	ωΒ2Ρ	PLYP'/def2-SVP/C	C-PCM	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S1	1.3030	1.2670	0.0360	0.0000
S2	1.1480	0.9660	0.1820	0.0020
S3	1.7000	1.5900	0.1100	0.0018
S4	1.9740	1.8970	0.0770	0.0064
S5	1.8260	1.3930	0.4330	0.0000
S6	1.7280	1.4910	0.2370	0.0000
S7	2.0920	1.9210	0.1710	0.0020
S8	1.5640	1.3150	0.2490	0.0046
S9	1.7570	1.6130	0.1440	0.0012
S10	2.1290	1.7580	0.3710	0.0010
S11	1.9320	1.8510	0.0810	0.0081
S12	2.2310	2.1870	0.0440	0.0052
S13	2.2960	2.1630	0.1330	0.0119
S14	2.5290	2.4490	0.0800	0.0150
S15	1.9060	1.6130	0.2930	0.0036
S16	2.2350	1.9790	0.2560	0.0007
S17	2.0430	1.8070	0.2360	0.0028
S18	2.2870	2.1340	0.1530	0.0007
S19	1.6260	1.2790	0.3470	0.0070
S20	1.7430	1.4420	0.3010	0.0205
S21	0.9930	0.7500	0.2430	0.0017
S22	1.5360	1.1110	0.4250	0.0065
S23	1.8830	1.2360	0.6470	0.0022
S24	1.8000	1.3270	0.4730	0.0117
S25	1.9970	1.6090	0.3880	0.0097
S26	1.8350	1.5630	0.2720	0.0119
S27	2.1240	1.7540	0.3700	0.0268
S28	1.8060	1.2770	0.5290	0.0028
S29	2.1340	1.5940	0.5400	0.0055
S30	1.6070	1.3020	0.3050	0.0017
S31	1.8860	1.5540	0.3320	0.0110
S32	2.2640	1.7500	0.5140	0.0018
S33	2.2010	1.8420	0.3590	0.0121
S34	1.6730	1.4060	0.2670	0.0016
S35	2.4380	1.7550	0.6830	0.0002
S36	2.4090	1.8710	0.5380	0.0037
S37	2.0040	1.7710	0.2330	0.0079
S38	2.3970	1.9610	0.4360	0.0087
S39	2.4310	2.0730	0.3580	0.0204
S40	1.6730	1.4630	0.2100	0.0006
S41	1.9730	1.7130	0.2600	0.0040
S42	2.2540	1.8290	0.4250	0.0018
S43	2.2830	1.9810	0.3020	0.0026
S44	1.8970	1.8960	0.0010	0.0004
S45	1.7430	1.4980	0.2450	0.0044
S46	2.4650	2.2740	0.1910	0.0000

	ωΒ2Ρ	LYP'/def2-SVP/C	C-PCM	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S47	2.2660	2.2390	0.0270	0.0014
S48	2.0450	1.7710	0.2740	0.0021
S49	2.1530	1.8780	0.2750	0.0074
S50	2.1310	1.8890	0.2420	0.0066
S51	2.6190	2.5560	0.0630	0.0043
S52	2.5650	2.5000	0.0650	0.0087
S53	2.8590	2.8870	-0.0280	0.0057
S54	2.7070	2.3300	0.3770	0.0027
S55	2.3220	2.0570	0.2650	0.0060
S56	2.6340	2.3530	0.2810	0.0008
S57	2.2530	1.5780	0.6750	0.0058
S58	1.4390	1.1010	0.3380	0.0054
S59	1.8670	1.4470	0.4200	0.0127
S60	2.5580	2.0920	0.4660	0.0018
S61	2.5580	2.2230	0.3350	0.0144
S62	2.7690	2.1030	0.6660	0.0007
S63	2.0400	1.6310	0.4090	0.0015
S64	2.4310	2.0100	0.4210	0.0064
S65	2.2050	1.9880	0.2170	0.0111
S66	1.9950	1.6130	0.3820	0.0026
