Kohn-Sham composition of the excitations:

BFPF

```
B3LYP 6-31G*
1: 3.6005 eV  344.35 nm  f=0.5477         50 -> 54    -0.14271
                                          53 -> 54     0.59708
2: 3.6014 eV  344.27 nm  f=0.0003         52 -> 54     0.69295
3: 4.1793 eV  296.66 nm  f=0.0091         51 -> 54     0.65976
                                          53 -> 55    -0.20474
4: 4.4311 eV  279.80 nm  f=0.2157         50 -> 54     0.65095
                                          53 -> 54     0.11367
                                          53 -> 56    -0.10975
5: 5.0390 eV  246.05 nm  f=0.0001         49 -> 54     0.69024
6: 5.1798 eV  239.36 nm  f=0.0440         51 -> 54     0.16243
                                          51 -> 56    -0.17622
                                          53 -> 55     0.63828
7: 5.5464 eV  223.54 nm  f=0.0400         48 -> 54     0.42478
                                          53 -> 56     0.54080
8: 6.0300 eV  205.61 nm  f=0.1076         48 -> 54     0.46623
                                          51 -> 55    -0.27751
                                          53 -> 56    -0.32890
                                          53 -> 57     0.11752

B3LYP 631+G*
1: 3.5205 eV  352.17 nm  f=0.5599         50 -> 54    -0.13098
                                          53 -> 54     0.60273
2: 3.6268 eV  341.85 nm  f=0.0003         52 -> 54     0.69347
3: 4.1224 eV  300.76 nm  f=0.0094         51 -> 54     0.65787
                                          53 -> 55     0.20985
4: 4.3653 eV  284.02 nm  f=0.1951         50 -> 54     0.65303
                                          53 -> 54     0.10281
                                          53 -> 55    -0.10808
5: 5.0189 eV  247.03 nm  f=0.0560         51 -> 54    -0.17145
                                          51 -> 57    -0.15996
                                          53 -> 55     0.63725
6: 5.0457 eV  245.72 nm  f=0.0001         49 -> 54     0.69022
7: 5.1418 eV  241.13 nm  f=0.0001         53 -> 56     0.69417
8: 5.4174 eV  228.86 nm  f=0.0241         48 -> 54    -0.36729
                                          53 -> 57     0.58004

B3LYP 631+G* PCM (Methanol)
1: 3.4188 eV  362.65 nm  f=0.6562         50 -> 54     0.10675
                                          53 -> 54     0.61840
2: 3.7758 eV  328.37 nm  f=0.0003         51 -> 54     0.69503
3: 4.0523 eV  305.96 nm  f=0.0127         52 -> 54     0.66603
                                          53 -> 55     0.17531
4: 4.2681 eV  290.49 nm  f=0.2086         50 -> 54     0.66304
5: 5.0795 eV  244.09 nm  f=0.0599         52 -> 54    -0.14076
                                          52 -> 56     0.16682
                                          53 -> 55     0.65097
6: 5.1637 eV  240.11 nm  f=0.0001         48 -> 54     0.69042
7: 5.4371 eV  228.04 nm  f=0.0414         49 -> 54    -0.44190
                                          53 -> 56     0.53363
8: 5.4470 eV  227.62 nm  f=0.0000         53 -> 57     0.69058
```

$\mathbf{BFP}_{\delta}$

```
B3LYP 631G*
1: 3.5926 eV  345.11 nm  f=0.6090         50 -> 51     0.58772
2: 3.7730 eV  328.61 nm  f=0.0003         49 -> 51     0.69337
3: 4.3670 eV  283.91 nm  f=0.0940         48 -> 51     0.65289
4: 4.4782 eV  276.86 nm  f=0.0000         47 -> 51     0.70161
5: 4.9813 eV  248.90 nm  f=0.0050         46 -> 51     0.67452
6: 5.4003 eV  229.59 nm  f=0.0003         44 -> 51     0.69037
7: 5.6532 eV  219.31 nm  f=0.0183         45 -> 51    -0.25030
                                          50 -> 52     0.63166
8: 5.9882 eV  207.05 nm  f=0.0398         43 -> 51    -0.13849
                                          45 -> 51     0.36193
                                          50 -> 52     0.13608
                                          50 -> 53     0.54264

B3LYP 631+G*
1: 3.5076 eV  353.47 nm  f=0.6197         50 -> 51     0.59302
2: 3.8023 eV  326.08 nm  f=0.0003         49 -> 51     0.69406
3: 4.3172 eV  287.18 nm  f=0.0938         46 -> 51     0.10003
                                          48 -> 51     0.65588
4: 4.5119 eV  274.79 nm  f=0.0000         47 -> 51     0.70169
5: 4.9033 eV  252.86 nm  f=0.0000         50 -> 52     0.69068
                                          50 -> 53    -0.10947
6: 4.9567 eV  250.13 nm  f=0.0037         46 -> 51     0.67294
7: 5.3617 eV  231.24 nm  f=0.0005         50 -> 52     0.11173
                                          50 -> 53     0.68561
8: 5.3995 eV  229.62 nm  f=0.0003         44 -> 51     0.68970

B3LYP 631+G* PCM (Methanol)
