	FNO-F	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0\text{-}S_1)$
S1	1.1777	1.2635	-0.0858	0.0000
S2	1.0151	1.0384	-0.0233	0.0010
S3	1.6040	1.6068	-0.0028	0.0011
S4	1.8594	1.9048	-0.0454	0.0042
S5	1.7715	1.5026	0.2689	0.0001
S6	1.5866	1.5931	-0.0065	0.0000
S7	2.0261	1.9495	0.0766	0.0010
S8	1.4755	1.4055	0.0700	0.0026
S9	1.6264	1.6632	-0.0368	0.0003
S10	2.1211	1.8603	0.2608	0.0011
S11	1.7942	1.8380	-0.0438	0.0053
S12	2.1107	2.1491	-0.0384	0.0035
S13	2.1791	2.1761	0.0030	0.0074
S14	2.3915	2.4255	-0.0340	0.0094
S15	1.7485	1.6614	0.0871	0.0020
S16	2.1195	2.0291	0.0904	0.0004
S17	1.9159	1.9023	0.0136	0.0024
S18	2.1392	2.1843	-0.0451	0.0005
S19	1.5518	1.3915	0.1603	0.0032
S20	1.6035	1.5291	0.0744	0.0116
S21	0.8547	0.8490	0.0057	0.0007
S22	1.4940	1.2610	0.2330	0.0031
S23	1.8698	1.4074	0.4624	0.0007
S24	1.6586	1.4371	0.2215	0.0056
S25	1.9533	1.7391	0.2142	0.0048
S26	1.7107	1.6592	0.0515	0.0067
S27	2.0008	1.8709	0.1299	0.0150
S28	1.7855	1.4182	0.3673	0.0018
S29	2.1480	1.7601	0.3879	0.0029
S30	1.4573	1.4166	0.0407	0.0006
S31	1.7650	1.6793	0.0857	0.0064
S32	2.2220	1.8642	0.3578	0.0004
S33	2.0899	1.9116	0.1783	0.0066
S34	1.5419	1.4661	0.0758	0.0010
S35	2.4419	1.9007	0.5412	0.0005
S36	2.3067	1.9556	0.3511	0.0022
S37	1.8524	1.8143	0.0381	0.0050
S38	2.2682	2.0437	0.2245	0.0044
S39	2.2576	2.1286	0.1290	0.0114
S40	1.4671	1.4569	0.0102	0.0003
S41	1.8235	1.7439	0.0796	0.0029
S42	2.1440	1.9119	0.2321	0.0024
S43	2.0923	2.0104	0.0819	0.0012
S44	1.7759	1.8592	-0.0833	0.0004
S45	1.6185	1.5656	0.0529	0.0028
S46	2.4179	2.3002	0.1177	-0.0000

	FNO-F	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{S}_1)~\mathrm{[eV]}$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0\text{-}S_1)$
S47	2.1659	2.2173	-0.0514	0.0009
S48	1.9515	1.8804	0.0711	0.0012
S49	2.0423	1.9794	0.0629	0.0032
S50	2.0573	1.9783	0.0790	0.0050
S51	2.5263	2.5303	-0.0040	0.0031
S52	2.4473	2.4948	-0.0475	0.0050
S53	2.7418	2.8204	-0.0786	0.0033
S54	2.6085	2.4135	0.1950	0.0011
S55	2.1902	2.1598	0.0304	0.0031
S56	2.5092	2.5034	0.0058	0.0004
S57	2.2467	1.7533	0.4934	0.0024
S58	1.3211	1.2412	0.0799	0.0030
S59	1.7768	1.5780	0.1988	0.0070
S60	2.5534	2.2157	0.3377	0.0008
S61	2.4963	2.3112	0.1851	0.0090
S62	2.7851	2.2571	0.5280	0.0002
S63	2.0303	1.7972	0.2331	0.0016
S64	2.4442	2.1581	0.2861	0.0049
S65	2.0648	2.0490	0.0158	0.0066
S66	1.9123	1.7528	0.1595	0.0005
S67	1.9532	1.8803	0.0729	0.0037
S68	2.3139	2.2202	0.0937	0.0038
S69	2.4216	2.3950	0.0266	0.0106
S70	2.5433	2.2677	0.2756	0.0024
S71	1.9278	1.9287	-0.0009	0.0001
S72	2.2484	2.2208	0.0276	0.0034
S73	2.3904	2.4920	-0.1016	0.0002
S74	2.2148	2.2056	0.0092	0.0019
S75	1.5531	1.4665	0.0866	0.0075
S76	2.1771	1.8468	0.3303	0.0096
S77	2.2742	2.1734	0.1008	0.0125
