

EOM-CCSD/cc-pVDZ				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S843	2.1534	2.1707	-0.0173	0.0011
S844	2.2950	2.2963	-0.0013	0.0029
S845	2.3653	2.3821	-0.0168	0.0007
S846	2.5099	2.4921	0.0178	0.0052
S847	2.0583	1.9577	0.1006	0.0015
S848	2.2029	2.1328	0.0701	0.0004
S849	2.1448	2.0595	0.0853	0.0043
S850	2.2983	2.2457	0.0526	0.0011
S851	2.2854	2.2041	0.0813	0.0025
S852	2.3311	2.2448	0.0863	0.0046
S853	2.5083	2.3986	0.1097	0.0015
S854	2.5741	2.4620	0.1121	0.0068
S855	2.1766	2.0680	0.1086	0.0041
S856	2.2273	2.1705	0.0568	0.0002
S857	2.3322	2.2105	0.1217	0.0076
S858	2.4180	2.3513	0.0667	0.0003
S859	2.1233	2.0508	0.0725	0.0044
S860	2.4605	2.4045	0.0560	0.0038
S861	2.4353	2.4062	0.0291	0.0016
S862	2.6146	2.5669	0.0477	0.0046
S863	2.2228	1.9788	0.2440	0.0003
S864	2.3923	2.1629	0.2294	0.0005
S865	2.1750	1.9927	0.1823	0.0031
S866	2.3527	2.1955	0.1572	0.0014
S867	2.5535	2.3955	0.1580	0.0053
S868	2.6197	2.4058	0.2139	0.0081
S869	2.7099	2.5596	0.1503	0.0037
S870	2.7989	2.5951	0.2038	0.0086
S871	2.4702	2.2014	0.2688	0.0022
S872	2.5332	2.2579	0.2753	0.0017
S873	2.4518	2.1967	0.2551	0.0068
S874	2.5566	2.3203	0.2363	0.0005
S875	2.2313	2.1114	0.1199	0.0060
S876	2.2840	2.2522	0.0318	0.0015
S877	2.1451	1.9652	0.1799	0.0108
S878	2.2891	2.1478	0.1413	0.0026
S879	2.3743	2.1546	0.2197	0.0156
S880	1.9697	1.9193	0.0504	0.0003
S881	2.0623	1.9475	0.1148	0.0051
S882	2.0912	2.0212	0.0700	0.0017
S883	2.1861	2.0970	0.0891	0.0037
S884	2.1791	1.9333	0.2458	0.0094
S885	2.4680	2.1820	0.2860	0.0006
S886	2.4503	2.1580	0.2923	0.0139
S887	2.1277	1.9658	0.1619	0.0014
S888	2.0842	1.8944	0.1898	0.0033

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S889	2.3333	2.1495	0.1838	0.0047
S890	2.3414	2.1290	0.2124	0.0021
S891	2.3284	2.2661	0.0623	0.0034
S892	2.5288	2.5036	0.0252	0.0021
S893	2.4587	2.3822	0.0765	0.0031
S894	2.3218	2.0456	0.2762	0.0141
S895	2.3380	2.2267	0.1113	0.0034
S896	2.4750	2.2050	0.2700	0.0155
S897	2.2740	2.0247	0.2493	0.0081
S898	2.0789	1.9725	0.1064	0.0009
S899	2.2255	2.1486	0.0769	0.0032
S900	2.4592	2.1043	0.3549	0.0146
S901	2.6404	2.3584	0.2820	0.0016
S902	2.6567	2.2818	0.3749	0.0164
S903	2.3922	2.1793	0.2129	0.0000
S904	2.3767	2.0525	0.3242	0.0079
S905	2.3937	2.2062	0.1875	0.0035
S906	2.4318	2.1957	0.2361	0.0014
S907	2.4589	2.3252	0.1337	0.0070
S908	2.6830	2.6170	0.0660	0.0034
