

Supporting Information for:

The Effect of Explicit Solvent on  
Photodegradation of Decabromodiphenyl  
Ether in Toluene: Insights from Theoretical  
Study

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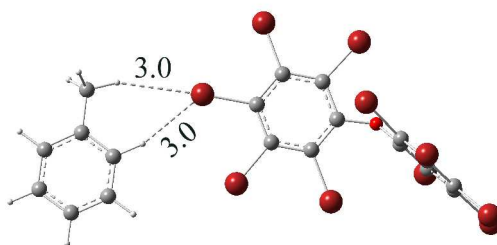
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Total 10 pages, including 1 table and 2 figures

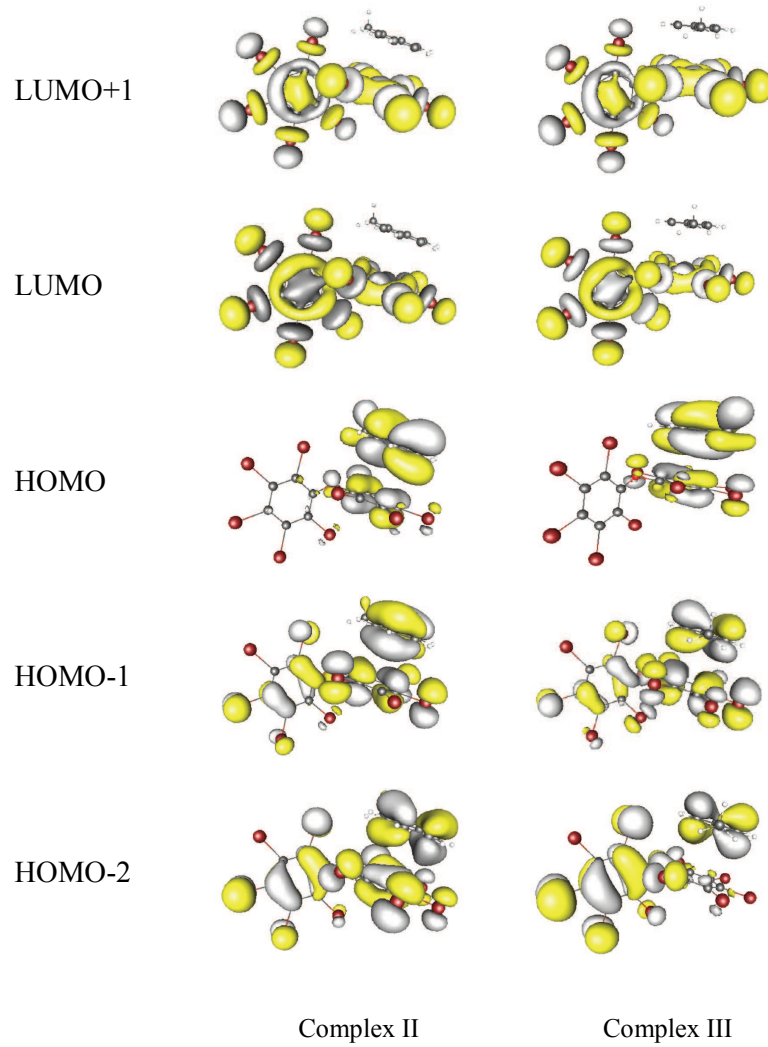
**Table 1s.** Properties of low-lying transitions for BDE209 and Complex I in the toluene solvent using fine and ultrafine integration grids, respectively.