1: 3.3790 eV  366.93 nm  f=0.6904         50 -> 51     0.60831
2: 3.9321 eV  315.31 nm  f=0.0004         48 -> 51     0.69571
3: 4.2146 eV  294.18 nm  f=0.1274         49 -> 51     0.66324
4: 4.8473 eV  255.78 nm  f=0.0000         46 -> 51     0.70017
5: 5.0196 eV  247.00 nm  f=0.0071         47 -> 51     0.67136
6: 5.2396 eV  236.63 nm  f=0.0000         50 -> 52     0.68597
                                          50 -> 53     0.13232
7: 5.4121 eV  229.09 nm  f=0.0002         44 -> 51     0.69130
8: 5.6571 eV  219.17 nm  f=0.0119         45 -> 51     0.37258
                                          50 -> 54     0.57201
                                          50 -> 55    -0.11529
```

$\mathbf{BFP}_{\epsilon}$

```
B3LYP 631G*
1: 3.6186 eV  342.63 nm  f=0.0003         49 -> 51     0.69435
2: 3.7410 eV  331.42 nm  f=0.4660         46 -> 51    -0.10210
                                          48 -> 51    -0.17489
                                          50 -> 51     0.58457
3: 4.5545 eV  272.22 nm  f=0.2528         48 -> 51     0.64376
                                          50 -> 51     0.13953
                                          50 -> 52     0.12008
4: 4.7682 eV  260.02 nm  f=0.0004         45 -> 51    -0.14722
                                          47 -> 51     0.68074
5: 5.1759 eV  239.54 nm  f=0.0011         45 -> 51     0.67501
                                          47 -> 51     0.15666
6: 5.2835 eV  234.66 nm  f=0.1152         46 -> 51     0.60027
                                          50 -> 52    -0.32320
7: 5.5849 eV  222.00 nm  f=0.0216         46 -> 51     0.30158
                                          50 -> 52     0.58223
8: 6.0279 eV  205.68 nm  f=0.0022         43 -> 51     0.14526
                                          44 -> 51    -0.28350
                                          50 -> 53     0.61223

B3LYP 631+G*
1: 3.6396 eV  340.65 nm  f=0.0003         49 -> 51     0.69492
2: 3.6500 eV  339.68 nm  f=0.4741         48 -> 51    -0.16163
                                          50 -> 51     0.59195
3: 4.4888 eV  276.21 nm  f=0.2398         48 -> 51     0.64730
                                          50 -> 51     0.12779
                                          50 -> 54    -0.12080
4: 4.6516 eV  266.54 nm  f=0.0001         50 -> 52     0.69865
5: 4.7723 eV  259.80 nm  f=0.0003         45 -> 51    -0.14510
                                          47 -> 51     0.68111
6: 5.0351 eV  246.24 nm  f=0.0002         50 -> 53     0.69374
7: 5.1349 eV  241.45 nm  f=0.0830         46 -> 51     0.38438
                                          50 -> 54     0.56629
8: 5.1900 eV  238.89 nm  f=0.0008         45 -> 51     0.67587
                                          47 -> 51     0.15410

B3LYP 631+G* PCM (Methanol)
1: 3.5596 eV  348.31 nm  f=0.6608         50 -> 51     0.61369
2: 3.9202 eV  316.27 nm  f=0.0003         49 -> 51     0.69524
3: 4.3864 eV  282.66 nm  f=0.1565         48 -> 51     0.66280
4: 4.9130 eV  252.36 nm  f=0.0007         46 -> 51     0.69207
5: 5.1153 eV  242.38 nm  f=0.0712         47 -> 51     0.65761
                                          50 -> 53     0.17638
6: 5.2169 eV  237.66 nm  f=0.0000         50 -> 52     0.68527
                                          50 -> 54    -0.11978
7: 5.4736 eV  226.51 nm  f=0.0010         45 -> 51     0.68544
8: 5.5243 eV  224.44 nm  f=0.0390         47 -> 51    -0.15147
                                          50 -> 53     0.65405
```

CFP

```
B3LYP 631G*
1: 3.4172 eV  362.82 nm  f=0.6248         63 -> 64     0.60567
2: 3.7472 eV  330.87 nm  f=0.0003         60 -> 64     0.69289
3: 3.9348 eV  315.10 nm  f=0.0099         61 -> 64    -0.13332
                                          62 -> 64     0.63597
                                          63 -> 65     0.23492
4: 4.1268 eV  300.44 nm  f=0.0045         59 -> 64     0.11013
                                          61 -> 64     0.65056
                                          62 -> 64     0.15565
5: 4.4036 eV  281.55 nm  f=0.0715         62 -> 64    -0.19556
                                          63 -> 65     0.63130
6: 4.9438 eV  250.79 nm  f=0.0972         59 -> 64     0.40896
                                          61 -> 65    -0.11680
                                          62 -> 65    -0.39893
                                          63 -> 66     0.36479
7: 5.0441 eV  245.80 nm  f=0.1642         59 -> 64     0.51797
                                          62 -> 65     0.18178
