

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]	$f_{12}(S_0-S_1)$
S1169	3.2730	3.0440	0.2290	0.0320
S1170	3.4610	2.9470	0.5140	0.2786
S1171	3.1360	2.9710	0.1650	0.0357
S1172	2.9800	2.7200	0.2600	0.0554
S1173	3.2150	2.9590	0.2560	0.0631
S1174	3.2070	2.8480	0.3590	0.2981
S1175	2.3250	2.1930	0.1320	0.0313
S1176	3.0600	2.7600	0.3000	0.0856
S1177	3.0670	2.6160	0.4510	0.3470
S1178	3.2830	2.8970	0.3860	0.5791
S1179	2.5040	2.3690	0.1350	0.0355
S1180	2.3410	2.2500	0.0910	0.0200
S1181	3.1400	2.6860	0.4540	0.4872
S1182	2.5120	2.4130	0.0990	0.0222
S1183	3.2950	2.8430	0.4520	0.0242
S1184	3.2050	2.9930	0.2120	0.0251
S1185	3.0990	2.7340	0.3650	0.0526
S1186	3.1750	2.9530	0.2220	0.0368
S1187	3.1270	2.7190	0.4080	0.0514
S1188	3.4750	2.9190	0.5560	0.2927
S1189	3.4120	2.8170	0.5950	0.3981
S1190	3.3660	3.0400	0.3260	0.0825
S1191	3.2680	2.9410	0.3270	0.0465
S1192	3.2150	2.9080	0.3070	0.0848
S1193	3.5110	2.5110	1.0000	1.2392
S1194	3.3290	2.5860	0.7430	0.3713
S1195	3.3580	2.5390	0.8190	0.6153
S1196	3.2860	3.0010	0.2850	0.0233
S1197	3.1590	3.0230	0.1360	0.0096
S1198	3.1210	3.0060	0.1150	0.0070
S1199	3.0810	3.0150	0.0660	0.0039
S1200	3.0430	2.9780	0.0650	0.0023
S1201	3.1950	3.0250	0.1700	0.0126
S1202	3.2190	2.9660	0.2530	0.0182
S1203	3.2490	2.8610	0.3880	0.0010
S1204	3.0870	3.0040	0.0830	0.0050
S1205	3.1990	3.0260	0.1730	0.0130
S1206	3.1580	3.0170	0.1410	0.0096
S1207	3.1030	2.8010	0.3020	0.0055
S1208	3.1970	3.0160	0.1810	0.0129
S1209	3.3680	3.0000	0.3680	0.0340
S1210	3.3270	2.9990	0.3280	0.0243
S1211	3.1220	2.9930	0.1290	0.0068
S1212	3.1730	2.9930	0.1800	0.0108
S1213	3.1500	3.0150	0.1350	0.0089
S1214	3.1870	2.8050	0.3820	1.2665

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S1215	3.1720	2.7760	0.3960	1.4075
S1216	3.1270	2.7650	0.3620	0.9495
S1217	3.1400	2.8400	0.3000	1.2265
S1218	3.1280	2.7680	0.3600	1.5079
S1219	2.9760	2.6920	0.2840	1.5312
S1220	2.9190	2.6500	0.2690	1.3874
S1221	3.1430	2.9690	0.1740	0.1648
S1222	3.0370	2.7430	0.2940	1.4362
S1223	3.1770	2.8560	0.3210	0.4103
S1224	3.1330	2.8300	0.3030	1.3457
S1225	3.0900	2.8150	0.2750	0.9693
S1226	3.1500	2.8240	0.3260	0.5469
S1227	3.1520	2.8510	0.3010	1.1018
S1228	3.1180	2.8220	0.2960	1.1136
S1229	3.1120	2.8100	0.3020	1.2109
S1230	3.1090	2.8390	0.2700	0.9135
S1231	2.8930	2.6430	0.2500	1.4317
S1232	3.1710	2.8490	0.3220	1.2450
S1233	3.1880	2.8600	0.3280	0.3579
S1234	3.0320	2.4880	0.5440	0.1642
S1235	3.0970	2.7060	0.3910	1.2825
