

FNO-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	2.1941	2.2133	-0.0192	0.0019
S844	2.3304	2.3300	0.0004	0.0034
S845	2.4056	2.4259	-0.0203	0.0012
S846	2.5489	2.5301	0.0188	0.0060
S847	2.0859	1.9858	0.1001	0.0015
S848	2.2364	2.1711	0.0653	0.0003
S849	2.1769	2.0947	0.0822	0.0043
S850	2.3339	2.2828	0.0511	0.0012
S851	2.3275	2.2543	0.0732	0.0029
S852	2.3724	2.2991	0.0733	0.0046
S853	2.5507	2.4534	0.0973	0.0018
S854	2.6167	2.5186	0.0981	0.0072
S855	2.2127	2.0956	0.1171	0.0044
S856	2.2722	2.2132	0.0590	0.0001
S857	2.3709	2.2434	0.1275	0.0080
S858	2.4847	2.3968	0.0879	0.0003
S859	2.1576	2.0798	0.0778	0.0049
S860	2.4982	2.4417	0.0565	0.0041
S861	2.4837	2.4629	0.0208	0.0021
S862	2.6566	2.6062	0.0504	0.0052
S863	2.2513	2.0156	0.2357	0.0004
S864	2.4321	2.2175	0.2146	0.0007
S865	2.2040	2.0287	0.1753	0.0032
S866	2.4338	2.2662	0.1676	0.0017
S867	2.6022	2.4655	0.1367	0.0077
S868	2.6679	2.4756	0.1923	0.0084
S869	2.7632	2.6340	0.1292	0.0048
S870	2.9764	2.6670	0.3094	0.0227
S871	2.5129	2.2470	0.2659	0.0034
S872	2.5817	2.3193	0.2624	0.0012
S873	2.5079	2.2499	0.2580	0.0079
S874	2.6776	2.4018	0.2758	0.0005
S875	2.2676	2.1434	0.1242	0.0069
S876	2.3109	2.2740	0.0369	0.0025
S877	2.1690	1.9854	0.1836	0.0110
S878	2.3274	2.1770	0.1504	0.0035
S879	2.4125	2.1803	0.2322	0.0162
S880	1.9906	1.9375	0.0531	0.0001
S881	2.0855	1.9722	0.1133	0.0051
S882	2.1255	2.0550	0.0705	0.0017
S883	2.2359	2.1365	0.0994	0.0042
S884	2.2127	1.9686	0.2441	0.0095
S885	2.5099	2.2225	0.2874	0.0013
S886	2.5114	2.2033	0.3081	0.0166
S887	2.1538	2.0017	0.1521	0.0016
S888	2.1190	1.9366	0.1824	0.0031

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S889	2.3764	2.2014	0.1750	0.0045
S890	2.4122	2.1869	0.2253	0.0020
S891	2.3682	2.2996	0.0686	0.0041
S892	2.5713	2.5413	0.0300	0.0023
S893	2.5127	2.4328	0.0799	0.0032
S894	2.3612	2.0693	0.2919	0.0162
S895	2.3857	2.2564	0.1293	0.0043
S896	2.6148	2.2451	0.3697	0.0271
S897	2.3074	2.0565	0.2509	0.0090
S898	2.1220	2.0180	0.1040	0.0007
S899	2.3274	2.2155	0.1119	0.0038
S900	2.4994	2.1462	0.3532	0.0161
S901	2.7183	2.4172	0.3011	0.0034
S902	2.8041	2.3349	0.4692	0.0329
S903	2.4306	2.2467	0.1839	0.0001
S904	2.4309	2.1080	0.3229	0.0079
S905	2.4513	2.2708	0.1805	0.0034
S906	2.5266	2.2458	0.2808	0.0015
S907	2.5014	2.3575	0.1439	0.0084
S908	2.8021	2.7026	0.0995	0.0055
