Molecule	ωB2PLYP'/def2-SV(P) (adiabatic) $\Delta E(S_0\text{-}S_1)$ [eV]	$\Delta E(S_0\text{-}T_1)$ [eV]	$\Delta E(S_1\text{-}T_1)$ [eV]	$f_{12}(S_0\text{-}S_1)$
S1	1.2961	1.2410	0.0551	-
S2	1.1556	0.9799	0.1757	-
S3	1.6136	1.5375	0.0761	-
S4	1.8833	1.8155	0.0678	-
S5	1.5458	1.3105	0.2353	-
S6	1.6076	1.4369	0.1706	-
S7	1.9330	1.8374	0.0956	-
S8	1.4923	1.3181	0.1742	-
S9	1.7231	1.5929	0.1302	-
S10	1.8545	1.6687	0.1858	-
S11	1.8624	1.7857	0.0767	-
S12	2.1407	2.1113	0.0294	-
S13	2.1731	2.0734	0.0998	-
S14	2.4306	2.3742	0.0564	-
S15	1.7579	1.5407	0.2173	-
S16	2.0576	1.9179	0.1398	-
S17	1.9090	1.7599	0.1491	-
S18	2.1836	2.1097	0.0739	-
S19	1.5032	1.2447	0.2585	-
S20	1.7128	1.4190	0.2939	-
S21	1.0170	0.7899	0.2271	-
S22	1.3933	1.1224	0.2709	-
S23	1.4694	1.1057	0.3637	-
S24	1.6332	1.2841	0.3491	-
S25	1.8246	1.5566	0.2680	-
S26	1.7629	1.5016	0.2613	-
S27	2.0404	1.7136	0.3268	-
S28	1.4567	1.2206	0.2361	-
S29	1.7793	1.5287	0.2506	-
S30	1.4976	1.2526	0.2450	-
S31	1.7875	1.5316	0.2560	-
S32	1.9088	1.5821	0.3268	-
S33	2.0161	1.7476	0.2686	-
S34	1.5729	1.3841	0.1888	-
S35	1.9086	1.5339	0.3746	-
S36	2.0182	1.7174	0.3008	-
S37	1.9383	1.7345	0.2038	-
S38	2.1375	1.7904	0.3471	-
S39	2.3003	1.9788	0.3215	-
S40	1.5736	1.4071	0.1665	-
S41	1.8500	1.6823	0.1677	-
S42	1.9229	1.6876	0.2353	-
S43	2.1045	1.8906	0.2139	-
S44	1.8408	1.8235	0.0173	-
S45	1.6563	1.4622	0.1941	-
S46	2.2476	2.1745	0.0731	-

Molecule	ωB2PLYP'/def2-SV(P) (adiabatic) $\Delta E(S_0\text{-}S_1)$ [eV]	$\Delta E(S_0\text{-}T_1)$ [eV]	$\Delta E(S_1\text{-}T_1)$ [eV]	$f_{12}(S_0\text{-}S_1)$
S47	2.1543	2.1326	0.0217	-
S48	1.8902	1.6600	0.2302	-
S49	2.0505	1.8026	0.2478	-
S50	1.9889	1.8053	0.1836	-
S51	2.4657	2.4506	0.0152	-
S52	2.4361	2.3881	0.0480	-
S53	2.7322	2.7698	-0.0376	-
S54	2.4329	2.1634	0.2695	-
S55	2.1771	1.9131	0.2639	-
S56	2.4933	1.9084	0.5850	-
S57	1.8227	1.4149	0.4078	-
S58	1.3857	1.1084	0.2773	-
S59	1.7564	1.4440	0.3124	-
S60	2.2052	1.9384	0.2668	-
S61	2.3388	2.0927	0.2461	-
S62	2.2298	1.8912	0.3385	-
S63	1.7686	1.5037	0.2649	-
S64	2.1166	1.8887	0.2279	-
S65	2.1150	1.9142	0.2008	-
S66	1.8050	1.5136	0.2914	-
S67	1.9733	1.7518	0.2215	-
S68	2.2087	2.0472	0.1615	-
S69	2.4474	1.9302	0.5171	-
S70	2.2319	2.0271	0.2048	-
S71	1.9373	1.7688	0.1686	-
S72	2.2445	1.7759	0.4686	-
S73	2.4148	2.4617	-0.0469	-
S74	2.2541	2.0894	0.1647	-