S78	2.0306	1.8782	0.1524	0.0040
S79	2.0381	1.9480	0.0901	0.0057
S80	2.7296	2.3728	0.3568	0.0039
S81	2.6544	2.5396	0.1148	0.0075
S82	2.0016	2.0147	-0.0131	0.0014
S83	2.5657	2.4246	0.1411	0.0008
S84	3.0406	3.2073	-0.1667	0.0000
S85	2.7262	2.6105	0.1157	0.0066
S86	1.9833	1.8200	0.1633	0.0141
S87	2.4272	2.2768	0.1504	0.0090
S88	2.4489	2.4099	0.0390	0.0048
S89	0.6935	0.6783	0.0152	0.0000
S90	1.9389	1.3677	0.5712	0.0017
S91	1.2780	1.2035	0.0745	0.0023
S92	2.5195	1.8461	0.6734	0.0022

	FNO-F	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S93	1.2940	1.2507	0.0433	0.0007
S94	2.1341	1.7653	0.3688	0.0003
S95	2.1449	1.7765	0.3684	0.0062
S96	1.7707	1.7503	0.0204	0.0006
S97	1.1877	1.1436	0.0441	0.0006
S98	3.0674	2.3549	0.7125	0.0000
S99	2.1021	1.6844	0.4177	0.0048
S100	1.6857	1.6716	0.0141	0.0006
S101	2.8059	2.3126	0.4933	0.0032
S102	1.7675	1.7055	0.0620	0.0031
S103	2.5125	2.2663	0.2462	0.0024
S104	2.1869	2.2542	-0.0673	0.0000
S105	1.2369	1.3279	-0.0910	0.0000
S106	1.2485	1.2902	-0.0417	0.0000
S107	1.4547	1.5319	-0.0772	0.0020
S108	1.3410	1.2376	0.1034	0.0006
S109	1.4045	1.4896	-0.0851	0.0013
S110	1.3462	1.2132	0.1330	0.0005
S111	1.3059	1.4038	-0.0979	0.0004
S112	1.2057	1.2073	-0.0016	0.0002
S113	1.2611	1.3575	-0.0964	0.0000
S114	1.1656	1.2067	-0.0411	0.0004
S115	1.2123	1.3036	-0.0913	-0.0000
S116	1.1537	1.2330	-0.0793	0.0001
S117	1.1960	1.2828	-0.0868	0.0000
S118	1.1586	1.2412	-0.0826	0.0002
S119	1.5090	1.5655	-0.0565	0.0031
S120	1.1865	1.2211	-0.0346	0.0002
S121	1.1586	1.1992	-0.0406	0.0006
S122	1.2093	1.2892	-0.0799	0.0005
S123	1.0298	0.9999	0.0299	0.0011
S124	1.5241	1.5639	-0.0398	0.0005
S125	1.0783	1.1402	-0.0619	0.0004
S126	1.2522	1.3259	-0.0737	0.0005
S127	1.1293	1.2024	-0.0731	0.0002
S128	1.2272	1.3088	-0.0816	0.0004
S129	1.0412	1.0698	-0.0286	0.0006
S130	1.3586	1.4106	-0.0520	0.0003
S131	1.5104	1.5700	-0.0596	0.0032
S132	1.1496	1.2275	-0.0779	0.0000
S133	0.9987	1.0119	-0.0132	0.0008
S134	1.4989	1.5310	-0.0321	0.0005
S135	1.1693	1.2243	-0.0550	0.0001
S136	1.2568	1.3433	-0.0865	0.0002
S137	0.9875	0.9769	0.0106	0.0007
S138	1.5780	1.5864	-0.0084	0.0006

	FNO-E	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S139	1.0984	1.1557	-0.0573	0.0003
S140	1.3086	1.3865	-0.0779	0.0001
S141	3.1052	3.2731	-0.1679	0.0002
S142	3.4242	3.5063	-0.0821	0.0120
S143	3.3275	3.4556	-0.1281	0.0063
S144	3.2227	3.3878	-0.1651	0.0021
S145	3.1584	3.3297	-0.1713	0.0003
S146	3.0983	3.2697	-0.1714	0.0001
S147	3.0766	3.2435	-0.1669	0.0000
S148	3.4657	3.5235	-0.0578	0.0147
S149	3.0261	3.1840	-0.1579	0.0002
S150	2.9024	3.0021	-0.0997	0.0015
S151	2.9612	3.1028	-0.1416	0.0007
S152	3.0203	3.1736	-0.1533	0.0002
S153	2.9182	3.0218	-0.1036	0.0014
S154	3.4921	3.5401	-0.0480	0.0186
S155	2.9178	3.0316	-0.1138	0.0010
