

SA-SF-PBE50/def2-SVP				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S1	1.0948	1.2039	-0.1091	-
S2	0.9089	0.9895	-0.0806	-
S3	1.4314	1.5233	-0.0919	-
S4	1.6770	1.7772	-0.1002	-
S5	1.4530	1.4459	0.0071	-
S6	1.4406	1.5241	-0.0835	-
S7	1.7811	1.8615	-0.0804	-
S8	1.2523	1.3175	-0.0652	-
S9	1.4576	1.5701	-0.1125	-
S10	1.7860	1.7818	0.0042	-
S11	1.6347	1.7424	-0.1077	-
S12	1.9397	2.0652	-0.1255	-
S13	1.9570	2.0477	-0.0907	-
S14	2.1969	2.3082	-0.1113	-
S15	1.5390	1.5849	-0.0459	-
S16	1.8906	1.9543	-0.0637	-
S17	1.7322	1.8184	-0.0862	-
S18	1.9963	2.1120	-0.1157	-
S19	1.2896	1.3170	-0.0274	-
S20	1.4060	1.4334	-0.0274	-
S21	0.7604	0.8083	-0.0479	-
S22	1.1955	1.1814	0.0141	-
S23	1.4475	1.3477	0.0998	-
S24	1.3956	1.3577	0.0379	-
S25	1.6120	1.6350	-0.0230	-
S26	1.4869	1.5312	-0.0443	-
S27	1.7413	1.7251	0.0162	-
S28	1.4071	1.3490	0.0581	-
S29	1.7191	1.6741	0.0450	-
S30	1.2800	1.3369	-0.0569	-
S31	1.5171	1.5718	-0.0547	-
S32	1.8355	1.8009	0.0346	-
S33	1.8042	1.8152	-0.0110	-
S34	1.3560	1.3988	-0.0428	-
S35	1.9539	1.8593	0.0946	-
S36	1.9163	1.8827	0.0336	-
S37	1.6603	1.7299	-0.0696	-
S38	1.9658	1.9436	0.0222	-
S39	2.0265	2.0041	0.0224	-
S40	1.3374	1.3982	-0.0608	-
S41	1.5840	1.6786	-0.0946	-
S42	1.8268	1.8378	-0.0110	-
S43	1.8397	1.9276	-0.0879	-
S44	1.6647	1.7809	-0.1162	-
S45	1.4287	1.4992	-0.0705	-
S46	2.1634	2.2166	-0.0532	-

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Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S47	1.9877	2.1025	-0.1148	-
S48	1.7446	1.8233	-0.0787	-
S49	1.7652	1.8413	-0.0761	-
S50	1.7794	1.8520	-0.0726	-
S51	2.3159	2.4227	-0.1068	-
S52	2.2104	2.3392	-0.1288	-
S53	2.5176	2.6901	-0.1725	-
S54	2.2642	2.3089	-0.0447	-
S55	1.9879	2.0723	-0.0844	-
S56	2.2680	2.4244	-0.1564	-
S57	1.7900	1.6779	0.1121	-
S58	1.1671	1.1940	-0.0269	-
S59	1.5293	1.4935	0.0358	-
S60	2.1355	2.1322	0.0033	-
S61	2.1277	2.1560	-0.0283	-
S62	2.3066	2.2083	0.0983	-
S63	1.7194	1.7189	0.0005	-
S64	2.0658	2.0532	0.0126	-
S65	1.8871	1.9872	-0.1001	-
S66	1.6468	1.6833	-0.0365	-
S67	1.7602	1.8124	-0.0522	-
S68	2.0518	2.1432	-0.0914	-
S69	2.1995	2.2862	-0.0867	-
S70	2.2080	2.2089	-0.0009	-
S71	1.7600	1.8532	-0.0932	-
S72	2.0304	2.1494	-0.1190	-
S73	2.2639	2.3952	-0.1313	-
S74	1.9611	2.0786	-0.1175	-