                                          63 -> 66    -0.39119
8: 5.2198 eV  237.53 nm  f=0.0002         58 -> 64     0.68805

B3LYP 631+G*
1: 3.3165 eV  373.84 nm  f=0.5986         63 -> 64     0.61074
2: 3.7715 eV  328.74 nm  f=0.0004         60 -> 64     0.69381
3: 3.8674 eV  320.59 nm  f=0.0142         61 -> 64    -0.13907
                                          62 -> 64     0.63142
                                          63 -> 65     0.24261
4: 4.0575 eV  305.57 nm  f=0.0048         59 -> 64     0.11059
                                          61 -> 64     0.65029
                                          62 -> 64     0.16174
5: 4.2520 eV  291.59 nm  f=0.0668         62 -> 64    -0.20798
                                          63 -> 65     0.63230
6: 4.4951 eV  275.82 nm  f=0.0002         63 -> 66     0.69873
7: 4.7469 eV  261.19 nm  f=0.0000         63 -> 67     0.69247
8: 4.8312 eV  256.63 nm  f=0.0346         59 -> 64     0.28853
                                          61 -> 65    -0.10967
                                          61 -> 68    -0.10596
                                          62 -> 65    -0.43267
                                          63 -> 68     0.44212

B3LYP 631+G* PCM (Methanol)
1: 3.1547 eV  393.02 nm  f=0.6987         63 -> 64     0.62483
2: 3.7427 eV  331.27 nm  f=0.0267         61 -> 64     0.10043
                                          62 -> 64     0.67119
                                          63 -> 65     0.13674
3: 3.9701 eV  312.30 nm  f=0.0007         60 -> 64     0.68669
                                          61 -> 64    -0.10715
4: 3.9740 eV  311.99 nm  f=0.0095         59 -> 64    -0.12439
                                          60 -> 64     0.11435
                                          61 -> 64     0.64315
                                          62 -> 64    -0.11369
5: 4.3304 eV  286.31 nm  f=0.0737         62 -> 64    -0.10780
                                          63 -> 65     0.66149
6: 4.7813 eV  259.31 nm  f=0.2220         59 -> 64     0.60634
                                          62 -> 65    -0.28988
                                          63 -> 67     0.13267
7: 4.9064 eV  252.70 nm  f=0.0002         63 -> 66     0.68023
                                          63 -> 68    -0.13088
                                          63 -> 71    -0.10656
```

GFP_N

```
B3LYP 6-31G*
1: 3.5354 eV  350.69 nm  f=0.6975         57 -> 58     0.60185
2: 3.6628 eV  338.49 nm  f=0.0003         56 -> 58     0.69321
3: 4.2212 eV  293.72 nm  f=0.0795         53 -> 58     0.10202
                                          55 -> 58     0.64962
                                          57 -> 60     0.12022
4: 4.3798 eV  283.08 nm  f=0.0074         54 -> 58     0.56240
                                          55 -> 58    -0.10275
                                          57 -> 59     0.40248
5: 4.9464 eV  250.65 nm  f=0.0711         54 -> 58    -0.37440
                                          54 -> 60     0.13249
                                          55 -> 59     0.10460
                                          57 -> 59     0.53203
6: 5.1060 eV  242.82 nm  f=0.0002         52 -> 58     0.68966
7: 5.4628 eV  226.96 nm  f=0.0854         53 -> 58     0.50821
                                          57 -> 60    -0.45705
8: 5.8277 eV  212.75 nm  f=0.1013         51 -> 58     0.13700
                                          53 -> 58     0.37921
                                          54 -> 59    -0.18488
                                          55 -> 59    -0.14660
                                          57 -> 60     0.41525
                                          57 -> 61    -0.20435

B3LYP 6-31+G*
1: 3.4593 eV  358.41 nm  f=0.6918         57 -> 58     0.60579
2: 3.6902 eV  335.99 nm  f=0.0003         55 -> 58     0.69376
3: 4.1686 eV  297.43 nm  f=0.0755         53 -> 58     0.10084
                                          56 -> 58     0.64860
                                          57 -> 59    -0.10740
                                          57 -> 62    -0.11718
4: 4.3032 eV  288.12 nm  f=0.0046         54 -> 58     0.52077
                                          56 -> 58    -0.12239
                                          57 -> 59    -0.44978
5: 4.8017 eV  258.21 nm  f=0.0000         56 -> 60    -0.10027
                                          57 -> 60     0.69574
6: 4.8095 eV  257.79 nm  f=0.0853         54 -> 58     0.42847
                                          54 -> 62     0.11285