S67	2.0820	1.8010	0.2810	0.0062
S68	2.3850	2.1250	0.2600	0.0044
S69	2.5580	2.3300	0.2280	0.0160
S70	2.6050	2.1670	0.4380	0.0027
S71	2.0880	1.8480	0.2400	0.0000
S72	2.3870	2.1760	0.2110	0.0042
S73	2.5060	2.5720	-0.0660	0.0005
S74	2.3460	2.1610	0.1850	0.0032
S75	1.6780	1.3530	0.3250	0.0140
S76	2.2850	1.7040	0.5810	0.0196
S77	2.4100	2.0400	0.3700	0.0241
S78	2.1030	1.7790	0.3240	0.0064
S79	2.1840	1.8210	0.3630	0.0129
S80	2.8070	2.2750	0.5320	0.0067
S81	2.7900	2.4690	0.3210	0.0140
S82	2.1650	2.0180	0.1470	0.0021
S83	2.7080	2.3720	0.3360	0.0028
S84	3.1650	3.4010	-0.2360	0.0000
S85	2.8850	2.2480	0.6370	0.0099
S86	2.1150	1.7080	0.4070	0.0234
S87	2.5380	2.2020	0.3360	0.0150
S88	2.6400	2.1670	0.4730	0.0073
S89	0.8300	0.5620	0.2680	0.0000
S90	1.9120	1.1620	0.7500	0.0029
S91	1.4610	1.1470	0.3140	0.0054
S92	2.4960	1.6470	0.8490	0.0039
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	ωΒ2Ρ	LYP'/def2-SVP/C	C-PCM	
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	1.4430	1.1360	0.3070	0.0017
S94	2.1270	1.5790	0.5480	0.0000
S95	2.2070	1.6330	0.5740	0.0084
S96	1.9380	1.6620	0.2760	0.0024
S97	1.3190	1.0320	0.2870	0.0009
S98	3.0610	2.1770	0.8840	0.0000
S99	2.1640	1.5290	0.6350	0.0082
S100	1.8410	1.6320	0.2090	0.0011
S101	2.8130	2.1590	0.6540	0.0030
S102	1.9760	1.6760	0.3000	0.0063
S103	2.5970	2.1270	0.4700	0.0024
S104	2.4020	2.1080	0.2940	0.0000
S105	1.3670	1.3480	0.0190	0.0001
S106	1.3470	1.2670	0.0800	0.0000
S107	1.6270	1.5640	0.0630	0.0047
S108	1.3700	1.1330	0.2370	0.0009
S109	1.5560	1.5150	0.0410	0.0026
S110	1.3700	1.1070	0.2630	0.0009
S111	1.4500	1.4220	0.0280	0.0006
S112	1.2860	1.1650	0.1210	0.0004
S113	1.3970	1.3760	0.0210	0.0001
S114	1.2750	1.2010	0.0740	0.0004
S115	1.3410	1.3030	0.0380	0.0000
S116	1.2810	1.2450	0.0360	0.0001
S117	1.3190	1.2740	0.0450	0.0000
S118	1.2990	1.2680	0.0310	0.0002
S119	1.6690	1.5840	0.0850	0.0061
S120	1.2810	1.1910	0.0900	0.0002
S121	1.2690	1.2060	0.0630	0.0007
S122	1.3290	1.2940	0.0350	0.0006
S123	1.0830	0.8700	0.2130	0.0026
S124	1.6760	1.5890	0.0870	0.0016
S125	1.1890	1.1050	0.0840	0.0007
S126	1.3970	1.3620	0.0350	0.0008
S127	1.2210	1.1530	0.0680	0.0005
S128	1.3900	1.3420	0.0480	0.0007
S129	1.1160	0.9330	0.1830	0.0020
S130	1.5460	1.4710	0.0750	0.0012
S131	1.6590	1.5810	0.0780	0.0057
S132	1.2710	1.2270	0.0440	0.0000
