$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		$\omega \mathrm{B2PLYP/def2\text{-}SVP}$					
S2 1.1690 1.0160 0.1530 0.0016 S3 1.6860 1.5770 0.1090 0.0016 S4 1.9250 1.8610 0.0640 0.0060 S5 1.8060 1.4110 0.3950 0.0001 S6 1.6950 1.5630 0.1320 0.0001 S7 2.0630 1.8920 0.1710 0.0018 S8 1.5680 1.3410 0.2270 0.0037 S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0667 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.014 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.005	Molecule				$f_{12}(S_0-S_1)$		
S3 1.6860 1.5770 0.1090 0.0016 S4 1.9250 1.8610 0.0640 0.0060 S5 1.8060 1.4110 0.3950 0.0001 S6 1.6950 1.5630 0.1320 0.0001 S7 2.0630 1.8920 0.1710 0.0018 S8 1.5680 1.3410 0.2270 0.0037 S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.033 S16 2.1720 1.9780 0.1940 0.0055 S17 2.040 1.8680 0.1360 0.0027	S1	1.3160	1.2740	0.0420	0.0000		
S4 1.9250 1.8610 0.0640 0.0060 S5 1.8060 1.4110 0.3950 0.0001 S6 1.6950 1.5530 0.1320 0.0001 S7 2.0630 1.8920 0.1710 0.0018 S8 1.5680 1.3410 0.2270 0.0037 S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0667 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0055 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009	S2	1.1690	1.0160	0.1530	0.0016		
S5 1.8060 1.4110 0.3950 0.0001 S6 1.6950 1.5630 0.1320 0.0001 S7 2.0630 1.8920 0.1710 0.0018 S8 1.5680 1.3410 0.2270 0.0037 S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0330 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0002 S17 2.0040 1.8880 0.1360 0.0027 S18 2.2210 2.810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0016	S3	1.6860	1.5770	0.1090	0.0016		
S6 1.6950 1.5630 0.1320 0.0001 S7 2.0630 1.8920 0.1710 0.0018 S8 1.5680 1.3410 0.2270 0.0037 S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162	S4	1.9250	1.8610	0.0640	0.0060		
S7 2.0630 1.8920 0.1710 0.0018 S8 1.5680 1.3410 0.2270 0.0037 S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.033 S16 2.1720 1.9780 0.1940 0.0033 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013	S5	1.8060	1.4110	0.3950	0.0001		
S8 1.5680 1.3410 0.2270 0.0037 S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 <t< td=""><td>S6</td><td>1.6950</td><td>1.5630</td><td>0.1320</td><td>0.0001</td></t<>	S6	1.6950	1.5630	0.1320	0.0001		
S9 1.7340 1.6190 0.1150 0.0011 S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0114 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 <	S7	2.0630	1.8920	0.1710	0.0018		
S10 2.1320 1.7580 0.3740 0.0008 S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0005 S17 2.0040 1.8680 0.1360 0.027 S18 2.2210 2.1810 0.0400 0.0005 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0013 <	S8	1.5680	1.3410	0.2270	0.0037		
S11 1.8810 1.8290 0.0520 0.0067 S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076	S9	1.7340	1.6190	0.1150	0.0011		