S909	2.5273	2.4960	0.0313	0.0014
S910	2.7698	2.7768	-0.0070	0.0002
S911	2.2577	2.1039	0.1538	0.0067
S912	2.5175	2.3837	0.1338	0.0122
S913	2.2238	1.9452	0.2786	0.0022
S914	2.1728	2.0013	0.1715	0.0060
S915	2.4583	2.1876	0.2707	0.0059
S916	2.4653	2.2970	0.1683	0.0054
S917	2.6679	2.5222	0.1457	0.0096
S918	2.1608	1.9697	0.1911	0.0033
S919	2.3093	2.1836	0.1257	0.0073
S920	2.4261	2.1742	0.2519	0.0073
S921	2.1730	2.0166	0.1564	0.0103
S922	2.5239	2.2756	0.2483	0.0170
S923	2.4748	2.2408	0.2340	0.0033
S924	2.0946	1.9859	0.1087	0.0039
S925	2.4791	2.2477	0.2314	0.0093
S926	2.4250	2.2462	0.1788	0.0122
S927	2.7275	2.4636	0.2639	0.0175
S928	2.4494	2.2943	0.1551	0.0001
S929	2.2867	2.1885	0.0982	0.0013
S930	2.5390	2.3240	0.2150	0.0016
S931	2.5334	2.5598	-0.0264	0.0012
S932	2.5654	2.6210	-0.0556	0.0002
S933	2.7379	2.7788	-0.0409	0.0033
S934	2.4584	2.3329	0.1255	0.0011

EOM-CCSD/cc-pVDZ				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S935	2.3409	2.2345	0.1064	0.0062
S936	2.5217	2.4347	0.0870	0.0030
S937	2.5162	2.4849	0.0313	0.0029
S938	2.6585	2.6210	0.0375	0.0008
S939	2.7546	2.7278	0.0268	0.0049
S940	2.4201	2.3695	0.0506	0.0002
S941	2.4658	2.3526	0.1132	0.0077
S942	2.5784	2.5107	0.0677	0.0013
S943	2.0520	1.9085	0.1435	0.0025
S944	1.9884	1.8742	0.1142	0.0001
S945	2.2706	2.1004	0.1702	0.0029
S946	2.0820	1.8516	0.2304	0.0107
S947	2.3215	2.0572	0.2643	0.0136
S948	2.7019	2.6348	0.0671	0.0021
S949	2.8557	2.8541	0.0016	0.0032
S950	2.6569	2.3821	0.2748	0.0007
S951	2.4130	2.1947	0.2183	0.0047
S952	2.6104	2.4165	0.1939	0.0032
S953	2.7896	2.6267	0.1629	0.0061
S954	2.8718	2.7564	0.1154	0.0021
S955	2.9795	2.8558	0.1237	0.0069
S956	2.7224	2.4556	0.2668	0.0014
S957	2.6341	2.3670	0.2671	0.0069
S958	2.7559	2.5224	0.2335	0.0011
S959	2.1811	2.0915	0.0896	0.0013
S960	2.0368	1.8455	0.1913	0.0055
S961	2.4161	2.3371	0.0790	0.0002
S962	2.1651	2.0461	0.1190	0.0023
S963	2.0523	1.9977	0.0546	0.0000
S964	2.4203	2.2538	0.1665	0.0050
S965	2.3273	2.1670	0.1603	0.0123
S966	2.5027	2.3401	0.1626	0.0182
S967	2.2842	2.1464	0.1378	0.0071
S968	2.1387	2.0767	0.0620	0.0021
S969	2.3068	2.2149	0.0919	0.0069
S970	2.2151	2.0239	0.1912	0.0152
S971	2.4515	2.2470	0.2045	0.0206
S972	2.1283	1.9856	0.1427	0.0094
S973	2.2532	2.1308	0.1224	0.0017
S974	2.2971	2.1787	0.1184	0.0071
S975	2.1187	2.0332	0.0855	0.0037
S976	2.0765	2.0033	0.0732	0.0006