S909	2.5911	2.5388	0.0523	0.0032
S910	2.8982	2.8562	0.0420	0.0015
S911	2.2920	2.1383	0.1537	0.0074
S912	2.5579	2.4141	0.1438	0.0142
S913	2.2510	1.9803	0.2707	0.0026
S914	2.2027	2.0228	0.1799	0.0066
S915	2.4971	2.2345	0.2626	0.0084
S916	2.5043	2.3416	0.1627	0.0063
S917	2.7374	2.5879	0.1495	0.0134
S918	2.1993	2.0198	0.1795	0.0033
S919	2.3507	2.2211	0.1296	0.0075
S920	2.4983	2.2411	0.2572	0.0098
S921	2.2165	2.0613	0.1552	0.0109
S922	2.5803	2.3383	0.2420	0.0190
S923	2.5047	2.2709	0.2338	0.0031
S924	2.1361	2.0343	0.1018	0.0038
S925	2.5324	2.3185	0.2139	0.0082
S926	2.4977	2.3033	0.1944	0.0155
S927	2.9745	2.5717	0.4028	0.0333
S928	2.5721	2.3629	0.2092	0.0006
S929	2.4085	2.3050	0.1035	0.0019
S930	2.6803	2.3904	0.2899	0.0017
S931	2.5788	2.6148	-0.0360	0.0011
S932	2.6053	2.6646	-0.0593	0.0004
S933	2.7879	2.8353	-0.0474	0.0033
S934	2.5014	2.3696	0.1318	0.0011

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S935	2.3802	2.2670	0.1132	0.0063
S936	2.5987	2.4928	0.1059	0.0038
S937	2.5744	2.5648	0.0096	0.0025
S938	2.7132	2.6954	0.0178	0.0010
S939	2.8974	2.8352	0.0622	0.0080
S940	2.4805	2.4034	0.0771	0.0001
S941	2.5247	2.4044	0.1203	0.0078
S942	2.6560	2.5566	0.0994	0.0016
S943	2.0769	1.9303	0.1466	0.0027
S944	2.0152	1.8905	0.1247	0.0005
S945	2.3035	2.1259	0.1776	0.0042
S946	2.1053	1.8730	0.2323	0.0112
S947	2.3765	2.0852	0.2913	0.0168
S948	2.7464	2.6985	0.0479	0.0019
S949	3.1032	3.0075	0.0957	0.0050
S950	2.7105	2.4300	0.2805	0.0006
S951	2.4864	2.2514	0.2350	0.0064
S952	2.7651	2.5033	0.2618	0.0061
S953	2.8606	2.7374	0.1232	0.0052
S954	3.0383	2.8608	0.1775	0.0066
S955	3.2312	2.9924	0.2388	0.0199
S956	2.7917	2.5169	0.2748	0.0003
S957	2.7518	2.4440	0.3078	0.0099
S958	3.0459	2.6229	0.4230	0.0190
S959	2.2103	2.1191	0.0912	0.0012
S960	2.0650	1.8728	0.1922	0.0055
S961	2.4705	2.3758	0.0947	0.0003
S962	2.2009	2.0737	0.1272	0.0027
S963	2.0916	2.0328	0.0588	0.0001
S964	2.5372	2.3292	0.2080	0.0066
S965	2.3625	2.2040	0.1585	0.0123
S966	2.6129	2.3989	0.2140	0.0247
S967	2.3262	2.1929	0.1333	0.0072
S968	2.1870	2.1198	0.0672	0.0021
S969	2.3814	2.2837	0.0977	0.0077
S970	2.2510	2.0648	0.1862	0.0153
S971	2.5523	2.3034	0.2489	0.0268
S972	2.1692	2.0311	0.1381	0.0091
S973	2.3047	2.1916	0.1131	0.0015
S974	2.3613	2.2431	0.1182	0.0073
S975	2.1478	2.0660	0.0818	0.0035
S976	2.1212	2.0441	0.0771	0.0006