S75	1.6381	1.3466	0.2915	-
S76	2.0219	1.5909	0.4309	-
S77	2.3173	1.9798	0.3376	-
S78	1.9212	1.7307	0.1906	-
S79	2.0693	1.7381	0.3312	-
S80	2.3770	2.0811	0.2959	-
S81	2.6238	2.3404	0.2834	-
S82	2.0939	1.9772	0.1166	-
S83	2.4504	1.7849	0.6655	-
S84	3.0447	3.2325	-0.1878	-
S85	2.7854	1.8239	0.9615	-
S86	2.0855	1.7021	0.3833	-
S87	2.3622	1.7993	0.5629	-
S88	2.5622	1.7583	0.8040	-
S89	0.8749	0.6377	0.2372	-
S90	1.3904	1.0402	0.3502	-
S91	1.4143	1.1311	0.2832	-
S92	1.8533	1.4116	0.4417	-

Molecule	ωB2PLYP'/def2-SV(P) (adiabatic) $\Delta E(S_0\text{-}S_1)$ [eV]	$\Delta E(S_0\text{-}T_1)$ [eV]	$\Delta E(S_1\text{-}T_1)$ [eV]	$f_{12}(S_0\text{-}S_1)$
S93	1.3694	1.1251	0.2444	-
S94	1.7229	1.4147	0.3082	-
S95	1.8242	1.5268	0.2973	-
S96	1.8294	1.6330	0.1963	-
S97	1.2868	1.0325	0.2543	-
S98	2.3134	1.9027	0.4107	-
S99	1.7726	1.4583	0.3143	-
S100	1.7861	1.5931	0.1930	-
S101	2.2071	1.9514	0.2558	-
S102	1.9031	1.6424	0.2607	-
S103	2.2288	1.7369	0.4919	-
S104	2.3554	1.7028	0.6526	-
S105	1.3585	1.3194	0.0391	-
S106	1.3188	1.2557	0.0631	-
S107	1.6194	1.5404	0.0790	-
S108	1.1883	1.0503	0.1380	-
S109	1.5651	1.4983	0.0668	-
S110	1.1814	1.0489	0.1325	-
S111	1.4648	1.4163	0.0485	-
S112	1.2057	1.1282	0.0775	-
S113	1.4066	1.3687	0.0379	-
S114	1.2233	1.1618	0.0615	-
S115	1.3442	1.2963	0.0479	-
S116	1.2586	1.2068	0.0518	-
S117	1.3189	1.2637	0.0551	-
S118	1.2765	1.2299	0.0466	-
S119	1.6391	1.5516	0.0875	-
S120	1.2355	1.1503	0.0851	-
S121	1.2446	1.1927	0.0519	-
S122	1.3133	1.2589	0.0543	-
S123	1.0758	0.8777	0.1980	-
S124	1.5819	1.4972	0.0847	-
S125	1.2003	1.1126	0.0877	-
S126	1.3701	1.3217	0.0484	-
S127	1.2458	1.1833	0.0625	-
S128	1.3504	1.2880	0.0624	-
S129	1.1486	0.9848	0.1638	-
S130	1.4633	1.3997	0.0636	-
S131	1.6323	1.5418	0.0905	-
S132	1.2682	1.2036	0.0647	-
S133	1.0942	0.9218	0.1723	-
S134	1.5540	1.4639	0.0902	-
S135	1.2638	1.1760	0.0878	-
S136	1.3933	1.3561	0.0372	-
S137	1.0726	0.7931	0.2796	-
S138	1.6187	1.5278	0.0910	-

	ωB2PLYP'/def2-SV(P) (adiabatic)			
Molecule	**ΔE(S_0-S_1) [eV]**	**ΔE(S_0-T_1) [eV]**	**ΔE(S_1-T_1) [eV]**	**f_{12}(S_0-S_1)**
S139	1.2200	1.1093	0.1108	-
S140	1.4224	1.3714	0.0510	-
S141	3.1161	3.3085	-0.1924	-
S142	3.4487	3.4654	-0.0166	-
S143	3.3643	3.4572	-0.0929	-
S144	3.2619	3.4214	-0.1595	-
S145	3.1969	3.3785	-0.1816	-
S146	3.1307	3.3292	-0.1985	-
S147	3.1031	3.3021	-0.1990	-