S156	3.0409	3.1944	-0.1535	0.0000
S157	3.0258	3.1728	-0.1470	0.0001
S158	2.9821	3.1215	-0.1394	0.0004
S159	1.8549	1.9116	-0.0567	0.0045
S160	1.8539	1.8900	-0.0361	0.0080
S161	1.8119	1.8325	-0.0206	0.0062
S162	1.7937	1.8159	-0.0222	0.0060
S163	2.1161	2.2011	-0.0850	0.0004
S164	2.1024	2.0594	0.0430	0.0171
S165	1.7633	1.6913	0.0720	0.0091
S166	1.7302	1.6988	0.0314	0.0055
S167	2.0372	2.1272	-0.0900	0.0011
S168	2.0623	2.0297	0.0326	0.0141
S169	1.7543	1.7268	0.0275	0.0081
S170	1.7343	1.6784	0.0559	0.0062
S171	1.9194	2.0085	-0.0891	0.0027
S172	1.9521	1.9676	-0.0155	0.0088
S173	1.7162	1.7183	-0.0021	0.0076
S174	1.7274	1.7320	-0.0046	0.0059
S175	1.8704	1.9398	-0.0694	0.0043
S176	1.8879	1.9154	-0.0275	0.0101
S177	1.7996	1.8490	-0.0494	0.0061
S178	1.8290	1.8708	-0.0418	0.0044
S179	1.8091	1.8663	-0.0572	0.0052
S180	1.8475	1.8828	-0.0353	0.0075
S181	1.7302	1.7653	-0.0351	0.0072
S182	1.7486	1.7860	-0.0374	0.0042
S183	1.7891	1.8369	-0.0478	0.0057
S184	1.8305	1.8650	-0.0345	0.0075

	FNO-F	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0\text{-}S_1)$
S185	1.7354	1.7751	-0.0397	0.0072
S186	1.7556	1.7941	-0.0385	0.0042
S187	2.1765	2.2474	-0.0709	0.0002
S188	2.1765	2.0785	0.0980	0.0210
S189	1.7490	1.7458	0.0032	0.0075
S190	1.7726	1.7096	0.0630	0.0055
S191	1.7284	1.7371	-0.0087	0.0081
S192	1.7805	1.8041	-0.0236	0.0102
S193	1.7687	1.8026	-0.0339	0.0082
S194	1.7683	1.8098	-0.0415	0.0031
S195	1.5728	1.4978	0.0750	0.0104
S196	1.7073	1.6657	0.0416	0.0064
S197	1.9131	1.9408	-0.0277	0.0086
S198	1.9353	1.9690	-0.0337	0.0019
S199	1.6745	1.6724	0.0021	0.0084
S200	1.7128	1.7372	-0.0244	0.0073
S201	1.7955	1.8370	-0.0415	0.0091
S202	1.8165	1.8627	-0.0462	0.0024
S203	1.7061	1.7283	-0.0222	0.0076
S204	1.7683	1.7995	-0.0312	0.0067
S205	1.7750	1.8217	-0.0467	0.0085
S206	1.8119	1.8615	-0.0496	0.0024
S207	1.6121	1.5713	0.0408	0.0097
S208	1.7068	1.6943	0.0125	0.0055
S209	1.8553	1.9007	-0.0454	0.0080
S210	1.9164	1.9605	-0.0441	0.0024
S211	2.1715	2.2424	-0.0709	0.0001
S212	2.1608	2.0850	0.0758	0.0234
S213	1.7608	1.7546	0.0062	0.0079
S214	1.7599	1.7700	-0.0101	0.0052
S215	1.5930	1.5345	0.0585	0.0095
S216	1.6618	1.6521	0.0097	0.0065
S217	1.9438	1.9747	-0.0309	0.0087
S218	2.0405	2.0658	-0.0253	0.0025
S219	1.7464	1.7617	-0.0153	0.0063
S220	1.8119	1.8265	-0.0146	0.0081
S221	1.8321	1.8887	-0.0566	0.0060
S222	1.8364	1.8864	-0.0500	0.0042
S223	1.5591	1.4773	0.0818	0.0094
S224	1.6919	1.6743	0.0176	0.0051
S225	1.9848	2.0120	-0.0272	0.0071
S226	2.0620	2.0920	-0.0300	0.0024
S227	1.6813	1.6784	0.0029	0.0080
S228	1.7658	1.7776	-0.0118	0.0048
S229	1.8536	1.9130	-0.0594	0.0055
S230	1.9148	1.9583	-0.0435	0.0044

	FNO-F	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$
S231	2.2339	2.2462	-0.0123	0.0067