S12 2.1740 2.1510 0.0230 0.0037 S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105	S10	2.1320	1.7580	0.3740	0.0008		
S13 2.2260 2.1230 0.1030 0.0104 S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0016	S11	1.8810	1.8290	0.0520	0.0067		
S14 2.4400 2.4100 0.0300 0.0116 S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 <	S12	2.1740	2.1510	0.0230	0.0037		
S15 1.8280 1.6140 0.2140 0.0033 S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041	S13	2.2260	2.1230	0.1030	0.0104		
S16 2.1720 1.9780 0.1940 0.0005 S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017	S14	2.4400	2.4100	0.0300	0.0116		
S17 2.0040 1.8680 0.1360 0.0027 S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094	S15	1.8280	1.6140	0.2140	0.0033		
S18 2.2210 2.1810 0.0400 0.0009 S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018	S16	2.1720	1.9780	0.1940	0.0005		
S19 1.6230 1.3080 0.3150 0.0058 S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097	S17	2.0040	1.8680	0.1360	0.0027		
S20 1.7160 1.4690 0.2470 0.0162 S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014	S18	2.2210	2.1810	0.0400	0.0009		
S21 1.0230 0.8110 0.2120 0.0013 S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003	S19	1.6230	1.3080	0.3150	0.0058		
S22 1.5550 1.1500 0.4050 0.0053 S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035	S20	1.7160	1.4690	0.2470	0.0162		
S23 1.8660 1.2560 0.6100 0.0021 S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 <td< td=""><td>S21</td><td>1.0230</td><td>0.8110</td><td>0.2120</td><td>0.0013</td></td<>	S21	1.0230	0.8110	0.2120	0.0013		
S24 1.7410 1.3440 0.3970 0.0097 S25 1.9910 1.6270 0.3640 0.0076 S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0055 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 <td< td=""><td>S22</td><td>1.5550</td><td>1.1500</td><td>0.4050</td><td>0.0053</td></td<>	S22	1.5550	1.1500	0.4050	0.0053		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S23	1.8660	1.2560	0.6100	0.0021		
S26 1.7920 1.5670 0.2250 0.0105 S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005	S24	1.7410	1.3440	0.3970	0.0097		
S27 2.0760 1.7620 0.3140 0.0216 S28 1.8040 1.2850 0.5190 0.0016 S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 <td< td=""><td>S25</td><td>1.9910</td><td>1.6270</td><td>0.3640</td><td>0.0076</td></td<>	S25	1.9910	1.6270	0.3640	0.0076		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S26	1.7920	1.5670	0.2250	0.0105		
S29 2.1430 1.6040 0.5390 0.0041 S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 <t< td=""><td>S27</td><td>2.0760</td><td>1.7620</td><td>0.3140</td><td>0.0216</td></t<>	S27	2.0760	1.7620	0.3140	0.0216		
S30 1.5720 1.3510 0.2210 0.0017 S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033 <td>S28</td> <td>1.8040</td> <td>1.2850</td> <td>0.5190</td> <td>0.0016</td>	S28	1.8040	1.2850	0.5190	0.0016		