S75	1.3501	1.3443	0.0058	-
S76	1.8323	1.7216	0.1107	-
S77	2.0158	1.9825	0.0333	-
S78	1.7528	1.7595	-0.0067	-
S79	1.7965	1.8311	-0.0346	-
S80	2.3070	2.2656	0.0414	-
S81	2.3446	2.3564	-0.0118	-
S82	1.8622	1.9379	-0.0757	-
S83	2.2323	2.3344	-0.1021	-
S84	2.9088	3.0900	-0.1812	-
S85	3.0212	2.1311	0.8901	-
S86	1.7804	1.6869	0.0935	-
S87	2.1521	2.1492	0.0029	-
S88	2.2650	2.3924	-0.1274	-
S89	0.6168	0.6382	-0.0214	-
S90	1.4481	1.2991	0.1490	-
S91	1.1285	1.1383	-0.0098	-
S92	1.9511	1.7967	0.1544	-

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S93	1.1255	1.1607	-0.0352	-
S94	1.7528	1.6960	0.0568	-
S95	1.7268	1.6771	0.0497	-
S96	1.5725	1.6548	-0.0823	-
S97	1.0566	1.1011	-0.0445	-
S98	2.5413	2.3485	0.1928	-
S99	1.6797	1.6046	0.0751	-
S100	1.5612	1.6336	-0.0724	-
S101	2.3209	2.2488	0.0721	-
S102	1.5620	1.6015	-0.0395	-
S103	2.1561	2.1867	-0.0306	-
S104	2.0500	2.1920	-0.1420	-
S105	1.1534	1.2700	-0.1166	-
S106	1.1281	1.2225	-0.0944	-
S107	1.3773	1.5030	-0.1257	-
S108	1.0928	1.1348	-0.0420	-
S109	1.3256	1.4528	-0.1272	-
S110	1.0734	1.1060	-0.0326	-
S111	1.2377	1.3632	-0.1255	-
S112	1.0351	1.1195	-0.0844	-
S113	1.1940	1.3179	-0.1239	-
S114	1.5789	1.3141	0.2648	-
S115	1.1379	1.2536	-0.1157	-
S116	1.0599	1.1677	-0.1078	-
S117	1.1155	1.2277	-0.1122	-
S118	1.0760	1.1855	-0.1095	-
S119	1.4063	1.5251	-0.1188	-
S120	1.0519	1.1422	-0.0903	-
S121	0.9002	0.7298	0.1704	-
S122	1.1153	1.2264	-0.1111	-
S123	0.6195	0.4299	0.1896	-
S124	1.4108	1.4981	-0.0873	-
S125	0.9588	1.0682	-0.1094	-
S126	1.0804	0.9556	0.1248	-
S127	1.0216	1.1314	-0.1098	-
S128	1.1378	1.2462	-0.1084	-
S129	0.8940	0.9839	-0.0899	-
S130	1.2644	1.3650	-0.1006	-
S131	1.3973	1.5188	-0.1215	-
S132	1.0590	1.1650	-0.1060	-
S133	0.6483	0.4821	0.1662	-
S134	1.3834	1.4679	-0.0845	-
S135	1.0583	1.1548	-0.0965	-
S136	1.1815	1.2950	-0.1135	-
S137	0.7797	0.8428	-0.0631	-
S138	1.4730	1.5392	-0.0662	-

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S139	0.9917	1.0874	-0.0957	-
S140	1.2321	1.3396	-0.1075	-
S141	2.9773	3.1706	-0.1933	-
S142	3.2979	3.3866	-0.0887	-
S143	3.1901	3.3448	-0.1547	-
S144	3.0828	3.2801	-0.1973	-
S145	3.0425	3.2480	-0.2055	-
S146	2.9950	3.1871	-0.1921	-
S147	2.9775	3.1643	-0.1868	-
S148	3.3336	3.4017	-0.0681	-
S149	2.9114	3.1080	-0.1966	-