S232	2.2397	2.2346	0.0051	0.0120
S233	2.2236	2.2120	0.0116	0.0091
S234	2.1349	2.1231	0.0118	0.0086
S235	2.2192	2.1671	0.0521	0.0086
S236	2.2135	2.1692	0.0443	0.0090
S237	2.4938	2.5244	-0.0306	0.0016
S238	2.4190	2.3698	0.0492	0.0231
S239	2.4990	2.3728	0.1262	0.0285
S240	2.0063	1.9306	0.0757	0.0121
S241	2.1781	1.9586	0.2195	0.0130
S242	2.1743	2.0416	0.1327	0.0103
S243	2.4208	2.4528	-0.0320	0.0027
S244	2.3442	2.3309	0.0133	0.0155
S245	2.4478	2.3506	0.0972	0.0221
S246	1.9901	1.9106	0.0795	0.0133
S247	2.2279	2.0467	0.1812	0.0108
S248	2.1946	2.0339	0.1607	0.0111
S249	2.2969	2.3386	-0.0417	0.0046
S250	2.2579	2.2844	-0.0265	0.0094
S251	2.3604	2.3077	0.0527	0.0154
S252	2.0415	2.0133	0.0282	0.0111
S253	2.1762	2.0869	0.0893	0.0097
S254	2.1327	2.0760	0.0567	0.0088
S255	2.2554	2.2824	-0.0270	0.0066
S256	2.2129	2.2226	-0.0097	0.0163
S257	2.2816	2.2578	0.0238	0.0112
S258	2.0367	2.0044	0.0323	0.0104
S259	2.1443	2.0501	0.0942	0.0138
S260	2.2026	2.2005	0.0021	0.0053
S261	2.1937	2.2089	-0.0152	0.0077
S262	2.1775	2.1912	-0.0137	0.0107
S263	2.0875	2.0797	0.0078	0.0094
S264	2.1232	2.0990	0.0242	0.0111
S265	2.1534	2.1195	0.0339	0.0063
S266	2.2461	2.2310	0.0151	0.0092
S267	2.1752	2.1820	-0.0068	0.0083
S268	2.1612	2.1697	-0.0085	0.0110
S269	2.2288	2.2166	0.0122	0.0087
S270	2.0982	2.0919	0.0063	0.0091
S271	2.1253	2.1074	0.0179	0.0120
S272	2.1517	2.1252	0.0265	0.0059
S273	2.5637	2.5674	-0.0037	0.0008
S274	2.4451	2.3660	0.0791	0.0256
S275	2.5510	2.3875	0.1635	0.0321
S276	2.0065	1.9080	0.0985	0.0127

	FNO-F	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0\text{-}S_1)$
S277	2.2345	1.9434	0.2911	0.0147
S278	2.1711	2.0969	0.0742	0.0084
S279	2.1412	2.1120	0.0292	0.0094
S280	2.1872	2.1145	0.0727	0.0211
S281	2.1147	2.1408	-0.0261	0.0063
S282	2.1348	2.1240	0.0108	0.0084
S283	2.0819	2.0297	0.0522	0.0184
S284	2.1439	2.1312	0.0127	0.0043
S285	1.9455	1.8431	0.1024	0.0138
S286	2.1506	1.9827	0.1679	0.0141
S287	2.0185	2.0304	-0.0119	0.0040
S288	2.2839	2.2908	-0.0069	0.0062
S289	2.1840	2.2455	-0.0615	0.0008
S290	2.2319	2.2264	0.0055	0.0162
S291	2.0671	2.0293	0.0378	0.0116
S292	2.1162	2.0416	0.0746	0.0168
S293	2.0869	2.1031	-0.0162	0.0046
S294	2.1615	2.1674	-0.0059	0.0090
S295	2.1331	2.1109	0.0222	0.0170
S296	2.1586	2.1706	-0.0120	0.0029
S297	2.0970	2.0830	0.0140	0.0109
S298	2.1455	2.1066	0.0389	0.0125
S299	2.1695	2.1710	-0.0015	0.0063
S300	2.1352	2.1448	-0.0096	0.0088
S301	2.1345	2.1176	0.0169	0.0156
S302	2.1726	2.1733	-0.0007	0.0031
S303	2.0035	1.9242	0.0793	0.0134
S304	2.1228	1.9961	0.1267	0.0111
S305	2.0761	2.0730	0.0031	0.0042
S306	2.2253	2.2417	-0.0164	0.0077
S307	2.1687	2.1700	-0.0013	0.0168
S308	2.2120	2.2513	-0.0393	0.0018
S309	2.5473	2.5567	-0.0094	0.0014
S310	2.4639	2.3886	0.0753	0.0324