S133	1.0830	0.9280	0.1550	0.0018
S134	1.6390	1.5510	0.0880	0.0014
S135	1.2760	1.2020	0.0740	0.0002
S136	1.3970	1.3720	0.0250	0.0003
S137	1.0650	0.8210	0.2440	0.0026
S138	1.7740	1.6040	0.1700	0.0027

	ωΒ2Ρ	LYP'/def2-SVP/C	C-PCM	
Molecule	$\Delta E(S_0\text{-}S_1)~[eV]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1)~[\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S139	1.2110	1.1080	0.1030	0.0007
S140	1.4660	1.4250	0.0410	0.0004
S141	3.1950	3.4290	-0.2340	0.0005
S142	3.5440	3.5940	-0.0500	0.0171
S143	3.4700	3.6300	-0.1600	0.0082
S144	3.3200	3.5350	-0.2150	0.0024
S145	3.2940	3.5360	-0.2420	0.0009
S146	3.1950	3.4300	-0.2350	0.0002
S147	3.1710	3.4040	-0.2330	0.0001
S148	3.6110	3.6410	-0.0300	0.0205
S149	3.1630	3.2780	-0.1150	0.0001
S150	3.0020	2.9610	0.0410	0.0029
S151	3.0460	3.2500	-0.2040	0.0009
S152	3.0970	3.3210	-0.2240	0.0004
S153	2.9850	3.0740	-0.0890	0.0029
S154	3.5740	3.6000	-0.0260	0.0182
S155	3.0270	3.1690	-0.1420	0.0019
S156	3.1720	3.4040	-0.2320	0.0001
S157	3.1530	2.8190	0.3340	0.0007
S158	3.0710	3.2490	-0.1780	0.0008
S159	2.0010	1.9560	0.0450	0.0060
S160	2.0010	1.9160	0.0850	0.0127
S161	1.9310	1.8190	0.1120	0.0089
S162	1.9220	1.8280	0.0940	0.0088
S163	2.3070	2.2690	0.0380	0.0001
S164	2.2800	2.0370	0.2430	0.0303
S165	1.8350	1.5980	0.2370	0.0140
S166	1.8170	1.6670	0.1500	0.0083
S167	2.1950	2.1820	0.0130	0.0013
S168	2.2140	2.0180	0.1960	0.0222
S169	1.8390	1.6640	0.1750	0.0119
S170	1.8230	1.6490	0.1740	0.0091
S171	2.0640	2.0440	0.0200	0.0044
S172	2.1050	1.9740	0.1310	0.0132
S173	1.8320	1.7070	0.1250	0.0113
S174	1.8560	1.7420	0.1140	0.0087
S175	2.0250	1.9930	0.0320	0.0059
S176	2.0340	1.9300	0.1040	0.0150
S177	1.9420	1.8900	0.0520	0.0089
S178	1.9800	1.9150	0.0650	0.0065
S179	1.9500	1.8870	0.0630	0.0084
S180	1.9890	1.8880	0.1010	0.0104
S181	1.8700	1.7950	0.0750	0.0104
S182	1.8990	1.8260	0.0730	0.0063
S183	1.9260	1.8500	0.0760	0.0093

ωB2PLYP'/def2-SVP/C-PCM				
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	1.8850	1.8200	0.0650	0.0104
S186	1.9160	1.8490	0.0670	0.0060
S187	2.3560	2.2990	0.0570	0.0001
S188	2.3340	2.0370	0.2970	0.0353
S189	1.8660	1.7270	0.1390	0.0114
S190	1.8430	1.6700	0.1730	0.0079
S191	1.8790	1.7910	0.0880	0.0110
S192	1.9190	1.8240	0.0950	0.0170
S193	1.8920	1.8060	0.0860	0.0124
S194	1.9020	1.8320	0.0700	0.0040
