|          | ADC(2  | 2)/cc-pVDZ/IEFP  | CM(T1)   |                   |
|----------|--|--|--|-------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \overset{\cdot}{\mathrm{E}}(\overset{\cdot}{\mathrm{S}_1}\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $f_{12}(S_0-S_1)$ |
| S1       | 1.0209   | 1.1938   | -0.1729  | 0.0000            |
| S2       | 0.9222   | 1.0459   | -0.1237  | 0.0006            |
| S3       | 1.3804   | 1.4912   | -0.1107  | 0.0005            |
| S4       | 1.6235   | 1.7745   | -0.1509  | 0.0023            |
| S5       | 1.5177   | 1.4277   | 0.0900   | 0.0001            |
| S6       | 1.3599   | 1.4992   | -0.1394  | 0.0002            |
| S7       | 1.7317   | 1.7968   | -0.0651  | 0.0006            |
| S8       | 1.2853   | 1.3514   | -0.0661  | 0.0024            |
| S9       | 1.4256   | 1.5748   | -0.1492  | 0.0003            |
| S10      | 1.8155   | 1.7417   | 0.0738   | 0.0012            |
| S11      | 1.5362   | 1.6859   | -0.1498  | 0.0025            |
| S12      | 1.8027   | 1.9607   | -0.1580  | 0.0016            |
| S13      | 1.8626   | 1.9908   | -0.1282  | 0.0038            |
| S14      | 2.0412   | 2.2121   | -0.1709  | 0.0045            |
| S15      | 1.4790   | 1.5381   | -0.0591  | 0.0008            |
| S16      | 1.8052   | 1.8681   | -0.0629  | 0.0000            |
| S17      | 1.6339   | 1.7647   | -0.1308  | 0.0017            |
| S18      | 1.8182   | 2.0021   | -0.1839  | 0.0000            |
| S19      | 1.3486   | 1.3544   | -0.0058  | 0.0021            |
| S20      | 1.3970   | 1.4771   | -0.0802  | 0.0064            |
| S21      | 0.8086   | 0.9141   | -0.1055  | 0.0005            |
| S22      | 1.3172   | 1.2661   | 0.0510   | 0.0023            |
| S23      | 1.6135   | 1.3711   | 0.2423   | 0.0005            |
| S24      | 1.4216   | 1.3843   | 0.0373   | 0.0032            |
| S25      | 1.6883   | 1.6649   | 0.0234   | 0.0033            |
| S26      | 1.4853   | 1.5769   | -0.0916  | 0.0039            |
| S27      | 1.7351   | 1.7890   | -0.0538  | 0.0086            |
| S28      | 1.5609   | 1.3938   | 0.1671   | 0.0010            |
| S29      | 1.8650   | 1.7011   | 0.1639   | 0.0021            |
| S30      | 1.2663   | 1.3792   | -0.1129  | 0.0003            |
| S31      | 1.5268   | 1.6150   | -0.0882  | 0.0040            |
| S32      | 1.8977   | 1.7521   | 0.1457   | 0.0005            |
| S33      | 1.7684   | 1.7684   | 0.0051   | 0.0000            |
| S34      | 1.3426   | 1.4105   | -0.0679  | 0.0010            |
| S35      | 2.1180   | 1.8201   | 0.2979   | 0.0002            |
| S36      | 1.9718   | 1.8354   | 0.1364   | 0.0014            |
| S37      | 1.5709   | 1.6879   | -0.1170  | 0.0035            |
| S38      | 1.9220   | 1.8985   | 0.0236   | 0.0025            |
| S39      | 1.9078   | 1.9741   | -0.0663  | 0.0076            |
| S40      | 1.2191   | 1.3430   | -0.1239  | 0.0000            |
| S41      | 1.5459   | 1.6382   | -0.0923  | 0.0017            |
| S42      | 1.8335   | 1.8074   | 0.0261   | 0.0018            |
| S43      | 1.7758   | 1.8771   | -0.1013  | 0.0004            |
| S44      | 1.5292   | 1.7042   | -0.1750  | 0.0002            |
| S45      | 1.3842   | 1.4706   | -0.0865  | 0.0024            |
| S46      | 2.0624   | 2.1014   | -0.0390  | 0.0000            |

|          | ADC(2  | 2)/cc-pVDZ/IEFP  | CM(T1)                                  |                   |
|----------|--|--|---|-------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \dot{E}(\dot{S_1}-T_1) \; [eV]$ | $f_{12}(S_0-S_1)$ |
| S47      | 1.8524   | 2.0150   | -0.1626                                 | 0.0006            |
| S48      | 1.6620   | 1.7581   | -0.0960                                 | 0.0016            |
| S49      | 1.7703   | 1.8677   | -0.0975                                 | 0.0021            |
| S50      | 1.7509   | 1.8228   | -0.0719                                 | 0.0042            |
| S51      | 2.1527   | 2.2927   | -0.1400                                 | 0.0017            |
| S52      | 2.0927   | 2.2665   | -0.1738                                 | 0.0024            |
| S53      | 2.3326   | 2.5414   | -0.2088                                 | 0.0017            |
| S54      | 2.2186   | 2.2233   | -0.0047                                 | 0.0010            |
| S55      | 1.8594   | 1.9969   | -0.1375                                 | 0.0025            |
| S56      | 2.1257   | 2.2943   | -0.1686                                 | 0.0011            |
| S57      | 1.9330   | 1.6844   | 0.2486                                  | 0.0021            |
| S58      | 1.1270   | 1.2007   | -0.0737                                 | 0.0027            |
| S59      | 1.4915   | 1.4913   | 0.0002                                  | 0.0057            |
| S60      | 2.1763   | 2.0575   | 0.1188                                  | 0.0012            |
