

| Molecule | ADC(2)/cc-pVDZ | | | |
|----------|--------------------------|--------------------------|--------------------------|-------------------|
| | $\Delta E(S_0-S_1)$ [eV] | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S843 | 2.0617 | 2.1469 | -0.0852 | 0.0009 |
| S844 | 2.1793 | 2.2697 | -0.0904 | 0.0024 |
| S845 | 2.2494 | 2.3475 | -0.0981 | 0.0006 |
| S846 | 2.3697 | 2.4635 | -0.0939 | 0.0035 |
| S847 | 1.9749 | 1.9798 | -0.0049 | 0.0023 |
| S848 | 2.1008 | 2.1566 | -0.0558 | 0.0003 |
| S849 | 2.0325 | 2.0653 | -0.0328 | 0.0056 |
| S850 | 2.1602 | 2.2345 | -0.0742 | 0.0017 |
| S851 | 2.1765 | 2.1998 | -0.0233 | 0.0022 |
| S852 | 2.1989 | 2.2177 | -0.0188 | 0.0065 |
| S853 | 2.3733 | 2.3980 | -0.0247 | 0.0016 |
| S854 | 2.4175 | 2.4335 | -0.0160 | 0.0073 |
| S855 | 2.0894 | 2.1008 | -0.0114 | 0.0027 |
| S856 | 2.1211 | 2.1991 | -0.0780 | 0.0008 |
| S857 | 2.2029 | 2.2207 | -0.0178 | 0.0082 |
| S858 | 2.2702 | 2.3619 | -0.0917 | 0.0003 |
| S859 | 2.0534 | 2.0696 | -0.0162 | 0.0035 |
| S860 | 2.3280 | 2.3888 | -0.0608 | 0.0020 |
| S861 | 2.3168 | 2.3772 | -0.0604 | 0.0015 |
| S862 | 2.4672 | 2.5536 | -0.0864 | 0.0016 |
| S863 | 2.0858 | 1.9868 | 0.0990 | 0.0023 |
| S864 | 2.2422 | 2.1661 | 0.0761 | 0.0007 |
| S865 | 2.0429 | 2.0049 | 0.0380 | 0.0067 |
| S866 | 2.1936 | 2.1803 | 0.0133 | 0.0044 |
| S867 | 2.4063 | 2.4443 | -0.0379 | 0.0046 |
| S868 | 2.4607 | 2.4343 | 0.0264 | 0.0082 |
| S869 | 2.5590 | 2.6263 | -0.0673 | 0.0034 |
| S870 | 2.6349 | 2.6242 | 0.0106 | 0.0062 |
| S871 | 2.2979 | 2.2108 | 0.0870 | 0.0039 |
| S872 | 2.3670 | 2.3142 | 0.0529 | 0.0003 |
| S873 | 2.2977 | 2.2338 | 0.0639 | 0.0106 |
| S874 | 2.3911 | 2.2869 | 0.1042 | 0.0029 |
| S875 | 2.1036 | 2.1041 | -0.0005 | 0.0051 |
| S876 | 2.1492 | 2.2325 | -0.0833 | 0.0029 |
| S877 | 2.0486 | 2.0122 | 0.0364 | 0.0095 |
| S878 | 2.1814 | 2.1717 | 0.0097 | 0.0029 |
| S879 | 2.2516 | 2.1965 | 0.0551 | 0.0128 |
| S880 | 1.9033 | 1.9357 | -0.0324 | 0.0005 |
| S881 | 1.9865 | 2.0093 | -0.0228 | 0.0034 |
| S882 | 1.9924 | 2.0359 | -0.0435 | 0.0017 |
| S883 | 2.0682 | 2.1165 | -0.0483 | 0.0027 |
| S884 | 2.0341 | 1.9353 | 0.0987 | 0.0133 |
| S885 | 2.3102 | 2.1949 | 0.1152 | 0.0024 |
| S886 | 2.2785 | 2.1576 | 0.1208 | 0.0165 |
| S887 | 2.0178 | 1.9756 | 0.0422 | 0.0001 |
| S888 | 1.9691 | 1.9164 | 0.0527 | 0.0063 |