S195	1.6650	1.4040	0.2610	0.0188
S196	1.7980	1.5800	0.2180	0.0119
S197	2.0680	2.0090	0.0590	0.0115
S198	2.1120	2.0390	0.0730	0.0029
S199	1.8080	1.6670	0.1410	0.0135
S200	1.8440	1.7230	0.1210	0.0132
S201	1.9380	1.8850	0.0530	0.0132
S202	1.9730	1.9170	0.0560	0.0031
S202 S203	1.8190	1.7090	0.1100	0.0031
S204	1.8870	1.7780	0.1090	0.0128 $0.0112$
S204	1.9320	1.8640	0.0680	0.0112 $0.0127$
S206	1.9810	1.9090	0.0720	0.0127 $0.0032$
S200 S207	1.7050	1.4530	0.0720 $0.2520$	0.0032 $0.0186$
S208	1.8050	1.5930	0.2120	0.0099
S209	2.0340	1.9860	0.0480	0.0115
S210	2.1050	2.0370	0.0680	0.0032
S211	2.3380	2.2850	0.0530	0.0000
S212	2.3100	2.0510	0.2590	0.0368
S213	1.8790	1.7490	0.1300	0.0109
S214	1.8820	1.7830	0.0990	0.0077
S215	1.6990	1.4710	0.2280	0.0168
S216	1.7700	1.5950	0.1750	0.0111
S217	2.0800	2.0250	0.0550	0.0111
S218	2.1770	2.0890	0.0880	0.0034
S219	1.8680	1.7590	0.1090	0.0108
S220	1.9460	1.8280	0.1180	0.0117
S221	1.9700	1.9300	0.0400	0.0092
S222	1.9940	1.9400	0.0540	0.0060
S223	1.6260	1.2860	0.3400	0.0202
S224	1.7910	1.5360	0.2550	0.0103
S225	2.1540	2.0460	0.1080	0.0113
S226	2.2480	2.1570	0.0910	0.0026
S227	1.8080	1.6430	0.1650	0.0141
S228	1.9000	1.7570	0.1430	0.0073
S229	2.0090	1.9730	0.0360	0.0080
S230	2.0810	2.0070	0.0740	0.0065

	ωΒ2Ρ	PLYP'/def2-SVP/C	C-PCM	
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	2.3610	2.2620	0.0990	0.0097
S232	2.3650	2.2370	0.1280	0.0186
S233	2.3530	2.2090	0.1440	0.0159
S234	2.2520	2.0970	0.1550	0.0137
S235	2.3100	2.1230	0.1870	0.0126
S236	2.3120	2.1430	0.1690	0.0133
S237	2.6620	2.5380	0.1240	0.0033
S238	2.5850	2.3190	0.2660	0.0366
S239	2.6750	2.3260	0.3490	0.0504
S240	2.0850	1.8130	0.2720	0.0207
S241	2.1710	1.7680	0.4030	0.0188
S242	2.2170	1.9480	0.2690	0.0155
S243	2.5570	2.4650	0.0920	0.0046
S244	2.4860	2.3110	0.1750	0.0230
S245	2.5970	2.3140	0.2830	0.0357
S246	2.0880	1.8290	0.2590	0.0217
S247	2.2420	1.9120	0.3300	0.0152
S248	2.2460	1.9550	0.2910	0.0165
S249	2.4230	2.3500	0.0730	0.0080
S250	2.3970	2.2820	0.1150	0.0136
S251	2.5080	2.2830	0.2250	0.0236
S252	2.1620	1.9940	0.1680	0.0173
S253	2.2740	2.0550	0.2190	0.0148
S254	2.1650	1.9990	0.1660	0.0118
S255	2.3930	2.3090	0.0840	0.0099
S256	2.3450	2.2220	0.1230	0.0241
S257	2.4130	2.2390	0.1740	0.0184
S258	2.1110	1.9710	0.1400	0.0148
S259	2.2180	2.0030	0.2150	0.0189