S1236	3.0440	2.7760	0.2680	1.0305
S1237	3.2730	2.9160	0.3570	0.4918
S1238	3.2880	2.9170	0.3710	0.4596
S1239	3.2440	2.6930	0.5510	1.8293
S1240	3.1890	2.9430	0.2460	0.0622
S1241	3.2290	2.6770	0.5520	1.8381
S1242	3.2620	2.8190	0.4430	0.2058
S1243	3.3050	2.8530	0.4520	0.4735
S1244	3.3260	2.8160	0.5100	0.7148
S1245	3.3410	2.9120	0.4290	0.5639
S1246	3.1890	2.6380	0.5510	1.9792
S1247	3.1360	3.0060	0.1300	0.0317
S1248	3.0720	2.9140	0.1580	0.0563
S1249	3.2000	2.9980	0.2020	0.0813
S1250	3.0670	2.8880	0.1790	0.0407
S1251	3.1300	2.9290	0.2010	0.1354
S1252	3.0750	2.7900	0.2850	0.6765
S1253	3.1320	2.8550	0.2770	0.3867
S1254	3.0980	2.8030	0.2950	0.6137
S1255	3.0870	2.7730	0.3140	0.7890
S1256	3.0970	2.8950	0.2020	0.0863
S1257	3.0200	2.7260	0.2940	0.6366
S1258	2.9980	2.7390	0.2590	0.5214
S1259	3.0220	2.7270	0.2950	0.6422
S1260	3.0100	2.7490	0.2610	0.5128

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]	$f_{12}(S_0-S_1)$
S1261	3.1450	2.8440	0.3010	0.9037
S1262	2.9980	2.6190	0.3790	0.7865
S1263	3.0840	2.9150	0.1690	0.0377
S1264	3.0470	2.7660	0.2810	0.7134
S1265	3.0630	2.7640	0.2990	0.6247
S1266	3.0320	2.7690	0.2630	0.5390
S1267	3.0360	2.7620	0.2740	0.5576
S1268	2.9510	2.5130	0.4380	0.7721
S1269	3.0930	2.8110	0.2820	0.5800
S1270	3.0570	2.7820	0.2750	0.5912
S1271	3.0410	2.7950	0.2460	0.4638
S1272	3.0130	2.7670	0.2460	0.4970
S1273	3.0340	2.6910	0.3430	0.6911
S1274	3.1190	2.9260	0.1930	0.0775
S1275	2.9740	2.7020	0.2720	0.6887
S1276	2.9170	2.6880	0.2290	0.4849
S1277	2.9480	2.6820	0.2660	0.6938
S1278	2.8570	2.5890	0.2680	0.4497
S1279	3.1270	2.8080	0.3190	1.3786
S1280	3.1170	2.8230	0.2940	1.1951
S1281	2.9920	2.7210	0.2710	0.6644
S1282	2.9220	2.6870	0.2350	0.5197
S1283	3.2830	3.0090	0.2740	0.0310
S1284	3.4610	2.9480	0.5130	0.2780
S1285	3.3660	3.0400	0.3260	0.0825
S1286	3.3630	3.0270	0.3360	0.1524
S1287	3.3820	3.0380	0.3440	0.1137
S1288	3.4260	2.9810	0.4450	0.2539
S1289	3.3750	3.0170	0.3580	0.2329
S1290	3.3250	2.9860	0.3390	0.2075
S1291	3.2910	3.0120	0.2790	0.4017
S1292	3.1990	2.9650	0.2340	0.7353
S1293	3.2290	2.9650	0.2640	0.5677
S1294	3.1900	2.9460	0.2440	0.5825
S1295	3.1650	3.0010	0.1640	0.6973
S1296	3.1320	2.9390	0.1930	0.4186
S1297	2.9650	2.9180	0.0470	0.7236
S1298	3.1420	2.9560	0.1860	0.5367
S1299	3.1160	2.9430	0.1730	0.6139
S1300	3.0570	2.9380	0.1190	0.6813
S1301	3.1960	2.9590	0.2370	0.3625
S1302	3.1750	2.9550	0.2200	0.4404
S1303	3.1640	2.9650	0.1990	0.5006