| S61      | 2.1134   | 2.1226   | -0.0092                                 | 0.0072            |
| S62      | 2.4029   | 2.1324   | 0.2705                                  | 0.0003            |
| S63      | 1.7246   | 1.6950   | 0.0295                                  | 0.0022            |
| S64      | 2.0664   | 2.0084   | 0.0580                                  | 0.0050            |
| S65      | 1.7493   | 1.8985   | -0.1492                                 | 0.0060            |
| S66      | 1.6458   | 1.6840   | -0.0381                                 | 0.0007            |
| S67      | 1.6446   | 1.7503   | -0.1057                                 | 0.0038            |
| S68      | 1.9641   | 2.0520   | -0.0879                                 | 0.0038            |
| S69      | 2.0458   | 2.1993   | -0.1535                                 | 0.0086            |
| S70      | 2.1797   | 2.1357   | 0.0440                                  | 0.0022            |
| S71      | 1.6294   | 1.8024   | -0.1730                                 | 0.0007            |
| S72      | 1.8978   | 2.0618   | -0.1640                                 | 0.0035            |
| S73      | 2.0370   | 2.2464   | -0.2094                                 | 0.0001            |
| S74      | 1.8800   | 2.0230   | -0.1430                                 | 0.0020            |
| S75      | 1.3709   | 1.4355   | -0.0646                                 | 0.0044            |
| S76      | 1.8611   | 1.7567   | 0.1043                                  | 0.0063            |
| S77      | 1.9699   | 2.0620   | -0.0921                                 | 0.0068            |
| S78      | 1.7496   | 1.7728   | -0.0231                                 | 0.0030            |
| S79      | 1.7535   | 1.8547   | -0.1012                                 | 0.0033            |
| S80      | 2.3287   | 2.2050   | 0.1236                                  | 0.0033            |
| S81      | 2.2453   | 2.3332   | -0.0879                                 | 0.0060            |
| S82      | 1.6986   | 1.8669   | -0.1683                                 | 0.0009            |
| S83      | 2.1816   | 2.2561   | -0.0745                                 | 0.0005            |
| S84      | 2.5780   | 2.8559   | -0.2779                                 | 0.0000            |
| S85      | 2.3000   | 2.2651   | 0.0349                                  | 0.0064            |
| S86      | 1.6502   | 1.6907   | -0.0405                                 | 0.0100            |
| S87      | 2.0364   | 2.0534   | -0.0171                                 | 0.0082            |
| S88      | 2.0596   | 2.0124   | 0.0471                                  | 0.0046            |
| S89      | 0.6932   | 0.7907   | -0.0974                                 | 0.0000            |
| S90      | 1.7001   | 1.3645   | 0.3356                                  | 0.0011            |
| S91      | 1.0765   | 1.1510   | -0.0746                                 | 0.0010            |
| S92      | 2.2112   | 1.8077   | 0.4035                                  | 0.0018            |

|          | ADC(2  | 2)/cc-pVDZ/IEFP  | CM(T1)                                  |                   |
|----------|--|--|---|-------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \dot{E}(\dot{S_1}-T_1) \; [eV]$ | $f_{12}(S_0-S_1)$ |
| S93      | 1.1436   | 1.2541   | -0.1105                                 | 0.0001            |
| S94      | 1.8463   | 1.7146   | 0.1317                                  | 0.0004            |
| S95      | 1.8582   | 1.7243   | 0.1340                                  | 0.0045            |
| S96      | 1.5176   | 1.6748   | -0.1572                                 | 0.0000            |
| S97      | 1.0368   | 1.1344   | -0.0976                                 | 0.0008            |
| S98      | 2.7007   | 2.2808   | 0.4199                                  | 0.0000            |
| S99      | 1.8001   | 1.6257   | 0.1743                                  | 0.0038            |
| S100     | 1.4161   | 1.5691   | -0.1531                                 | 0.0010            |
| S101     | 2.4308   | 2.2076   | 0.2232                                  | 0.0033            |
| S102     | 1.4762   | 1.5971   | -0.1209                                 | 0.0018            |
| S103     | 2.1410   | 2.0564   | 0.0846                                  | 0.0026            |
| S104     | 1.8341   | 1.9302   | -0.0961                                 | 0.0000            |
| S105     | 1.0650   | 1.2420   | -0.1770                                 | 0.0000            |
| S106     | 1.0772   | 1.2182   | -0.1410                                 | 0.0000            |
| S107     | 1.3084   | 1.4621   | -0.1537                                 | 0.0031            |