S148	3.4785	3.4751	0.0034	-
S149	3.0564	3.2732	-0.2169	-
S150	2.9026	2.7073	0.1953	-
S151	2.9889	3.1610	-0.1721	-
S152	3.0478	3.2491	-0.2013	-
S153	2.9404	3.0041	-0.0638	-
S154	3.4896	3.4798	0.0098	-
S155	2.9331	2.7733	0.1598	-
S156	3.0556	3.2648	-0.2092	-
S157	3.0263	1.7618	1.2645	-
S158	3.0004	3.1476	-0.1472	-
S159	1.9259	1.8916	0.0343	-
S160	1.9347	1.8489	0.0857	-
S161	1.8590	1.7646	0.0944	-
S162	1.8536	1.7656	0.0881	-
S163	2.2141	2.2141	0.0000	-
S164	2.2120	1.9781	0.2339	-
S165	1.6824	1.4023	0.2801	-
S166	1.6538	1.4833	0.1705	-
S167	2.1354	2.1439	-0.0085	-
S168	2.1517	1.9424	0.2093	-
S169	1.7160	1.5241	0.1919	-
S170	1.6811	1.5238	0.1573	-
S171	2.0263	2.0253	0.0010	-
S172	2.0501	1.9172	0.1329	-
S173	1.7386	1.6034	0.1352	-
S174	1.7396	1.6373	0.1022	-
S175	1.9708	1.8241	0.1468	-
S176	1.9848	1.8809	0.1040	-
S177	1.8821	1.8087	0.0734	-
S178	1.9106	1.8487	0.0620	-
S179	1.9048	1.8554	0.0495	-
S180	1.9247	1.8410	0.0837	-
S181	1.7982	1.7120	0.0862	-
S182	1.8074	1.7383	0.0691	-
S183	1.8785	1.8115	0.0671	-
S184	1.9004	1.8203	0.0801	-

	ωB2PLYP'/def2-SV(P) (adiabatic)			
Molecule	**ΔE(S_0-S_1) [eV]**	**ΔE(S_0-T_1) [eV]**	**ΔE(S_1-T_1) [eV]**	**f_{12}(S_0-S_1)**
S185	1.8155	1.7412	0.0743	-
S186	1.8270	1.7646	0.0625	-
S187	2.2428	2.2282	0.0146	-
S188	2.2303	1.9752	0.2551	-
S189	1.7678	1.5879	0.1798	-
S190	1.6653	1.4970	0.1683	-
S191	1.8040	1.7174	0.0866	-
S192	1.8633	1.7874	0.0759	-
S193	1.8362	1.7343	0.1020	-
S194	1.8383	1.7735	0.0647	-
S195	1.6245	1.3354	0.2891	-
S196	1.7148	1.5307	0.1841	-
S197	1.9855	1.9307	0.0548	-
S198	2.0014	1.9572	0.0442	-
S199	1.7666	1.6259	0.1407	-
S200	1.7862	1.6920	0.0942	-
S201	1.8826	1.8162	0.0665	-
S202	1.8996	1.8485	0.0511	-
S203	1.7993	1.7042	0.0952	-
S204	1.8392	1.7651	0.0741	-
S205	1.8668	1.7801	0.0867	-
S206	1.8895	1.8218	0.0677	-
S207	1.7003	1.4602	0.2400	-
S208	1.7511	1.5811	0.1700	-
S209	1.9562	1.8955	0.0607	-
S210	1.9930	1.9444	0.0486	-
S211	2.2245	2.2108	0.0137	-
S212	2.2282	1.9877	0.2406	-
S213	1.7850	1.6123	0.1727	-
S214	1.7761	1.6781	0.0980	-
S215	1.6558	1.3948	0.2610	-
S216	1.7092	1.5292	0.1800	-
S217	2.0097	1.9233	0.0864	-
S218	2.0639	1.9927	0.0712	-
S219	1.8139	1.6797	0.1341	-
S220	1.8713	1.7617	0.1096	-
S221	1.9263	1.8897	0.0367	-
S222	1.9323	1.8772	0.0550	-
S223	1.6295	1.2592	0.3703	-
S224	1.7385	1.5011	0.2374	-