S977	2.3191	2.2143	0.1048	0.0050
S978	2.1317	2.0812	0.0505	0.0005
S979	2.2880	2.1064	0.1816	0.0095
S980	2.2729	2.0976	0.1753	0.0052

EOM-CCSD/cc-pVDZ				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S981	2.4761	2.3132	0.1629	0.0129
S982	2.5481	2.2907	0.2574	0.0180
S983	2.6671	2.4277	0.2394	0.0213
S984	2.5547	2.3101	0.2446	0.0126
S985	2.4651	2.3292	0.1359	0.0073
S986	2.4859	2.1897	0.2962	0.0251
S987	2.6833	2.3820	0.3013	0.0286
S988	2.4337	2.1725	0.2612	0.0198
S989	2.4270	2.3334	0.0936	0.0008
S990	2.4872	2.3358	0.1514	0.0088
S991	2.2741	2.2452	0.0289	-0.0000
S992	2.1529	2.0083	0.1446	0.0027
S993	2.5015	2.4379	0.0636	0.0006
S994	2.3156	2.2179	0.0977	0.0036
S995	2.3603	2.2909	0.0694	0.0016
S996	2.2760	2.2142	0.0618	0.0004
S997	2.5781	2.4916	0.0865	0.0050
S998	2.3931	2.3550	0.0381	0.0019
S999	2.4824	2.2519	0.2305	0.0089
S1000	2.0086	1.7503	0.2583	0.0114
S1001	2.3564	1.9778	0.3786	0.0185
S1002	2.3555	1.9874	0.3681	0.0197
S1003	2.6953	2.5312	0.1641	0.0051
S1004	2.6820	2.5001	0.1819	0.0124
S1005	2.0820	1.8936	0.1884	0.0140
S1006	2.5773	2.2812	0.2961	0.0173
S1007	2.3888	2.1094	0.2794	0.0248
S1008	2.3753	2.2935	0.0818	0.0029
S1009	2.5396	2.4576	0.0820	0.0058
S1010	2.2752	2.0756	0.1996	0.0034
S1011	2.2718	2.0906	0.1812	0.0020
S1012	2.4097	2.1650	0.2447	0.0036
S1013	2.6209	2.5404	0.0805	0.0033
S1014	2.7363	2.6611	0.0752	0.0039
S1015	2.2965	2.1898	0.1067	0.0053
S1016	2.5462	2.3990	0.1472	0.0014
S1017	2.4765	2.2953	0.1812	0.0067
S1018	2.4705	2.5236	-0.0531	0.0006
S1019	2.7083	2.7275	-0.0192	0.0020
S1020	2.3306	2.1487	0.1819	0.0059
S1021	2.5169	2.3661	0.1508	0.0062
S1022	2.5450	2.4634	0.0816	0.0006
S1023	2.8046	2.7088	0.0958	0.0023
S1024	2.4175	2.1670	0.2505	0.0027
S1025	2.6789	2.4407	0.2382	0.0050
S1026	2.4105	2.2982	0.1123	0.0051

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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]	$f_{12}(S_0-S_1)$
S1027	2.6546	2.4296	0.2250	0.0084
S1028	2.7260	2.7170	0.0090	0.0005
S1029	2.3957	2.1348	0.2609	0.0072
S1030	2.4336	2.2441	0.1895	0.0110
S1031	2.7386	2.4883	0.2503	0.0001
S1032	2.9306	2.7251	0.2055	0.0001
S1033	2.5807	2.2031	0.3776	0.0044
S1034	2.6438	2.3474	0.2964	0.0132
S1035	2.3666	2.2567	0.1099	0.0071
S1036	2.5700	2.5134	0.0566	0.0013
S1037	2.5832	2.3481	0.2351	0.0115
S1038	2.2037	2.0664	0.1373	0.0043