| S108     | 1.1218   | 1.1468   | -0.0251                                 | 0.0007            |
| S109     | 1.2540   | 1.4221   | -0.1680                                 | 0.0019            |
| S110     | 1.1170   | 1.1225   | -0.0055                                 | 0.0009            |
| S111     | 1.1664   | 1.3489   | -0.1826                                 | 0.0006            |
| S112     | 1.0140   | 1.1125   | -0.0985                                 | 0.0004            |
| S113     | 1.0936   | 1.2735   | -0.1799                                 | 0.0001            |
| S114     | 0.9905   | 1.1325   | -0.1420                                 | 0.0004            |
| S115     | 1.0523   | 1.2248   | -0.1725                                 | 0.0000            |
| S116     | 0.9981   | 1.1544   | -0.1563                                 | 0.0002            |
| S117     | 1.0353   | 1.2033   | -0.1680                                 | 0.0000            |
| S118     | 1.0045   | 1.1633   | -0.1588                                 | 0.0002            |
| S119     | 1.3498   | 1.4878   | -0.1380                                 | 0.0042            |
| S120     | 1.0051   | 1.1393   | -0.1343                                 | 0.0002            |
| S121     | 0.9596   | 1.0985   | -0.1389                                 | 0.0009            |
| S122     | 1.0375   | 1.2061   | -0.1686                                 | 0.0005            |
| S123     | 0.8165   | 0.8817   | -0.0652                                 | 0.0018            |
| S124     | 1.3377   | 1.4788   | -0.1411                                 | 0.0008            |
| S125     | 0.9038   | 1.0472   | -0.1433                                 | 0.0006            |
| S126     | 1.0885   | 1.2536   | -0.1651                                 | 0.0006            |
| S127     | 0.9298   | 1.0730   | -0.1432                                 | 0.0006            |
| S128     | 1.0981   | 1.2654   | -0.1673                                 | 0.0006            |
| S129     | 0.8676   | 0.9604   | -0.0928                                 | 0.0011            |
| S130     | 1.2254   | 1.3642   | -0.1389                                 | 0.0005            |
| S131     | 1.3418   | 1.4838   | -0.1420                                 | 0.0041            |
| S132     | 0.9883   | 1.1561   | -0.1678                                 | 0.0000            |
| S133     | 0.8024   | 0.8999   | -0.0975                                 | 0.0013            |
| S134     | 1.3115   | 1.4479   | -0.1363                                 | 0.0007            |
| S135     | 0.9961   | 1.1377   | -0.1416                                 | 0.0001            |
| S136     | 1.0886   | 1.2616   | -0.1729                                 | 0.0003            |
| S137     | 0.7971   | 0.8463   | -0.0492                                 | 0.0014            |
| S138     | 1.4206   | 1.5274   | -0.1068                                 | 0.0010            |

|          | ADC(2  | 2)/cc-pVDZ/IEFP  | CM(T1)   |                   |
|----------|--|--|--|-------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \dot{\mathrm{E}}(\dot{\mathrm{S_1-T_1}}) \; [\mathrm{eV}]$ | $f_{12}(S_0-S_1)$ |
| S139     | 0.9457   | 1.0805   | -0.1349  | 0.0004            |
| S140     | 1.1656   | 1.3303   | -0.1647  | 0.0002            |
| S141     | 2.6291   | 2.9075   | -0.2784  | 0.0001            |
| S142     | 2.9648   | 3.1741   | -0.2093  | 0.0142            |
| S143     | 2.8799   | 3.1287   | -0.2487  | 0.0078            |
| S144     | 2.7894   | 3.0666   | -0.2773  | 0.0031            |
| S145     | 2.6933   | 2.9736   | -0.2803  | 0.0007            |
| S146     | 2.6437   | 2.9239   | -0.2802  | 0.0001            |
| S147     | 2.6195   | 2.8962   | -0.2767  | 0.0000            |
| S148     | 2.9909   | 3.1876   | -0.1967  | 0.0160            |
| S149     | 2.5581   | 2.8238   | -0.2657  | 0.0002            |
| S150     | 2.4438   | 2.6696   | -0.2258  | 0.0015            |
| S151     | 2.4998   | 2.7560   | -0.2562  | 0.0006            |
| S152     | 2.5625   | 2.8273   | -0.2648  | 0.0002            |
| S153     | 2.4716   | 2.7011   | -0.2295  | 0.0013            |
| S154     | 3.0751   | 3.2488   | -0.1737  | 0.0202            |
| S155     | 2.4912   | 2.7244   | -0.2332  | 0.0023            |
| S156     | 1.8961   | 2.4063   | -0.5102  | 0.0436            |
| S157     | 2.6469   | 2.8957   | -0.2488  | 0.0004            |
| S158     | 2.5920   | 2.8455   | -0.2535  | 0.0009            |
| S159     | 1.6147   | 1.7737   | -0.1590  | 0.0025            |
| S160     | 1.6114   | 1.7593   | -0.1480  | 0.0052            |
| S161     | 1.5727   | 1.7070   | -0.1343  | 0.0035            |
| S162     | 1.5537   | 1.6929   | -0.1392  | 0.0037            |
| S163     | 1.9193   | 2.0734   | -0.1542  | 0.0002            |