S311	2.5488	2.3968	0.1520	0.0330
S312	2.0851	2.0487	0.0364	0.0105
S313	2.1707	2.0132	0.1575	0.0137
S314	2.1892	2.1120	0.0772	0.0084
S315	1.9818	1.8886	0.0932	0.0119
S316	2.0768	1.9489	0.1279	0.0140
S317	2.0308	2.0473	-0.0165	0.0036
S318	2.2874	2.3042	-0.0168	0.0078
S319	2.3170	2.3479	-0.0309	0.0012
S320	2.2008	2.1974	0.0034	0.0162
S321	2.1108	2.0908	0.0200	0.0105
S322	2.2023	2.1540	0.0483	0.0127

	FNO-F	EOM-CCSD/aug-c	c-pVDZ	
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1 ext{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0\text{-}S_1)$
S323	2.2064	2.1889	0.0175	0.0081
S324	2.1886	2.2020	-0.0134	0.0064
S325	2.2035	2.2174	-0.0139	0.0049
S326	2.2308	2.2265	0.0043	0.0124
S327	1.9590	1.8390	0.1200	0.0130
S328	2.0956	1.9685	0.1271	0.0098
S329	2.1717	2.1602	0.0115	0.0063
S330	2.3217	2.3424	-0.0207	0.0057
S331	2.3002	2.3577	-0.0575	0.0006
S332	2.2084	2.2267	-0.0183	0.0161
S333	2.0788	2.0335	0.0453	0.0109
S334	2.1865	2.1107	0.0758	0.0078
S335	2.1488	2.1384	0.0104	0.0053
S336	2.2232	2.2450	-0.0218	0.0070
S337	2.2090	2.2229	-0.0139	0.0104
S338	2.2617	2.2828	-0.0211	0.0039
S339	2.5100	2.5755	-0.0655	0.0038
S340	2.5103	2.5458	-0.0355	0.0073
S341	2.4349	2.4477	-0.0128	0.0057
S342	2.7771	2.8754	-0.0983	-0.0000
S343	2.7868	2.7006	0.0862	0.0249
S344	2.2903	2.1378	0.1525	0.0102
S345	2.6768	2.7846	-0.1078	0.0004
S346	2.7197	2.6765	0.0432	0.0174
S347	2.2979	2.2103	0.0876	0.0095
S348	2.5676	2.6741	-0.1065	0.0020
S349	2.6274	2.6358	-0.0084	0.0101
S350	2.3428	2.3423	0.0005	0.0072
S351	2.5316	2.6172	-0.0856	0.0036
S352	2.5455	2.5725	-0.0270	0.0100
S353	2.3269	2.2934	0.0335	0.0101
S354	2.4716	2.5405	-0.0689	0.0048
S355	2.3619	2.3887	-0.0268	0.0075
S356	2.5073	2.5459	-0.0386	0.0065
S357	2.4512	2.5082	-0.0570	0.0054
S358	2.4877	2.5266	-0.0389	0.0063
S359	2.3718	2.4025	-0.0307	0.0078
S360	2.8169	2.8981	-0.0812	0.0002
S361	2.8262	2.7202	0.1060	0.0307
S362	2.2665	2.1512	0.1153	0.0109
S363	2.4045	2.4220	-0.0175	0.0078
S364	2.3885	2.4421	-0.0536	0.0056
S365	2.3990	2.4116	-0.0126	0.0086
S366	2.2638	2.1785	0.0853	0.0113
S367	2.2934	2.3086	-0.0152	0.0041
S368	2.4880	2.5441	-0.0561	0.0089

Molecule AE(S ₀ -S ₁) [eV] AE(S ₀ -T ₁) [eV] AE(S ₁ -T ₁) [eV] f ₁₂ (S ₀ -S ₁) S369 2.3569 2.3535 0.0034 0.0090 S370 2.3935 2.4286 -0.0361 0.0097 S371 2.3935 2.4286 -0.0351 0.0081 S373 2.4281 2.4662 -0.0381 0.0054 S374 2.3882 2.4296 -0.0414 0.0089 S375 2.2947 2.2418 0.0529 0.0111 S376 2.3331 2.3448 -0.0117 0.0044 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S381 2.2850 2.2137 0.0713 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0525 S384 2.4090 2		FNO-F	EOM-CCSD/aug-c	c-pVDZ	