S31 1.8670 1.5960 0.2710 0.0094 S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S29	2.1430	1.6040	0.5390	0.0041		
S32 2.2210 1.7410 0.4800 0.0018 S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S30	1.5720	1.3510	0.2210	0.0017		
S33 2.1490 1.8470 0.3020 0.0097 S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S31	1.8670	1.5960	0.2710	0.0094		
S34 1.6470 1.4160 0.2310 0.0014 S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S32	2.2210	1.7410	0.4800	0.0018		
S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S33	2.1490	1.8470	0.3020	0.0097		
S35 2.4090 1.7320 0.6770 0.0003 S36 2.3300 1.8420 0.4880 0.0035 S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S34	1.6470	1.4160	0.2310	0.0014		
S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	o	2.4090	1.7320	0.6770	0.0003		
S37 1.9480 1.7880 0.1600 0.0061 S38 2.2900 1.9310 0.3590 0.0084 S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S36	2.3300	1.8420	0.4880	0.0035		
S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S37		1.7880	0.1600	0.0061		
S39 2.3190 2.0580 0.2610 0.0166 S40 1.5730 1.4310 0.1420 0.0005 S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033		2.2900	1.9310	0.3590	0.0084		
S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033	S39	2.3190	2.0580	0.2610	0.0166		
S41 1.9110 1.6920 0.2190 0.0026 S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033							
S42 2.1900 1.8040 0.3860 0.0015 S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033		1.9110		0.2190			
S43 2.1750 1.9550 0.2200 0.0031 S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033		2.1900					
S44 1.8680 1.8690 -0.0010 0.0001 S45 1.7230 1.5390 0.1840 0.0033							
S45 1.7230 1.5390 0.1840 0.0033							
	S46		2.2270	0.1940	0.0000		

$\omega \mathrm{B2PLYP/def2 ext{-}SVP}$					
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
S47	2.2130	2.1840	0.0290	0.0016	
S48	2.0260	1.8330	0.1930	0.0011	
S49	2.1040	1.8700	0.2340	0.0065	
S50	2.1120	1.9150	0.1970	0.0054	
S51	2.5450	2.4920	0.0530	0.0037	
S52	2.4790	2.4350	0.0440	0.0080	
S53	2.7550	2.8060	-0.0510	0.0045	
S54	2.6130	2.3020	0.3110	0.0028	
S55	2.2560	2.1100	0.1460	0.0050	
S56	2.5580	2.2360	0.3220	0.0005	
S57	2.2290	1.5860	0.6430	0.0051	
S58	1.4570	1.1930	0.2640	0.0037	
S59	1.8640	1.4970	0.3670	0.0096	
S60	2.5280	2.0870	0.4410	0.0013	
S61	2.5160	2.2160	0.3000	0.0115	
S62	2.7350	2.0790	0.6560	0.0004	
S63	2.0680	1.6910	0.3770	0.0009	
S64	2.4610	2.0420	0.4190	0.0050	
S65	2.1620	2.0420	0.1200	0.0075	
S66	1.9750	1.6500	0.3250	0.0019	
S67	2.0500	1.8440	0.2060	0.0044	
S68	2.3670	2.1730	0.1940	0.0027	
S69	2.4900	2.2630	0.2270	0.0115	
S70	2.5600	2.1480	0.4120	0.0009	
S71	2.0270	1.8950	0.1320	0.0000	
S72	2.3360	2.1110	0.2250	0.0029	
