

Molecule	ω B2PLYP'/def2-SVP			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S843	2.3250	2.2230	0.1020	0.0020
S844	2.4850	2.3370	0.1480	0.0036
S845	2.5460	2.4270	0.1190	0.0021
S846	2.7080	2.5050	0.2030	0.0106
S847	2.2020	1.9020	0.3000	0.0037
S848	2.3700	2.0670	0.3030	0.0009
S849	2.3120	2.0470	0.2650	0.0046
S850	2.4850	2.2440	0.2410	0.0020
S851	2.4500	2.2270	0.2230	0.0041
S852	2.5280	2.2880	0.2400	0.0059
S853	2.6790	2.4000	0.2790	0.0034
S854	2.7750	2.4840	0.2910	0.0133
S855	2.3190	1.9710	0.3480	0.0061
S856	2.4060	2.0650	0.3410	0.0001
S857	2.4850	2.1450	0.3400	0.0059
S858	2.6010	2.2720	0.3290	0.0009
S859	2.2650	2.0150	0.2500	0.0096
S860	2.6360	2.3740	0.2620	0.0037
S861	2.6200	2.4740	0.1460	0.0035
S862	2.8080	2.5350	0.2730	0.0091
S863	2.3440	1.9300	0.4140	0.0023
S864	2.5310	2.1070	0.4240	0.0004
S865	2.3370	1.9740	0.3630	0.0048
S866	2.5320	2.2010	0.3310	0.0017
S867	2.7210	2.3550	0.3660	0.0096
S868	2.8160	2.3730	0.4430	0.0094
S869	2.8930	2.5280	0.3650	0.0075
S870	3.0080	2.5620	0.4460	0.0161
S871	2.6050	2.1270	0.4780	0.0056
S872	2.7030	2.1690	0.5340	0.0004
S873	2.6190	2.1360	0.4830	0.0082
S874	2.7510	2.2230	0.5280	0.0004
S875	2.3970	2.1020	0.2950	0.0087
S876	2.4710	2.2880	0.1830	0.0015
S877	2.3150	1.8690	0.4460	0.0182
S878	2.4450	2.0720	0.3730	0.0084
S879	2.5540	2.0350	0.5190	0.0319
S880	2.0850	1.8640	0.2210	0.0002
S881	2.2100	1.8330	0.3770	0.0074
S882	2.2350	1.9770	0.2580	0.0013
S883	2.3540	2.0060	0.3480	0.0088
S884	2.3440	1.8770	0.4670	0.0164
S885	2.6010	2.1150	0.4860	0.0058
S886	2.6210	2.0820	0.5390	0.0293
S887	2.2240	1.9080	0.3160	0.0008
S888	2.2290	1.8140	0.4150	0.0052

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S889	2.4510	2.0800	0.3710	0.0019
S890	2.4920	2.0500	0.4420	0.0074
S891	2.4850	2.2290	0.2560	0.0084
S892	2.6980	2.4830	0.2150	0.0053
S893	2.6330	2.4290	0.2040	0.0032
S894	2.4780	1.8970	0.5810	0.0204
S895	2.5000	2.1170	0.3830	0.0088
S896	2.6530	2.0450	0.6080	0.0315
S897	2.3940	1.8550	0.5390	0.0088
S898	2.2240	1.9350	0.2890	0.0006
S899	2.3880	2.0220	0.3660	0.0065
S900	2.6280	1.9960	0.6320	0.0228
S901	2.7980	2.2660	0.5320	0.0075
S902	2.8440	2.1610	0.6830	0.0353
S903	2.4940	2.0880	0.4060	0.0003
S904	2.5220	1.9250	0.5970	0.0091
S905	2.5370	2.1260	0.4110	0.0019
S906	2.6070	2.0770	0.5300	0.0046
S907	2.6350	2.2940	0.3410	0.0129