S370 2.3534 2.3944 -0.0410 0.0059 S371 2.3935 2.4286 -0.0351 0.0097 S372 2.3853 2.4124 -0.0271 0.0081 S373 2.4281 2.4662 -0.0381 0.0054 S374 2.3882 2.4296 -0.0414 0.0089 S375 2.2947 2.2418 0.0529 0.0111 S376 2.3331 2.3448 -0.0117 0.0044 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S378 2.8394 2.7159 0.1235 0.0323 S381 2.2850 2.2137 0.0175 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0267	Molecule				$f_{12}(S_0-S_1)$
S371 2.3935 2.4286 -0.0351 0.0097 S372 2.3853 2.4124 -0.0271 0.0081 S373 2.4281 2.4662 -0.0381 0.0054 S374 2.3882 2.4296 -0.0414 0.0089 S375 2.2947 2.2418 0.0529 0.0111 S376 2.3331 2.3448 -0.0117 0.0044 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S384 2.4090 2.4296 -0.0206 0.063 S385 2.4705 2.4940 -0.0235 0.0667 S386 2.4744 2.5270 -0.0526 0	S369	2.3569	2.3535	0.0034	0.0090
S372 2.3853 2.4124 -0.0271 0.0081 S373 2.4281 2.4662 -0.0381 0.0054 S374 2.3882 2.4296 -0.0414 0.0089 S375 2.2947 2.2418 0.0529 0.0111 S376 2.3331 2.3448 -0.0117 0.0044 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.063 S385 2.4705 2.4940 -0.0225 0.0067 S386 2.4744 2.5270 -0.0526 0	S370	2.3534	2.3944	-0.0410	0.0059
S373 2.4281 2.4662 -0.0381 0.0054 S374 2.3882 2.4296 -0.0414 0.0089 S375 2.2947 2.2418 0.0529 0.0111 S376 2.3331 2.3448 -0.0117 0.0044 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0	S371	2.3935	2.4286	-0.0351	0.0097
S374 2.3882 2.4296 -0.0414 0.0089 S375 2.2947 2.2418 0.0529 0.0111 S376 2.3331 2.3448 -0.0117 0.0044 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S384 2.4090 2.4296 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4957 2.5652 -0.0695 0	S372	2.3853	2.4124	-0.0271	0.0081
S375 2.2947 2.2418 0.0529 0.0111 S376 2.3331 2.3448 -0.017 0.0048 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.	S373	2.4281	2.4662	-0.0381	0.0054
S376 2.3331 2.3448 -0.0117 0.0044 S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.	S374	2.3882	2.4296	-0.0414	0.0089
S377 2.4518 2.5088 -0.0570 0.0086 S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.47444 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.083 S391 2.4076 2.4359 -0.0283 0	S375	2.2947	2.2418	0.0529	0.0111
S378 2.8201 2.8924 -0.0723 0.0002 S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0	S376	2.3331	2.3448	-0.0117	0.0044
S379 2.8394 2.7159 0.1235 0.0323 S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0206 0.0063 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0	S377	2.4518	2.5088	-0.0570	0.0086
S380 2.3104 2.2029 0.1075 0.0108 S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0118 S395 2.3767 2.3738 0.0029 0	S378	2.8201	2.8924	-0.0723	0.0002
S381 2.2850 2.2137 0.0713 0.0101 S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029	S379	2.8394	2.7159	0.1235	0.0323
S382 2.3129 2.3338 -0.0209 0.0052 S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254	S380	2.3104	2.2029	0.1075	0.0108