                                          56 -> 59     0.10706
                                          57 -> 59     0.49317
7: 4.9640 eV  249.77 nm  f=0.0001         57 -> 61     0.69305
8: 5.1138 eV  242.45 nm  f=0.0001         52 -> 58     0.68947

B3LYP 6-31+G* PCM (methanol)
1: 3.3464 eV  370.50 nm  f=0.8299         57 -> 58     0.62266
2: 3.8783 eV  319.69 nm  f=0.0004         55 -> 58     0.69460
3: 4.1102 eV  301.65 nm  f=0.0526         53 -> 58     0.11814
                                          56 -> 58     0.65958
4: 4.2740 eV  290.09 nm  f=0.0098         54 -> 58     0.60859
                                          57 -> 59    -0.33090
5: 4.8339 eV  256.49 nm  f=0.0973         54 -> 58     0.30438
                                          54 -> 61     0.13160
                                          57 -> 59     0.58387
6: 5.1968 eV  238.58 nm  f=0.0000         57 -> 60     0.68530
7: 5.2824 eV  234.71 nm  f=0.0001         52 -> 58     0.68919
8: 5.3473 eV  231.86 nm  f=0.0896         53 -> 58     0.53029
                                          57 -> 61     0.43413
```

$\mathbf{GFP}_{\mathrm{A}}$

```
B3LYP 6-31G*
1: 3.0914 eV  401.06 nm  f=0.0000         56 -> 58     0.68715
2: 3.1942 eV  388.15 nm  f=0.9840         57 -> 58     0.57114
3: 4.1633 eV  297.80 nm  f=0.0004         53 -> 58     0.69617
4: 4.3215 eV  286.90 nm  f=0.0031         52 -> 58     0.13186
                                          54 -> 58     0.12181
                                          55 -> 58     0.62124
                                          57 -> 62    -0.16694
5: 4.3781 eV  283.19 nm  f=0.0110         54 -> 58     0.48722
                                          57 -> 59    -0.46669
6: 4.4777 eV  276.89 nm  f=0.0564         54 -> 58     0.46736
                                          57 -> 59     0.46943
7: 4.7508 eV  260.97 nm  f=0.0718         52 -> 58     0.14138
                                          57 -> 60     0.65497
8: 4.9796 eV  248.98 nm  f=0.0001         56 -> 59     0.69072
                                          56 -> 60     0.12056

B3LYP 6-31+G*
1: 2.9725 eV  417.10 nm  f=0.0001         57 -> 59     0.70341
2: 3.0762 eV  403.04 nm  f=0.9867         57 -> 58     0.57913
3: 3.2146 eV  385.69 nm  f=0.0000         56 -> 58     0.68818
4: 3.5813 eV  346.20 nm  f=0.0007         57 -> 60     0.70378
5: 3.8618 eV  321.05 nm  f=0.0001         57 -> 61     0.69751
6: 4.0540 eV  305.83 nm  f=0.0003         57 -> 62     0.70178
7: 4.1520 eV  298.61 nm  f=0.0010         57 -> 64     0.69466
8: 4.1704 eV  297.29 nm  f=0.0525         54 -> 58    -0.21023
                                          57 -> 63     0.63386

B3LYP 6-31+G* PCM (methanol) [optimized with 6-31G* PCM (methanol)]
1: 3.1490 eV  393.72 nm  f=0.9349         57 -> 58     0.58802
2: 3.8654 eV  320.75 nm  f=0.0000         53 -> 58     0.14197
                                          55 -> 58     0.67893
3: 4.0528 eV  305.92 nm  f=0.0035         53 -> 58     0.58184
                                          55 -> 58    -0.12767
                                          56 -> 58    -0.33137
4: 4.0715 eV  304.52 nm  f=0.0082         52 -> 58    -0.13531
                                          53 -> 58     0.35444
                                          54 -> 58    -0.10275
                                          56 -> 58     0.54232
5: 4.2248 eV  293.46 nm  f=0.0055         54 -> 58     0.49279
                                          56 -> 58     0.10548
                                          57 -> 59    -0.47052
6: 4.3936 eV  282.19 nm  f=0.0001         57 -> 60     0.68746
                                          57 -> 61     0.12760
7: 4.4985 eV  275.61 nm  f=0.0876         54 -> 58     0.46373
                                          57 -> 59     0.47150
8: 4.7881 eV  258.94 nm  f=0.0012         57 -> 60    -0.11225
                                          57 -> 61     0.67966
                                          57 -> 64    -0.11149
```

ORN_A

```
B3LYP 6-31+G*
1: 2.6480 eV  468.22 nm  f=0.8748         71 -> 72     0.56865
2: 2.7853 eV  445.14 nm  f=0.0000         70 -> 72     0.67912
                                          70 -> 73    -0.12395
3: 3.6045 eV  343.97 nm  f=0.0313         69 -> 72     0.51596
                                          71 -> 73    -0.44206
4: 3.6236 eV  342.16 nm  f=0.0003         68 -> 72     0.69759
5: 3.9919 eV  310.59 nm  f=0.1351         66 -> 72    -0.16347
