	$\omega ext{B2PLYP'/def2-SVP}$				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
S1	1.3160	1.2740	0.0420	0.0000	
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	0.0067	
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	
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	
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	
S46	2.4210	2.2270	0.1940	0.0000	

	$\omega ext{B2PLYP'/def2-SVP}$				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1)~[\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S_1}\text{-}\mathrm{T_1}) \; [\mathrm{eV}]$	$f_{12}(S_0\text{-}S_1)$	
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	0.0115	
S88	2.5370	2.0190	0.5180	0.0052	
S89	0.8700	0.6270	0.2430	0.0000	
S90	1.9100	1.1760	0.7340	0.0025	
S91	1.3970	1.1440	0.2530	0.0042	
S92	2.4710	1.6330	0.8380	0.0036	

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
S133	1.1180	0.9880	0.1300	0.0001
S134	1.6000	1.5200	0.0800	0.0010
S134 S135	1.2970	1.2150	0.0820	0.0010
S136	1.4050	1.3810	0.0240	0.0002
	1.0960	0.8860	0.0240 0.2100	0.0003
S137				

		B2PLYP'/def2-SV	/ P	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
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
S151	2.9670	3.1760	-0.2090	0.0005
S152	3.0290	3.2600	-0.2310	0.0000
S153	2.9260	3.0630	-0.1370	0.0016
S154	3.4880	3.5390	-0.0510	0.0175
S155	2.9240	3.0810	-0.1570	0.0011
S156	3.0520	3.2770	-0.2250	0.0000
S157	3.0420	2.7350	0.3070	0.0002
S158	2.9880	3.1710	-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	0.0092
S182	1.8340	1.7870	0.0470	0.0055
~ = 0 =				
S183	1.8930	1.8480	0.0450	0.0070

	$\omega ext{B2PLYP'/def2-SVP}$				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
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	
S203	1.8030	1.7380	0.0650	0.0096	
S204	1.8590	1.8050	0.0540	0.0089	
S205	1.8700	1.8120	0.0580	0.0111	
S206	1.9010	1.8550	0.0460	0.0032	
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	

	$\omega ext{B2PLYP'/def2-SVP}$				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
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	
S271	2.1760	2.0720	0.1040	0.0154	
S272	2.2020	2.0930	0.1090	0.0085	
S273	2.6180	2.5550	0.0630	0.0022	
S274	2.5430	2.3130	0.2300	0.0351	
S275	2.6350	2.3060	0.3290	0.0464	
S276	2.0170	1.7900	0.2270	0.0186	

	$\omega ext{B2PLYP'/def2-SVP}$				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
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	

$\omega B2PLYP'/def2-SVP$ Molecule $\Delta E(S_0-S_1)$ [eV] $\Delta E(S_0-T_1)$ [eV] $\Delta E(S_1-T_1)$ [eV] $f_{12}(S_0-S_1)$				
	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
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	0.0111
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
S360	2.8570	2.9310	-0.0740	0.0001
S361	2.8960	2.6200	0.2760	0.0407
S362	2.2490	2.0020	0.2470	0.0407
S363	2.2490 2.4480	2.3970	0.2470 0.0510	0.0109 0.0104
S364	2.4460	2.4360	0.0310 0.0100	0.0104 0.0102
S365	2.4400 2.4180	2.4500 2.3420	0.0760	0.0102 0.0117
S366				0.0117 0.0189
S367	2.2910 2.3250	$2.0500 \\ 2.2750$	$0.2410 \\ 0.0500$	0.0189 0.0072
2901	2.5250 2.5380	2.2750 2.5530	-0.0150	0.0072 0.0109

	$\omega ext{B2PLYP'/def2-SVP}$				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
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	

	$\omega \mathrm{B2PLYP'/def2\text{-}SVP}$					
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$		
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		