S1304	3.1560	2.9100	0.2460	0.4543
S1305	3.1550	2.9390	0.2160	0.4525
S1306	3.1970	2.9670	0.2300	0.4463

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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]	$f_{12}(S_0-S_1)$
S1307	3.1860	2.9650	0.2210	0.3843
S1308	3.1770	2.9620	0.2150	0.4268
S1309	2.6020	1.8730	0.7290	0.0104
S1310	3.1520	2.9530	0.1990	0.3629
S1311	3.1630	2.9680	0.1950	0.4132
S1312	3.1580	2.9240	0.2340	0.3060
S1313	3.2230	2.9810	0.2420	0.2135
S1314	3.1970	2.9640	0.2330	0.3766
S1315	3.2210	2.9490	0.2720	0.2961
S1316	3.1470	2.9620	0.1850	0.5257
S1317	3.1740	2.9670	0.2070	0.4586
S1318	3.1220	2.9330	0.1890	0.3892
S1319	3.1080	2.7710	0.3370	0.3711
S1320	3.1570	2.9620	0.1950	0.5039
S1321	3.1760	2.9690	0.2070	0.4403
S1322	3.1400	2.9440	0.1960	0.4387
S1323	3.0720	2.9070	0.1650	0.5123
S1324	2.9970	2.6040	0.3930	0.5738
S1325	2.7960	2.8390	-0.0430	0.7560
S1326	3.2040	2.9720	0.2320	0.3618
S1327	3.1470	2.9530	0.1940	0.0803
S1328	3.0830	2.9170	0.1660	0.5551
S1329	3.1320	2.9820	0.1500	0.6160
S1330	3.1400	2.9680	0.1720	0.7439
S1331	3.0310	2.9640	0.0670	0.6326
S1332	3.2270	2.8930	0.3340	0.1587
S1333	3.2560	3.0020	0.2540	0.0372
S1334	3.1870	2.9970	0.1900	0.3292
S1335	3.1190	2.9860	0.1330	0.4232
S1336	3.1920	2.9840	0.2080	0.4253
S1337	3.2250	3.0110	0.2140	0.2063
S1338	3.1050	2.8790	0.2260	0.2064
S1339	3.0410	2.9330	0.1080	0.8803
S1340	3.1350	2.9270	0.2080	1.0158
S1341	3.1470	2.9350	0.2120	1.0476
S1342	3.1890	2.9260	0.2630	1.0291
S1343	3.1720	2.9330	0.2390	1.0445
S1344	2.8810	2.8510	0.0300	0.3476
S1345	3.2670	3.0310	0.2360	0.0835
S1346	3.1750	2.9310	0.2440	1.0107
S1347	3.1790	2.9390	0.2400	1.0310
S1348	3.0440	2.8990	0.1450	0.9345
S1349	3.0320	2.9000	0.1320	0.9649
S1350	3.1880	2.9260	0.2620	1.0204
S1351	3.1740	2.9320	0.2420	1.0373
S1352	3.0850	2.9300	0.1550	0.8039

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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]	$f_{12}(S_0-S_1)$
S1353	3.0820	2.9340	0.1480	0.8213
S1354	2.9110	2.9050	0.0060	0.7164
S1355	3.1870	3.0300	0.1570	0.0328
S1356	2.9690	2.8620	0.1070	0.3652
S1357	3.0190	2.8970	0.1220	0.8764
S1358	3.0440	2.9090	0.1350	0.9068
S1359	3.1880	2.9950	0.1930	0.5857
S1360	3.2630	2.9760	0.2870	0.8119
S1361	3.1600	2.9930	0.1670	0.6417
S1362	3.1910	2.9790	0.2120	0.7217
S1363	3.1650	2.9770	0.1880	0.7758
S1364	3.0480	2.9460	0.1020	0.7505
S1365	3.2000	2.9900	0.2100	0.8117
S1366	3.1500	2.9520	0.1980	0.9824