                                          67 -> 72     0.44564
                                          69 -> 72     0.28931
                                          71 -> 73     0.33209
6: 4.0556 eV  305.71 nm  f=0.1361         66 -> 72     0.14619
                                          67 -> 72     0.52488
                                          69 -> 72    -0.23054
                                          71 -> 73    -0.28162
7: 4.4650 eV  277.68 nm  f=0.0583         71 -> 74     0.67154
8: 4.4881 eV  276.25 nm  f=0.0000         70 -> 72     0.14592
                                          70 -> 73     0.67513
                                          70 -> 75    -0.11372
```


```
B3LYP 6-31+G*
1: 2.6480 eV  468.22 nm  f=0.8748         71 -> 72     0.56865
2: 2.7853 eV  445.14 nm  f=0.0000         70 -> 72     0.67912
                                          70 -> 73    -0.12395
3: 3.6045 eV  343.97 nm  f=0.0313         69 -> 72     0.51596
                                          71 -> 73    -0.44206
4: 3.6236 eV  342.16 nm  f=0.0003         68 -> 72     0.69759
5: 3.9919 eV  310.59 nm  f=0.1351         66 -> 72    -0.16347
                                          67 -> 72     0.44564
                                          69 -> 72     0.28931
                                          71 -> 73     0.33209
6: 4.0556 eV  305.71 nm  f=0.1361         66 -> 72     0.14619
                                          67 -> 72     0.52488
                                          69 -> 72    -0.23054
                                          71 -> 73    -0.28162
7: 4.4650 eV  277.68 nm  f=0.0583         71 -> 74     0.67154
8: 4.4881 eV  276.25 nm  f=0.0000         70 -> 72     0.14592
                                          70 -> 73     0.67513
                                          70 -> 75    -0.11372
```


```
B3LYP 6-31+G* PCM (methanol) [optimized with 6-31G* PCM (methanol)]
1: 2.5637 eV  483.61 nm  f=1.0460         71 -> 72     0.60405
2: 3.2921 eV  376.62 nm  f=0.0000         70 -> 72     0.68654
                                          70 -> 73    -0.10084
3: 3.6991 eV  335.17 nm  f=0.0160         69 -> 72     0.57480
                                          71 -> 73     0.35139
4: 3.7856 eV  327.51 nm  f=0.0004         67 -> 72     0.69649
5: 3.9011 eV  317.82 nm  f=0.1966         65 -> 72     0.13480
                                          66 -> 72    -0.21793
                                          68 -> 72     0.23058
                                          69 -> 72    -0.25181
                                          71 -> 73     0.50785
6: 4.0061 eV  309.49 nm  f=0.0454         66 -> 72     0.12268
                                          68 -> 72     0.63651
                                          69 -> 72     0.10949
                                          71 -> 73    -0.13845
                                          71 -> 74     0.12159
7: 4.2198 eV  293.81 nm  f=0.0726         65 -> 72     0.10649
                                          66 -> 72     0.64285
                                          69 -> 72    -0.11047
                                          71 -> 73     0.15571
8: 4.3487 eV  285.11 nm  f=0.0905         68 -> 72    -0.11395
                                          71 -> 74     0.66333
```

$\mathbf{ASF}_{\mathrm{A}}$

```
B3LYP 6-31+G*
1: 2.5804 eV  480.49 nm  f=0.7969         64 -> 65     0.57170
2: 2.8754 eV  431.19 nm  f=0.0000         63 -> 65     0.68131
                                          63 -> 66    -0.11886
3: 3.4341 eV  361.04 nm  f=0.0001         59 -> 65    -0.17434
                                          61 -> 65     0.66611
4: 3.5327 eV  350.97 nm  f=0.0135         62 -> 65     0.57014
                                          64 -> 66    -0.36687
5: 3.7672 eV  329.11 nm  f=0.0003         59 -> 65     0.63435
                                          59 -> 66     0.16095
                                          61 -> 65     0.20097
6: 3.8948 eV  318.33 nm  f=0.1480         58 -> 65     0.16919
                                          60 -> 65     0.43762
                                          62 -> 65     0.22458
                                          64 -> 66     0.40300
7: 3.9457 eV  314.22 nm  f=0.0000         64 -> 67     0.69209
8: 3.9805 eV  311.48 nm  f=0.1488         58 -> 65    -0.14525
                                          60 -> 65     0.53132
                                          62 -> 65    -0.18664
                                          64 -> 66    -0.31253