S73	2.4300	2.5010	-0.0710	0.0002	
S74	2.2770	2.1620	0.1150	0.0026	
S75	1.6480	1.3640	0.2840	0.0121	
S76	2.2070	1.6920	0.5150	0.0165	
S77	2.3330	2.0300	0.3030	0.0196	
S78	2.0790	1.7660	0.3130	0.0056	
S79	2.1200	1.8440	0.2760	0.0107	
S80	2.7230	2.2250	0.4980	0.0059	
S81	2.6790	2.4370	0.2420	0.0114	
S82	2.0850	1.9780	0.1070	0.0018	
S83	2.6030	2.2020	0.4010	0.0026	
S84	3.0280	3.2460	-0.2180	0.0000	
S85	2.7730	2.1530	0.6200	0.0069	
S86	2.0650	1.7250	0.3400	0.0199	
S87	2.4840	2.1360	0.3480	0.0133	
S88	2.5370	2.0190	0.5180	0.0113 0.0052	
S89	0.8700	0.6270	0.3180 0.2430	0.0002	
S90	1.9100	1.1760	0.2450 0.7340	0.0005	
S90 S91	1.3970	1.1440	0.7540 0.2530	0.0025 0.0042	
S92	2.4710	1.6330	0.8380	0.0042 0.0036	
004	4.4110	1.0000	0.0300	0.0000	

ω B2PLYP/def2-SVP				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S93	1.4180	1.1710	0.2470	0.0019
S94	2.1450	1.6060	0.5390	0.0002
S95	2.1820	1.6140	0.5680	0.0073
S96	1.8820	1.6800	0.2020	0.0023
S97	1.3280	1.0920	0.2360	0.0005
S98	3.0030	2.1320	0.8710	0.0000
S99	2.1340	1.5310	0.6030	0.0057
S100	1.8070	1.6470	0.1600	0.0006
S101	2.7920	2.1280	0.6640	0.0021
S102	1.8740	1.6440	0.2300	0.0056
S103	2.5570	2.0500	0.5070	0.0021
S104	2.3050	1.9730	0.3320	0.0000
S105	1.3770	1.3530	0.0240	0.0001
S106	1.3660	1.2810	0.0850	0.0000
S107	1.6290	1.5750	0.0540	0.0042
S108	1.3890	1.1470	0.2420	0.0009
S109	1.5740	1.5300	0.0440	0.0027
S110	1.3840	1.1040	0.2800	0.0010
S111	1.4720	1.4400	0.0320	0.0008
S112	1.2880	1.1580	0.1300	0.0004
S113	1.4170	1.3930	0.0240	0.0002
S114	1.2820	1.1930	0.0890	0.0005
S115	1.3620	1.3240	0.0380	0.0000
S116	1.2830	1.2370	0.0460	0.0001
S117	1.3390	1.2950	0.0440	0.0000
S118	1.2970	1.2620	0.0350	0.0001
S119	1.6660	1.5930	0.0730	0.0054
S120	1.2940	1.1940	0.1000	0.0003
S121	1.2810	1.2160	0.0650	0.0007
S122	1.3400	1.2990	0.0410	0.0005
S123	1.1220	0.9450	0.1770	0.0022
S124	1.6250	1.5510	0.0740	0.0010
S125	1.2110	1.1380	0.0730	0.0006
S126	1.3860	1.3500	0.0360	0.0007
S127	1.2590	1.2090	0.0500	0.0003
S128	1.3630	1.3140	0.0490	0.0005
S129	1.1640	1.0270	0.1370	0.0014
S130	1.4920	1.4310	0.0610	0.0007
S131	1.6540	1.5900	0.0640	0.0051
S132	1.2830	1.2320	0.0510	0.0001
S132 S133	1.1180	0.9880	0.1300	0.0001
S133	1.6000	1.5200	0.0800	0.0013
S134 S135	1.2970	1.2150	0.0820	0.0010
S136	1.4050	1.3810	0.0820 0.0240	0.0002 0.0003
S130 S137	1.0960	0.8860	0.0240 0.2100	0.0003
S137 S138	1.6790	1.5840	0.0950	0.0023 0.0014
DIO	1.0190	1.0040	0.0300	0.0014

$\omega \mathrm{B2PLYP/def2} ext{-SVP}$				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S139	1.2310	1.1390	0.0920	0.0005
S140	1.4540	1.4140	0.0400	0.0003
S141	3.1010	3.3330	-0.2320	0.0004
S142	3.4440	3.5240	-0.0800	0.0157
S143	3.3450	3.5010	-0.1560	0.0081
S144	3.2360	3.4440	-0.2080	0.0027
S145	3.1730	3.3990	-0.2260	0.0011
S146	3.1140	3.3430	-0.2290	0.0002