S1367	3.0560	2.9150	0.1410	0.9510
S1368	3.0960	2.9620	0.1340	0.7772
S1369	3.0480	2.9270	0.1210	0.8112
S1370	2.9520	2.8860	0.0660	0.8009
S1371	3.0970	2.9850	0.1120	0.6281
S1372	3.1310	2.9700	0.1610	0.7718
S1373	3.1800	2.9810	0.1990	0.7536
S1374	3.2330	2.9950	0.2380	0.4849
S1375	3.3100	2.9730	0.3370	0.7988
S1376	3.3230	2.9840	0.3390	0.8131
S1377	3.1980	2.9840	0.2140	0.8075
S1378	3.1490	2.9710	0.1780	0.7578
S1379	3.0290	2.9640	0.0650	0.4880
S1380	3.0890	2.9840	0.1050	0.6373
S1381	3.1460	2.9770	0.1690	0.7639
S1382	3.1920	2.9880	0.2040	0.7484
S1383	3.2790	3.0040	0.2750	0.4037
S1384	3.0500	2.9330	0.1170	0.6426
S1385	3.0810	2.9420	0.1390	0.6045
S1386	3.0590	2.9290	0.1300	0.6212
S1387	2.9850	2.9240	0.0610	0.5462
S1388	2.9880	2.9200	0.0680	0.6417
S1389	2.9970	2.9180	0.0790	0.6096
S1390	3.2980	2.9810	0.3170	0.9861
S1391	3.1990	2.9780	0.2210	0.6716
S1392	3.3400	2.9780	0.3620	0.8978
S1393	2.9440	2.9430	0.0010	0.6836
S1394	3.0420	2.9470	0.0950	0.5919
S1395	3.0610	2.9450	0.1160	0.7827
S1396	2.9200	2.9020	0.0180	0.8216
S1397	3.4980	3.2980	0.2000	0.0182
S1398	3.5340	3.1430	0.3910	0.0094

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S1399	3.5100	2.9260	0.5840	0.0269
S1400	3.5100	2.9260	0.5840	0.0269
S1401	3.3510	2.8620	0.4890	0.1488
S1402	3.3380	2.8950	0.4430	0.3356
S1403	3.2630	2.8920	0.3710	0.3959
S1404	3.1700	2.8430	0.3270	0.4608
S1405	3.0420	2.7800	0.2620	0.5382
S1406	2.9630	2.7190	0.2440	0.5313
S1407	2.9490	2.7150	0.2340	0.5559
S1408	2.8490	2.6470	0.2020	0.5068
S1409	3.0750	2.7910	0.2840	0.5899
S1410	2.9880	2.7310	0.2570	0.5368
S1411	3.0990	2.8100	0.2890	0.5856
S1412	3.0900	2.7940	0.2960	0.5285
S1413	3.1060	2.8150	0.2910	0.5829
S1414	3.0970	2.7990	0.2980	0.5255
S1415	3.3420	3.1060	0.2360	0.0399
S1416	3.4540	3.2750	0.1790	0.0129
S1417	3.5170	3.2990	0.2180	0.0176
S1418	3.4390	3.2640	0.1750	0.0196
S1419	3.5290	3.1490	0.3800	0.0331
S1420	3.5040	3.1690	0.3350	0.0141
S1421	3.5920	2.9010	0.6910	0.0136
S1422	3.4890	3.2830	0.2060	0.0170
S1423	3.3490	3.1790	0.1700	0.0279
S1424	3.4710	3.2750	0.1960	0.0204
S1425	3.4020	3.1490	0.2530	0.0281
S1426	3.3780	2.9960	0.3820	0.0221
S1427	3.3980	3.0910	0.3070	0.0385
S1428	3.3190	3.0730	0.2460	0.0421
S1429	3.4010	2.8220	0.5790	0.0246
S1430	3.1860	2.8750	0.3110	0.0286
S1431	3.4150	3.2350	0.1800	0.0241
S1432	3.5490	2.8700	0.6790	0.0250
S1433	3.4470	3.2580	0.1890	0.0214
S1434	3.2220	3.0570	0.1650	0.0279
S1435	3.5250	3.2170	0.3080	0.0465