B3LYP 6-31+G* PCM (methanol)
1: 2.4998 eV  495.99 nm  f=0.9394         64 -> 65     0.59789
2: 3.2066 eV  386.65 nm  f=0.0000         62 -> 65     0.68377
                                          62 -> 66    -0.10764
3: 3.4554 eV  358.81 nm  f=0.0001         59 -> 65     0.19618
                                          59 -> 66     0.11952
                                          61 -> 65     0.64680
4: 3.5708 eV  347.22 nm  f=0.0145         63 -> 65     0.60763
                                          64 -> 66    -0.28780
5: 3.7941 eV  326.78 nm  f=0.0005         59 -> 65     0.63112
                                          59 -> 66     0.11887
                                          61 -> 65    -0.23478
                                          61 -> 66     0.10951
6: 3.8607 eV  321.14 nm  f=0.1692         58 -> 65     0.15011
                                          60 -> 65     0.40783
                                          63 -> 65     0.16279
                                          64 -> 66     0.47813
7: 3.9377 eV  314.86 nm  f=0.1412         58 -> 65    -0.12791
                                          60 -> 65     0.55051
                                          63 -> 65    -0.15527
                                          64 -> 66    -0.31964
8: 4.4065 eV  281.37 nm  f=0.0837         64 -> 67     0.67426
```

$\mathbf{ZFP}_{\mathrm{A}}$

```
B3LYP 631G*
1: 2.6360 eV  470.34 nm  f=0.8595         75 -> 76     0.57358
                                          75 -> 77     0.12154
2: 2.8410 eV  436.41 nm  f=0.0000         74 -> 76     0.67894
                                          74 -> 77    -0.12713
3: 3.6130 eV  343.16 nm  f=0.0684         73 -> 76    -0.47956
                                          75 -> 77     0.47570
4: 3.6566 eV  339.07 nm  f=0.0005         72 -> 76     0.69524
5: 3.9687 eV  312.40 nm  f=0.2256         69 -> 76    -0.20514
                                          71 -> 76    -0.17874
                                          73 -> 76     0.41069
                                          75 -> 77     0.39092
6: 4.1003 eV  300.38 nm  f=0.0311         71 -> 76     0.66487
                                          75 -> 77     0.10594
7: 4.2150 eV  294.15 nm  f=0.0009         70 -> 76     0.66317
                                          70 -> 77     0.17338
8: 4.4287 eV  279.95 nm  f=0.0615         75 -> 78     0.66963

B3LYP 631+G*
1: 2.5672 eV  482.95 nm  f=0.8587         75 -> 76     0.58139
2: 2.9731 eV  417.01 nm  f=0.0000         74 -> 76     0.67990
                                          74 -> 78    -0.11038
3: 3.0959 eV  400.47 nm  f=0.0386         75 -> 77     0.69091
4: 3.5673 eV  347.56 nm  f=0.0695         73 -> 76    -0.39095
                                          75 -> 78     0.54429
                                          75 -> 79    -0.13130
5: 3.6674 eV  338.07 nm  f=0.0017         73 -> 76    -0.26781
                                          75 -> 79     0.63916
6: 3.6870 eV  336.27 nm  f=0.0006         72 -> 76     0.69463
7: 3.7829 eV  327.75 nm  f=0.0014         75 -> 80    -0.35516
                                          75 -> 81     0.57628
8: 3.8133 eV  325.14 nm  f=0.0041         75 -> 80     0.58586
                                          75 -> 81     0.37368

B3LYP 631+G* PCM (methanol)
1: 2.6223 eV  472.81 nm  f=1.0830         75 -> 76     0.60548
2: 3.4384 eV  360.59 nm  f=0.0000         73 -> 76     0.68682
3: 3.6365 eV  340.94 nm  f=0.0008         72 -> 76     0.66926
                                          72 -> 77     0.14326
4: 3.7532 eV  330.34 nm  f=0.0152         74 -> 76     0.57502
                                          75 -> 77     0.34773
5: 3.8883 eV  318.86 nm  f=0.0026         71 -> 76     0.68200
6: 3.9399 eV  314.69 nm  f=0.2041         69 -> 76     0.20515
                                          70 -> 76     0.11222
                                          74 -> 76    -0.27900
                                          75 -> 77     0.54826
7: 4.1378 eV  299.64 nm  f=0.0095         70 -> 76     0.59724
                                          75 -> 78     0.32597
8: 4.3104 eV  287.64 nm  f=0.1014         70 -> 76    -0.30680
                                          75 -> 78     0.58562
                                          75 -> 79     0.11135
```

$\mathbf{DSR}_{\mathrm{A}}$

```
B3LYP 631G*
1: 2.4252 eV  511.24 nm  f=0.9336         75 -> 76     0.55989
2: 2.6343 eV  470.64 nm  f=0.0001         74 -> 76     0.67570