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| | $\Delta E(S_0-S_1)$ [eV] | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S889 | 2.1935 | 2.1603 | 0.0331 | 0.0026 |
| S890 | 2.1833 | 2.1296 | 0.0537 | 0.0028 |
| S891 | 2.2352 | 2.2741 | -0.0389 | 0.0028 |
| S892 | 2.4103 | 2.4905 | -0.0802 | 0.0017 |
| S893 | 2.2978 | 2.3297 | -0.0319 | 0.0038 |
| S894 | 2.2177 | 2.1356 | 0.0820 | 0.0095 |
| S895 | 2.2367 | 2.2662 | -0.0295 | 0.0018 |
| S896 | 2.3566 | 2.2894 | 0.0672 | 0.0092 |
| S897 | 2.1608 | 2.1412 | 0.0196 | 0.0024 |
| S898 | 1.9725 | 1.9893 | -0.0168 | 0.0026 |
| S899 | 2.0984 | 2.1430 | -0.0445 | 0.0023 |
| S900 | 2.2896 | 2.1395 | 0.1501 | 0.0179 |
| S901 | 2.4739 | 2.3977 | 0.0762 | 0.0020 |
| S902 | 2.4873 | 2.3297 | 0.1577 | 0.0168 |
| S903 | 2.2059 | 2.1924 | 0.0134 | 0.0000 |
| S904 | 2.2110 | 2.1085 | 0.1025 | 0.0074 |
| S905 | 2.2341 | 2.2434 | -0.0093 | 0.0043 |
| S906 | 2.2749 | 2.1614 | 0.1135 | 0.0011 |
| S907 | 2.3078 | 2.3138 | -0.0059 | 0.0055 |
| S908 | 2.4998 | 2.5578 | -0.0581 | 0.0036 |
| S909 | 2.3628 | 2.4590 | -0.0962 | 0.0025 |
| S910 | 2.5758 | 2.6946 | -0.1188 | 0.0012 |
| S911 | 2.1650 | 2.1289 | 0.0361 | 0.0059 |
| S912 | 2.3821 | 2.3454 | 0.0367 | 0.0102 |
| S913 | 2.0957 | 1.9653 | 0.1304 | 0.0039 |
| S914 | 2.0976 | 2.0461 | 0.0514 | 0.0043 |
| S915 | 2.2932 | 2.1781 | 0.1150 | 0.0067 |
| S916 | 2.3471 | 2.3232 | 0.0239 | 0.0050 |
| S917 | 2.5337 | 2.5312 | 0.0025 | 0.0081 |
| S918 | 2.0549 | 2.0124 | 0.0425 | 0.0061 |
| S919 | 2.1977 | 2.1991 | -0.0014 | 0.0074 |
| S920 | 2.2920 | 2.2250 | 0.0671 | 0.0099 |
| S921 | 2.0416 | 2.0113 | 0.0303 | 0.0113 |
| S922 | 2.3519 | 2.2755 | 0.0764 | 0.0161 |
| S923 | 2.3092 | 2.2439 | 0.0652 | 0.0006 |
| S924 | 1.9895 | 1.9971 | -0.0076 | 0.0046 |
| S925 | 2.2995 | 2.2626 | 0.0369 | 0.0062 |
| S926 | 2.2669 | 2.2288 | 0.0380 | 0.0126 |
| S927 | 2.5575 | 2.4764 | 0.0811 | 0.0162 |
| S928 | 2.2938 | 2.3085 | -0.0147 | 0.0009 |
| S929 | 2.1534 | 2.1982 | -0.0448 | 0.0017 |
| S930 | 2.3841 | 2.2840 | 0.1001 | 0.0007 |
| S931 | 2.3859 | 2.4962 | -0.1103 | 0.0017 |
| S932 | 2.4238 | 2.5587 | -0.1349 | 0.0002 |
| S933 | 2.5655 | 2.7071 | -0.1415 | 0.0028 |
| S934 | 2.3252 | 2.3559 | -0.0307 | 0.0008 |

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|----------|--------------------------|--------------------------|--------------------------|-------------------|