S1436	3.4800	3.2860	0.1940	0.0406
S1437	3.3320	1.9560	1.3760	0.0018
S1438	3.4060	3.1410	0.2650	0.0902
S1439	3.3960	3.1960	0.2000	0.0456
S1440	3.3490	3.1690	0.1800	0.0165
S1441	3.4750	3.0320	0.4430	0.0237
S1442	3.5790	3.2580	0.3210	0.0768
S1443	3.5040	3.0860	0.4180	0.0257
S1444	3.5260	3.2620	0.2640	0.0983

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S1445	3.5680	3.1220	0.4460	0.0529
S1446	3.4730	3.0190	0.4540	0.0218
S1447	3.4080	3.2160	0.1920	0.0208
S1448	3.5610	3.0290	0.5320	0.0522
S1449	3.4760	3.0380	0.4380	0.0338
S1450	3.3940	3.2010	0.1930	0.0212
S1451	3.4690	3.2810	0.1880	0.0319
S1452	3.4790	3.2800	0.1990	0.0364
S1453	3.4650	3.2800	0.1850	0.0386
S1454	3.3380	3.1270	0.2110	0.0390
S1455	3.4970	3.2880	0.2090	0.0496
S1456	3.4830	3.2860	0.1970	0.0420
S1457	3.4820	3.2870	0.1950	0.0457
S1458	3.3900	3.2340	0.1560	0.0318
S1459	3.4980	3.2690	0.2290	0.0824
S1460	3.4980	3.2530	0.2450	0.0443
S1461	3.4780	3.2670	0.2110	0.0685
S1462	3.4380	3.2130	0.2250	0.2925
S1463	3.5200	3.2910	0.2290	0.0626
S1464	3.4960	3.2850	0.2110	0.0427
S1465	3.4710	3.2770	0.1940	0.0493
S1466	3.5260	3.2380	0.2880	0.3895
S1467	3.5080	3.2920	0.2160	0.0466
S1468	3.4700	3.2860	0.1840	0.0363
S1469	3.4630	3.2730	0.1900	0.0419
S1470	3.2630	3.1200	0.1430	0.0327
S1471	3.2870	3.1860	0.1010	0.6774
S1472	3.4400	2.8450	0.5950	0.0449
S1473	3.4390	2.8380	0.6010	0.0391
S1474	3.4390	2.7730	0.6660	0.0429
S1475	3.2390	2.8390	0.4000	0.0285
S1476	3.4550	3.2700	0.1850	0.0393
S1477	3.4550	3.2750	0.1800	0.0388
S1478	3.4540	3.2640	0.1900	0.0396
S1479	3.3180	3.1990	0.1190	0.0220
S1480	2.6440	2.9920	-0.3480	0.4862
S1481	2.7230	3.0310	-0.3080	0.3478
S1482	2.7270	3.0340	-0.3070	0.3394
S1483	2.8890	3.1260	-0.2370	0.6037
S1484	2.8710	3.1070	-0.2360	0.4574
S1485	2.8740	3.1090	-0.2350	0.4664
S1486	3.1180	3.1860	-0.0680	0.6613
S1487	3.5050	3.0620	0.4430	0.1188
S1488	3.4200	3.1630	0.2570	0.0593
S1489	3.4730	3.1830	0.2900	0.0876
S1490	3.4970	2.8080	0.6890	0.0941

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]	$f_{12}(S_0-S_1)$
S1491	3.3870	3.1400	0.2470	0.0481
S1492	3.3570	3.1480	0.2090	0.0408
S1493	3.4850	2.7340	0.7510	0.0958
S1494	3.3790	3.1190	0.2600	0.0735
S1495	3.3810	3.1470	0.2340	0.0702
S1496	3.3840	3.1400	0.2440	0.0693
S1497	3.4030	3.1390	0.2640	0.0757
S1498	3.3820	3.1240	0.2580	0.0870
S1499	3.3200	3.1370	0.1830	0.0390
S1500	3.4090	3.1400	0.2690	0.1028
S1501	3.4090	3.1430	0.2660	0.0943