                                          74 -> 77     0.14280
3: 3.2663 eV  379.59 nm  f=0.0007         71 -> 76    -0.45346
                                          71 -> 77     0.11700
                                          72 -> 76     0.50984
4: 3.2746 eV  378.62 nm  f=0.0145         73 -> 76     0.54397
                                          75 -> 77     0.41613
5: 3.3159 eV  373.91 nm  f=0.0032         71 -> 76     0.49445
                                          71 -> 77    -0.10444
                                          72 -> 76     0.47448
6: 3.7787 eV  328.11 nm  f=0.2069         69 -> 76    -0.22281
                                          70 -> 76    -0.35476
                                          73 -> 76    -0.28597
                                          75 -> 77     0.39091
7: 3.8533 eV  321.76 nm  f=0.0993         69 -> 76    -0.14036
                                          70 -> 76     0.59028
                                          73 -> 76    -0.16007
                                          75 -> 77     0.23345
8: 4.2201 eV  293.79 nm  f=0.0000         74 -> 76    -0.16391
                                          74 -> 77     0.66861

B3LYP 631+G*
1: 2.3639 eV  524.48 nm  f=0.9581         75 -> 76     0.56817
2: 2.7435 eV  451.92 nm  f=0.0000         74 -> 76     0.67719
                                          74 -> 77    -0.14220
3: 3.2446 eV  382.13 nm  f=0.0192         73 -> 76     0.53778
                                          75 -> 77    -0.42601
4: 3.2887 eV  377.01 nm  f=0.0008         71 -> 76     0.42359
                                          71 -> 77     0.11489
                                          72 -> 76     0.53584
5: 3.3542 eV  369.64 nm  f=0.0041         71 -> 76     0.52055
                                          71 -> 77     0.10506
                                          72 -> 76    -0.44403
6: 3.6906 eV  335.94 nm  f=0.2326         69 -> 76     0.21221
                                          70 -> 76     0.26424
                                          73 -> 76     0.32036
                                          75 -> 77     0.42120
7: 3.8017 eV  326.13 nm  f=0.0600         70 -> 76     0.63395
                                          73 -> 76    -0.11944
                                          75 -> 77    -0.16525
8: 3.8849 eV  319.15 nm  f=0.0143         75 -> 78     0.67910

B3LYP 631+G* PCM (methanol)
1: 2.2948 eV  540.29 nm  f=1.0857         75 -> 76     0.59737
2: 3.0984 eV  400.15 nm  f=0.0000         73 -> 76     0.67991
                                          73 -> 77    -0.13467
3: 3.2311 eV  383.72 nm  f=0.0020         72 -> 76     0.66380
                                          72 -> 77     0.15594
4: 3.3324 eV  372.06 nm  f=0.0307         74 -> 76     0.53454
                                          75 -> 77    -0.42692
5: 3.4831 eV  355.96 nm  f=0.0037         71 -> 76     0.68436
6: 3.6460 eV  340.06 nm  f=0.2786         69 -> 76     0.20202
                                          70 -> 76     0.19352
                                          74 -> 76     0.34712
                                          75 -> 77     0.45906
7: 3.7963 eV  326.59 nm  f=0.0485         70 -> 76     0.66048
                                          75 -> 77    -0.12097
8: 4.2653 eV  290.68 nm  f=0.0184         68 -> 76     0.62482
                                          68 -> 77     0.13676
                                          69 -> 76    -0.21082
```

$\mathbf{KAE_A}$

```
B3LYP 6-31G*
1: 2.2459 eV  552.05 nm  f=0.8227         77 -> 78     0.57171
                                          77 -> 79     0.10858
2: 2.6585 eV  466.36 nm  f=0.0000         76 -> 78     0.67384
                                          76 -> 79    -0.16055
3: 3.1782 eV  390.11 nm  f=0.1435         75 -> 78     0.45790
                                          77 -> 79     0.50167
4: 3.5658 eV  347.70 nm  f=0.0004         74 -> 78     0.69510
5: 3.7379 eV  331.70 nm  f=0.2563         72 -> 78    -0.31275
                                          75 -> 78     0.41754
                                          77 -> 79    -0.32023
                                          77 -> 80    -0.11223
6: 3.8490 eV  322.12 nm  f=0.0104         73 -> 78     0.68521
7: 3.9923 eV  310.56 nm  f=0.0000         76 -> 78     0.18237
                                          76 -> 79     0.66893
8: 4.2169 eV  294.02 nm  f=0.0399         72 -> 78    -0.18330
                                          77 -> 80     0.65847