S1039	2.4221	2.3048	0.1173	0.0058
S1040	2.6844	2.3771	0.3073	0.0121
S1041	2.2861	2.0296	0.2565	0.0032
S1042	2.6200	2.3794	0.2406	0.0049
S1043	2.4454	2.1333	0.3121	0.0019
S1044	2.6171	2.5165	0.1006	0.0035
S1045	2.7004	2.4635	0.2369	0.0013
S1046	2.8752	2.7285	0.1467	0.0046
S1047	2.5997	2.3524	0.2473	0.0057
S1048	2.3176	2.1828	0.1348	0.0068
S1049	2.7932	2.4116	0.3816	0.0062
S1050	2.4313	2.0431	0.3882	0.0021
S1051	2.5382	2.2540	0.2842	0.0083
S1052	2.2827	1.9867	0.2960	0.0151
S1053	2.6155	2.5078	0.1077	0.0077
S1054	2.5390	2.3039	0.2351	0.0061
S1055	2.8243	2.8043	0.0200	0.0009
S1056	2.6157	2.3274	0.2883	0.0044
S1057	2.8285	2.7170	0.1115	0.0071
S1058	2.3872	2.1579	0.2293	0.0043
S1059	2.6062	2.3361	0.2701	0.0071
S1060	2.6461	2.4604	0.1857	0.0060
S1061	2.9001	2.7254	0.1747	0.0125
S1062	2.6847	2.4788	0.2059	0.0008
S1063	2.7233	2.5236	0.1997	0.0003
S1064	2.9405	2.9954	-0.0549	0.0029
S1065	2.7190	2.5443	0.1747	0.0131
S1066	2.9872	3.0045	-0.0173	0.0021
S1067	2.8249	2.5902	0.2347	0.0102
S1068	2.1520	1.9300	0.2220	0.0018
S1069	2.3270	2.1698	0.1572	0.0047
S1070	2.0789	1.9568	0.1221	0.0003
S1071	2.3637	1.9807	0.3830	0.0143
S1072	2.5277	2.1443	0.3834	0.0190

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S1073	2.3399	2.1084	0.2315	0.0045
S1074	2.6887	2.4882	0.2005	0.0178
S1075	3.1389	3.0160	0.1229	0.0006
S1076	2.8520	2.5613	0.2907	0.0175
S1077	1.9323	1.7200	0.2123	0.0054
S1078	2.2956	2.2291	0.0665	0.0019
S1079	2.0187	1.8618	0.1569	0.0089
S1080	2.1943	2.0533	0.1410	-0.0000
S1081	2.4630	2.2693	0.1937	0.0027
S1082	2.1886	2.1397	0.0489	0.0015
S1083	2.5126	2.3953	0.1173	0.0095
S1084	2.5557	2.4323	0.1234	0.0091
S1085	2.3260	2.1076	0.2184	0.0035
S1086	2.4506	2.3402	0.1104	0.0066
S1087	2.2521	2.1125	0.1396	0.0004
S1088	2.6215	2.3111	0.3104	0.0146
S1089	2.7279	2.4499	0.2780	0.0191
S1090	2.5850	2.3883	0.1967	0.0072
S1091	2.2777	2.0395	0.2382	0.0002
S1092	2.3631	2.1043	0.2588	0.0215
S1093	2.6107	2.4900	0.1207	0.0073
S1094	2.3780	2.2107	0.1673	0.0025
S1095	2.1820	1.9406	0.2414	0.0028
S1096	2.4678	2.4450	0.0228	0.0002
S1097	2.1798	2.0716	0.1082	0.0055
S1098	2.5334	2.3309	0.2025	0.0002
S1099	2.7148	2.5671	0.1477	0.0033
S1100	2.4762	2.3892	0.0870	0.0027
S1101	2.5720	2.1733	0.3987	0.0224
S1102	2.3241	2.1300	0.1941	0.0181
S1103	2.6065	2.3228	0.2837	0.0282
S1104	2.6185	2.3584	0.2601	0.0038