S260	2.3290	2.2210	0.1080	0.0086
S261	2.3170	2.2080	0.1090	0.0127
S262	2.3070	2.1820	0.1250	0.0158
S263	2.2170	2.0960	0.1210	0.0144
S264	2.2380	2.1010	0.1370	0.0161
S265	2.2750	2.1270	0.1480	0.0101
S266	2.3790	2.2140	0.1650	0.0144
S267	2.2950	2.1720	0.1230	0.0139
S268	2.2880	2.1570	0.1310	0.0172
S269	2.3570	2.1980	0.1590	0.0132
S270	2.2340	2.1240	0.1100	0.0136
S271	2.2500	2.1260	0.1240	0.0174
S272	2.2820	2.1500	0.1320	0.0092
S273	2.7130	2.5510	0.1620	0.0028
S274	2.5910	2.2950	0.2960	0.0404
S275	2.7060	2.3260	0.3800	0.0529
S276	2.0590	1.7970	0.2620	0.0198

	ωΒ2Ρ	LYP'/def2-SVP/C	C-PCM	
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	2.1930	1.7320	0.4610	0.0207
S278	2.2570	2.0570	0.2000	0.0130
S279	2.2680	2.1390	0.1290	0.0131
S280	2.3050	2.0890	0.2160	0.0363
S281	2.2340	2.1570	0.0770	0.0112
S282	2.2320	2.0960	0.1360	0.0135
S283	2.2000	2.0190	0.1810	0.0286
S284	2.2530	2.1140	0.1390	0.0063
S285	2.0410	1.7400	0.3010	0.0256
S286	2.2240	1.8570	0.3670	0.0272
S287	2.0810	1.9660	0.1150	0.0052
S288	2.4060	2.3560	0.0500	0.0088
S289	2.3460	2.3220	0.0240	0.0013
S290	2.3760	2.2600	0.1160	0.0213
S291	2.1400	1.9810	0.1590	0.0160
S292	2.2300	1.9830	0.2470	0.0300
S293	2.1840	2.0860	0.0980	0.0075
S294	2.2790	2.1930	0.0860	0.0132
S295	2.2630	2.1330	0.1300	0.0247
S296	2.2860	2.1930	0.0930	0.0048
S297	2.1980	2.0470	0.1510	0.0179
S298	2.2480	2.0460	0.2020	0.0229
S299	2.2570	2.1350	0.1220	0.0090
S300	2.2740	2.1730	0.1010	0.0137
S301	2.2730	2.1330	0.1400	0.0231
S302	2.3080	2.1930	0.1150	0.0053
S303	2.0540	1.7890	0.2650	0.0214
S304	2.2070	1.8570	0.3500	0.0232
S305	2.1360	1.9770	0.1590	0.0051
S306	2.3740	2.3230	0.0510	0.0103
S307	2.3440	2.2290	0.1150	0.0250
S308	2.3740	2.3270	0.0470	0.0025
S309	2.6870	2.5460	0.1410	0.0035
S310	2.5950	2.3240	0.2710	0.0463
S311	2.6920	2.3340	0.3580	0.0512
S312	2.1930	2.0220	0.1710	0.0159
S313	2.2090	1.9280	0.2810	0.0183
S314	2.2760	2.0820	0.1940	0.0125
S315	2.0830	1.8130	0.2700	0.0216
S316	2.1710	1.8530	0.3180	0.0250
S317	2.1140	2.0150	0.0990	0.0048
S318	2.4040	2.3550	0.0490	0.0102
S319	2.4350	2.3720	0.0630	0.0026
S320	2.3430	2.2330	0.1100	0.0219
S321	2.2300	2.0750	0.1550	0.0172
S322	2.3140	2.1270	0.1870	0.0201

Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$ m ^{O}CYP'/def2 ext{-}SVP/OO$ $ m \Delta E(S_0 ext{-}T_1)~[eV]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S323	2.3230	2.1710	0.1520	0.0114
