2     0.00 !
  HP   CAP  CAP  HP       2.5000  2     0.00 !
  HE2  CC2  CC2  HE2      1.0000  2     0.00 !
  CPT  CA   CA   N        3.0000  2     0.00 !
  CA   CA   N    CT1      3.0000  2     0.00 !
  CA   CA   CA   N        3.0000  2     0.00 !
  N    CA   CA   HP       2.5000  2     0.00 !
```

```
CT1  N    CA   HA       3.0000  2     0.00 !
CAP  CAP  CAP  NR2      0.80  2   180.00 ! pyridine
CAP  CAP  NR2  CAP      1.20  2   180.00 ! pyridine
CC2  CAP  CAP  NR2      1.00  2   180.00 ! pyridine
HP   CAP  CAP  NR2      2.80  2   180.00 ! pyridine
HP   CAP  NR2  CAP      5.80  2   180.00 ! pyridine
HP   CAP  NR2  CT2      5.80  2   180.00 ! pyridine
CA   CBD  CA   HP       3.5000  2   180.00 !
CA   CBN  CA   HP       3.5000  2   180.00 !
CBD  CA   CA   HP       3.5000  2   180.00 !
CA   CBN  CBN  CA       3.1000  2   180.00 !
CA   CBN  CA   CA       3.1000  2   180.00 !
CA   CBD  CC2  CC2      3.1000  2   180.00 !
CA   CBD  CC2  HE2      3.5000  2   180.00 !
CBD  CA   CBN  CBN      3.1000  2   180.00 !
CBD  CA   CBN  CA       3.1000  2   180.00 !
CBD  CA   CA   CBN      3.1000  2   180.00 !
CBD  CC2  CC2  HE2      3.5000  2   180.00 !
CBD  CC2  CC2  CAP      3.1000  2   180.00 !
CA   CBD  CA   CBN      3.1000  2   180.00 !
CA   CA   CBN  CBN      3.1000  2   180.00 !
CA   CA   CBD  CC2      3.1000  2   180.00 !
CBN  CA   CA   HP       3.5000  2   180.00 !
CBN  CBN  CA   HP       3.5000  2   180.00 !
CBN  CA   CBD  CC2      3.1000  2   180.00 !
HP   CA   CBD  CC2      3.5000  2   180.00 !
CBN  CA   CBD  N        2.8000  2   180.00 !
CA   CA   CBD  N        2.8000  2   180.00 !
CA   CBD  N    CT1      2.5000  2   180.00 ! Guess
CBD  N    CT1  CT1      0.0400  3     0.00 !
CBD  N    CT1  HA       2.5000  2   180.00 !
HP   CA   CBD  N        3.0000  2   180.00 !
OSD  S    CT1  CT1      0.1000  3   180.00 !
HA   CT1  S    OSD      0.1000  3   180.00 !
!extra stuff
X    CT1  CT1  X        0.2000  3     0.00 ! ALLOW   ALI
X    CT1  CT2  X        0.2000  3     0.00 ! ALLOW   ALI


IMPROPER
!atom types           Kpsi                   psi0
!
CD    OC    OC    OC         107.00               0             0.0000  !  carbonate
```

5. CHARMM excited state charges for di-8-ANEPPS

```
RESI DIA          0.00  !  Di-8-ANEPPS EXCITED STATE CHARGES.
GROUP                   ! Naphthalene group
ATOM CE3  CA     -0.12  !
ATOM CZ3  CBD     0.09  ! was CBD
ATOM CH2  CA     -0.11
ATOM CZ2  CA     -0.09
ATOM CE2  CBN     0.04
ATOM CD2  CBN     0.06
ATOM CZ1  CA     -0.14
ATOM CD3  CBD     0.28
ATOM CE4  CA     -0.17
ATOM CD4  CA     -0.06
ATOM HC7  HP      0.14
ATOM HC8  HP      0.14
ATOM HC9  HP      0.13
ATOM HC10 HP      0.13
ATOM HC11 HP      0.13
ATOM HC12 HP      0.13
GROUP                   !Ethylene group
ATOM CC1  CC2    -0.19
ATOM CC2  CC2    -0.13
ATOM HC5  HE2     0.12
ATOM HC6  HE2     0.12
GROUP                   !Pyridinium group
ATOM CP1  CAP    -0.01
ATOM CP2  CAP    -0.16
ATOM CP3  CAP     0.03
ATOM NP   NR2    -0.42
ATOM CP4  CAP     0.05
ATOM CP5  CAP    -0.18
ATOM HC1  HP      0.16
ATOM HC2  HP      0.15
ATOM HC3  HP      0.14
ATOM HC4  HP      0.16
GROUP                   !Alkyl group before SO3-
ATOM CA1  CT2     0.03
ATOM CA2  CT1     0.25
ATOM CA3  CT1    -0.15
ATOM HC13 HA      0.01
ATOM HC14 HA      0.07
ATOM HC15 HA     -0.03
ATOM HC16 HA     -0.07
ATOM HC17 HA      0.03
ATOM HC18 HA      0.04
GROUP                   !SO3- group
ATOM S    S       0.95
ATOM OS1  OSD    -0.65
ATOM OS2  OSD    -0.65
ATOM OS3  OSD    -0.65
GROUP
ATOM NA1  N       0.00  !Amine Nitrogen
GROUP
ATOM CB1  CT1     0.33
ATOM CB2  CT1     0.06
ATOM CB3  CT1     0.01
ATOM CB4  CT1     0.16
ATOM HD16 HA     -0.07
ATOM HD17 HA     -0.03
ATOM HD18 HA     -0.03
ATOM HD19 HA     -0.05
ATOM HD20 HA     -0.03
ATOM HE1  HA     -0.03
ATOM HE2  HA     -0.05
ATOM HE3  HA     -0.04
```

```
GROUP
ATOM CB5  CT1     0.01
ATOM CB6  CT1     0.07
ATOM CB7  CT1     0.23
ATOM CB8  CT1    -0.16
ATOM HE4  HA     -0.03
ATOM HE5  HA     -0.02
ATOM HE6  HA     -0.03
ATOM HE7  HA     -0.05
ATOM HE8  HA     -0.06
ATOM HE9  HA     -0.06
ATOM HE10 HA      0.02
ATOM HE11 HA      0.02
ATOM HE12 HA      0.03
GROUP
ATOM CF1  CT1     0.41
ATOM CF2  CT1     0.02
ATOM CF3  CT1     0.01
ATOM CF4  CT1     0.14
ATOM HC19 HA     -0.08
ATOM HC20 HA     -0.06
ATOM HD1  HA     -0.03
ATOM HD2  HA     -0.04
ATOM HD3  HA     -0.04
ATOM HD4  HA     -0.02
ATOM HD5  HA     -0.04
ATOM HD6  HA     -0.03
GROUP
ATOM CF5  CT1     0.00
ATOM CF6  CT1     0.06
ATOM CF7  CT1     0.19
ATOM CF8  CT1    -0.07
ATOM HD7  HA     -0.02
ATOM HD8  HA     -0.03
ATOM HD9  HA     -0.03
ATOM HD10 HA     -0.03
ATOM HD11 HA     -0.06
ATOM HD12 HA     -0.05
ATOM HD13 HA      0.00
ATOM HD14 HA      0.00
ATOM HD15 HA      0.00
```