| | $\Delta E(S_0-S_1)$ [eV] | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S935 | 2.2014 | 2.2348 | -0.0334 | 0.0069 |
| S936 | 2.3523 | 2.4200 | -0.0677 | 0.0035 |
| S937 | 2.3613 | 2.4189 | -0.0576 | 0.0058 |
| S938 | 2.5094 | 2.5891 | -0.0796 | 0.0008 |
| S939 | 2.5754 | 2.6559 | -0.0805 | 0.0066 |
| S940 | 2.2911 | 2.3940 | -0.1029 | 0.0008 |
| S941 | 2.3220 | 2.3635 | -0.0415 | 0.0073 |
| S942 | 2.4100 | 2.3849 | 0.0251 | 0.0008 |
| S943 | 1.9897 | 1.9491 | 0.0406 | 0.0030 |
| S944 | 1.9410 | 1.9108 | 0.0302 | 0.0000 |
| S945 | 2.1855 | 2.1430 | 0.0425 | 0.0030 |
| S946 | 1.9813 | 1.9075 | 0.0738 | 0.0081 |
| S947 | 2.1931 | 2.1060 | 0.0870 | 0.0101 |
| S948 | 2.5366 | 2.6042 | -0.0676 | 0.0016 |
| S949 | 2.6743 | 2.7924 | -0.1181 | 0.0015 |
| S950 | 2.4780 | 2.3826 | 0.0954 | 0.0011 |
| S951 | 2.2511 | 2.2024 | 0.0487 | 0.0078 |
| S952 | 2.4162 | 2.3397 | 0.0765 | 0.0058 |
| S953 | 2.6154 | 2.6317 | -0.0163 | 0.0089 |
| S954 | 2.7184 | 2.8266 | -0.1082 | 0.0022 |
| S955 | 2.7990 | 2.8511 | -0.0521 | 0.0074 |
| S956 | 2.5443 | 2.5138 | 0.0305 | 0.0011 |
| S957 | 2.4746 | 2.4140 | 0.0606 | 0.0095 |
| S958 | 2.5738 | 2.2637 | 0.3101 | 0.0022 |
| S959 | 2.0685 | 2.0906 | -0.0220 | 0.0008 |
| S960 | 1.9573 | 1.9189 | 0.0384 | 0.0024 |
| S961 | 2.2733 | 2.3097 | -0.0365 | 0.0006 |
| S962 | 2.0565 | 2.0896 | -0.0331 | 0.0028 |
| S963 | 1.9746 | 2.0429 | -0.0683 | 0.0001 |
| S964 | 2.2810 | 2.2920 | -0.0111 | 0.0042 |
| S965 | 2.1708 | 2.1546 | 0.0162 | 0.0139 |
| S966 | 2.3213 | 2.3229 | -0.0016 | 0.0180 |
| S967 | 2.1468 | 2.1531 | -0.0063 | 0.0066 |
| S968 | 2.0080 | 2.0712 | -0.0632 | 0.0025 |
| S969 | 2.1323 | 2.1532 | -0.0208 | 0.0064 |
| S970 | 2.0526 | 2.0034 | 0.0492 | 0.0200 |
| S971 | 2.2612 | 2.2175 | 0.0437 | 0.0240 |
| S972 | 1.9941 | 1.9845 | 0.0096 | 0.0125 |
| S973 | 2.1039 | 2.1290 | -0.0251 | 0.0018 |
| S974 | 2.1186 | 2.0818 | 0.0368 | 0.0086 |
| S975 | 2.0337 | 2.0618 | -0.0281 | 0.0046 |
| S976 | 2.0056 | 2.0389 | -0.0333 | 0.0006 |
| S977 | 2.2066 | 2.2357 | -0.0291 | 0.0054 |
| S978 | 2.0320 | 2.1001 | -0.0680 | 0.0012 |
| S979 | 2.1223 | 2.0827 | 0.0396 | 0.0095 |
| S980 | 2.1311 | 2.1013 | 0.0297 | 0.0035 |

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|----------|--------------------------|--------------------------|--------------------------|-------------------|
| | $\Delta E(S_0-S_1)$ [eV] | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S981 | 2.2837 | 2.2724 | 0.0112 | 0.0121 |