| S164     | 1.8914   | 1.9476   | -0.0562  | 0.0156            |
| S165     | 1.4709   | 1.5304   | -0.0595  | 0.0057            |
| S166     | 1.4390   | 1.5253   | -0.0863  | 0.0031            |
| S167     | 1.7908   | 1.9783   | -0.1875  | 0.0000            |
| S168     | 1.8206   | 1.9074   | -0.0869  | 0.0106            |
| S169     | 1.4559   | 1.5486   | -0.0927  | 0.0048            |
| S170     | 1.4276   | 1.4952   | -0.0676  | 0.0035            |
| S171     | 1.6908   | 1.8803   | -0.1895  | 0.0004            |
| S172     | 1.7254   | 1.8512   | -0.1258  | 0.0063            |
| S173     | 1.4260   | 1.5399   | -0.1139  | 0.0048            |
| S174     | 1.4346   | 1.5528   | -0.1182  | 0.0031            |
| S175     | 1.6141   | 1.7852   | -0.1711  | 0.0016            |
| S176     | 1.6352   | 1.7748   | -0.1397  | 0.0053            |
| S177     | 1.5410   | 1.6979   | -0.1569  | 0.0033            |
| S178     | 1.5655   | 1.7162   | -0.1507  | 0.0017            |
| S179     | 1.5596   | 1.7206   | -0.1610  | 0.0023            |
| S180     | 1.5964   | 1.7398   | -0.1434  | 0.0036            |
| S181     | 1.4636   | 1.6089   | -0.1453  | 0.0041            |
| S182     | 1.4803   | 1.6261   | -0.1458  | 0.0018            |
| S183     | 1.5389   | 1.6926   | -0.1537  | 0.0027            |
| S184     | 1.5774   | 1.7198   | -0.1424  | 0.0036            |

| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$  |          | ADC(2  | 2)/cc-pVDZ/IEFP | CM(T1)  |                   |
|---|----------|--------|-----------------|---------|-------------------|
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | Molecule |        |                 |         | $f_{12}(S_0-S_1)$ |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S185     | 1.4698 | 1.6182          | -0.1483 | 0.0042            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S186     | 1.4878 | 1.6359          | -0.1481 | 0.0016            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S187     | 1.9700 | 2.1093          | -0.1393 | 0.0008            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S188     | 1.9474 | 1.9644          | -0.0170 | 0.0185            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S189     | 1.4983 | 1.6116          | -0.1132 | 0.0052            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S190     | 1.4464 | 1.5244          | -0.0780 | 0.0034            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S191     | 1.4593 | 1.5954          | -0.1361 | 0.0067            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S192     | 1.5308 | 1.6607          | -0.1299 | 0.0072            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S193     | 1.5231 | 1.6657          | -0.1426 | 0.0058            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S194     | 1.5261 | 1.6770          | -0.1509 | 0.0012            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S195     | 1.2820 | 1.3433          | -0.0613 | 0.0094            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S196     | 1.4466 | 1.5010          | -0.0544 | 0.0041            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S197     | 1.6412 | 1.7847          | -0.1435 | 0.0053            |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | S198     | 1.6657 | 1.8132          | -0.1474 | 0.0006            |
| S201       1.5509       1.7074       -0.1566       0.0066         S202       1.5863       1.7415       -0.1552       0.0007         S203       1.4245       1.5504       -0.1259       0.0068         S204       1.5159       1.6355       -0.1196       0.0041         S205       1.5228       1.6729       -0.1501       0.0051         S206       1.5525       1.7051       -0.1526       0.0007 | S199     | 1.4153 | 1.5360          | -0.1207 | 0.0068            |
| S202     1.5863     1.7415     -0.1552     0.0007       S203     1.4245     1.5504     -0.1259     0.0068       S204     1.5159     1.6355     -0.1196     0.0041       S205     1.5228     1.6729     -0.1501     0.0051       S206     1.5525     1.7051     -0.1526     0.0007   | S200     | 1.4757 | 1.5958          | -0.1201 | 0.0044            |
| S203       1.4245       1.5504       -0.1259       0.0068         S204       1.5159       1.6355       -0.1196       0.0041         S205       1.5228       1.6729       -0.1501       0.0051         S206       1.5525       1.7051       -0.1526       0.0007   | S201     | 1.5509 | 1.7074          | -0.1566 | 0.0066            |
| S204       1.5159       1.6355       -0.1196       0.0041         S205       1.5228       1.6729       -0.1501       0.0051         S206       1.5525       1.7051       -0.1526       0.0007   | S202     | 1.5863 | 1.7415          | -0.1552 | 0.0007            |
| S205       1.5228       1.6729       -0.1501       0.0051         S206       1.5525       1.7051       -0.1526       0.0007   | S203     | 1.4245 | 1.5504          | -0.1259 | 0.0068            |