S147	3.0890	3.3170	-0.2280	0.0001
S148	3.4760	3.5330	-0.0570	0.0176
S149	3.0360	3.2820	-0.2460	0.0001
S150	2.8990	2.9310	-0.0320	0.0018
S150 S151	2.9670	3.1760	-0.2090	0.0013 0.0005
S151	3.0290	3.2600	-0.2310	0.0000
S152 S153	2.9260	3.0630	-0.1370	0.0006
S155 S154	3.4880	3.5390	-0.1570 -0.0510	0.0010 0.0175
S154 S155	$\frac{3.4880}{2.9240}$	3.0810	-0.0510 -0.1570	0.0175 0.0011
S155 S156	3.0520	3.2770	-0.1370	0.0011
S150 S157	3.0420			0.0000
		2.7350 3.1710	0.3070	
S158	2.9880		-0.1830	0.0004
S159	1.9460	1.9320	0.0140	0.0049
S160	1.9510	1.8950	0.0560	0.0105
S161	1.8890	1.8070	0.0820	0.0074
S162	1.8790	1.8090	0.0700	0.0076
S163	2.2330	2.2600	-0.0270	0.0001
S164	2.2330	2.0430	0.1900	0.0259
S165	1.7990	1.5930	0.2060	0.0122
S166	1.7820	1.6500	0.1320	0.0074
S167	2.1490	2.1790	-0.0300	0.0008
S168	2.1810	2.0110	0.1700	0.0206
S169	1.7980	1.6540	0.1440	0.0099
S170	1.7750	1.6120	0.1630	0.0081
S171	2.0330	2.0460	-0.0130	0.0028
S172	2.0680	1.9640	0.1040	0.0124
S173	1.7760	1.6660	0.1100	0.0098
S174	1.7900	1.7000	0.0900	0.0075
S175	1.9830	1.9840	-0.0010	0.0044
S176	2.0030	1.9230	0.0800	0.0130
S177	1.9010	1.8710	0.0300	0.0073
S178	1.9280	1.8890	0.0390	0.0057
S179	1.9170	1.8870	0.0300	0.0062
S180	1.9510	1.8820	0.0690	0.0092
S181	1.8160	1.7590	0.0570	0.0090
S182	1.8340	1.7870	0.0470	0.0055
S183	1.8930	1.8480	0.0450	0.0070
S184	1.9300	1.8620	0.0680	0.0092

ω B2PLYP/def2-SVP					
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
S185	1.8310	1.7850	0.0460	0.0089	
S186	1.8510	1.8100	0.0410	0.0052	
S187	2.2750	2.2900	-0.0150	0.0001	
S188	2.2910	2.0510	0.2400	0.0305	
S189	1.8140	1.7000	0.1140	0.0101	
S190	1.8120	1.6550	0.1570	0.0074	
S191	1.8210	1.7590	0.0620	0.0095	
S192	1.8800	1.8230	0.0570	0.0137	
S193	1.8520	1.7900	0.0620	0.0107	
S194	1.8560	1.8110	0.0450	0.0036	
S195	1.6410	1.4280	0.2130	0.0157	
S196	1.7620	1.6300	0.1320	0.0085	
S197	2.0170	1.9870	0.0300	0.0086	
S198	2.0390	1.9970	0.0420	0.0037	
S199	1.7680	1.6610	0.1070	0.0111	
S200	1.8010	1.7340	0.0670	0.0101	
S201	1.8910	1.8540	0.0370	0.0112	
S202	1.9120	1.8810	0.0310	0.0030	
S202	1.8030	1.7380	0.0650	0.0096	
S204	1.8590	1.8050	0.0540	0.0089	
S204 S205	1.8700	1.8120	0.0540 0.0580	0.0033	
S205 S206	1.9010	1.8550	0.0360 0.0460	0.0111 0.0032	
S200 S207					
	1.7000	1.5110	0.1890	0.0145	
S208	1.7770	1.6560	0.1210	0.0075	
S209	1.9620	1.9300	0.0320	0.0097	
S210	2.0110	1.9750	0.0360	0.0032	
S211	2.2570	2.2730	-0.0160	0.0000	
S212	2.2660	2.0580	0.2080	0.0317	
S213	1.8320	1.7290	0.1030	0.0094	
S214	1.8340	1.7570	0.0770	0.0066	
S215	1.6700	1.4820	0.1880	0.0140	
S216	1.7400	1.6260	0.1140	0.0091	
S217	2.0270	1.9750	0.0520	0.0101	
S218	2.1010	2.0420	0.0590	0.0031	
S219	1.8300	1.7450	0.0850	0.0086	
S220	1.8920	1.8090	0.0830	0.0105	
S221	1.9340	1.9220	0.0120	0.0069	
S222	1.9390	1.9120	0.0270	0.0058	