|           | Transition                                 | Fine grid         |                       | Ultrafine grid    |                       |
|-----------|--------------------------------------------|-------------------|-----------------------|-------------------|-----------------------|
|           |                                            | Abs. <sup>a</sup> | <i>f</i> <sup>b</sup> | Abs. <sup>a</sup> | <i>f</i> <sup>b</sup> |
| BDE209    | $\pi_{\text{BDE209}} \rightarrow \sigma^*$ | 333               | 0.0136                | 333               | 0.0137                |
|           | $\pi_{\text{cpx}} \rightarrow \sigma^*$    | 342               | 0.0051                | 342               | 0.0050                |
| Complex I | $\pi_{\text{cpx}} \rightarrow \sigma^*$    | 333               | 0.0093                | 333               | 0.0092                |
|           | $\pi_{\text{tolu}} \rightarrow \sigma^*$   | 305               | 0.0102                | 305               | 0.0101                |

<sup>a</sup> Vertical excitation wavelength in nm; <sup>b</sup> oscillator strengths.



**Figure 1s.** Structure of H-bonding complex. Bond lengths are in Angstroms.



**Figure 2s.** Frontier molecular orbitals of BDE209-tolu Complex II and Complex III.

Cartesian coordinate for BDE209:

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.702551 | -0.942940 | -1.134529 |
| C  | -1.423096 | -0.381974 | -1.039550 |
| C  | -1.202112 | 0.695375  | -0.182778 |
| C  | -2.266800 | 1.256756  | 0.526978  |
| C  | -3.544462 | 0.710022  | 0.425929  |
| C  | -3.762742 | -0.404475 | -0.396487 |
| O  | -0.004320 | 1.326779  | -0.055391 |
| Br | 0.005673  | -1.044459 | -2.095988 |
| Br | -1.885935 | 2.723915  | 1.657005  |
| Br | -5.492175 | -1.171760 | -0.509129 |
| Br | -4.966259 | 1.468642  | 1.418360  |
| Br | -2.993066 | -2.425744 | -2.276301 |
| C  | 1.198453  | 0.721587  | 0.136114  |
| C  | 2.256063  | 1.216958  | -0.631878 |
| C  | 1.432793  | -0.263351 | 1.094517  |
| C  | 3.534666  | 0.680322  | -0.497507 |
| C  | 2.710695  | -0.823263 | 1.214861  |
| C  | 3.761074  | -0.359062 | 0.415574  |
| Br | 0.021080  | -0.817745 | 2.232785  |
| Br | 3.013283  | -2.200264 | 2.480449  |
| Br | 5.489246  | -1.122714 | 0.567990  |
| Br | 4.946748  | 1.347753  | -1.566313 |
| Br | 1.863769  | 2.578093  | -1.884409 |

Cartesian coordinate for BDE209-tolu Complex I:

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.290911  | -0.466936 | 1.442506  |
| C  | 1.067337  | 0.006807  | 0.956776  |
| C  | 0.849216  | 0.080713  | -0.417141 |
| C  | 1.875601  | -0.239441 | -1.307422 |
| C  | 3.099276  | -0.699553 | -0.830316 |
| C  | 3.309774  | -0.815886 | 0.550253  |
| O  | -0.294097 | 0.565283  | -0.974075 |
| Br | -0.282704 | 0.609456  | 2.144176  |
| Br | 1.530703  | -0.019754 | -3.153376 |
| Br | 4.989809  | -1.405157 | 1.203092  |
| Br | 4.467006  | -1.156937 | -2.057313 |
| Br | 2.577760  | -0.585450 | 3.310552  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.557522 | 0.193536  | -0.640357 |
| C  | -2.487193 | 1.229136  | -0.515714 |
| C  | -1.973709 | -1.132893 | -0.527381 |
| C  | -3.813817 | 0.948698  | -0.193650 |
| C  | -3.298244 | -1.417698 | -0.175155 |
| C  | -4.217001 | -0.378346 | 0.005910  |
| Br | -0.737770 | -2.526935 | -0.878273 |
| Br | -3.841184 | -3.220036 | 0.033799  |
| Br | -6.003747 | -0.764577 | 0.506908  |
| Br | -5.053858 | 2.368647  | -0.015748 |
| Br | -1.868451 | 3.001113  | -0.753057 |
| H  | 6.246536  | 1.439868  | 0.186385  |
| C  | 5.786383  | 2.107948  | -0.550120 |
| H  | 5.773735  | 1.588706  | -1.514320 |
| H  | 6.449186  | 2.976087  | -0.656217 |
| C  | 4.411156  | 2.532920  | -0.135311 |
| C  | 4.077373  | 2.663954  | 1.212575  |
| C  | 3.439152  | 2.835180  | -1.087858 |
| C  | 2.816473  | 3.097135  | 1.598561  |
| H  | 4.819824  | 2.415666  | 1.971681  |
| C  | 2.177571  | 3.274148  | -0.707901 |
| H  | 3.673572  | 2.714015  | -2.146329 |
| C  | 1.863602  | 3.413071  | 0.638083  |
| H  | 2.571949  | 3.182506  | 2.655985  |
| H  | 1.431181  | 3.500841  | -1.468418 |
| H  | 0.873998  | 3.752174  | 0.939206  |