| S206 1.5525 1.7051 -0.1526 0.0007   | S204     | 1.5159 | 1.6355          | -0.1196 | 0.0041            |
|   | S205     | 1.5228 | 1.6729          | -0.1501 | 0.0051            |
| S207 1.3669 1.4456 -0.0788 0.0062   | S206     | 1.5525 | 1.7051          | -0.1526 | 0.0007            |
|   | S207     | 1.3669 | 1.4456          | -0.0788 | 0.0062            |
| S208 1.4659 1.5316 -0.0657 0.0027   | S208     | 1.4659 | 1.5316          | -0.0657 | 0.0027            |
| S209 1.6321 1.7894 -0.1573 0.0061   | S209     | 1.6321 | 1.7894          | -0.1573 | 0.0061            |
| S210 1.6506 1.8004 -0.1498 0.0005   | S210     | 1.6506 | 1.8004          | -0.1498 | 0.0005            |
| S211 1.9531 2.0952 -0.1421 0.0005   | S211     | 1.9531 | 2.0952          | -0.1421 | 0.0005            |
| S212 1.9186 1.9617 -0.0431 0.0200   | S212     | 1.9186 | 1.9617          | -0.0431 | 0.0200            |
| S213 1.5050 1.6171 -0.1121 0.0051   | S213     | 1.5050 | 1.6171          | -0.1121 | 0.0051            |
| S214 1.4901 1.6175 -0.1274 0.0028   | S214     | 1.4901 | 1.6175          | -0.1274 | 0.0028            |
| S215 1.3079 1.3811 -0.0732 0.0084   | S215     | 1.3079 | 1.3811          | -0.0732 | 0.0084            |
| S216 1.4085 1.4878 -0.0794 0.0041   | S216     | 1.4085 | 1.4878          | -0.0794 | 0.0041            |
| S217 1.6831 1.8370 -0.1539 0.0068   | S217     | 1.6831 | 1.8370          | -0.1539 | 0.0068            |
| S218 1.7892 1.9280 -0.1387 0.0003   | S218     | 1.7892 | 1.9280          | -0.1387 | 0.0003            |
| S219 1.4915 1.6205 -0.1290 0.0047   | S219     | 1.4915 | 1.6205          | -0.1290 | 0.0047            |
| S220 1.5727 1.6938 -0.1212 0.0046   | S220     | 1.5727 | 1.6938          | -0.1212 | 0.0046            |
| S221 1.5797 1.7427 -0.1629 0.0042   | S221     | 1.5797 | 1.7427          | -0.1629 | 0.0042            |
| S222 1.5948 1.7557 -0.1609 0.0016   | S222     | 1.5948 | 1.7557          | -0.1609 | 0.0016            |
| S223 1.2758 1.3117 -0.0359 0.0084   | S223     | 1.2758 | 1.3117          | -0.0359 | 0.0084            |
| S224 1.4661 1.5114 -0.0453 0.0030   | S224     | 1.4661 | 1.5114          | -0.0453 | 0.0030            |
| S225 1.7409 1.8833 -0.1423 0.0065   | S225     | 1.7409 | 1.8833          | -0.1423 | 0.0065            |
| S226 1.8472 1.9794 -0.1322 0.0001   |          |        |                 |         |                   |
| S227 1.4414 1.5521 -0.1107 0.0061   |          |        |                 |         |                   |
| S228 1.5434 1.6497 -0.1063 0.0024   |          |        |                 |         |                   |
| S229 1.6243 1.7932 -0.1689 0.0035   |          |        |                 |         |                   |
| S230 1.6978 1.8503 -0.1525 0.0018   | S230     | 1.6978 | 1.8503          | -0.1525 | 0.0018            |

| N.α - 1 1 |  | 2)/cc-pVDZ/IEFP  |  | £ (C C )          |
|-----------|--|--|--|-------------------|
| Molecule  | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $f_{12}(S_0-S_1)$ |
| S231      | 1.9540   | 2.0882   | -0.1343  | 0.0035            |
| S232      | 1.9575   | 2.0844   | -0.1269  | 0.0079            |
| S233      | 1.9393   | 2.0633   | -0.1240  | 0.0055            |
| S234      | 1.8273   | 1.9538   | -0.1265  | 0.0042            |
| S235      | 1.8937   | 1.9900   | -0.0963  | 0.0042            |
| S236      | 1.8894   | 1.9891   | -0.0997  | 0.0048            |
| S237      | 2.1773   | 2.3290   | -0.1517  | 0.0007            |
| S238      | 2.1351   | 2.2214   | -0.0863  | 0.0168            |
| S239      | 2.2005   | 2.2253   | -0.0248  | 0.0235            |
| S240      | 1.6725   | 1.7388   | -0.0663  | 0.0077            |
| S241      | 1.7907   | 1.7498   | 0.0410   | 0.0090            |
| S242      | 1.8097   | 1.8327   | -0.0230  | 0.0064            |
| S243      | 2.1147   | 2.2710   | -0.1562  | 0.0007            |
| S244      | 2.0591   | 2.1756   | -0.1165  | 0.0109            |
| S245      | 2.1544   | 2.2043   | -0.0499  | 0.0176            |
| S246      | 1.6488   | 1.7090   | -0.0602  | 0.0092            |
| S247      | 1.8328   | 1.8218   | 0.0109   | 0.0076            |
| S248      | 1.8199   | 1.8224   | -0.0025  | 0.0070            |
| S249      | 2.0063   | 2.1730   | -0.1668  | 0.0013            |
| S250      | 1.9822   | 2.1307   | -0.1485  | 0.0058            |
| S251      | 2.0781   | 2.1628   | -0.0847  | 0.0119            |
| S252      | 1.7038   | 1.8069   | -0.1031  | 0.0073            |
| S253      | 1.8174   | 1.8772   | -0.0597  | 0.0058            |
| S254      | 1.7737   | 1.8563   | -0.0826  | 0.0057            |
| S255      | 1.9413   | 2.0931   | -0.1518  | 0.0028            |
| S256      | 1.9093   | 2.0493   | -0.1400  | 0.0088            |