S225	2.0435	1.9901	0.0535	-
S226	2.0902	2.0341	0.0562	-
S227	1.7780	1.6049	0.1731	-
S228	1.8303	1.7108	0.1195	-
S229	1.9448	1.8940	0.0508	-
S230	1.9836	1.9133	0.0703	-

	ωB2PLYP'/def2-SV(P) (adiabatic)			
Molecule	**ΔE(S_0-S_1) [eV]**	**ΔE(S_0-T_1) [eV]**	**ΔE(S_1-T_1) [eV]**	**f_{12}(S_0-S_1)**
S231	2.2346	2.1603	0.0743	-
S232	2.2447	2.1518	0.0929	-
S233	2.2416	2.1089	0.1327	-
S234	2.1450	2.0127	0.1324	-
S235	2.1590	2.0352	0.1238	-
S236	2.1741	2.0522	0.1218	-
S237	2.5109	2.4157	0.0952	-
S238	2.4860	2.2317	0.2544	-
S239	2.5767	2.2314	0.3453	-
S240	1.9204	1.5709	0.3494	-
S241	1.9119	1.5309	0.3810	-
S242	1.9703	1.6648	0.3054	-
S243	2.4331	2.3503	0.0828	-
S244	2.3966	2.2026	0.1940	-
S245	2.5094	2.2103	0.2991	-
S246	1.9546	1.6804	0.2743	-
S247	2.0000	1.7560	0.2441	-
S248	2.0265	1.7609	0.2656	-
S249	2.3267	2.2767	0.0500	-
S250	2.3123	2.2027	0.1096	-
S251	2.4066	2.1931	0.2135	-
S252	2.0334	1.8611	0.1723	-
S253	2.0776	1.8967	0.1808	-
S254	2.0439	1.9046	0.1392	-
S255	2.2844	2.1546	0.1298	-
S256	2.2598	2.1623	0.0975	-
S257	2.3204	2.1562	0.1641	-
S258	2.1400	1.9830	0.1570	-
S259	2.0261	1.8609	0.1652	-
S260	2.2025	2.1068	0.0957	-
S261	2.2181	2.1474	0.0708	-
S262	2.2070	2.1197	0.0873	-
S263	2.0980	1.9863	0.1117	-
S264	2.0928	1.9858	0.1070	-
S265	2.1183	1.9998	0.1186	-
S266	2.2603	2.1334	0.1269	-
S267	2.1938	2.1096	0.0842	-
S268	2.1851	2.0906	0.0945	-
S269	2.2333	2.1194	0.1139	-
S270	2.1152	2.0198	0.0954	-
S271	2.1105	2.0164	0.0940	-
S272	2.1310	2.0282	0.1028	-
S273	2.5303	2.4143	0.1160	-
S274	2.4732	2.2135	0.2597	-
S275	2.5975	2.2304	0.3671	-
S276	1.9161	1.5639	0.3522	-

	ωB2PLYP'/def2-SV(P) (adiabatic)			
Molecule	**ΔE(S_0-S_1) [eV]**	**ΔE(S_0-T_1) [eV]**	**ΔE(S_1-T_1) [eV]**	**f_{12}(S_0-S_1)**
S277	1.9139	1.5480	0.3659	-
S278	2.0655	1.7386	0.3270	-
S279	2.1354	2.0429	0.0925	-
S280	2.1876	2.0137	0.1739	-
S281	2.1493	2.0929	0.0564	-
S282	2.1242	2.0262	0.0979	-
S283	2.0838	1.8610	0.2228	-
S284	2.1312	1.9934	0.1378	-
S285	1.9690	1.6590	0.3100	-
S286	2.0660	1.7348	0.3311	-
S287	1.9821	1.9126	0.0695	-
S288	2.2737	2.2578	0.0159	-
S289	2.2465	2.2370	0.0095	-
S290	2.2702	2.1577	0.1125	-
S291	2.0976	1.9437	0.1539	-
S292	2.1096	1.8953	0.2143	-
S293	2.0847	2.0366	0.0481	-
S294	2.1743	2.1153	0.0590	-
S295	2.1511	2.0148	0.1363	-
S296	2.1751	2.1077	0.0674	-
S297	2.1270	2.0211	0.1059	-
S298	2.1452	1.9954	0.1498	-