S150	2.6934	2.8762	-0.1828	-
S151	2.8126	3.0105	-0.1979	-
S152	2.9044	3.0912	-0.1868	-
S153	2.7312	2.9185	-0.1873	-
S154	3.3491	3.4105	-0.0614	-
S155	2.7307	2.9211	-0.1904	-
S156	3.6313	3.2509	0.3804	-
S157	2.9028	3.0832	-0.1804	-
S158	2.8356	3.0219	-0.1863	-
S159	1.7115	1.8305	-0.1190	-
S160	1.6997	1.8038	-0.1041	-
S161	1.6314	1.7285	-0.0971	-
S162	1.6310	1.7264	-0.0954	-
S163	2.0341	2.1702	-0.1361	-
S164	1.9599	1.9821	-0.0222	-
S165	1.5018	1.5421	-0.0403	-
S166	1.5255	1.5866	-0.0611	-
S167	1.9451	2.0807	-0.1356	-
S168	1.9014	1.9473	-0.0459	-
S169	1.5225	1.5923	-0.0698	-
S170	1.5146	1.5647	-0.0501	-
S171	1.8174	1.9509	-0.1335	-
S172	1.7970	1.8858	-0.0888	-
S173	1.5165	1.5977	-0.0812	-
S174	1.5460	1.6330	-0.0870	-
S175	1.7588	1.8896	-0.1308	-
S176	1.7449	1.8466	-0.1017	-
S177	1.6628	1.7779	-0.1151	-
S178	1.6863	1.7954	-0.1091	-
S179	1.6787	1.7996	-0.1209	-
S180	1.6973	1.8027	-0.1054	-
S181	1.5676	1.6714	-0.1038	-
S182	1.5952	1.6991	-0.1039	-
S183	1.6491	1.7641	-0.1150	-
S184	1.6801	1.7844	-0.1043	-

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S185	1.5845	1.6915	-0.1070	-
S186	1.6109	1.7171	-0.1062	-
S187	2.0704	2.2043	-0.1339	-
S188	2.0147	2.0046	0.0101	-
S189	1.5452	1.6265	-0.0813	-
S190	1.5502	1.5934	-0.0432	-
S191	1.5478	1.6421	-0.0943	-
S192	1.6235	1.7327	-0.1092	-
S193	1.5926	1.7032	-0.1106	-
S194	1.6106	1.7205	-0.1099	-
S195	1.3353	1.3397	-0.0044	-
S196	1.4870	1.5586	-0.0716	-
S197	1.7782	1.8891	-0.1109	-
S198	1.7935	1.9132	-0.1197	-
S199	1.4917	1.5704	-0.0787	-
S200	1.5483	1.6521	-0.1038	-
S201	1.6361	1.7547	-0.1186	-
S202	1.6662	1.7796	-0.1134	-
S203	1.5430	1.6392	-0.0962	-
S204	1.6121	1.7158	-0.1037	-
S205	1.6131	1.7275	-0.1144	-
S206	1.6560	1.7674	-0.1114	-
S207	1.4070	1.4499	-0.0429	-
S208	1.5140	1.5972	-0.0832	-
S209	1.7117	1.8355	-0.1238	-
S210	1.7638	1.8798	-0.1160	-
S211	2.0522	2.1839	-0.1317	-
S212	1.9955	2.0005	-0.0050	-
S213	1.5647	1.6482	-0.0835	-
S214	1.5857	1.6724	-0.0867	-
S215	1.3687	1.3884	-0.0197	-
S216	1.4692	1.5516	-0.0824	-
S217	1.7908	1.8935	-0.1027	-
S218	1.8574	1.9624	-0.1050	-
S219	1.5717	1.6624	-0.0907	-
S220	1.6456	1.7350	-0.0894	-
S221	1.6967	1.8162	-0.1195	-
S222	1.6938	1.8097	-0.1159	-
S223	1.3153	1.3007	0.0146	-
S224	1.4880	1.5587	-0.0707	-