S977	2.3639	2.2655	0.0984	0.0045
S978	2.1888	2.1367	0.0521	0.0003
S979	2.3344	2.1510	0.1834	0.0097
S980	2.3229	2.1491	0.1738	0.0048

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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]	$f_{12}(S_0-S_1)$
S981	2.5617	2.3875	0.1742	0.0135
S982	2.5880	2.3307	0.2573	0.0186
S983	2.8104	2.4953	0.3151	0.0316
S984	2.6087	2.3694	0.2393	0.0121
S985	2.5573	2.4171	0.1402	0.0074
S986	2.5370	2.2403	0.2967	0.0272
S987	2.9187	2.4534	0.4653	0.0724
S988	2.4849	2.2328	0.2521	0.0188
S989	2.4925	2.3986	0.0939	0.0005
S990	2.6001	2.4287	0.1714	0.0161
S991	2.3152	2.2801	0.0351	0.0000
S992	2.2334	2.0826	0.1508	0.0019
S993	2.6640	2.5172	0.1468	0.0034
S994	2.3938	2.2970	0.0968	0.0028
S995	2.4462	2.3487	0.0975	0.0031
S996	2.3447	2.2804	0.0643	0.0003
S997	2.8988	2.5999	0.2989	0.0272
S998	2.4651	2.4277	0.0374	0.0023
S999	2.5172	2.2828	0.2344	0.0087
S1000	2.0387	1.7824	0.2563	0.0114
S1001	2.3839	1.9999	0.3840	0.0190
S1002	2.3918	2.0249	0.3669	0.0205
S1003	2.7496	2.5806	0.1690	0.0050
S1004	2.9253	2.6256	0.2997	0.0225
S1005	2.1398	1.9480	0.1918	0.0144
S1006	2.6258	2.3354	0.2904	0.0156
S1007	2.6929	2.2768	0.4161	0.0414
S1008	2.4209	2.3399	0.0810	0.0033
S1009	2.5950	2.5300	0.0650	0.0072
S1010	2.3096	2.1096	0.2000	0.0036
S1011	2.3126	2.1244	0.1882	0.0022
S1012	2.4548	2.2149	0.2399	0.0045
S1013	2.7798	2.6660	0.1138	0.0059
S1014	3.0833	2.7592	0.3241	0.0135
S1015	2.4005	2.2508	0.1497	0.0087
S1016	2.6213	2.4376	0.1837	0.0028
S1017	2.8467	2.4552	0.3915	0.0114
S1018	2.5096	2.5587	-0.0491	0.0004
S1019	2.7559	2.7654	-0.0095	0.0022
S1020	2.3626	2.1715	0.1911	0.0060
S1021	2.5913	2.4114	0.1799	0.0085
S1022	2.5919	2.5072	0.0847	0.0005
S1023	2.8686	2.7883	0.0803	0.0025
S1024	2.4846	2.1919	0.2927	0.0047
S1025	2.7437	2.4835	0.2602	0.0074
S1026	2.4646	2.3456	0.1190	0.0070

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S1027	2.7261	2.4728	0.2533	0.0114
S1028	2.8968	2.7887	0.1081	0.0030
S1029	2.4517	2.1772	0.2745	0.0079
S1030	2.5259	2.3387	0.1872	0.0108
S1031	2.7986	2.5968	0.2018	0.0001
S1032	3.1806	2.8460	0.3346	0.0057
S1033	2.6458	2.2600	0.3858	0.0075
S1034	2.9301	2.4428	0.4873	0.0536
S1035	2.4363	2.3254	0.1109	0.0075
S1036	2.8104	2.6789	0.1315	0.0036
S1037	2.6721	2.3792	0.2929	0.0166
S1038	2.2679	2.0963	0.1716	0.0071