S324	2.3100	2.2380	0.1320 $0.0720$	0.0114 $0.0104$
S325	2.3360	2.2490	0.0870	0.0104 $0.0073$
S326	2.3500 $2.3500$	2.2350	0.1150	0.0073
S327	2.0240	1.6410	0.3830	0.0164 $0.0269$
S327 S328	2.0240 $2.1770$	1.7970	0.3800	0.0209 $0.0231$
S329	$\frac{2.1770}{2.2710}$	2.0950	0.3800 $0.1760$	0.0231 $0.0074$
S330	2.4590	2.4220	0.0370	0.0074
S331	2.4570	2.4340	0.0230	0.0006
S332	2.3790	2.2640	0.1150	0.0000 $0.0254$
S333	2.1880	1.9740	0.2140	0.0254 $0.0193$
S334	2.2990	2.0550	0.2140 $0.2440$	0.0193 $0.0137$
S335	2.2520	2.0990	0.2440 $0.1530$	0.0137 $0.0073$
S336	2.2520 $2.3600$	2.0990 $2.2970$	0.1630	0.0073 $0.0099$
S337	2.3550	2.2540	0.1010	0.0155
S338	2.4040	2.3210	0.0830	0.0066
S339	2.6310	2.6190	0.0120	0.0060
S340	2.6410	2.5580	0.0830	0.0135
S341	2.5350	2.4180	0.1170	0.0100
S342	2.9270	2.9400	-0.0130	0.0000
S343	2.9580	2.6440	0.3140	0.0422
S344	2.3010	1.9320	0.3690	0.0188
S345	2.8070	2.8600	-0.0530	0.0009
S346	2.8660	2.6430	0.2230	0.0271
S347	2.3630	2.1100	0.2530	0.0163
S348	2.6870	2.7300	-0.0430	0.0040
S349	2.7680	2.6210	0.1470	0.0157
S350	2.4480	2.3250	0.1230	0.0122
S351	2.6650	2.6770	-0.0120	0.0057
S352	2.6770	2.5720	0.1050	0.0167
S353	2.4250	2.2730	0.1520	0.0154
S354	2.5930	2.5590	0.0340	0.0089
S355	2.4840	2.4140	0.0700	0.0119
S356	2.6380	2.5470	0.0910	0.0111
S357	2.5710	2.5230	0.0480	0.0097
S358	2.6130	2.5290	0.0840	0.0109
S359	2.5020	2.4460	0.0560	0.0121
S360	2.9560	2.9540	0.0020	0.0002
S361	2.9820	2.6560	0.3260	0.0466
S362	2.3110	2.0330	0.2780	0.0178
S363	2.5460	2.4710	0.0750	0.0111
S364	2.5090	2.4830	0.0260	0.0124
S365	2.4920	2.4040	0.0880	0.0124
S366	2.3680	2.0690	0.2990	0.0222
S367	2.3590	2.2620	0.0970	0.0081
S368	2.6290	2.6190	0.0100	0.0139

	ωB2PLYP'/def2-SVP/C-PCM				
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	2.4860	2.3370	0.1490	0.0150	
S370	2.4580	2.3980	0.0600	0.0119	
S371	2.5150	2.4700	0.0450	0.0151	
S372	2.4930	2.3840	0.1090	0.0142	
S373	2.5190	2.4520	0.0670	0.0105	
S374	2.5280	2.4720	0.0560	0.0143	
S375	2.3960	2.1080	0.2880	0.0222	
S376	2.4010	2.2620	0.1390	0.0093	
S377	2.6150	2.6100	0.0050	0.0131	
S378	2.9460	2.9440	0.0020	0.0001	
S379	2.9780	2.6450	0.3330	0.0464	
S380	2.3580	2.1240	0.2340	0.0168	
S381	2.3990	2.1340	0.2650	0.0195	