S223	1.6340	1.3630	0.2710	0.0163	
S224	1.7700	1.6210	0.1490	0.0071	
S225	2.0770	2.0290	0.0480	0.0086	
S226	2.1450	2.0930	0.0520	0.0037	
S227	1.7760	1.6450	0.1310	0.0112	
S228	1.8470	1.7560	0.0910	0.0061	
S229	1.9590	1.9380	0.0210	0.0066	
S230	2.0090	1.9650	0.0440	0.0057	

ωB2PLYP/def2-SVP				
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	2.2860	2.2250	0.0610	0.0085
S232	2.2990	2.1980	0.1010	0.0161
S233	2.2840	2.1710	0.1130	0.0138
S234	2.1840	2.0680	0.1160	0.0119
S235	2.2510	2.0910	0.1600	0.0112
S236	2.2500	2.1070	0.1430	0.0119
S237	2.5690	2.5340	0.0350	0.0028
S238	2.5300	2.3280	0.2020	0.0313
S239	2.5970	2.3010	0.2960	0.0434
S240	2.0210	1.8010	0.2200	0.0186
S241	2.1320	1.7550	0.3770	0.0172
S242	2.1720	1.9210	0.2510	0.0147
S243	2.4930	2.4550	0.0380	0.0041
S244	2.4410	2.2920	0.1490	0.0218
S245	2.5340	2.2820	0.2520	0.0331
S246	2.0050	1.7780	0.2270	0.0203
S247	2.1900	1.8760	0.3140	0.0134
S248	2.1860	1.9010	0.2850	0.0157
S249	2.3700	2.3360	0.0340	0.0061
S250	2.3470	2.2590	0.0880	0.0129
S251	2.4380	2.2500	0.1880	0.0224
S252	2.0760	1.9300	0.1460	0.0159
S253	2.1900	1.9910	0.1990	0.0139
S254	2.1450	1.9800	0.1650	0.0114
S255	2.3300	2.2850	0.0450	0.0080
S256	2.2960	2.2040	0.0920	0.0209
S257	2.3600	2.2110	0.1490	0.0172
S258	2.0850	1.9460	0.1390	0.0152
S259	2.1540	1.9540	0.2000	0.0173
S260	2.2600	2.1780	0.0820	0.0077
S261	2.2620	2.1880	0.0740	0.0099
S262	2.2490	2.1650	0.0840	0.0138
S263	2.1410	2.0380	0.1030	0.0129
S264	2.1640	2.0450	0.1190	0.0142
S265	2.1940	2.0700	0.1240	0.0094
S266	2.3180	2.1870	0.1310	0.0138
S267	2.2390	2.1510	0.0880	0.0109
S268	2.2280	2.1410	0.0870	0.0150
S269	2.2970	2.1740	0.1230	0.0126
S270	2.1600	2.0680	0.0920	0.0122
S270	2.1760	2.0720	0.1040	0.0122 0.0154
S271	2.2020	2.0930	0.1090	0.0194 0.0085
S272	2.6180	2.5550	0.0630	0.0022
S273	2.5430	2.3130	0.2300	0.0022 0.0351
S274 S275	2.6350	2.3160 2.3060	0.2300 0.3290	0.0351 0.0464
	4.0000	4.0000	0.0400	0.0404

	$\omega ext{B2PLYP/def2-SVP}$					
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$		
S277	2.1770	1.7430	0.4340	0.0187		
S278	2.1920	2.0130	0.1790	0.0119		
S279	2.1940	2.0880	0.1060	0.0114		
S280	2.2430	2.0830	0.1600	0.0301		
S281	2.1870	2.1300	0.0570	0.0099		
S282	2.1760	2.0700	0.1060	0.0116		
S283	2.1330	1.9750	0.1580	0.0262		
S284	2.1910	2.0850	0.1060	0.0058		
S285	1.9900	1.7420	0.2480	0.0207		
S286	2.1550	1.8900	0.2650	0.0209		
S287	2.0640	1.9970	0.0670	0.0046		
S288	2.3470	2.3070	0.0400	0.0066		
S289	2.2720	2.2730	-0.0010	0.0017		
S290	2.2910	2.2000	0.0910	0.0191		
S291	2.1270	1.9790	0.1480	0.0153		
S292	2.1600	1.9870	0.1730	0.0242		
S293	2.1440	2.0750	0.0690	0.0067		
S294	2.2170	2.1470	0.0700	0.0117		
S295	2.1870	2.0750	0.1120	0.0224		
S296	2.2130	2.1490	0.0640	0.0046		
S297	2.1570	2.0540	0.1030	0.0138		
S298	2.1940	2.0690	0.1250	0.0182		