S225	1.8716	1.9365	-0.0649	-
S226	1.9036	2.0133	-0.1097	-
S227	1.5027	1.5787	-0.0760	-
S228	1.5989	1.6882	-0.0893	-
S229	1.7226	1.8456	-0.1230	-
S230	1.7616	1.8727	-0.1111	-

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S231	2.0296	2.1355	-0.1059	-
S232	2.0235	2.1104	-0.0869	-
S233	2.0177	2.0938	-0.0761	-
S234	1.9150	1.9936	-0.0786	-
S235	1.9634	2.0337	-0.0703	-
S236	1.9715	2.0390	-0.0675	-
S237	2.3085	2.4660	-0.1575	-
S238	2.2597	2.2501	0.0096	-
S239	2.3496	2.2500	0.0996	-
S240	1.7362	1.7443	-0.0081	-
S241	1.7912	1.7518	0.0394	-
S242	1.8759	1.8811	-0.0052	-
S243	2.2354	2.3824	-0.1470	-
S244	2.1632	2.2088	-0.0456	-
S245	2.2694	2.2247	0.0447	-
S246	1.7285	1.7273	0.0012	-
S247	1.8644	1.8614	0.0030	-
S248	1.8878	1.8798	0.0080	-
S249	2.1219	2.2545	-0.1326	-
S250	2.0701	2.1665	-0.0964	-
S251	2.1629	2.1799	-0.0170	-
S252	1.8089	1.8622	-0.0533	-
S253	1.9097	1.9514	-0.0417	-
S254	1.8597	1.9218	-0.0621	-
S255	2.0826	2.2031	-0.1205	-
S256	2.0320	2.1188	-0.0868	-
S257	2.0916	2.1473	-0.0557	-
S258	1.8057	1.8587	-0.0530	-
S259	1.8590	1.8923	-0.0333	-
S260	1.9970	2.0948	-0.0978	-
S261	2.0017	2.1086	-0.1069	-
S262	1.9875	2.0845	-0.0970	-
S263	1.8753	1.9552	-0.0799	-
S264	1.8891	1.9680	-0.0789	-
S265	1.9281	2.0033	-0.0752	-
S266	2.0454	2.1169	-0.0715	-
S267	1.9745	2.0735	-0.0990	-
S268	1.9713	2.0646	-0.0933	-
S269	2.0262	2.1036	-0.0774	-
S270	1.8949	1.9786	-0.0837	-
S271	1.9044	1.9861	-0.0817	-
S272	1.9377	2.0187	-0.0810	-
S273	2.3465	2.5010	-0.1545	-
S274	2.2761	2.2461	0.0300	-
S275	2.3875	2.2647	0.1228	-
S276	1.7334	1.7257	0.0077	-

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S277	1.8162	1.7396	0.0766	-
S278	1.9101	1.9551	-0.0450	-
S279	1.9027	1.9778	-0.0751	-
S280	1.9735	2.0289	-0.0554	-
S281	1.9127	2.0348	-0.1221	-
S282	1.8961	1.9863	-0.0902	-
S283	1.8537	1.9099	-0.0562	-
S284	1.9216	2.0083	-0.0867	-
S285	1.6832	1.6472	0.0360	-
S286	1.8635	1.8668	-0.0033	-
S287	1.8051	1.8980	-0.0929	-
S288	2.0943	2.2224	-0.1281	-
S289	2.0387	2.1764	-0.1377	-
S290	2.0499	2.1190	-0.0691	-
S291	1.8350	1.8870	-0.0520	-
S292	1.8875	1.9428	-0.0553	-
S293	1.8780	1.9892	-0.1112	-
S294	1.9491	2.0495	-0.1004	-
S295	1.9132	1.9891	-0.0759	-
S296	1.9581	2.0586	-0.1005	-
S297	1.8806	1.9539	-0.0733	-
S298	1.9336	2.0050	-0.0714	-