| S982 | 2.3735 | 2.3072 | 0.0663 | 0.0188 |
| S983 | 2.4764 | 2.4410 | 0.0354 | 0.0196 |
| S984 | 2.3815 | 2.3353 | 0.0463 | 0.0089 |
| S985 | 2.2684 | 2.1090 | 0.1593 | 0.0053 |
| S986 | 2.3101 | 2.2124 | 0.0977 | 0.0301 |
| S987 | 2.4939 | 2.3050 | 0.1888 | 0.0320 |
| S988 | 2.2666 | 2.1321 | 0.1345 | 0.0205 |
| S989 | 2.2709 | 2.1577 | 0.1132 | 0.0013 |
| S990 | 2.3110 | 2.0451 | 0.2659 | 0.0086 |
| S991 | 2.1433 | 2.2302 | -0.0868 | 0.0002 |
| S992 | 2.0478 | 2.0561 | -0.0084 | 0.0012 |
| S993 | 2.3419 | 2.4234 | -0.0814 | 0.0008 |
| S994 | 2.1452 | 2.1858 | -0.0407 | 0.0032 |
| S995 | 2.2002 | 2.2824 | -0.0822 | 0.0023 |
| S996 | 2.1386 | 2.2249 | -0.0863 | 0.0000 |
| S997 | 2.3943 | 2.3724 | 0.0220 | 0.0042 |
| S998 | 2.2122 | 2.0378 | 0.1744 | 0.0013 |
| S999 | 2.3273 | 2.2669 | 0.0604 | 0.0070 |
| S1000 | 1.8828 | 1.7800 | 0.1028 | 0.0129 |
| S1001 | 2.2256 | 2.0624 | 0.1632 | 0.0143 |
| S1002 | 2.1910 | 2.0302 | 0.1608 | 0.0194 |
| S1003 | 2.5066 | 2.4921 | 0.0145 | 0.0054 |
| S1004 | 2.4892 | 2.4621 | 0.0271 | 0.0144 |
| S1005 | 1.9232 | 1.8780 | 0.0452 | 0.0163 |
| S1006 | 2.3858 | 2.2792 | 0.1066 | 0.0177 |
| S1007 | 2.2063 | 2.1153 | 0.0910 | 0.0267 |
| S1008 | 2.2180 | 2.2702 | -0.0521 | 0.0056 |
| S1009 | 2.3600 | 2.4260 | -0.0660 | 0.0079 |
| S1010 | 2.1079 | 2.0751 | 0.0328 | 0.0075 |
| S1011 | 2.1489 | 2.1721 | -0.0232 | 0.0022 |
| S1012 | 2.2337 | 2.2030 | 0.0307 | 0.0060 |
| S1013 | 2.4326 | 2.4929 | -0.0602 | 0.0062 |
| S1014 | 2.5435 | 2.6362 | -0.0927 | 0.0060 |
| S1015 | 2.1276 | 2.1723 | -0.0447 | 0.0090 |
| S1016 | 2.3674 | 2.4029 | -0.0355 | 0.0018 |
| S1017 | 2.3016 | 2.1510 | 0.1506 | 0.0097 |
| S1018 | 2.3399 | 2.4811 | -0.1413 | 0.0002 |
| S1019 | 2.5491 | 2.6881 | -0.1390 | 0.0008 |
| S1020 | 2.2187 | 2.2009 | 0.0178 | 0.0049 |
| S1021 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1022 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1023 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1024 | 2.2995 | 2.2678 | 0.0317 | 0.0006 |
| S1025 | 2.4969 | 2.4013 | 0.0956 | 0.0046 |
| S1026 | 2.3097 | 2.3186 | -0.0089 | 0.0044 |

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|----------|--------------------------|--------------------------|--------------------------|-------------------|
| | $\Delta E(S_0-S_1)$ [eV] | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S1027 | 2.4944 | 2.4556 | 0.0388 | 0.0060 |