B3LYP 6-31+G*
1: 2.1471 eV  577.44 nm  f=0.7939         77 -> 78     0.58075
                                          77 -> 80     0.10328
2: 2.6359 eV  470.36 nm  f=0.0001         77 -> 79     0.70324
3: 2.7686 eV  447.81 nm  f=0.0000         76 -> 78     0.67465
                                          76 -> 80    -0.16355
4: 3.0996 eV  400.00 nm  f=0.1706         75 -> 78     0.42929
                                          77 -> 80     0.52456
5: 3.3976 eV  364.91 nm  f=0.0011         77 -> 81     0.69959
6: 3.5781 eV  346.50 nm  f=0.0005         74 -> 78     0.69464
7: 3.6040 eV  344.02 nm  f=0.2555         72 -> 78    -0.24890
                                          75 -> 78     0.45616
                                          77 -> 80    -0.30580
                                          77 -> 82     0.15439
8: 3.7861 eV  327.47 nm  f=0.0002         77 -> 83     0.61267
                                          77 -> 84    -0.30141
                                          77 -> 85     0.15226

B3LYP 6-31+G* PCM (methanol)
1: 2.2777 eV  544.33 nm  f=0.9791         77 -> 78     0.61100
2: 3.2310 eV  383.73 nm  f=0.1164         76 -> 78     0.40097
                                          77 -> 79     0.56052
3: 3.3854 eV  366.23 nm  f=0.0000         75 -> 78     0.68049
                                          75 -> 79    -0.13981
4: 3.7155 eV  333.69 nm  f=0.4097         74 -> 78    -0.28943
                                          76 -> 78     0.47307
                                          77 -> 79    -0.28242
5: 3.8239 eV  324.23 nm  f=0.0006         72 -> 78     0.43122
                                          73 -> 78     0.54251
6: 3.8902 eV  318.71 nm  f=0.4891         74 -> 78     0.60613
                                          76 -> 78     0.20234
                                          77 -> 79    -0.16352
7: 4.0462 eV  306.42 nm  f=0.0126         72 -> 78     0.45080
                                          73 -> 78    -0.35835
                                          77 -> 80     0.37365
8: 4.1497 eV  298.78 nm  f=0.0008         77 -> 81     0.67505
                                          77 -> 82    -0.18689

B3LYP 6-31+G* PCM (methanol) [optimized with 6-31G* PCM (methanol)]
1: 2.3076 eV  537.29 nm  f=0.9429         77 -> 78     0.61501
2: 3.2553 eV  380.87 nm  f=0.1224         76 -> 78    -0.42718
                                          77 -> 79     0.54289
3: 3.3595 eV  369.06 nm  f=0.0000         75 -> 78     0.68232
                                          75 -> 79    -0.13328
4: 3.6972 eV  335.35 nm  f=0.4418         74 -> 78    -0.26191
```

```
                                        76 -> 78     0.46277
                                        77 -> 79     0.32137
5: 3.8170 eV  324.82 nm  f=0.0006       72 -> 78     0.69228
6: 3.9114 eV  316.98 nm  f=0.4661       74 -> 78     0.61679
                                        76 -> 78     0.17021
                                        77 -> 79     0.16153
7: 4.0056 eV  309.53 nm  f=0.0078       73 -> 78     0.63000
                                        77 -> 80    -0.27537
8: 4.1868 eV  296.13 nm  f=0.0808       73 -> 78     0.27353
                                        77 -> 80     0.61507
```

Permanent and transition dipole moments for CFP (gas phase, 6-31G*)

	μ_x	μ_y	μ_z	$\lvert\mu\rvert$
$\overline{\mu} = \langle 0\lvert\mu\rvert 0\rangle$	-3.6952	-0.1602	-2.7317	4.5981
$\langle 1\lvert\mu\rvert 1\rangle - \overline{\mu}$	-1.7894	-0.0984	1.7383	2.4966
$\langle 2\lvert\mu\rvert 2\rangle - \overline{\mu}$	1.4173	0.0597	-3.8054	4.0613
$\langle 3\lvert\mu\rvert 3\rangle - \overline{\mu}$	-3.4892	-0.1552	3.6603	5.0592
$\langle 4\lvert\mu\rvert 4\rangle - \overline{\mu}$	-3.0044	-0.1364	2.6167	3.9865
$\langle 5\lvert\mu\rvert 5\rangle - \overline{\mu}$	5.0631	0.2185	-4.3567	6.6830
$\langle 1\lvert\mu\rvert 2\rangle$	0.0295	-0.0354	0.0605	0.0761
$\langle 1\lvert\mu\rvert 3\rangle$	1.8217	0.0774	-1.9602	**2.6772**
$\langle 2\lvert\mu\rvert 3\rangle$	-0.0356	-0.0533	0.0492	0.0808
$\langle 1\lvert\mu\rvert 4\rangle$	-2.6909	-0.1220	2.4560	**3.6453**
$\langle 2\lvert\mu\rvert 4\rangle$	0.0899	0.0735	-0.1034	0.1555
$\langle 3\lvert\mu\rvert 4\rangle$	-3.3651	-0.1506	3.6776	**4.9871**
$\langle 1\lvert\mu\rvert 5\rangle$	0.1829	0.0100	-0.2274	0.2920
$\langle 2\lvert\mu\rvert 5\rangle$	-0.1371	0.0057	0.14732	0.2013
$\langle 3\lvert\mu\rvert 5\rangle$	3.7596	0.1706	-3.8291	**5.3690**
$\langle 4\lvert\mu\rvert 5\rangle$	0.6781	0.0226	-0.5157	0.8522