S1502	3.4020	3.1320	0.2700	0.1004
S1503	3.3540	3.1180	0.2360	0.0768
S1504	3.4190	3.1190	0.3000	0.1382
S1505	3.4280	3.1400	0.2880	0.0991
S1506	3.4580	3.1120	0.3460	0.1122
S1507	3.4140	2.9780	0.4360	0.4954
S1508	3.4130	3.1260	0.2870	0.1121
S1509	3.4160	3.1500	0.2660	0.0860
S1510	3.4000	3.1310	0.2690	0.1056
S1511	3.4770	3.0380	0.4390	0.4797
S1512	3.4000	3.1280	0.2720	0.0930
S1513	3.3980	3.1470	0.2510	0.0790
S1514	3.3890	3.1270	0.2620	0.0922
S1515	3.3150	3.1250	0.1900	0.0559
S1516	3.3390	2.9390	0.4000	0.8943
S1517	3.3610	2.8530	0.5080	0.0988
S1518	3.3580	2.7900	0.5680	0.0971
S1519	3.3680	2.7860	0.5820	0.1012
S1520	3.2590	2.8330	0.4260	0.0466
S1521	3.3780	3.1260	0.2520	0.0869
S1522	3.3760	3.1250	0.2510	0.0889
S1523	3.3810	3.1140	0.2670	0.0878
S1524	3.2760	3.1120	0.1640	0.0453
S1525	2.9280	2.8480	0.0800	0.7498
S1526	3.0090	2.8690	0.1400	0.6951
S1527	3.0110	2.8710	0.1400	0.6037
S1528	3.1920	2.9020	0.2900	0.8776
S1529	3.2020	2.8960	0.3060	0.7943
S1530	3.2030	2.8970	0.3060	0.7951
S1531	3.3530	2.9530	0.4000	0.6765
S1532	3.3160	3.1670	0.1490	0.8091
S1533	3.1170	3.1090	0.0080	0.9386
S1534	3.1920	3.1660	0.0260	0.7452
S1535	3.2060	3.1400	0.0660	1.0358
S1536	3.4770	3.2090	0.2680	0.2168

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]	$f_{12}(S_0-S_1)$
S1537	3.0120	3.0670	-0.0550	1.0384
S1538	3.2160	3.1730	0.0430	0.6982
S1539	3.1480	3.1130	0.0350	1.1109
S1540	3.4180	3.2050	0.2130	0.4859
S1541	2.9420	3.1110	-0.1690	0.6581
S1542	2.7480	3.0200	-0.2720	0.5690
S1543	3.0520	3.1770	-0.1250	0.6314
S1544	3.1840	2.9250	0.2590	0.8537
S1545	2.7470	3.0090	-0.2620	0.5896
S1546	3.0980	3.1080	-0.0100	0.6577
S1547	3.3310	2.9140	0.4170	0.7510
S1548	3.0460	3.1570	-0.1110	0.6910
S1549	3.3220	2.9540	0.3680	0.8102
S1550	3.0220	3.1600	-0.1380	0.6673
S1551	3.3150	2.9410	0.3740	0.7952
S1552	2.9730	3.0350	-0.0620	1.0814
S1553	3.2550	3.1740	0.0810	0.9459
S1554	3.2250	3.1710	0.0540	0.7582
S1555	2.6520	2.9000	-0.2480	0.6661
S1556	3.2160	3.1450	0.0710	1.0440
S1557	3.3680	3.1910	0.1770	0.6902
S1558	3.4280	3.2070	0.2210	0.2953
S1559	3.1800	3.1820	-0.0020	0.6827
S1560	3.1310	3.1670	-0.0360	0.7196
S1561	3.0350	3.0810	-0.0460	1.0731
S1562	3.1730	3.1490	0.0240	0.9857
S1563	3.0540	3.1780	-0.1240	0.6449
S1564	3.0970	3.1830	-0.0860	0.6481
S1565	3.1480	3.1750	-0.0270	0.7153
S1566	2.6950	3.1660	-0.4710	0.1098
S1567	3.0690	3.1790	-0.1100	0.3520
S1568	3.0580	3.1280	-0.0700	0.8334
S1569	2.9770	3.1110	-0.1340	0.7348