| S1028 | 2.5563 | 2.6460 | -0.0897 | 0.0013 |
| S1029 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1030 | 2.2483 | 2.2058 | 0.0425 | 0.0163 |
| S1031 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1032 | 2.7500 | 2.7437 | 0.0063 | 0.0002 |
| S1033 | 2.4164 | 2.2573 | 0.1591 | 0.0067 |
| S1034 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1035 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1036 | 2.3972 | 2.4825 | -0.0853 | 0.0034 |
| S1037 | 2.4407 | 2.3948 | 0.0460 | 0.0085 |
| S1038 | 2.1155 | 2.1643 | -0.0488 | 0.0029 |
| S1039 | 2.2691 | 2.3054 | -0.0363 | 0.0046 |
| S1040 | 2.4904 | 2.3675 | 0.1229 | 0.0151 |
| S1041 | 2.1598 | 2.0844 | 0.0754 | 0.0046 |
| S1042 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1043 | 2.2998 | 2.1635 | 0.1363 | 0.0035 |
| S1044 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| S1045 | 2.5047 | 2.4545 | 0.0502 | 0.0003 |
| S1046 | 2.6804 | 2.7035 | -0.0231 | 0.0044 |
| S1047 | 2.4592 | 2.4451 | 0.0141 | 0.0016 |
| S1048 | 2.1627 | 2.1636 | -0.0009 | 0.0096 |
| S1049 | 2.6170 | 2.4651 | 0.1519 | 0.0054 |
| S1050 | 2.2822 | 2.1312 | 0.1510 | 0.0013 |
| S1051 | 2.3670 | 2.0367 | 0.3303 | 0.0093 |
| S1052 | 2.1256 | 2.0016 | 0.1240 | 0.0157 |
| S1053 | 2.4341 | 2.4509 | -0.0168 | 0.0100 |
| S1054 | 2.3392 | 2.2903 | 0.0489 | 0.0099 |
| S1055 | 2.6193 | 2.6205 | -0.0011 | 0.0032 |
| S1056 | 2.4617 | 2.3630 | 0.0987 | 0.0044 |
| S1057 | 2.6950 | 2.7366 | -0.0416 | 0.0062 |
| S1058 | 2.2551 | 2.1997 | 0.0554 | 0.0068 |
| S1059 | 2.4690 | 2.3908 | 0.0781 | 0.0089 |
| S1060 | 2.4493 | 2.4589 | -0.0096 | 0.0056 |
| S1061 | 2.7065 | 2.6933 | 0.0132 | 0.0147 |
| S1062 | 2.4976 | 2.3290 | 0.1686 | 0.0018 |
| S1063 | 2.5491 | 2.2582 | 0.2909 | 0.0003 |
| S1064 | 2.7503 | 2.9279 | -0.1776 | 0.0016 |
| S1065 | 2.5182 | 2.5363 | -0.0182 | 0.0128 |
| S1066 | 2.7864 | 2.9116 | -0.1252 | 0.0023 |
| S1067 | 2.6194 | 2.3277 | 0.2917 | 0.0077 |
| S1068 | 2.0468 | 1.9513 | 0.0955 | 0.0004 |
| S1069 | 2.2462 | 2.2251 | 0.0212 | 0.0030 |
| S1070 | 1.9976 | 2.0040 | -0.0064 | 0.0017 |
| S1071 | 2.2307 | 2.0825 | 0.1483 | 0.0066 |
| S1072 | 2.3911 | 2.2330 | 0.1582 | 0.0139 |

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| | $\Delta E(S_0-S_1)$ [eV] | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S1073 | 2.2119 | 2.1940 | 0.0178 | 0.0015 |
| S1074 | 2.4717 | 2.2523 | 0.2194 | 0.0213 |