S383 2.5035 2.5708 -0.0673 0.0065 S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.	S381	2.2850	2.2137	0.0713	0.0101
S384 2.4090 2.4296 -0.0206 0.0063 S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S490 2.6415 2.5738 0.0677 0.0	S382	2.3129	2.3338	-0.0209	0.0052
S385 2.4705 2.4940 -0.0235 0.0067 S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S400 2.6415 2.5738 0.0677 0.02	S383	2.5035	2.5708	-0.0673	0.0065
S386 2.4744 2.5270 -0.0526 0.0063 S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.01	S384	2.4090	2.4296	-0.0206	0.0063
S387 2.2576 2.1609 0.0967 0.0101 S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.01	S385	2.4705	2.4940	-0.0235	0.0067
S388 2.4270 2.4528 -0.0258 0.0042 S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197	S386	2.4744	2.5270	-0.0526	0.0063
S389 2.4957 2.5652 -0.0695 0.0077 S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 <	S387	2.2576	2.1609	0.0967	0.0101
S390 2.3579 2.3510 0.0069 0.0083 S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 <	S388	2.4270	2.4528	-0.0258	0.0042
S391 2.4076 2.4359 -0.0283 0.0039 S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138	S389	2.4957	2.5652	-0.0695	0.0077
S392 2.4844 2.5531 -0.0687 0.0057 S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0096	S390	2.3579	2.3510	0.0069	0.0083
S393 2.4629 2.4944 -0.0315 0.0124 S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119	S391	2.4076	2.4359	-0.0283	0.0039
S394 2.4421 2.4606 -0.0185 0.0118 S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S410 2.4578 2.4771 -0.0193 0.0109	S392	2.4844	2.5531	-0.0687	0.0057
S395 2.3767 2.3738 0.0029 0.0115 S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109	S393	2.4629	2.4944	-0.0315	0.0124
S396 2.7725 2.7471 0.0254 0.0148 S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134	S394	2.4421	2.4606	-0.0185	0.0118
S397 2.7037 2.5951 0.1086 0.0374 S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100	S395	2.3767	2.3738	0.0029	0.0115
S398 2.2663 2.1694 0.0969 0.0149 S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S396	2.7725	2.7471	0.0254	0.0148
S399 2.6747 2.6834 -0.0087 0.0109 S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S397	2.7037	2.5951	0.1086	0.0374
S400 2.6415 2.5738 0.0677 0.0286 S401 2.2668 2.1562 0.1106 0.0159 S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S398	2.2663	2.1694	0.0969	0.0149
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S399	2.6747	2.6834	-0.0087	0.0109
S402 2.5464 2.5975 -0.0511 0.0084 S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S400	2.6415	2.5738	0.0677	0.0286
S403 2.5621 2.5380 0.0241 0.0197 S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S401	2.2668	2.1562	0.1106	0.0159