S1570	3.1300	3.1820	-0.0520	0.6820
S1571	3.2250	3.1930	0.0320	0.6459
S1572	3.3170	3.1960	0.1210	0.6111
S1573	2.5910	2.8330	-0.2420	0.7648
S1574	2.9810	3.0890	-0.1080	0.9379
S1575	2.6680	3.0330	-0.3650	0.4554
S1576	2.6340	2.3610	0.2730	0.3496
S1577	2.5810	2.8100	-0.2290	0.8168
S1578	2.6850	3.0050	-0.3200	0.6632
S1579	2.9560	3.0720	-0.1160	0.9755
S1580	2.6140	2.8580	-0.2440	0.7960
S1581	2.6820	2.9640	-0.2820	0.7093
S1582	3.3580	3.2130	0.1450	0.4672

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]	$f_{12}(S_0-S_1)$
S1583	3.1420	3.1780	-0.0360	0.8999
S1584	2.9960	3.1050	-0.1090	0.9525
S1585	3.0900	3.1570	-0.0670	0.8914
S1586	3.4230	3.2100	0.2130	0.4501
S1587	3.2710	3.1830	0.0880	0.9404
S1588	2.6450	3.0020	-0.3570	0.6615
S1589	3.1060	3.1760	-0.0700	0.9132
S1590	3.2230	3.0890	0.1340	0.2218
S1591	3.0800	3.1050	-0.0250	0.9034
S1592	3.4350	3.2090	0.2260	0.3243
S1593	3.4190	3.2080	0.2110	0.4937
S1594	3.0960	3.1610	-0.0650	0.7198
S1595	3.2960	3.1720	0.1240	0.7030
S1596	3.2170	3.1710	0.0460	0.7461
S1597	3.2730	3.1100	0.1630	0.1049
S1598	3.2770	3.1160	0.1610	0.1350
S1599	2.9840	3.0670	-0.0830	1.0002
S1600	2.9440	3.0360	-0.0920	1.0426
S1601	3.2120	3.1660	0.0460	0.9069
S1602	3.2770	3.1750	0.1020	0.7453
S1603	3.1890	3.1660	0.0230	0.9301
S1604	3.3890	3.1950	0.1940	0.2975
S1605	3.0920	3.1420	-0.0500	0.9839
S1606	3.1460	3.1580	-0.0120	0.9027
S1607	3.0360	3.1310	-0.0950	0.9045
S1608	3.2530	3.1610	0.0920	1.0079
S1609	3.3290	3.1700	0.1590	0.8024
S1610	3.2460	3.1650	0.0810	0.9873
S1611	3.2100	3.1620	0.0480	1.0130
S1612	3.2870	3.1710	0.1160	0.8481
S1613	3.1760	3.1630	0.0130	0.9815
S1614	3.2670	2.9970	0.2700	0.0333
S1615	3.2430	3.0890	0.1540	0.3861
S1616	3.2980	3.1730	0.1250	0.9272
S1617	3.0620	3.1430	-0.0810	0.9505
S1618	3.2270	3.0680	0.1590	0.0469
S1619	3.4190	3.2060	0.2130	0.4933
S1620	3.3700	3.1640	0.2060	0.1218
S1621	2.9800	3.1130	-0.1330	0.8956
S1622	3.2420	3.1620	0.0800	1.0078
S1623	3.2180	3.1720	0.0460	0.9291
S1624	3.1980	3.1700	0.0280	0.9996
S1625	3.2620	3.1760	0.0860	0.8518
S1626	3.3500	2.8880	0.4620	0.5803
S1627	3.3180	3.1800	0.1380	0.6843
S1628	3.3890	3.1630	0.2260	0.9281

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]	$f_{12}(S_0-S_1)$
S1629	3.4790	3.2250	0.2540	0.0908
S1630	3.4690	3.1780	0.2910	0.2892
S1631	3.4650	3.2520	0.2130	0.0356
S1632	3.5760	3.2790	0.2970	0.1891
S1633	3.4640	3.2340	0.2300	0.0878
S1634	3.4570	3.2490	0.2080	0.0360