S1039	2.5117	2.3711	0.1406	0.0082
S1040	2.8456	2.4205	0.4251	0.0310
S1041	2.3436	2.0628	0.2808	0.0048
S1042	2.6811	2.4248	0.2563	0.0065
S1043	2.5000	2.1881	0.3119	0.0032
S1044	2.7276	2.5945	0.1331	0.0069
S1045	2.7737	2.5069	0.2668	0.0001
S1046	3.0754	2.9059	0.1695	0.0030
S1047	2.7542	2.3749	0.3793	0.0158
S1048	2.4353	2.3295	0.1058	0.0082
S1049	3.1653	2.4895	0.6758	0.0604
S1050	2.4831	2.2114	0.2717	0.0029
S1051	3.0204	2.4939	0.5265	0.0153
S1052	2.4116	2.0851	0.3265	0.0168
S1053	2.9040	2.7113	0.1927	0.0114
S1054	2.6510	2.3971	0.2539	0.0064
S1055	3.0980	3.0135	0.0845	0.0030
S1056	2.6827	2.3944	0.2883	0.0070
S1057	3.1437	2.8781	0.2656	0.0195
S1058	2.4871	2.2267	0.2604	0.0079
S1059	2.9432	2.5002	0.4430	0.0200
S1060	3.0137	2.5967	0.4170	0.0122
S1061	3.2335	2.8735	0.3600	0.0308
S1062	2.8278	2.5420	0.2858	0.0043
S1063	3.1435	2.7672	0.3763	0.0025
S1064	3.0244	3.0691	-0.0447	0.0030
S1065	2.8754	2.5947	0.2807	0.0269
S1066	3.5090	3.2474	0.2616	0.0068
S1067	3.0023	2.6239	0.3784	0.0303
S1068	2.1778	1.9560	0.2218	0.0021
S1069	2.3800	2.2025	0.1775	0.0063
S1070	2.1269	2.0077	0.1192	0.0002
S1071	2.3915	2.0257	0.3658	0.0136
S1072	2.6801	2.2366	0.4435	0.0230

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S1073	2.4245	2.1962	0.2283	0.0033
S1074	2.9617	2.5912	0.3705	0.0485
S1075	3.6981	3.2331	0.4650	0.0019
S1076	3.3457	2.8910	0.4547	0.0376
S1077	1.9648	1.7573	0.2075	0.0050
S1078	2.3703	2.3168	0.0535	0.0016
S1079	2.0748	1.9237	0.1511	0.0080
S1080	2.2290	2.0862	0.1428	-0.0000
S1081	2.8249	2.3590	0.4659	0.0247
S1082	2.5721	2.3092	0.2629	0.0000
S1083	2.6113	2.4635	0.1478	0.0135
S1084	2.6504	2.5161	0.1343	0.0117
S1085	2.3736	2.1722	0.2014	0.0043
S1086	2.6007	2.4272	0.1735	0.0146
S1087	2.3104	2.1814	0.1290	0.0002
S1088	2.6727	2.3751	0.2976	0.0111
S1089	3.0316	2.5887	0.4429	0.0528
S1090	2.9315	2.5930	0.3385	0.0201
S1091	2.6084	2.1091	0.4993	0.0038
S1092	2.6294	2.2454	0.3840	0.0351
S1093	3.0668	2.7893	0.2775	0.0160
S1094	2.7860	2.3380	0.4480	0.0025
S1095	2.2646	2.0359	0.2287	0.0017
S1096	2.8627	2.5612	0.3015	0.0032
S1097	2.3932	2.2467	0.1465	0.0062
S1098	2.9736	2.4749	0.4987	0.0001
S1099	3.0495	2.6524	0.3971	0.0288
S1100	2.9390	2.6524	0.2866	0.0037
S1101	2.8416	2.2759	0.5657	0.0519
S1102	2.6508	2.2979	0.3529	0.0418
S1103	2.9476	2.5550	0.3926	0.0519
S1104	2.9877	2.5210	0.4667	0.0230