S299	2.2250	2.1360	0.0890	0.0092		
S300	2.1940	2.1010	0.0930	0.0126		
S301	2.1870	2.0620	0.1250	0.0204		
S302	2.2200	2.1260	0.0940	0.0055		
S303	2.0590	1.8290	0.2300	0.0197		
S304	2.1470	1.9040	0.2430	0.0182		
S305	2.1230	2.0230	0.1000	0.0052		
S306	2.2890	2.2400	0.0490	0.0094		
S307	2.2430	2.1590	0.0840	0.0212		
S308	2.2790	2.2490	0.0300	0.0030		
S309	2.5880	2.5420	0.0460	0.0028		
S310	2.5450	2.3320	0.2130	0.0401		
S311	2.6280	2.3160	0.3120	0.0452		
S312	2.1230	1.9870	0.1360	0.0142		
S313	2.1680	1.9060	0.2620	0.0168		
S314	2.2130	2.0410	0.1720	0.0116		
S315	2.0300	1.8020	0.2280	0.0173		
S316	2.1090	1.8650	0.2440	0.0210		
S317	2.0930	2.0310	0.0620	0.0046		
S318	2.3370	2.2850	0.0520	0.0097		
S319	2.3560	2.3070	0.0490	0.0026		
S320	2.2620	2.1710	0.0910	0.0196		
S321	2.1640	2.0370	0.1270	0.0148		
S322	2.2410	2.0900	0.1510	0.0183		

ω B2PLYP/def2-SVP					
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
S323	2.2710	2.1530	0.1180	0.0109	
S324	2.2520	2.2050	0.0470	0.0080	
S325	2.2650	2.2050	0.0600	0.0069	
S326	2.2930	2.2130	0.0800	0.0152	
S327	2.0040	1.6910	0.3130	0.0214	
S328	2.1240	1.8620	0.2620	0.0166	
S329	2.2330	2.1090	0.1240	0.0080	
S330	2.3800	2.3510	0.0290	0.0069	
S331	2.3650	2.3550	0.0100	0.0010	
S332	2.2870	2.2260	0.0610	0.0197	
S333	2.1350	1.9570	0.1780	0.0156	
S334	2.2230	2.0380	0.1850	0.0118	
S335	2.2040	2.0890	0.1150	0.0073	
S336	2.2880	2.2360	0.0520	0.0088	
S337	2.2820	2.2110	0.0710	0.0132	
S338	2.3200	2.2560	0.0640	0.0062	
S339	2.5440	2.5550	-0.0110	0.0056	
S340	2.5550	2.4940	0.0610	0.0122	
S341	2.4570	2.3650	0.0920	0.0091	
S342	2.8300	2.9160	-0.0860	0.0000	
S343	2.8680	2.6060	0.2620	0.0368	
S344	2.2480	1.9200	0.3280	0.0177	
S345	2.7310	2.8230	-0.0920	0.0007	
S346	2.7910	2.5890	0.2020	0.0264	
S347	2.2830	2.0470	0.2360	0.0160	
S348	2.6200	2.6850	-0.0650	0.0031	
S349	2.6920	2.5650	0.1270	0.0158	
S350	2.3500	2.2390	0.1110	0.0116	
S351	2.5850	2.6250	-0.0400	0.0048	
S352	2.6100	2.5210	0.0890	0.0158	
S353	2.3400	2.2020	0.1380	0.0150	
S354	2.5180	2.5140	0.0040	0.0071	
S355	2.3900	2.3300	0.0600	0.0011	
S356	2.5670	2.4990	0.0680	0.0111	
S357	2.4960	2.4710	0.0250	0.0081	
S358	2.5430	2.4820	0.0610	0.0106	
S359	2.4070	2.3630	0.0440	0.0100 0.0112	
S360	2.8570	2.9310	-0.0740	0.00112	
S361	2.8960	2.6200	0.2760	0.0407	
S362	2.2490	2.0020	0.2470	0.0467	
S363	2.2490	2.3970	0.2470 0.0510	0.0109 0.0104	
	2.4480 2.4460				
S364		2.4360	0.0100	0.0102	
S365	2.4180	2.3420	0.0760	0.0117	
S366	2.2910	2.0500	0.2410	0.0189	
S367	2.3250	2.2750	0.0500	0.0072	
S368	2.5380	2.5530	-0.0150	0.0109	

	$\omega ext{B2PLYP/def2-SVP}$					
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$		
S369	2.3990	2.2880	0.1110	0.0130		
S370	2.3980	2.3700	0.0280	0.0101		
S371	2.4260	2.3910	0.0350	0.0141		
S372	2.4260	2.3710	0.0550	0.0112		
S373	2.4730	2.4360	0.0370	0.0096		