S299	2.1586	2.0918	0.0668	-
S300	2.1617	2.0715	0.0902	-
S301	2.1490	2.0201	0.1289	-
S302	2.1775	2.0749	0.1026	-
S303	2.0377	1.7778	0.2599	-
S304	2.0841	1.7733	0.3108	-
S305	2.0396	1.9558	0.0838	-
S306	2.2496	2.2094	0.0403	-
S307	2.2315	2.1216	0.1099	-
S308	2.2545	2.2098	0.0447	-
S309	2.5161	2.4098	0.1064	-
S310	2.4956	2.2436	0.2520	-
S311	2.6064	2.2480	0.3584	-
S312	2.0414	1.7759	0.2654	-
S313	1.9445	1.6351	0.3093	-
S314	2.0874	1.8784	0.2090	-
S315	1.9987	1.7228	0.2759	-
S316	2.0392	1.6993	0.3399	-
S317	2.0163	1.9671	0.0492	-
S318	2.2906	2.2329	0.0578	-
S319	2.3143	2.2501	0.0641	-
S320	2.2040	2.1004	0.1037	-
S321	2.1318	1.9822	0.1496	-
S322	2.1887	2.0169	0.1718	-

Molecule	ωB2PLYP'/def2-SV(P) (adiabatic) $\Delta E(S_0\text{-}S_1)$ [eV]	$\Delta E(S_0\text{-}T_1)$ [eV]	$\Delta E(S_1\text{-}T_1)$ [eV]	$f_{12}(S_0\text{-}S_1)$
S323	2.1972	2.1050	0.0923	-
S324	2.2160	2.1559	0.0601	-
S325	2.2278	2.1675	0.0603	-
S326	2.2351	2.1658	0.0693	-
S327	1.9805	1.5869	0.3936	-
S328	2.0637	1.6816	0.3821	-
S329	2.1133	1.9887	0.1246	-
S330	2.3368	2.2939	0.0429	-
S331	2.3409	2.2847	0.0562	-
S332	2.2600	2.1867	0.0733	-
S333	2.1045	1.9129	0.1917	-
S334	2.1606	1.9566	0.2040	-
S335	2.1316	2.0469	0.0847	-
S336	2.2458	2.1871	0.0586	-
S337	2.2456	2.1705	0.0750	-
S338	2.2768	2.1949	0.0819	-
S339	2.4917	2.5001	-0.0084	-
S340	2.5170	2.4426	0.0745	-
S341	2.3938	2.3091	0.0846	-
S342	2.7556	2.8114	-0.0558	-
S343	2.8443	2.5189	0.3255	-
S344	2.0634	1.6714	0.3919	-
S345	2.6729	2.7457	-0.0727	-
S346	2.7608	2.5062	0.2546	-
S347	2.1818	1.9220	0.2598	-
S348	2.5802	2.6466	-0.0664	-
S349	2.6620	2.5094	0.1527	-
S350	2.2855	2.1529	0.1326	-
S351	2.5469	2.4695	0.0775	-
S352	2.5762	2.4670	0.1091	-
S353	2.2501	2.0999	0.1501	-
S354	2.4855	2.4801	0.0054	-
S355	2.3359	2.2662	0.0697	-
S356	2.5168	2.4479	0.0690	-
S357	2.4629	2.4326	0.0303	-
S358	2.4887	2.4297	0.0590	-
S359	2.3560	2.3044	0.0516	-
S360	2.7706	2.8134	-0.0428	-
S361	2.8708	2.5416	0.3291	-
S362	1.9846	1.6005	0.3840	-
S363	2.4194	2.3431	0.0764	-
S364	2.3976	2.3985	-0.0009	-
S365	2.3554	2.2409	0.1144	-
S366	2.2791	1.9544	0.3248	-
S367	2.2434	2.1064	0.1370	-
S368	2.5067	2.4654	0.0413	-

Molecule	ωB2PLYP'/def2-SV(P) (adiabatic) $\Delta E(S_0\text{-}S_1)$ [eV]	$\Delta E(S_0\text{-}T_1)$ [eV]	$\Delta E(S_1\text{-}T_1)$ [eV]	$f_{12}(S_0\text{-}S_1)$