| S1075 | 2.9400 | 2.9883 | -0.0483 | 0.0001 |
| S1076 | 2.6505 | 2.1564 | 0.4941 | 0.0208 |
| S1077 | 1.8359 | 1.7679 | 0.0679 | 0.0071 |
| S1078 | 2.1609 | 2.2012 | -0.0403 | 0.0034 |
| S1079 | 1.8881 | 1.8695 | 0.0186 | 0.0099 |
| S1080 | 2.0625 | 2.0668 | -0.0043 | 0.0019 |
| S1081 | 2.3247 | 2.3507 | -0.0260 | 0.0014 |
| S1082 | 2.0519 | 2.1381 | -0.0861 | 0.0036 |
| S1083 | 2.3042 | 2.3512 | -0.0471 | 0.0084 |
| S1084 | 2.3348 | 1.9821 | 0.3527 | 0.0093 |
| S1085 | 2.1993 | 2.1425 | 0.0568 | 0.0013 |
| S1086 | 2.3279 | 2.3582 | -0.0303 | 0.0066 |
| S1087 | 2.1302 | 2.1483 | -0.0181 | 0.0006 |
| S1088 | 2.4412 | 2.3312 | 0.1100 | 0.0103 |
| S1089 | 2.5174 | 2.4453 | 0.0721 | 0.0193 |
| S1090 | 2.3887 | 2.1219 | 0.2668 | 0.0053 |
| S1091 | 2.1169 | 2.0891 | 0.0278 | 0.0010 |
| S1092 | 2.1906 | 2.0160 | 0.1746 | 0.0195 |
| S1093 | 2.3771 | 1.9338 | 0.4433 | 0.0000 |
| S1094 | 2.2118 | 1.9846 | 0.2272 | 0.0026 |
| S1095 | 2.0489 | 1.9781 | 0.0708 | 0.0040 |
| S1096 | 2.3116 | 2.3715 | -0.0599 | 0.0005 |
| S1097 | 2.0162 | 2.0189 | -0.0027 | 0.0071 |
| S1098 | 2.3422 | 2.3260 | 0.0162 | 0.0008 |
| S1099 | 2.5202 | 2.3329 | 0.1872 | 0.0020 |
| S1100 | 2.2790 | 1.9690 | 0.3100 | 0.0032 |
| S1101 | 2.4107 | 2.2294 | 0.1813 | 0.0214 |
| S1102 | 2.1347 | 2.0952 | 0.0395 | 0.0198 |
| S1103 | 2.4118 | 2.1997 | 0.2121 | 0.0311 |
| S1104 | 2.4308 | 2.3990 | 0.0318 | 0.0051 |
| S1105 | 2.7434 | 2.5818 | 0.1616 | 0.0042 |
| S1106 | 2.3541 | 2.2125 | 0.1415 | 0.0122 |
| S1107 | 2.5033 | 2.1260 | 0.3772 | 0.0109 |
| S1108 | 2.2252 | 2.1403 | 0.0848 | 0.0010 |
| S1109 | 2.2355 | 2.1821 | 0.0534 | 0.0030 |
| S1110 | 2.2786 | 2.1284 | 0.1502 | 0.0003 |
| S1111 | 2.1257 | 2.0080 | 0.1176 | 0.0001 |
| S1112 | 2.2538 | 2.1641 | 0.0897 | 0.0026 |
| S1113 | 2.2804 | 1.9902 | 0.2901 | 0.0114 |
| S1114 | 2.2882 | 1.9020 | 0.3862 | 0.0004 |
| S1115 | 2.7779 | 2.9526 | -0.1748 | 0.0025 |
| S1116 | 2.9845 | 3.0388 | -0.0543 | 0.0204 |
| S1117 | 2.9380 | 3.0442 | -0.1062 | 0.0136 |
| S1118 | 2.8894 | 3.0281 | -0.1387 | 0.0083 |

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| | $\Delta E(S_0-S_1)$ [eV] | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S1119 | 2.8075 | 2.9725 | -0.1650 | 0.0041 |
| S1120 | 2.7860 | 2.9536 | -0.1676 | 0.0026 |
| S1121 | 2.7684 | 2.9369 | -0.1685 | 0.0020 |
| S1122 | 2.7998 | 2.9782 | -0.1784 | 0.0014 |