| S257      | 1.9690   | 2.0798   | -0.1107  | 0.0068            |
| S258      | 1.7176   | 1.8239   | -0.1063  | 0.0069            |
| S259      | 1.7861   | 1.8465   | -0.0603  | 0.0086            |
| S260      | 1.8786   | 2.0110   | -0.1324  | 0.0022            |
| S261      | 1.8840   | 2.0265   | -0.1425  | 0.0037            |
| S262      | 1.8744   | 2.0160   | -0.1416  | 0.0051            |
| S263      | 1.7681   | 1.8943   | -0.1262  | 0.0057            |
| S264      | 1.8314   | 1.9501   | -0.1187  | 0.0075            |
| S265      | 1.8205   | 1.9288   | -0.1083  | 0.0030            |
| S266      | 1.9399   | 2.0554   | -0.1155  | 0.0054            |
| S267      | 1.8643   | 1.9997   | -0.1354  | 0.0041            |
| S268      | 1.8556   | 1.9939   | -0.1383  | 0.0054            |
| S269      | 1.9193   | 2.0360   | -0.1167  | 0.0049            |
| S270      | 1.8183   | 1.9501   | -0.1318  | 0.0062            |
| S271      | 1.7899   | 1.9086   | -0.1187  | 0.0072            |
| S272      | 1.8196   | 1.9346   | -0.1150  | 0.0027            |
| S273      | 2.3075   | 2.3930   | -0.0856  | 0.0011            |
| S274      | 2.1752   | 2.2057   | -0.0305  | 0.0221            |
| S275      | 2.2821   | 2.2696   | 0.0125   | 0.0292            |
| S276      | 1.6842   | 1.7160   | -0.0319  | 0.0090            |
| ~         | = : 5 O <b>1 =</b>   |  | 0.0010   | 0.000             |

|          | ADC(2  | 2)/cc-pVDZ/IEFP  | CM(T1)   |                   |
|----------|--|--|--|-------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $f_{12}(S_0-S_1)$ |
| S277     | 1.8104   | 1.7129   | 0.0975   | 0.0125            |
| S278     | 1.8522   | 1.9278   | -0.0755  | 0.0050            |
| S279     | 1.8320   | 1.9493   | -0.1173  | 0.0076            |
| S280     | 1.9039   | 1.9732   | -0.0692  | 0.0153            |
| S281     | 1.8087   | 1.9560   | -0.1473  | 0.0036            |
| S282     | 1.8413   | 1.9600   | -0.1187  | 0.0061            |
| S283     | 1.7967   | 1.8912   | -0.0946  | 0.0125            |
| S284     | 1.8554   | 1.9713   | -0.1159  | 0.0017            |
| S285     | 1.6323   | 1.6833   | -0.0510  | 0.0129            |
| S286     | 1.8531   | 1.8307   | 0.0223   | 0.0090            |
| S287     | 1.6936   | 1.7975   | -0.1038  | 0.0024            |
| S288     | 1.9519   | 2.0900   | -0.1382  | 0.0037            |
| S289     | 1.8704   | 2.0456   | -0.1752  | 0.0003            |
| S290     | 1.9003   | 2.0339   | -0.1336  | 0.0096            |
| S291     | 1.7719   | 1.8763   | -0.1044  | 0.0093            |
| S292     | 1.8446   | 1.9006   | -0.0560  | 0.0096            |
| S293     | 1.7845   | 1.9096   | -0.1251  | 0.0023            |
| S294     | 1.8404   | 1.9744   | -0.1340  | 0.0058            |
| S295     | 1.8491   | 1.9732   | -0.1240  | 0.0111            |
| S296     | 1.8781   | 2.0113   | -0.1333  | 0.0011            |
| S297     | 1.7786   | 1.8907   | -0.1120  | 0.0067            |
| S298     | 1.8561   | 1.9278   | -0.0717  | 0.0075            |
| S299     | 1.8592   | 1.9697   | -0.1105  | 0.0028            |
| S300     | 1.8271   | 1.9632   | -0.1361  | 0.0053            |
| S301     | 1.8170   | 1.9359   | -0.1189  | 0.0092            |
| S302     | 1.8523   | 1.9830   | -0.1307  | 0.0011            |
| S303     | 1.7019   | 1.7647   | -0.0628  | 0.0087            |
| S304     | 1.7999   | 1.8430   | -0.0431  | 0.0053            |
| S305     | 1.7703   | 1.8847   | -0.1144  | 0.0020            |
| S306     | 1.9023   | 2.0426   | -0.1402  | 0.0047            |
| S307     | 1.8490   | 1.9828   | -0.1338  | 0.0104            |
| S308     | 1.8941   | 2.0528   | -0.1587  | 0.0005            |
| S309     | 2.2811   | 2.3775   | -0.0964  | 0.0012            |
| S310     | 2.1761   | 2.2196   | -0.0435  | 0.0283            |
| S311     | 2.2637   | 2.2666   | -0.0029  | 0.0280            |
| S312     | 1.7927   | 1.8847   | -0.0920  | 0.0067            |
| S313     | 1.7906   | 1.7947   | -0.0041  | 0.0110            |
| S314     | 1.8525   | 1.9266   | -0.0741  | 0.0047            |
| S315     | 1.6677   | 1.7273   | -0.0596  | 0.0109            |
| S316     | 1.7903   | 1.7931   | -0.0028  | 0.0086            |
| S317     | 1.7136   | 1.8268   | -0.1132  | 0.0016            |
| S318     | 1.9809   | 2.1324   | -0.1516  | 0.0060            |
| S319     | 2.0252   | 2.1696   | -0.1444  | 0.0007            |
| S320     | 1.9173   | 2.0558   | -0.1385  | 0.0104            |
| S321     | 1.8254   | 1.9387   | -0.1132  | 0.0071            |
| S322     | 1.9226   | 2.0117   | -0.0891  | 0.0068            |

|          | ADC(2  | 2)/cc-pVDZ/IEFP  | CM(T1)   |                   |
|----------|--|--|--|-------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \overset{\cdot}{\mathrm{E}}(\overset{\cdot}{\mathrm{S}_1}\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $f_{12}(S_0-S_1)$ |