S369	2.3860	2.2516	0.1344	-
S370	2.3512	2.3011	0.0501	-
S371	2.3932	2.3048	0.0883	-
S372	2.4144	2.3378	0.0766	-
S373	2.4169	2.3761	0.0408	-
S374	2.3993	2.3154	0.0839	-
S375	2.3391	2.0796	0.2595	-
S376	2.3023	2.1691	0.1332	-
S377	2.4911	2.4471	0.0439	-
S378	2.7583	2.8004	-0.0420	-
S379	2.8757	2.5311	0.3446	-
S380	2.0895	1.7613	0.3282	-
S381	2.3023	2.0138	0.2884	-
S382	2.2836	2.1697	0.1138	-
S383	2.5127	2.5159	-0.0032	-
S384	2.4163	2.2992	0.1171	-
S385	2.4663	2.3861	0.0802	-
S386	2.4706	2.4720	-0.0014	-
S387	2.2941	1.8880	0.4061	-
S388	2.3722	2.1955	0.1767	-
S389	2.5245	2.5216	0.0029	-
S390	2.3874	2.2137	0.1738	-
S391	2.4027	2.3108	0.0918	-
S392	2.5072	2.5019	0.0053	-
S393	2.5054	2.4611	0.0443	-
S394	2.4963	2.4126	0.0837	-
S395	2.4052	2.3105	0.0947	-
S396	2.8099	2.6112	0.1988	-
S397	2.8093	2.5181	0.2912	-
S398	2.1404	1.7586	0.3818	-
S399	2.7117	2.5695	0.1422	-
S400	2.7383	2.5064	0.2319	-
S401	2.2076	1.9317	0.2759	-
S402	2.6081	2.5497	0.0584	-
S403	2.6472	2.4798	0.1675	-
S404	2.2886	2.1383	0.1503	-
S405	2.5506	2.4997	0.0509	-
S406	2.5728	2.4542	0.1187	-
S407	2.4380	2.3312	0.1067	-
S408	2.4858	2.4476	0.0382	-
S409	2.3462	2.2675	0.0787	-
S410	2.5147	2.4284	0.0863	-
S411	2.4600	2.4144	0.0456	-
S412	2.4896	2.4161	0.0735	-
S413	2.3619	2.3037	0.0582	-
S414	2.8103	2.5984	0.2119	-

	ωB2PLYP'/def2-SV(P) (adiabatic)			
Molecule	**ΔE(S_0-S_1) [eV]**	**ΔE(S_0-T_1) [eV]**	**ΔE(S_1-T_1) [eV]**	**f_{12}(S_0-S_1)**
S415	2.8361	2.5259	0.3102	-
S416	2.2544	1.9630	0.2914	-
S417	2.4372	2.3321	0.1050	-
S418	2.4276	2.3980	0.0297	-
S419	2.3608	2.2120	0.1487	-
S420	2.2799	2.0178	0.2621	-
S421	2.2779	2.2766	0.0013	-
S422	2.5167	2.5631	-0.0464	-
S423	2.3578	2.2073	0.1505	-
S424	2.3643	2.3579	0.0065	-
S425	2.4174	2.3931	0.0243	-
S426	2.3998	2.3169	0.0829	-
S427	2.4313	2.4008	0.0304	-
S428	2.4136	2.3561	0.0575	-
S429	2.3118	2.0600	0.2518	-
S430	2.3212	2.3039	0.0173	-
S431	2.5067	2.5228	-0.0161	-
S432	2.8193	2.6170	0.2024	-
S433	2.8444	2.5343	0.3101	-
S434	2.2601	1.9608	0.2993	-
S435	2.2776	1.9891	0.2885	-
S436	2.3096	2.3118	-0.0022	-
S437	2.5544	2.5466	0.0079	-
S438	2.4294	2.3108	0.1186	-
S439	2.4587	2.4067	0.0520	-
S440	2.4716	2.4685	0.0031	-
S441	2.2989	1.9620	0.3369	-
S442	2.4071	2.3552	0.0520	-
S443	2.5923	2.6204	-0.0281	-
S444	2.3910	2.2365	0.1545	-
S445	2.3985	2.3631	0.0355	-
S446	2.5221	2.5080	0.0141	-