S299	1.9517	2.0515	-0.0998	-
S300	1.9237	2.0199	-0.0962	-
S301	1.9067	1.9860	-0.0793	-
S302	1.9610	2.0565	-0.0955	-
S303	1.7525	1.7601	-0.0076	-
S304	1.8625	1.8924	-0.0299	-
S305	1.8604	1.9478	-0.0874	-
S306	2.0356	2.1492	-0.1136	-
S307	1.9830	2.0629	-0.0799	-
S308	2.0356	2.1573	-0.1217	-
S309	2.3203	2.4749	-0.1546	-
S310	2.2800	2.2549	0.0251	-
S311	2.3849	2.2683	0.1166	-
S312	1.8444	1.9014	-0.0570	-
S313	1.8470	1.8545	-0.0075	-
S314	1.9299	1.9732	-0.0433	-
S315	1.7214	1.7054	0.0160	-
S316	1.8188	1.8385	-0.0197	-
S317	1.8340	1.9336	-0.0996	-
S318	2.0800	2.2038	-0.1238	-
S319	2.1118	2.2325	-0.1207	-
S320	2.0140	2.0876	-0.0736	-
S321	1.8882	1.9535	-0.0653	-
S322	1.9744	2.0358	-0.0614	-

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S323	1.9958	2.0819	-0.0861	-
S324	2.0009	2.1062	-0.1053	-
S325	2.0009	2.1091	-0.1082	-
S326	2.0244	2.1180	-0.0936	-
S327	1.6789	1.6227	0.0562	-
S328	1.8289	1.8440	-0.0151	-
S329	1.9471	2.0354	-0.0883	-
S330	2.1324	2.2591	-0.1267	-
S331	2.1226	2.2716	-0.1490	-
S332	2.0483	2.1196	-0.0713	-
S333	1.8391	1.8892	-0.0501	-
S334	1.9470	2.0021	-0.0551	-
S335	1.9309	2.0214	-0.0905	-
S336	2.0430	2.1499	-0.1069	-
S337	2.0181	2.1213	-0.1032	-
S338	2.0557	2.1714	-0.1157	-
S339	2.2970	2.4407	-0.1437	-
S340	2.2828	2.3920	-0.1092	-
S341	2.1749	2.2788	-0.1039	-
S342	2.6715	2.8108	-0.1393	-
S343	2.6325	2.5282	0.1043	-
S344	1.9479	1.8967	0.0512	-
S345	2.5711	2.7097	-0.1386	-
S346	2.5328	2.5049	0.0279	-
S347	1.9935	1.9964	-0.0029	-
S348	2.4207	2.5733	-0.1526	-
S349	2.4169	2.4712	-0.0543	-
S350	2.0788	2.1605	-0.0817	-
S351	2.3586	2.5176	-0.1590	-
S352	2.3415	2.4291	-0.0876	-
S353	2.0568	2.1053	-0.0485	-
S354	2.2639	2.4125	-0.1486	-
S355	2.1218	2.2282	-0.1064	-
S356	2.2923	2.4052	-0.1129	-
S357	2.2347	2.3741	-0.1394	-
S358	2.2723	2.3904	-0.1181	-
S359	2.1401	2.2508	-0.1107	-
S360	2.6921	2.8284	-0.1363	-
S361	2.6680	2.5432	0.1248	-
S362	1.9543	1.9378	0.0165	-
S363	2.1714	2.2643	-0.0929	-
S364	2.1792	2.3264	-0.1472	-
S365	2.1314	2.2371	-0.1057	-
S366	2.0019	1.9472	0.0547	-
S367	2.0843	2.1730	-0.0887	-
S368	2.2867	2.4255	-0.1388	-

SA-SF-PBE50/def2-SVP				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S369	2.1168	2.1825	-0.0657	-
S370	2.1480	2.2703	-0.1223	-
S371	2.1473	2.2687	-0.1214	-