| S323     | 1.9195   | 2.0205   | -0.1010  | 0.0044            |
| S324     | 1.8921   | 2.0380   | -0.1459  | 0.0042            |
| S325     | 1.9117   | 2.0575   | -0.1458  | 0.0016            |
| S326     | 1.9304   | 2.0556   | -0.1252  | 0.0084            |
| S327     | 1.6407   | 1.6616   | -0.0209  | 0.0118            |
| S328     | 1.7874   | 1.8251   | -0.0377  | 0.0045            |
| S329     | 1.9129   | 1.9903   | -0.0774  | 0.0032            |
| S330     | 1.9837   | 2.1261   | -0.1424  | 0.0035            |
| S331     | 1.9705   | 2.1414   | -0.1709  | 0.0008            |
| S332     | 1.8822   | 2.0290   | -0.1468  | 0.0096            |
| S333     | 1.7937   | 1.8850   | -0.0913  | 0.0084            |
| S334     | 1.9205   | 1.9765   | -0.0560  | 0.0038            |
| S335     | 1.8762   | 1.9713   | -0.0951  | 0.0027            |
| S336     | 1.9465   | 2.1021   | -0.1556  | 0.0041            |
| S337     | 1.9399   | 2.0836   | -0.1437  | 0.0067            |
| S338     | 1.9964   | 2.1468   | -0.1505  | 0.0011            |
| S339     | 2.1396   | 2.3239   | -0.1843  | 0.0018            |
| S340     | 2.1455   | 2.3128   | -0.1672  | 0.0042            |
| S341     | 2.0751   | 2.2267   | -0.1516  | 0.0028            |
| S342     | 2.4126   | 2.6099   | -0.1973  | 0.0008            |
| S343     | 2.4502   | 2.5198   | -0.0696  | 0.0210            |
| S344     | 1.8791   | 1.8959   | -0.0168  | 0.0073            |
| S345     | 2.3253   | 2.5373   | -0.2121  | 0.0001            |
| S346     | 2.3882   | 2.4933   | -0.1050  | 0.0141            |
| S347     | 1.9002   | 1.9666   | -0.0665  | 0.0073            |
| S348     | 2.2302   | 2.4487   | -0.2186  | 0.0002            |
| S349     | 2.3084   | 2.4520   | -0.1436  | 0.0079            |
| S350     | 1.9526   | 2.0858   | -0.1332  | 0.0051            |
| S351     | 2.1736   | 2.3741   | -0.2006  | 0.0013            |
| S352     | 2.2324   | 2.3937   | -0.1612  | 0.0056            |
| S353     | 1.9501   | 2.0633   | -0.1132  | 0.0066            |
| S354     | 2.1176   | 2.3077   | -0.1901  | 0.0021            |
| S355     | 1.9922   | 2.1517   | -0.1595  | 0.0046            |
| S356     | 2.1629   | 2.3284   | -0.1655  | 0.0036            |
| S357     | 2.0987   | 2.2809   | -0.1822  | 0.0025            |
| S358     | 2.1402   | 2.3055   | -0.1653  | 0.0033            |
| S359     | 1.9976   | 2.1596   | -0.1620  | 0.0048            |
| S360     | 2.5061   | 2.6481   | -0.1420  | 0.0030            |
| S361     | 2.5317   | 2.5699   | -0.0382  | 0.0288            |
| S362     | 1.8634   | 1.9030   | -0.0396  | 0.0080            |
| S363     | 2.0924   | 2.2512   | -0.1588  | 0.0054            |
| S364     | 2.0452   | 2.2187   | -0.1736  | 0.0031            |
| S365     | 2.0582   | 2.2107   | -0.1525  | 0.0046            |
| S366     | 1.9140   | 1.9854   | -0.0714  | 0.0080            |
| S367     | 1.9381   | 2.0754   | -0.1373  | 0.0024            |
| S368     | 2.1175   | 2.2991   | -0.1816  | 0.0056            |

|          | ADC(2  | 2)/cc-pVDZ/IEFP  | CM(T1)   |                   |
|----------|--|--|--|-------------------|
| Molecule | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $f_{12}(S_0-S_1)$ |
| S369     | 2.0056   | 2.1412   | -0.1356  | 0.0054            |
| S370     | 1.9997   | 2.1618   | -0.1621  | 0.0032            |
| S371     | 2.0251   | 2.1905   | -0.1654  | 0.0061            |
| S372     | 2.0263   | 2.1806   | -0.1543  | 0.0049            |
| S373     | 2.0745   | 2.2358   | -0.1614  | 0.0028            |
| S374     | 2.0306   | 2.2006   | -0.1699  | 0.0051            |
| S375     | 1.9545   | 2.0547   | -0.1002  | 0.0070            |
| S376     | 1.9885   | 2.1264   | -0.1379  | 0.0023            |
| S377     | 2.0853   | 2.2679   | -0.1826  | 0.0054            |
| S378     | 2.4975   | 2.6395   | -0.1420  | 0.0027            |
| S379     | 2.5240   | 2.5535   | -0.0296  | 0.0288            |
| S380     | 1.8626   | 1.9104   | -0.0478  | 0.0087            |
| S381     | 1.9632   | 2.0491   | -0.0859  | 0.0087            |
| S382     | 1.9596   | 2.0813   | -0.1218  | 0.0036            |
| S383     | 2.1706   | 2.3672   | -0.1966  | 0.0040            |
| S384     | 2.0904   | 2.2474   | -0.1570  | 0.0040            |
| S385     | 2.1564   | 2.2978   | -0.1414  | 0.0026            |
| S386     | 2.1366   | 2.3151   | -0.1785  | 0.0038            |
| S387     | 1.9236   | 1.9890   | -0.0654  | 0.0067            |
| S388     | 2.0933   | 2.2413   | -0.1480  | 0.0020            |
| S389     | 2.1194   | 2.3125   | -0.1931  | 0.0044            |
| S390     | 2.0537   | 2.1875   | -0.1339  | 0.0058            |
| S391     | 2.1073   | 2.2400   | -0.1327  | 0.0016            |
| S392     | 2.1770   | 2.3768   | -0.1998  | 0.0029            |