Cartesian coordinate for BDE209-tolu Complex II:

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.286051  | -0.656577 | 1.356571  |
| C  | 1.074921  | -0.104675 | 0.924390  |
| C  | 0.875158  | 0.142733  | -0.432702 |
| C  | 1.918516  | -0.051495 | -1.339749 |
| C  | 3.139539  | -0.563575 | -0.907774 |
| C  | 3.315751  | -0.898073 | 0.441100  |
| O  | -0.269339 | 0.672812  | -0.947269 |
| Br | -0.268814 | 0.380713  | 2.169668  |
| Br | 1.598300  | 0.390716  | -3.151288 |
| Br | 4.963493  | -1.627039 | 1.028074  |
| Br | 4.552952  | -0.783596 | -2.147535 |
| Br | 2.536350  | -1.036869 | 3.195048  |
| C  | -1.526390 | 0.254460  | -0.643106 |
| C  | -2.463169 | 1.258482  | -0.386875 |
| C  | -1.925315 | -1.081761 | -0.671233 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -3.780792 | 0.928438  | -0.077596 |
| C  | -3.239820 | -1.420418 | -0.329507 |
| C  | -4.166704 | -0.417962 | -0.022939 |
| Br | -0.684304 | -2.414232 | -1.197842 |
| Br | -3.756947 | -3.241937 | -0.296603 |
| Br | -5.943037 | -0.877130 | 0.454823  |
| Br | -5.032013 | 2.302275  | 0.284302  |
| Br | -1.861293 | 3.051438  | -0.422995 |
| H  | 2.451060  | 3.450830  | -2.354656 |
| C  | 2.093374  | 3.838211  | -1.394957 |
| H  | 1.018563  | 3.634341  | -1.330734 |
| H  | 2.210010  | 4.929351  | -1.420362 |
| C  | 2.842330  | 3.242457  | -0.243880 |
| C  | 4.131151  | 2.739676  | -0.413042 |
| C  | 2.280447  | 3.200459  | 1.032005  |
| C  | 4.842942  | 2.217115  | 0.659182  |
| H  | 4.581234  | 2.750950  | -1.406318 |
| C  | 2.989288  | 2.683025  | 2.107961  |
| H  | 1.265005  | 3.570981  | 1.181551  |
| C  | 4.274806  | 2.189148  | 1.925782  |
| H  | 5.841264  | 1.812959  | 0.499611  |
| H  | 2.529235  | 2.653899  | 3.094082  |
| H  | 4.821836  | 1.764334  | 2.765372  |

Cartesian coordinate for BDE209-tolu Complex III:

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.409118  | -0.199638 | 1.398222  |
| C  | 1.154750  | 0.130950  | 0.871548  |
| C  | 0.895563  | -0.084003 | -0.480458 |
| C  | 1.899363  | -0.575539 | -1.317243 |
| C  | 3.154352  | -0.887601 | -0.801939 |
| C  | 3.409651  | -0.708644 | 0.564047  |
| O  | -0.261680 | 0.278526  | -1.097817 |
| Br | -0.180732 | 0.925745  | 1.958203  |
| Br | 1.484085  | -0.773848 | -3.150843 |
| Br | 5.121596  | -1.116266 | 1.266060  |
| Br | 4.510358  | -1.519187 | -1.962092 |
| Br | 2.753618  | 0.078322  | 3.240128  |
| C  | -1.521274 | 0.005278  | -0.670272 |
| C  | -2.433791 | 1.061364  | -0.746926 |
| C  | -1.951893 | -1.260591 | -0.274835 |
| C  | -3.759767 | 0.876264  | -0.362128 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -3.276860 | -1.444395 | 0.139159  |
| C  | -4.180698 | -0.377122 | 0.103262  |
| Br | -0.738824 | -2.716326 | -0.324178 |
| Br | -3.843506 | -3.154081 | 0.727836  |
| Br | -5.974630 | -0.625891 | 0.662423  |
| Br | -4.973945 | 2.325360  | -0.458346 |
| Br | -1.786153 | 2.738395  | -1.339412 |
| H  | 1.534885  | 3.634885  | 2.426951  |
| C  | 2.578017  | 3.828220  | 2.154210  |
| H  | 3.215423  | 3.353124  | 2.907306  |
| H  | 2.734684  | 4.911622  | 2.232329  |
| C  | 2.889185  | 3.334327  | 0.775549  |
| C  | 1.930111  | 3.384591  | -0.235685 |
| C  | 4.150576  | 2.830922  | 0.463646  |
| C  | 2.227078  | 2.960830  | -1.523794 |
| H  | 0.929657  | 3.753437  | -0.004969 |
| C  | 4.454267  | 2.406971  | -0.823679 |
| H  | 4.906137  | 2.765859  | 1.247020  |
| C  | 3.494098  | 2.475081  | -1.824544 |
| H  | 1.458122  | 2.992884  | -2.294768 |
| H  | 5.443897  | 2.008631  | -1.041416 |
| H  | 3.724202  | 2.130006  | -2.831020 |

Cartesian coordinate for BDE209  $\pi_{\text{BDE209}}\sigma^*$ :

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.478896 | -1.218618 | -0.957670 |
| C  | -1.242662 | -0.570364 | -1.006703 |
| C  | -1.123701 | 0.708170  | -0.465266 |
| C  | -2.237299 | 1.392524  | 0.016103  |
| C  | -3.475844 | 0.756199  | 0.051251  |
| C  | -3.592209 | -0.562992 | -0.413360 |
| O  | 0.060354  | 1.386880  | -0.472690 |
| Br | 0.258006  | -1.352946 | -1.858228 |
| Br | -1.967364 | 3.147652  | 0.656994  |
| Br | -5.262948 | -1.446587 | -0.329198 |
| Br | -4.974728 | 1.676615  | 0.741925  |
| Br | -2.637853 | -2.973525 | -1.647439 |
| C  | 1.190253  | 0.889338  | 0.058647  |
| C  | 2.398615  | 1.352468  | -0.544151 |
| C  | 1.249639  | 0.017036  | 1.164842  |
| C  | 3.535880  | 0.614978  | -0.372808 |
| C  | 2.409189  | -0.676369 | 1.361093  |
| C  | 3.433929  | -0.555980 | 0.398163  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Br | -0.220103 | -0.073537 | 2.438944  |
| Br | 2.747165  | -1.671760 | 2.996611  |
| Br | 4.457788  | -2.109099 | -0.078717 |
| Br | 5.239617  | 1.169048  | -1.103904 |
| Br | 2.335157  | 2.949186  | -1.587254 |

Cartesian coordinate for BDE209-tolu Complex I –  $\pi_{\text{CPX}}\sigma^*$ :