| S1123 | 3.0547 | 3.0610 | -0.0063 | 0.0299 |
| S1124 | 2.9931 | 3.0635 | -0.0704 | 0.0151 |
| S1125 | 2.9186 | 3.0520 | -0.1334 | 0.0059 |
| S1126 | 2.8453 | 3.0145 | -0.1692 | 0.0030 |
| S1127 | 2.8046 | 2.9851 | -0.1804 | 0.0019 |
| S1128 | 2.7843 | 2.9574 | -0.1731 | 0.0022 |
| S1129 | 2.7095 | 2.8769 | -0.1674 | 0.0020 |
| S1130 | 2.5486 | 2.5726 | -0.0240 | 0.0029 |
| S1131 | 2.6408 | 2.7462 | -0.1054 | 0.0021 |
| S1132 | 2.7349 | 2.8906 | -0.1557 | 0.0018 |
| S1133 | 2.6716 | 2.7911 | -0.1195 | 0.0033 |
| S1134 | 2.7512 | 2.9223 | -0.1711 | 0.0018 |
| S1135 | 2.7525 | 2.9240 | -0.1716 | 0.0021 |
| S1136 | 2.9968 | 3.0159 | -0.0191 | 0.0223 |
| S1137 | 2.7062 | 2.8839 | -0.1777 | 0.0007 |
| S1138 | 2.6279 | 2.7705 | -0.1426 | 0.0000 |
| S1139 | 2.6728 | 2.8444 | -0.1716 | 0.0001 |
| S1140 | 2.6537 | 2.7972 | -0.1435 | 0.0000 |
| S1141 | 2.7163 | 2.8842 | -0.1679 | 0.0006 |
| S1142 | 3.0636 | 3.0606 | 0.0029 | 0.0330 |
| S1143 | 2.6878 | 2.8190 | -0.1312 | 0.0064 |
| S1144 | 2.5254 | 2.5095 | 0.0158 | 0.0123 |
| S1145 | 2.6393 | 2.7267 | -0.0874 | 0.0074 |
| S1146 | 2.5991 | 2.6263 | -0.0272 | 0.0096 |
| S1147 | 2.6947 | 2.8023 | -0.1076 | 0.0059 |
| S1148 | 2.4477 | 2.4524 | -0.0048 | 0.0043 |
| S1149 | 2.6782 | 2.7085 | -0.0303 | 0.0065 |
| S1150 | 2.7696 | 2.8705 | -0.1009 | 0.0097 |
| S1151 | 2.7356 | 2.8450 | -0.1094 | 0.0063 |
| S1152 | 2.8001 | 2.9500 | -0.1499 | 0.0048 |
| S1153 | 2.7709 | 2.9378 | -0.1669 | 0.0026 |
| S1154 | 2.9991 | 2.9874 | 0.0117 | 0.0230 |
| S1155 | 2.6396 | 2.7924 | -0.1528 | 0.0001 |
| S1156 | 2.6878 | 2.8198 | -0.1320 | 0.0002 |
| S1157 | 2.7250 | 2.8842 | -0.1593 | 0.0013 |
| S1158 | 3.0470 | 3.0469 | 0.0000 | 0.0310 |
| S1159 | 2.5431 | 2.5467 | -0.0037 | 0.0110 |
| S1160 | 2.5993 | 2.5903 | 0.0090 | 0.0080 |
| S1161 | 2.6845 | 2.8086 | -0.1242 | 0.0026 |
| S1162 | 2.3410 | 2.2922 | 0.0488 | 0.0079 |
| S1163 | 2.7670 | 2.8679 | -0.1009 | 0.0092 |
| S1164 | 2.8476 | 2.9446 | -0.0970 | 0.0080 |

| Molecule | $\Delta E(S_0-S_1)$ [eV] | ADC(2)/cc-pVDZ | | |
|----------|--------------------------|--------------------------|--------------------------|-------------------|
| | | $\Delta E(S_0-T_1)$ [eV] | $\Delta E(S_1-T_1)$ [eV] | $f_{12}(S_0-S_1)$ |
| S1165 | 2.8006 | 2.9481 | -0.1475 | 0.0042 |
| S1166 | 2.7082 | 2.8708 | -0.1626 | 0.0004 |
| S1167 | 2.6677 | 2.7648 | -0.0971 | 0.0052 |
| S1168 | 2.8262 | 3.0036 | -0.1774 | 0.0017 |