S908	2.8690	2.6430	0.2260	0.0049
S909	2.7250	2.5210	0.2040	0.0024
S910	2.9780	2.4540	0.5240	0.0000
S911	2.3910	2.0520	0.3390	0.0135
S912	2.6570	2.3300	0.3270	0.0248
S913	2.3110	1.8550	0.4560	0.0060
S914	2.2760	1.8880	0.3880	0.0113
S915	2.5610	2.1000	0.4610	0.0144
S916	2.6120	2.2410	0.3710	0.0116
S917	2.8280	2.4530	0.3750	0.0206
S918	2.2930	1.9040	0.3890	0.0063
S919	2.4360	2.1150	0.3210	0.0076
S920	2.5660	2.0980	0.4680	0.0124
S921	2.3560	2.0230	0.3330	0.0152
S922	2.6990	2.2380	0.4610	0.0238
S923	2.5860	2.1790	0.4070	0.0016
S924	2.2590	1.9760	0.2830	0.0047
S925	2.6340	2.1620	0.4720	0.0096
S926	2.6170	2.2380	0.3790	0.0198
S927	2.9200	2.4130	0.5070	0.0278
S928	2.5910	2.2240	0.3670	0.0001
S929	2.4630	2.1450	0.3180	0.0018
S930	2.7130	2.1670	0.5460	0.0021
S931	2.7280	2.6650	0.0630	0.0007
S932	2.7550	2.7230	0.0320	0.0004
S933	2.9420	2.8660	0.0760	0.0052
S934	2.6340	2.2460	0.3880	0.0045

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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	2.5170	2.2100	0.3070	0.0098
S936	2.7150	2.4030	0.3120	0.0063
S937	2.7260	2.6170	0.1090	0.0018
S938	2.8470	2.6940	0.1530	0.0014
S939	2.9700	2.8520	0.1180	0.0067
S940	2.6150	2.2470	0.3680	0.0015
S941	2.6380	2.2780	0.3600	0.0099
S942	2.7800	2.4240	0.3560	0.0035
S943	2.1610	1.8190	0.3420	0.0068
S944	2.0620	1.7650	0.2970	0.0011
S945	2.3980	2.0000	0.3980	0.0095
S946	2.2240	1.7410	0.4830	0.0187
S947	2.4730	1.9290	0.5440	0.0277
S948	2.8810	2.6390	0.2420	0.0004
S949	3.0530	2.8820	0.1710	0.0041
S950	2.8040	2.3100	0.4940	0.0034
S951	2.5790	2.1660	0.4130	0.0100
S952	2.7910	2.2520	0.5390	0.0061
S953	3.0020	2.6310	0.3710	0.0032
S954	3.0750	2.7770	0.2980	0.0043
S955	3.2060	2.9010	0.3050	0.0081
S956	2.9110	2.3620	0.5490	0.0005
S957	2.8180	2.2980	0.5200	0.0123
S958	2.9890	2.1830	0.8060	0.0030
S959	2.3260	2.0740	0.2520	0.0012
S960	2.1610	1.7170	0.4440	0.0085
S961	2.5770	2.2650	0.3120	0.0004
S962	2.3310	1.9560	0.3750	0.0046
S963	2.1970	1.8890	0.3080	0.0003
S964	2.6000	2.1380	0.4620	0.0127
S965	2.5060	2.1400	0.3660	0.0158
S966	2.6950	2.2820	0.4130	0.0288
S967	2.4450	2.1080	0.3370	0.0088
S968	2.2980	2.0630	0.2350	0.0029
S969	2.4870	2.1980	0.2890	0.0117
S970	2.4180	2.0290	0.3890	0.0187
S971	2.6600	2.2380	0.4220	0.0316
S972	2.3180	1.9770	0.3410	0.0097
S973	2.3980	2.1000	0.2980	0.0020
S974	2.4880	2.1820	0.3060	0.0117