S1635	3.4670	3.1800	0.2870	0.2349
S1636	3.4570	3.2690	0.1880	0.0605
S1637	3.4560	3.2720	0.1840	0.0547
S1638	3.4520	3.2710	0.1810	0.0589
S1639	3.4510	3.2690	0.1820	0.0495
S1640	3.4470	3.2650	0.1820	0.0518
S1641	3.4550	3.2720	0.1830	0.0567
S1642	3.2560	3.1650	0.0910	0.7578
S1643	3.3330	3.1920	0.1410	0.7327
S1644	3.4500	3.1670	0.2830	0.9310
S1645	3.1890	3.1450	0.0440	0.7540
S1646	3.0590	3.1020	-0.0430	0.8192
S1647	2.9590	3.0730	-0.1140	0.7154
S1648	3.4670	3.2550	0.2120	0.0405
S1649	2.7360	2.4960	0.2400	0.6051
S1650	3.4560	3.2710	0.1850	0.0574
S1651	3.1870	3.1590	0.0280	0.9780
S1652	3.2500	3.1700	0.0800	0.8479
S1653	3.1660	3.1600	0.0060	0.9806
S1654	3.3290	3.1870	0.1420	0.6448
S1655	2.9260	3.0770	-0.1510	0.7125
S1656	3.1800	3.1550	0.0250	1.0142
S1657	3.1700	3.1640	0.0060	0.7550
S1658	3.2440	3.1760	0.0680	0.9948
S1659	3.3390	3.1530	0.1860	1.1480
S1660	3.1880	3.1310	0.0570	1.0984
S1661	3.0740	3.0950	-0.0210	1.0926
S1662	2.9950	3.0630	-0.0680	0.9397
S1663	3.4230	3.2020	0.2210	0.3827
S1664	3.4470	3.2640	0.1830	0.0594
S1665	3.2280	3.1870	0.0410	0.7676
S1666	3.1950	3.1610	0.0340	0.9719
S1667	3.1260	3.1510	-0.0250	0.7782
S1668	2.8840	2.4890	0.3950	0.9676
S1669	3.0090	3.0790	-0.0700	1.0027
S1670	3.1800	3.1560	0.0240	0.9556
S1671	3.1920	3.1710	0.0210	0.7880
S1672	3.2870	3.1620	0.1250	0.7983
S1673	3.1690	3.1570	0.0120	0.9757
S1674	3.3150	3.1850	0.1300	0.6529

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]	$f_{12}(S_0-S_1)$
S1675	3.4500	3.2650	0.1850	0.0558
S1676	3.2840	3.1990	0.0850	0.5156
S1677	3.2450	3.2110	0.0340	0.6365
S1678	3.2960	3.2240	0.0720	0.5096
S1679	3.4660	3.2610	0.2050	0.0489
S1680	3.2640	3.1810	0.0830	0.9589
S1681	3.3980	3.1480	0.2500	1.1146
S1682	3.2810	3.1870	0.0940	0.9309
S1683	3.2770	3.1840	0.0930	0.9298
S1684	3.4020	3.1450	0.2570	1.1164
S1685	3.2280	3.1330	0.0950	1.0528
S1686	3.1580	3.1120	0.0460	1.0621
S1687	3.1320	3.1250	0.0070	0.9642
S1688	3.2670	3.1810	0.0860	0.9381
S1689	3.4120	3.1470	0.2650	1.0939
S1690	3.4430	3.2240	0.2190	0.2448
S1691	3.2040	3.1990	0.0050	0.4935
S1692	3.2410	3.2120	0.0290	0.5820
S1693	3.2590	3.2030	0.0560	0.5665
S1694	3.1700	3.2090	-0.0390	0.5962
S1695	3.3380	3.1860	0.1520	0.6070
S1696	3.3470	3.2090	0.1380	0.4178
S1697	3.4390	3.2220	0.2170	0.2587
S1698	3.2500	3.1250	0.1250	0.9972
S1699	3.4420	3.2230	0.2190	0.2555
S1700	3.3040	3.2100	0.0940	0.4736
S1701	3.4560	3.2360	0.2200	0.2418
S1702	3.3260	3.1710	0.1550	0.0688