| S393     | 2.0986   | 2.2708   | -0.1722  | 0.0063            |
| S394     | 2.0805   | 2.2434   | -0.1629  | 0.0059            |
| S395     | 2.0254   | 2.1752   | -0.1498  | 0.0056            |
| S396     | 2.4303   | 2.5581   | -0.1278  | 0.0097            |
| S397     | 2.3661   | 2.4211   | -0.0550  | 0.0292            |
| S398     | 1.8763   | 1.9412   | -0.0649  | 0.0093            |
| S399     | 2.3376   | 2.4915   | -0.1539  | 0.0065            |
| S400     | 2.3073   | 2.3975   | -0.0902  | 0.0214            |
| S401     | 1.8684   | 1.9219   | -0.0535  | 0.0104            |
| S402     | 2.2268   | 2.4141   | -0.1873  | 0.0039            |
| S403     | 2.2418   | 2.3640   | -0.1221  | 0.0143            |
| S404     | 1.9055   | 2.0234   | -0.1179  | 0.0086            |
| S405     | 2.1794   | 2.3454   | -0.1660  | 0.0094            |
| S406     | 2.1423   | 2.2929   | -0.1506  | 0.0081            |
| S407     | 2.0375   | 2.2144   | -0.1769  | 0.0041            |
| S408     | 2.0863   | 2.2639   | -0.1776  | 0.0055            |
| S409     | 1.9507   | 2.1067   | -0.1560  | 0.0059            |
| S410     | 2.1127   | 2.2698   | -0.1570  | 0.0062            |
| S411     | 2.0644   | 2.2371   | -0.1727  | 0.0062            |
| S412     | 2.0916   | 2.2509   | -0.1593  | 0.0053            |
| S413     | 1.9561   | 2.1162   | -0.1602  | 0.0056            |
| S414     | 2.5234   | 2.5637   | -0.0403  | 0.0134            |

| $ m ADC(2)/cc	ext{-pVDZ/IEFPCM}(T1)$ |  |        |  |                   |  |
|--------------------------------------|--|--------|--|-------------------|--|
| Molecule                             | $\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$ |        | $\Delta \overset{\cdot}{\mathrm{E}}(\overset{\cdot}{\mathrm{S}_1}\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$ | $f_{12}(S_0-S_1)$ |  |
| S415                                 | 2.4301   | 2.4609 | -0.0308  | 0.0380            |  |
| S416                                 | 1.9771   | 2.0786 | -0.1014  | 0.0080            |  |
| S417                                 | 2.0585   | 2.1904 | -0.1319  | 0.0175            |  |
| S418                                 | 2.0406   | 2.2162 | -0.1756  | 0.0026            |  |
| S419                                 | 2.0123   | 2.1594 | -0.1471  | 0.0050            |  |
| S420                                 | 1.9289   | 1.9929 | -0.0640  | 0.0146            |  |
| S421                                 | 1.9251   | 2.0920 | -0.1669  | 0.0007            |  |
| S422                                 | 2.0981   | 2.3012 | -0.2031  | 0.0020            |  |
| S423                                 | 1.9479   | 2.0816 | -0.1337  | 0.0101            |  |
| S424                                 | 1.9694   | 2.1483 | -0.1789  | 0.0017            |  |
| S425                                 | 2.0084   | 2.1815 | -0.1731  | 0.0045            |  |
| S426                                 | 1.9912   | 2.1419 | -0.1507  | 0.0086            |  |
| S427                                 | 2.0425   | 2.2101 | -0.1676  | 0.0030            |  |
| S428                                 | 2.0070   | 2.1810 | -0.1740  | 0.0043            |  |
| S429                                 | 1.9166   | 2.0186 | -0.1020  | 0.0090            |  |
| S430                                 | 1.9659   | 2.1274 | -0.1615  | 0.0011            |  |
| S431                                 | 2.0814   | 2.2752 | -0.1938  | 0.0033            |  |
| S432                                 | 2.5121   | 2.5651 | -0.0529  | 0.0180            |  |
| S433                                 | 2.4280   | 2.4604 | -0.0324  | 0.0367            |  |
| S434                                 | 1.9581   | 2.0515 | -0.0934  | 0.0079            |  |
| S435                                 | 1.9148   | 1.9877 | -0.0729  | 0.0133            |  |
| S436                                 | 1.9449   | 2.0957 | -0.1507  | 0.0005            |  |
| S437                                 | 2.1971   | 2.3869 | -0.1898  | 0.0039            |  |
| S438                                 | 2.0751   | 2.2113 | -0.1362  | 0.0098            |  |
| S439                                 | 2.0990   | 2.2452 | -0.1462  | 0.0037            |  |
| S440                                 | 2.0781   | 2.2645 | -0.1864  | 0.0043            |  |
| S441                                 | 1.9189   | 2.0105 | -0.0916  | 0.0079            |  |
| S442                                 | 2.1244   | 2.2446 | -0.1202  | 0.0029            |  |
| S443                                 | 2.1641   | 2.3662 | -0.2022  | 0.0024            |  |
| S444                                 | 2.0350   | 2.1516 | -0.1165  | 0.0083            |  |
| S445                                 | 2.0635   | 2.2061 | -0.1426  | 0.0021            |  |
| S446                                 | 2.1643   | 2.3636 | -0.1993  | 0.0038            |  |