S1105	2.9522	2.9584	-0.0062	0.0018
S1106	2.5538	2.4205	0.1333	0.0094
S1107	2.6956	2.5090	0.1866	0.0092
S1108	2.4089	2.2274	0.1815	0.0017
S1109	2.3803	2.1993	0.1810	0.0027
S1110	2.4091	2.2985	0.1106	0.0000
S1111	2.3098	1.9766	0.3332	0.0137
S1112	2.3921	2.0988	0.2933	0.0043
S1113	2.4524	2.2747	0.1777	0.0111
S1114	2.4676	2.2538	0.2138	0.0008
S1115	2.9841	3.0251	-0.0410	0.0045
S1116	3.1942	3.0430	0.1512	0.0265
S1117	3.1438	3.0576	0.0862	0.0177
S1118	3.0847	3.0508	0.0339	0.0109

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S1119	3.0171	3.0263	-0.0092	0.0070
S1120	2.9918	3.0118	-0.0200	0.0048
S1121	2.9784	3.0029	-0.0245	0.0042
S1122	3.0076	3.0399	-0.0323	0.0030
S1123	3.2808	3.0964	0.1844	0.0313
S1124	3.2065	3.1135	0.0930	0.0153
S1125	3.1163	3.0933	0.0230	0.0067
S1126	3.0601	3.0713	-0.0112	0.0060
S1127	3.0119	3.0605	-0.0486	0.0036
S1128	2.9956	3.0416	-0.0460	0.0040
S1129	2.9033	2.9431	-0.0398	0.0035
S1130	2.8023	2.6926	0.1097	0.0046
S1131	2.8640	2.8433	0.0207	0.0037
S1132	2.9366	2.9818	-0.0452	0.0033
S1133	2.8845	2.8396	0.0449	0.0045
S1134	2.9483	2.9871	-0.0388	0.0033
S1135	2.9507	2.9923	-0.0416	0.0034
S1136	3.2116	3.0264	0.1852	0.0291
S1137	2.9218	2.9758	-0.0540	0.0024
S1138	2.8401	2.8654	-0.0253	0.0004
S1139	2.8807	2.9334	-0.0527	0.0011
S1140	2.8567	2.8743	-0.0176	0.0005
S1141	2.9281	2.9568	-0.0287	0.0020
S1142	3.2969	3.0946	0.2023	0.0347
S1143	2.9128	2.9081	0.0047	0.0077
S1144	2.7515	2.5761	0.1754	0.0115
S1145	2.8532	2.8042	0.0490	0.0080
S1146	2.8079	2.6802	0.1277	0.0101
S1147	2.9123	2.8926	0.0197	0.0066
S1148	2.7380	2.6245	0.1135	0.0051
S1149	2.8839	2.6718	0.2121	0.0068
S1150	2.9713	2.9252	0.0461	0.0079
S1151	2.9344	2.8345	0.0999	0.0066
S1152	2.9965	2.9992	-0.0027	0.0048
S1153	2.9700	2.9670	0.0030	0.0039
S1154	3.2180	3.0148	0.2032	0.0297
S1155	2.8564	2.8934	-0.0370	0.0007
S1156	2.8974	2.9008	-0.0034	0.0013
S1157	2.9518	2.9809	-0.0291	0.0032
S1158	3.2847	3.0835	0.2012	0.0341
S1159	2.7750	2.6244	0.1506	0.0105
S1160	2.8197	2.6605	0.1592	0.0081
S1161	2.9170	2.9236	-0.0066	0.0053
S1162	2.7047	2.5244	0.1803	0.0071
S1163	2.9684	2.9237	0.0447	0.0076
S1164	3.0468	3.0171	0.0297	0.0059

EOM-CCSD/cc-pVDZ				
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	3.0024	3.0226	-0.0202	0.0044
S1166	2.9123	2.9466	-0.0343	0.0015
S1167	2.8782	2.8437	0.0345	0.0059
S1168	3.0189	3.0795	-0.0606	0.0026