S975	2.2610	1.9890	0.2720	0.0053
S976	2.1940	1.9180	0.2760	0.0002
S977	2.4740	2.1720	0.3020	0.0086
S978	2.2660	2.0400	0.2260	0.0002
S979	2.4440	2.0870	0.3570	0.0122
S980	2.4170	2.0560	0.3610	0.0057

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S981	2.6450	2.2810	0.3640	0.0199
S982	2.7060	2.1870	0.5190	0.0185
S983	2.8470	2.3090	0.5380	0.0310
S984	2.6840	2.1850	0.4990	0.0111
S985	2.6230	2.1470	0.4760	0.0106
S986	2.6910	2.1290	0.5620	0.0270
S987	2.9010	2.2860	0.6150	0.0405
S988	2.6200	2.0890	0.5310	0.0170
S989	2.5860	2.1960	0.3900	0.0008
S990	2.6880	2.0990	0.5890	0.0118
S991	2.4400	2.2290	0.2110	0.0001
S992	2.2940	1.8920	0.4020	0.0062
S993	2.6790	2.3820	0.2970	0.0013
S994	2.4740	2.2080	0.2660	0.0055
S995	2.5430	2.2700	0.2730	0.0022
S996	2.4420	2.1370	0.3050	0.0021
S997	2.7770	2.4040	0.3730	0.0096
S998	2.5790	2.3330	0.2460	0.0054
S999	2.6240	2.1970	0.4270	0.0102
S1000	2.1570	1.6760	0.4810	0.0189
S1001	2.4750	1.8180	0.6570	0.0261
S1002	2.4980	1.8720	0.6260	0.0313
S1003	2.8480	2.5360	0.3120	0.0036
S1004	2.8770	2.5240	0.3530	0.0132
S1005	2.2670	1.8910	0.3760	0.0173
S1006	2.7140	2.1980	0.5160	0.0170
S1007	2.5730	2.0610	0.5120	0.0283
S1008	2.5550	2.3250	0.2300	0.0030
S1009	2.7380	2.4120	0.3260	0.0072
S1010	2.4180	2.0050	0.4130	0.0044
S1011	2.4280	1.9550	0.4730	0.0044
S1012	2.5820	2.0550	0.5270	0.0060
S1013	2.8130	2.4890	0.3240	0.0043
S1014	2.9540	2.4720	0.4820	0.0056
S1015	2.4910	2.1910	0.3000	0.0044
S1016	2.7140	2.3120	0.4020	0.0014
S1017	2.6880	2.2000	0.4880	0.0057
S1018	2.6740	2.5070	0.1670	0.0020
S1019	2.9190	2.7260	0.1930	0.0069
S1020	2.5180	2.0340	0.4840	0.0125
S1021	2.7110	2.3210	0.3900	0.0115
S1022	2.7480	2.4580	0.2900	0.0010
S1023	3.0110	2.7170	0.2940	0.0069
S1024	2.6040	2.0140	0.5900	0.0083
S1025	2.8640	2.3240	0.5400	0.0098
S1026	2.5650	2.2580	0.3070	0.0115

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S1027	2.8150	2.3550	0.4600	0.0139
S1028	2.9460	2.7020	0.2440	0.0028
S1029	2.5720	2.0640	0.5080	0.0124
S1030	2.6460	2.2590	0.3870	0.0135
S1031	2.9540	2.4530	0.5010	0.0000
S1032	3.1610	2.7090	0.4520	0.0030
S1033	2.7760	2.0860	0.6900	0.0097
S1034	2.8690	2.2200	0.6490	0.0141
S1035	2.5620	2.3230	0.2390	0.0083
S1036	2.7690	2.5230	0.2460	0.0022
S1037	2.7770	2.2060	0.5710	0.0273
S1038	2.3730	1.9160	0.4570	0.0096
S1039	2.6010	2.2130	0.3880	0.0140