S374	2.4240	2.3690	0.0550	0.0134		
S375	2.3350	2.1270	0.2080	0.0176		
S376	2.3700	2.3010	0.0690	0.0078		
S377	2.5000	2.5020	-0.0020	0.0118		
S378	2.8460	2.9180	-0.0720	0.0000		
S379	2.9020	2.6150	0.2870	0.0413		
S380	2.3020	2.0970	0.2050	0.0156		
S381	2.3180	2.1040	0.2140	0.0167		
S382	2.3560	2.3080	0.0480	0.0090		
S383	2.5470	2.5820	-0.0350	0.0076		
S384	2.4420	2.3660	0.0760	0.0101		
S385	2.5190	2.4490	0.0700	0.0111		
S386	2.5170	2.5220	-0.0050	0.0084		
S387	2.2880	1.9870	0.3010	0.0195		
S388	2.4750	2.4010	0.0740	0.0071		
S389	2.5440	2.5720	-0.0280	0.0097		
S390	2.3970	2.2560	0.1410	0.0133		
S391	2.4490	2.3860	0.0630	0.0071		
S392	2.5330	2.5430	-0.0100	0.0076		
S393	2.5180	2.5050	0.0130	0.0147		
S394	2.5010	2.4500	0.0510	0.0157		
S395	2.4220	2.3520	0.0700	0.0138		
S396	2.8510	2.7350	0.1160	0.0199		
S397	2.8040	2.5570	0.2470	0.0505		
S398	2.2710	2.0690	0.2020	0.0204		
S399	2.7460	2.6740	0.0720	0.0151		
S400	2.7290	2.5430	0.1860	0.0378		
S401	2.2710	2.0530	0.2180	0.0214		
S402	2.6210	2.6080	0.0130	0.0105		
S403	2.6410	2.5140	0.1270	0.0259		
S404	2.3190	2.2110	0.1080	0.0174		
S405	2.5630	2.5410	0.0220	0.0186		
S406	2.5710	2.4890	0.0820	0.0193		
S407	2.4550	2.4550	0.0000	0.0102		
S408	2.5000	2.4800	0.0200	0.0143		
S409	2.3620	2.3170	0.0450	0.0133		
S410	2.5280	2.4660	0.0620	0.0154		
S411	2.4750	2.4490	0.0260	0.0161		
S412	2.5070	2.4550	0.0520	0.0137		
S413	2.3770	2.3480	0.0290	0.0123		
S414	2.8820	2.7280	0.1540	0.0235		

	$\omega ext{B2PLYP/def2-SVP}$						
Molecule	$\Delta E(S_0\text{-}S_1)~[eV]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1)~[\mathrm{eV}]$	$f_{12}(S_0-S_1)$			
S415	2.8320	2.5640	0.2680	0.0535			
S416	2.3420	2.2260	0.1160	0.0160			
S417	2.4400	2.3820	0.0580	0.0288			
S418	2.4360	2.4280	0.0080	0.0102			
S419	2.3770	2.3290	0.0480	0.0102			
S420	2.2920	2.1360	0.1560	0.0240			
S421	2.3190	2.3230	-0.0040	0.0037			
S422	2.5280	2.5920	-0.0640	0.0048			
S423	2.3560	2.2710	0.0850	0.0244			
S424	2.3770	2.3820	-0.0050	0.0067			
S425	2.4190	2.4190	0.0000	0.0101			
S426	2.4020	2.3620	0.0400	0.0196			
S427	2.4500	2.4300	0.0200	0.0099			
S428	2.4100	2.3850	0.0250	0.0113			
S429	2.3100	2.1540	0.1560	0.0225			
S430	2.3560	2.3400	0.0160	0.0044			
S431	2.5000	2.5440	-0.0440	0.0073			
S432	2.8660	2.7330	0.1330	0.0276			
S433	2.8400	2.5710	0.2690	0.0528			
S434	2.3540	2.2490	0.1050	0.0153			
S435	2.2880	2.1280	0.1600	0.0235			
S436	2.3410	2.3480	-0.0070	0.0050			
S437	2.5630	2.5860	-0.0230	0.0074			
S438	2.4350	2.3610	0.0740	0.0204			
S439	2.4750	2.4380	0.0370	0.0116			
S440	2.4680	2.4960	-0.0280	0.0086			
S441	2.3020	2.1090	0.1930	0.0211			
S442	2.4670	2.4180	0.0490	0.0091			
S443	2.5900	2.6490	-0.0590	0.0050			
S444	2.3870	2.2880	0.0990	0.0160			
S445	2.4140	2.3890	0.0250	0.0077			
S446	2.5240	2.5490	-0.0250	0.0084			