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.187014 | -1.115489 | -1.092804 |
| C  | -0.976026 | -0.476464 | -0.818173 |
| C  | -0.864654 | 0.300156  | 0.334372  |
| C  | -1.953186 | 0.489767  | 1.183582  |
| C  | -3.159053 | -0.150583 | 0.915070  |
| C  | -3.274818 | -0.962363 | -0.222400 |
| O  | 0.256288  | 1.026337  | 0.612174  |
| Br | 0.480665  | -0.553921 | -2.027648 |
| Br | -1.700332 | 1.609972  | 2.681945  |
| Br | -4.920467 | -1.817331 | -0.606238 |
| Br | -4.627349 | 0.108100  | 2.079003  |
| Br | -2.361731 | -2.140706 | -2.673293 |
| C  | 1.492567  | 0.513210  | 0.672785  |
| C  | 2.538116  | 1.410428  | 0.285382  |
| C  | 1.816317  | -0.775768 | 1.132731  |
| C  | 3.745928  | 0.887433  | -0.083636 |
| C  | 3.056473  | -1.262334 | 0.834315  |
| C  | 3.888896  | -0.507014 | -0.019195 |
| Br | 0.562784  | -1.764643 | 2.246316  |
| Br | 3.774300  | -2.850138 | 1.708574  |
| Br | 4.969158  | -1.429216 | -1.316476 |
| Br | 5.216885  | 2.014052  | -0.652293 |
| Br | 2.154469  | 3.280469  | 0.272193  |
| H  | -5.717169 | 1.209432  | -1.695349 |
| C  | -5.356318 | 2.134422  | -1.232154 |
| H  | -5.568736 | 2.077036  | -0.158846 |
| H  | -5.962359 | 2.954899  | -1.636894 |
| C  | -3.899385 | 2.357421  | -1.497588 |
| C  | -3.302790 | 1.876805  | -2.663006 |
| C  | -3.109019 | 3.071713  | -0.598826 |
| C  | -1.961679 | 2.115699  | -2.930509 |
| H  | -3.903336 | 1.304307  | -3.370672 |
| C  | -1.764500 | 3.305106  | -0.856237 |
| H  | -3.555112 | 3.444430  | 0.324123  |
| C  | -1.185601 | 2.829244  | -2.025288 |
| H  | -1.515516 | 1.726741  | -3.844324 |

|   |           |          |           |
|---|-----------|----------|-----------|
| H | -1.159793 | 3.844754 | -0.128826 |
| H | -0.127195 | 2.997072 | -2.220022 |

Cartesian coordinate for BDE209-tolu Complex I -  $\pi_{\text{tolu}}\sigma^*\text{-P}$ :