S1040	2.8620	2.2850	0.5770	0.0264
S1041	2.4440	1.8870	0.5570	0.0074
S1042	2.7740	2.2630	0.5110	0.0135
S1043	2.5530	2.0370	0.5160	0.0078
S1044	2.7880	2.4860	0.3020	0.0082
S1045	2.8280	2.3460	0.4820	0.0000
S1046	3.0470	2.7060	0.3410	0.0054
S1047	2.8050	2.1820	0.6230	0.0195
S1048	2.5180	2.1560	0.3620	0.0114
S1049	3.0060	2.2850	0.7210	0.0219
S1050	2.6080	1.8910	0.7170	0.0054
S1051	2.7450	2.1560	0.5890	0.0111
S1052	2.4420	1.9040	0.5380	0.0279
S1053	2.8240	2.5680	0.2560	0.0103
S1054	2.6990	2.2160	0.4830	0.0120
S1055	3.0340	2.3750	0.6590	0.0002
S1056	2.7470	2.2210	0.5260	0.0137
S1057	3.0130	2.7160	0.2970	0.0158
S1058	2.5320	2.0970	0.4350	0.0101
S1059	2.7680	2.2570	0.5110	0.0147
S1060	2.8240	2.3730	0.4510	0.0031
S1061	3.1130	2.7520	0.3610	0.0150
S1062	2.8380	2.1930	0.6450	0.0020
S1063	2.9200	2.1320	0.7880	0.0003
S1064	3.1580	3.0370	0.1210	0.0084
S1065	2.9250	2.4470	0.4780	0.0253
S1066	3.2090	3.0370	0.1720	0.0057
S1067	3.0290	2.4490	0.5800	0.0225
S1068	2.2090	1.8130	0.3960	0.0030
S1069	2.4570	2.0440	0.4130	0.0120
S1070	2.1870	1.8700	0.3170	0.0005
S1071	2.4590	1.8010	0.6580	0.0159
S1072	2.6660	1.9740	0.6920	0.0343

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S1073	2.4560	1.9460	0.5100	0.0075
S1074	2.9060	2.2510	0.6550	0.0273
S1075	3.3800	3.0770	0.3030	0.0033
S1076	2.8990	2.1670	0.7320	0.0018
S1077	2.0590	1.6280	0.4310	0.0075
S1078	2.4760	2.2650	0.2110	0.0017
S1079	2.1930	1.8400	0.3530	0.0085
S1080	2.3110	1.8770	0.4340	0.0002
S1081	2.6440	2.1190	0.5250	0.0104
S1082	2.3660	2.1060	0.2600	0.0013
S1083	2.7090	2.3000	0.4090	0.0203
S1084	2.7530	2.1310	0.6220	0.0186
S1085	2.4200	1.9980	0.4220	0.0013
S1086	2.5990	2.2670	0.3320	0.0097
S1087	2.3700	2.0410	0.3290	0.0000
S1088	2.7430	2.2040	0.5390	0.0114
S1089	2.8800	2.3490	0.5310	0.0255
S1090	2.7150	2.0910	0.6240	0.0077
S1091	2.4240	1.8820	0.5420	0.0001
S1092	2.5370	2.0370	0.5000	0.0202
S1093	2.7640	2.0600	0.7040	0.0000
S1094	2.5680	2.1090	0.4590	0.0011
S1095	2.3220	1.8480	0.4740	0.0061
S1096	2.6620	2.3870	0.2750	0.0003
S1097	2.3620	2.0780	0.2840	0.0069
S1098	2.6670	2.2270	0.4400	0.0019
S1099	2.9060	2.3260	0.5800	0.0079
S1100	2.6560	2.0910	0.5650	0.0051
S1101	2.7390	2.0460	0.6930	0.0408
S1102	2.5190	2.1340	0.3850	0.0259
S1103	2.8090	2.2750	0.5340	0.0376
S1104	2.8150	2.2410	0.5740	0.0113