S372	2.1551	2.2541	-0.0990	-
S373	2.2095	2.3351	-0.1256	-
S374	2.1442	2.2653	-0.1211	-
S375	2.0452	2.0479	-0.0027	-
S376	2.1265	2.2202	-0.0937	-
S377	2.2344	2.3770	-0.1426	-
S378	2.6808	2.8153	-0.1345	-
S379	2.6747	2.5400	0.1347	-
S380	2.0056	2.0047	0.0009	-
S381	2.0277	1.9978	0.0299	-
S382	2.1120	2.2077	-0.0957	-
S383	2.2998	2.4572	-0.1574	-
S384	2.1658	2.2670	-0.1012	-
S385	2.2485	2.3602	-0.1117	-
S386	2.2615	2.3953	-0.1338	-
S387	1.9944	1.9188	0.0756	-
S388	2.2042	2.3182	-0.1140	-
S389	2.2948	2.4461	-0.1513	-
S390	2.1064	2.1742	-0.0678	-
S391	2.1876	2.3025	-0.1149	-
S392	2.2786	2.4293	-0.1507	-
S393	2.2764	2.3902	-0.1138	-
S394	2.2649	2.3468	-0.0819	-
S395	2.1711	2.2542	-0.0831	-
S396	2.6100	2.6617	-0.0517	-
S397	2.5908	2.4720	0.1188	-
S398	2.0010	1.9949	0.0061	-
S399	2.4916	2.5898	-0.0982	-
S400	2.5020	2.4495	0.0525	-
S401	2.0081	1.9936	0.0145	-
S402	2.3685	2.5047	-0.1362	-
S403	2.3994	2.4159	-0.0165	-
S404	2.0740	2.1279	-0.0539	-
S405	2.3268	2.4396	-0.1128	-
S406	2.3383	2.3943	-0.0560	-
S407	2.2230	2.3393	-0.1163	-
S408	2.2590	2.3789	-0.1199	-
S409	2.1235	2.2114	-0.0879	-
S410	2.2847	2.3687	-0.0840	-
S411	2.2369	2.3501	-0.1132	-
S412	2.2642	2.3581	-0.0939	-
S413	2.1398	2.2334	-0.0936	-
S414	2.6474	2.6695	-0.0221	-

SA-SF-PBE50/def2-SVP				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S415	2.6203	2.4829	0.1374	-
S416	2.0826	2.1304	-0.0478	-
S417	2.1973	2.2749	-0.0776	-
S418	2.1810	2.3212	-0.1402	-
S419	2.1212	2.2191	-0.0979	-
S420	2.0262	2.0400	-0.0138	-
S421	2.0896	2.2124	-0.1228	-
S422	2.3169	2.4747	-0.1578	-
S423	2.1028	2.1733	-0.0705	-
S424	2.1305	2.2769	-0.1464	-
S425	2.1751	2.2901	-0.1150	-
S426	2.1620	2.2518	-0.0898	-
S427	2.1970	2.3261	-0.1291	-
S428	2.1671	2.2775	-0.1104	-
S429	2.0446	2.0830	-0.0384	-
S430	2.1209	2.2445	-0.1236	-
S431	2.2775	2.4181	-0.1406	-
S432	2.6383	2.6612	-0.0229	-
S433	2.6315	2.4894	0.1421	-
S434	2.0942	2.1378	-0.0436	-
S435	2.0152	2.0387	-0.0235	-
S436	2.1018	2.2363	-0.1345	-
S437	2.3431	2.4825	-0.1394	-
S438	2.1924	2.2697	-0.0773	-
S439	2.2290	2.3373	-0.1083	-
S440	2.2366	2.3624	-0.1258	-
S441	2.0241	2.0416	-0.0175	-
S442	2.2032	2.3239	-0.1207	-
S443	2.3650	2.5409	-0.1759	-
S444	2.1362	2.2044	-0.0682	-
S445	2.1649	2.2922	-0.1273	-
S446	2.2942	2.4295	-0.1353	-