S1105	3.4652	3.3270	0.1382	0.0039
S1106	2.8162	2.4862	0.3300	0.0343
S1107	3.0968	2.7538	0.3430	0.0287
S1108	2.4462	2.2577	0.1885	0.0032
S1109	2.4373	2.2765	0.1608	0.0034
S1110	2.4748	2.4074	0.0674	0.0001
S1111	2.3507	2.0385	0.3122	0.0124
S1112	2.7023	2.1907	0.5116	0.0198
S1113	2.8977	2.5758	0.3219	0.0225
S1114	2.9680	2.7541	0.2139	0.0008
S1115	3.0721	3.1060	-0.0339	0.0057
S1116	3.2890	3.1041	0.1849	0.0286
S1117	3.2254	3.1222	0.1032	0.0199
S1118	3.5874	3.3610	0.2264	0.0178

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S1119	3.1352	3.1279	0.0073	0.0047
S1120	3.4917	3.3660	0.1257	0.0082
S1121	3.4731	3.3573	0.1158	0.0070
S1122	3.1326	3.1175	0.0151	0.0051
S1123	3.3637	3.1609	0.2028	0.0335
S1124	3.2908	3.2201	0.0707	0.0126
S1125	3.3526	3.2238	0.1288	0.0184
S1126	3.2113	3.2148	-0.0035	0.0020
S1127	3.5183	3.3691	0.1492	0.0067
S1128	3.4933	3.3321	0.1612	0.0075
S1129	2.9555	2.9954	-0.0399	0.0039
S1130	2.8655	2.7393	0.1262	0.0049
S1131	2.9956	2.9037	0.0919	0.0047
S1132	3.1328	3.1500	-0.0172	0.0022
S1133	3.0321	2.9181	0.1140	0.0042
S1134	3.4713	3.2858	0.1855	0.0067
S1135	3.4751	3.2828	0.1923	0.0068
S1136	3.2890	3.0725	0.2165	0.0314
S1137	2.9880	3.0407	-0.0527	0.0027
S1138	3.0329	3.0059	0.0270	0.0016
S1139	3.0316	3.0652	-0.0336	0.0000
S1140	3.0554	3.0231	0.0323	0.0000
S1141	3.0236	3.0389	-0.0153	0.0009
S1142	3.3727	3.1576	0.2151	0.0399
S1143	2.9807	2.9756	0.0051	0.0077
S1144	2.8084	2.6379	0.1705	0.0129
S1145	2.9105	2.8495	0.0610	0.0097
S1146	3.0839	2.8493	0.2346	0.0161
S1147	3.0168	2.9844	0.0324	0.0054
S1148	2.7877	2.6712	0.1165	0.0053
S1149	2.9372	2.7416	0.1956	0.0069
S1150	3.1758	3.0749	0.1009	0.0061
S1151	3.0958	2.9321	0.1637	0.0056
S1152	3.4454	3.1662	0.2792	0.0171
S1153	3.1532	3.1713	-0.0181	0.0017
S1154	3.2891	3.0570	0.2321	0.0319
S1155	2.9332	2.9640	-0.0308	0.0006
S1156	3.2924	3.1858	0.1066	0.0010
S1157	3.1135	3.1176	-0.0041	0.0015
S1158	3.3421	3.1259	0.2162	0.0346
S1159	2.8200	2.6673	0.1527	0.0116
S1160	3.1712	2.8683	0.3029	0.0203
S1161	3.0198	3.0222	-0.0024	0.0045
S1162	2.7634	2.5779	0.1855	0.0063
S1163	3.0976	2.9742	0.1234	0.0128
S1164	3.5686	3.3015	0.2671	0.0227

FNO-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	3.1806	3.1805	0.0001	0.0032
S1166	3.4034	3.3086	0.0948	0.0025
S1167	3.2507	3.0460	0.2047	0.0169
S1168	3.5311	3.3135	0.2176	0.0061