S1105	3.1860	2.3330	0.8530	0.0012
S1106	2.7600	2.2100	0.5500	0.0127
S1107	2.8860	2.1510	0.7350	0.0013
S1108	2.4720	2.1330	0.3390	0.0053
S1109	2.4920	2.1090	0.3830	0.0032
S1110	2.5440	2.2050	0.3390	0.0003
S1111	2.4320	1.8440	0.5880	0.0188
S1112	2.5410	1.9640	0.5770	0.0081
S1113	2.6380	2.0550	0.5830	0.0110
S1114	2.6860	2.0520	0.6340	0.0029
S1115	3.2080	3.0480	0.1600	0.0126
S1116	3.4290	3.0020	0.4270	0.0471
S1117	3.3690	3.0130	0.3560	0.0331
S1118	3.3000	3.0140	0.2860	0.0214

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S1119	3.2410	3.0130	0.2280	0.0167
S1120	3.2100	3.0120	0.1980	0.0122
S1121	3.1900	3.0090	0.1810	0.0105
S1122	3.2270	3.0560	0.1710	0.0087
S1123	3.5060	3.0780	0.4280	0.0393
S1124	3.4270	3.1200	0.3070	0.0195
S1125	3.3300	3.0930	0.2370	0.0108
S1126	3.2780	3.0710	0.2070	0.0133
S1127	3.2260	3.0720	0.1540	0.0100
S1128	3.2040	3.0550	0.1490	0.0113
S1129	3.1120	2.9560	0.1560	0.0095
S1130	2.9730	2.6330	0.3400	0.0099
S1131	3.0600	2.8140	0.2460	0.0089
S1132	3.1500	3.0050	0.1450	0.0078
S1133	3.0830	2.8070	0.2760	0.0098
S1134	3.1590	2.9860	0.1730	0.0083
S1135	3.1660	3.0000	0.1660	0.0085
S1136	3.4460	2.9910	0.4550	0.0505
S1137	3.1400	3.0200	0.1200	0.0081
S1138	3.0320	2.9450	0.0870	0.0017
S1139	3.0900	2.9990	0.0910	0.0045
S1140	3.0530	2.9350	0.1180	0.0022
S1141	3.1340	2.9850	0.1490	0.0071
S1142	3.5230	3.0700	0.4530	0.0450
S1143	3.1290	2.8960	0.2330	0.0181
S1144	2.9290	2.5260	0.4030	0.0237
S1145	3.0590	2.8100	0.2490	0.0185
S1146	3.0020	2.6350	0.3670	0.0221
S1147	3.1170	2.9270	0.1900	0.0147
S1148	2.9070	2.5970	0.3100	0.0103
S1149	3.0930	2.5410	0.5520	0.0148
S1150	3.1980	2.8950	0.3030	0.0141
S1151	3.1480	2.7410	0.4070	0.0148
S1152	3.2180	2.9560	0.2620	0.0106
S1153	3.1870	2.9160	0.2710	0.0101
S1154	3.4510	2.9890	0.4620	0.0508
S1155	3.0570	2.9750	0.0820	0.0028
S1156	3.0830	2.5120	0.5710	0.0029
S1157	3.1580	2.9980	0.1600	0.0085
S1158	3.5060	3.0630	0.4430	0.0437
S1159	2.9630	2.5950	0.3680	0.0221
S1160	2.9920	2.4750	0.5170	0.0221
S1161	3.1170	2.9400	0.1770	0.0146
S1162	2.8740	2.5190	0.3550	0.0123
S1163	3.1930	2.9070	0.2860	0.0136
S1164	3.2730	2.8180	0.4550	0.0127

ω 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]	$f_{12}(S_0-S_1)$
S1165	3.2260	3.0720	0.1540	0.0095
S1166	3.1160	2.9850	0.1310	0.0048
S1167	3.0810	2.8280	0.2530	0.0145
S1168	3.2380	3.0920	0.1460	0.0072