S404 2.2912 2.2633 0.0279 0.0137 S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S402	2.5464	2.5975	-0.0511	0.0084
S405 2.4871 2.5203 -0.0332 0.0158 S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S403	2.5621	2.5380	0.0241	0.0197
S406 2.4966 2.5031 -0.0065 0.0138 S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S404	2.2912	2.2633	0.0279	0.0137
S407 2.3928 2.4296 -0.0368 0.0086 S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S405	2.4871	2.5203	-0.0332	0.0158
S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S406	2.4966	2.5031	-0.0065	0.0138
S408 2.4274 2.4660 -0.0386 0.0119 S409 2.3120 2.3241 -0.0121 0.0105 S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102					
S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S408	2.4274	2.4660	-0.0386	0.0119
S410 2.4578 2.4771 -0.0193 0.0109 S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102	S409	2.3120	2.3241	-0.0121	0.0105
S411 2.4079 2.4402 -0.0323 0.0134 S412 2.4423 2.4665 -0.0242 0.0100 S413 2.3165 2.3327 -0.0162 0.0102			2.4771		0.0109
S413 2.3165 2.3327 -0.0162 0.0102	S411	2.4079	2.4402	-0.0323	0.0134
S413 2.3165 2.3327 -0.0162 0.0102	S412	2.4423	2.4665	-0.0242	0.0100
	S413	2.3165	2.3327	-0.0162	0.0102
S414 2.8243 2.7625 0.0618 0.0164	S414	2.8243	2.7625	0.0618	0.0164

	FNO-EOM-CCSD/aug-cc-pVDZ				
Molecule	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{S}_1)~[\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_0\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$\Delta \mathrm{E}(\mathrm{S}_1\text{-}\mathrm{T}_1) \; [\mathrm{eV}]$	$f_{12}(S_0-S_1)$	
S415	2.7375	2.6065	0.1310	0.0417	
S416	2.3160	2.2759	0.0401	0.0123	
S417	2.3749	2.3606	0.0143	0.0231	
S418	2.3706	2.4178	-0.0472	0.0068	
S419	2.3331	2.3496	-0.0165	0.0081	
S420	2.2542	2.1735	0.0807	0.0190	
S421	2.2775	2.3247	-0.0472	0.0029	
S422	2.4538	2.5319	-0.0781	0.0040	
S423	2.2964	2.2788	0.0176	0.0191	
S424	2.3232	2.3793	-0.0561	0.0048	
S425	2.3652	2.4062	-0.0410	0.0081	
S426	2.3401	2.3485	-0.0084	0.0163	
S427	2.3966	2.4354	-0.0388	0.0068	
S428	2.3550	2.3962	-0.0412	0.0082	
S429	2.2586	2.2005	0.0581	0.0167	
S430	2.3132	2.3545	-0.0413	0.0037	
S431	2.4380	2.5071	-0.0691	0.0065	
S432	2.8232	2.7670	0.0562	0.0216	
S433	2.7540	2.6147	0.1393	0.0433	
S434	2.3247	2.2781	0.0466	0.0122	
S435	2.2423	2.1756	0.0667	0.0177	
S436	2.2870	2.3378	-0.0508	0.0037	
S437	2.5254	2.5830	-0.0576	0.0063	
S438	2.3872	2.3809	0.0063	0.0158	
S439	2.4121	2.4395	-0.0274	0.0085	
S440	2.4059	2.4568	-0.0509	0.0074	
S441	2.2511	2.1839	0.0672	0.0147	
S442	2.4067	2.4352	-0.0285	0.0072	
S443	2.5310	2.6112	-0.0802	0.0047	
S444	2.3339	2.3159	0.0180	0.0126	
S445	2.3590	2.3983	-0.0393	0.0058	
S446	2.4640	2.5245	-0.0605	0.0074	