S382	2.3970	2.3110	0.0860	0.0098	
S383	2.6310	2.6450	-0.0140	0.0099	
S384	2.5240	2.4240	0.1000	0.0119	
S385	2.5900	2.4950	0.0950	0.0112	
S386	2.5950	2.5760	0.0190	0.0105	
S387	2.3470	1.9640	0.3830	0.0243	
S388	2.5250	2.4010	0.1240	0.0075	
S389	2.6490	2.6530	-0.0040	0.0122	
S390	2.4760	2.2950	0.1810	0.0161	
S391	2.5190	2.4150	0.1040	0.0076	
S392	2.6250	2.6230	0.0020	0.0086	
S393	2.6080	2.5390	0.0690	0.0192	
S394	2.5870	2.4850	0.1020	0.0200	
S395	2.5040	2.3790	0.1250	0.0175	
S396	2.9430	2.7050	0.2380	0.0259	
S397	2.8530	2.5730	0.2800	0.0569	
S398	2.3350	2.0670	0.2680	0.0245	
S399	2.8140	2.6770	0.1370	0.0178	
S400	2.8090	2.5660	0.2430	0.0443	
S401	2.3570	2.0940	0.2630	0.0250	
S402	2.6850	2.6190	0.0660	0.0136	
S403	2.6870	2.5390	0.1480	0.0283	
S404	2.4230	2.2780	0.1450	0.0208	
S405	2.6310	2.5500	0.0810	0.0251	
S406	2.6430	2.5130	0.1300	0.0225	
S407	2.5390	2.4980	0.0410	0.0132	
S408	2.5680	2.4900	0.0780	0.0195	
S409	2.4580	2.3780	0.0800	0.0163	
S410	2.5740	2.4930	0.0810	0.0170	
S411	2.5450	2.4600	0.0850	0.0218	
S412	2.5520	2.4820	0.0700	0.0150	
S413	2.4720	2.4090	0.0630	0.0151	
S414	2.9660	2.6870	0.2790	0.0301	

ωB2PLYP'/def2-SVP/C-PCM					
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	2.9130	2.5830	0.3300	0.0650	
S416	2.4270	2.2600	0.1670	0.0195	
S417	2.5240	2.3850	0.1390	0.0393	
S418	2.4790	2.4560	0.0230	0.0119	
S419	2.4520	2.3490	0.1030	0.0131	
S420	2.3700	2.1040	0.2660	0.0338	
S421	2.3470	2.3410	0.0060	0.0039	
S422	2.6110	2.6500	-0.0390	0.0066	
S423	2.4390	2.2710	0.1680	0.0340	
S424	2.4190	2.4120	0.0070	0.0076	
S425	2.5020	2.4640	0.0380	0.0127	
S426	2.4630	2.3370	0.1260	0.0281	
S427	2.4710	2.4430	0.0280	0.0101	
S428	2.5130	2.4620	0.0510	0.0134	
S429	2.3740	2.1020	0.2720	0.0315	
S430	2.3810	2.3490	0.0320	0.0044	
S431	2.6100	2.6390	-0.0290	0.0086	
S432	2.9550	2.7010	0.2540	0.0357	
S433	2.9140	2.5870	0.3270	0.0631	
S434	2.4320	2.2770	0.1550	0.0187	
S435	2.3620	2.1230	0.2390	0.0304	
S436	2.3870	2.3520	0.0350	0.0051	
S437	2.6570	2.6640	-0.0070	0.0090	
S438	2.5200	2.3980	0.1220	0.0256	
S439	2.5500	2.4600	0.0900	0.0131	
S440	2.5510	2.5410	0.0100	0.0116	
S441	2.3610	2.0530	0.3080	0.0303	
S442	2.5340	2.4190	0.1150	0.0090	
S443	2.6930	2.7410	-0.0480	0.0062	
S444	2.4730	2.3020	0.1710	0.0211	
S445	2.4880	2.4060	0.0820	0.0086	
S446	2.6240	2.6260	-0.0020	0.0106	