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.281593  | -0.520820 | 1.307503  |
| C  | 1.027703  | -0.073014 | 0.898543  |
| C  | 0.801778  | 0.143052  | -0.475924 |
| C  | 1.837190  | -0.045572 | -1.396685 |
| C  | 3.081878  | -0.461619 | -0.941332 |
| C  | 3.297073  | -0.678368 | 0.403565  |
| O  | -0.358441 | 0.637963  | -0.988437 |
| Br | -0.374017 | 0.270467  | 2.158099  |
| Br | 1.465515  | 0.312717  | -3.233552 |
| Br | 5.409887  | -1.442859 | 1.139144  |
| Br | 4.508657  | -0.738256 | -2.211450 |
| Br | 2.600711  | -0.858446 | 3.192333  |
| C  | -1.614895 | 0.243754  | -0.656959 |
| C  | -2.537652 | 1.265393  | -0.428408 |
| C  | -2.026504 | -1.088139 | -0.637272 |
| C  | -3.856787 | 0.963031  | -0.099766 |
| C  | -3.342101 | -1.399561 | -0.276759 |
| C  | -4.256442 | -0.376792 | 0.001872  |
| Br | -0.787612 | -2.441550 | -1.103207 |
| Br | -3.873661 | -3.213062 | -0.174129 |
| Br | -6.033419 | -0.799399 | 0.507499  |
| Br | -5.089908 | 2.363378  | 0.221040  |
| Br | -1.914242 | 3.051877  | -0.530908 |
| H  | 5.975764  | 0.980061  | 0.101351  |
| C  | 5.799350  | 2.050233  | -0.124164 |
| H  | 6.043744  | 2.233058  | -1.171799 |
| H  | 6.501957  | 2.590051  | 0.523634  |
| C  | 4.409012  | 2.381499  | 0.211904  |
| C  | 3.990663  | 2.327022  | 1.575337  |
| C  | 3.470719  | 2.755910  | -0.774742 |
| C  | 2.711768  | 2.665301  | 1.930357  |
| H  | 4.709299  | 1.995174  | 2.320972  |
| C  | 2.184546  | 3.069150  | -0.420829 |
| H  | 3.781352  | 2.778084  | -1.816405 |
| C  | 1.795825  | 3.020565  | 0.934491  |
| H  | 2.395049  | 2.619772  | 2.967663  |
| H  | 1.447855  | 3.334540  | -1.175333 |
| H  | 0.767330  | 3.249050  | 1.202636  |

Cartesian coordinate for BDE209-tolu Complex I -  $\pi_{\text{tolu}}\sigma^*\text{-M}$ :

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -3.286982 | -1.445110 | 0.089927  |
| C  | -1.981857 | -1.220594 | -0.361569 |
| C  | -1.588171 | 0.068989  | -0.716015 |
| C  | -2.522172 | 1.105076  | -0.728199 |
| C  | -3.830212 | 0.883444  | -0.304729 |
| C  | -4.210898 | -0.393860 | 0.128516  |
| O  | -0.343860 | 0.371137  | -1.171926 |
| Br | -0.737821 | -2.641444 | -0.510975 |
| Br | -1.927910 | 2.811727  | -1.298231 |
| Br | -5.978458 | -0.699744 | 0.737231  |
| Br | -5.070967 | 2.312431  | -0.310426 |
| Br | -3.798376 | -3.185219 | 0.635190  |
| C  | 0.823836  | 0.028004  | -0.564662 |
| C  | 1.851193  | -0.395713 | -1.428640 |
| C  | 1.090339  | 0.139452  | 0.808013  |
| C  | 3.077282  | -0.791353 | -0.912404 |
| C  | 2.294112  | -0.248097 | 1.315441  |
| C  | 3.263786  | -0.749329 | 0.483244  |
| Br | -0.289133 | 0.832034  | 1.993082  |
| Br | 2.905667  | 0.401290  | 3.523838  |
| Br | 4.873057  | -1.485031 | 1.246891  |
| Br | 4.471507  | -1.351894 | -2.085137 |
| Br | 1.490765  | -0.398127 | -3.291582 |
| H  | 5.801492  | 1.017343  | 0.665484  |
| C  | 5.760912  | 1.939065  | 0.055194  |
| H  | 6.177180  | 1.708296  | -0.927414 |
| H  | 6.407420  | 2.655946  | 0.575407  |
| C  | 4.368886  | 2.413682  | -0.007513 |
| C  | 3.753975  | 2.921355  | 1.177464  |
| C  | 3.620887  | 2.366319  | -1.197705 |
| C  | 2.447065  | 3.337802  | 1.169017  |
| H  | 4.337606  | 2.948489  | 2.093116  |
| C  | 2.311888  | 2.775007  | -1.203337 |
| H  | 4.084064  | 1.980516  | -2.103318 |
| C  | 1.713111  | 3.249301  | -0.012796 |
| H  | 1.975405  | 3.688694  | 2.081210  |
| H  | 1.717192  | 2.726049  | -2.112270 |
| H  | 0.667061  | 3.544106  | -0.028049 |