

Molecule	ADC(2)/cc-pVDZ			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S1	1.0381	1.1983	-0.1603	0.0000
S2	0.9222	1.0459	-0.1237	0.0006
S3	1.3804	1.4912	-0.1107	0.0005
S4	1.5935	1.7419	-0.1484	0.0022
S5	1.5177	1.4277	0.0900	0.0001
S6	1.3599	1.4992	-0.1394	0.0002
S7	1.7317	1.7968	-0.0651	0.0006
S8	1.2941	1.3597	-0.0655	0.0018
S9	1.4256	1.5748	-0.1492	0.0003
S10	1.8155	1.7417	0.0738	0.0012
S11	1.5362	1.6859	-0.1498	0.0025
S12	1.8027	1.9607	-0.1580	0.0016
S13	1.8626	1.9908	-0.1282	0.0038
S14	2.0412	2.2121	-0.1709	0.0045
S15	1.4790	1.5381	-0.0591	0.0008
S16	1.8052	1.8681	-0.0629	0.0000
S17	1.6339	1.7647	-0.1308	0.0017
S18	1.8182	2.0021	-0.1839	0.0000
S19	1.3486	1.3544	-0.0058	0.0021
S20	1.3970	1.4771	-0.0802	0.0064
S21	0.8086	0.9141	-0.1055	0.0005
S22	1.3172	1.2661	0.0510	0.0023
S23	1.6135	1.3711	0.2423	0.0005
S24	1.4216	1.3843	0.0373	0.0032
S25	1.6883	1.6649	0.0234	0.0033
S26	1.4853	1.5769	-0.0916	0.0039
S27	1.7351	1.7890	-0.0538	0.0086
S28	1.5609	1.3938	0.1671	0.0010
S29	1.8650	1.7011	0.1639	0.0021
S30	1.2663	1.3792	-0.1129	0.0003
S31	1.5268	1.6150	-0.0882	0.0040
S32	1.8977	1.7521	0.1457	0.0005
S33	1.7684	1.7728	-0.0044	0.0051
S34	1.3426	1.4105	-0.0679	0.0010
S35	2.1180	1.8201	0.2979	0.0002
S36	1.9718	1.8354	0.1364	0.0014
S37	1.5709	1.6879	-0.1170	0.0035
S38	1.9220	1.8985	0.0236	0.0025
S39	1.9078	1.9741	-0.0663	0.0076
S40	1.2191	1.3430	-0.1239	0.0000
S41	1.5459	1.6382	-0.0923	0.0017
S42	1.8335	1.8074	0.0261	0.0018
S43	1.7758	1.8771	-0.1013	0.0004
S44	1.5292	1.7042	-0.1750	0.0002
S45	1.3842	1.4706	-0.0865	0.0024
S46	2.0624	2.1014	-0.0390	0.0000

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S47	1.8524	2.0150	-0.1626	0.0006
S48	1.6620	1.7581	-0.0960	0.0016
S49	1.7703	1.8677	-0.0975	0.0021
S50	1.7509	1.8228	-0.0719	0.0042
S51	2.1527	2.2927	-0.1400	0.0017
S52	2.0927	2.2665	-0.1738	0.0024
S53	2.3326	2.5414	-0.2088	0.0017
S54	2.2186	2.2233	-0.0047	0.0010
S55	1.8594	1.9969	-0.1375	0.0025
S56	2.1257	2.2943	-0.1686	0.0011
S57	1.9330	1.6844	0.2486	0.0021
S58	1.1270	1.2007	-0.0737	0.0027
S59	1.4915	1.4913	0.0002	0.0057
S60	2.1763	2.0575	0.1188	0.0012
S61	2.1134	2.1226	-0.0092	0.0072
S62	2.4029	2.1324	0.2705	0.0003
S63	1.7246	1.6950	0.0295	0.0022
S64	2.0664	2.0084	0.0580	0.0050
S65	1.7493	1.8985	-0.1492	0.0060
S66	1.6458	1.6840	-0.0381	0.0007
S67	1.6446	1.7503	-0.1057	0.0038
S68	1.9641	2.0520	-0.0879	0.0038
S69	2.0458	2.1993	-0.1535	0.0086
S70	2.1797	2.1357	0.0440	0.0022
S71	1.6294	1.8024	-0.1730	0.0007
S72	1.8978	2.0618	-0.1640	0.0035
S73	2.0370	2.2464	-0.2094	0.0001
S74	1.8800	2.0230	-0.1430	0.0020
S75	1.3709	1.4355	-0.0646	0.0044
S76	1.8611	1.7567	0.1043	0.0063
S77	1.9699	2.0620	-0.0921	0.0068
S78	1.7496	1.7728	-0.0231	0.0030
S79	1.7535	1.8547	-0.1012	0.0033
S80	2.3287	2.2050	0.1236	0.0033
S81	2.2453	2.3332	-0.0879	0.0060
S82	1.6986	1.8669	-0.1683	0.0009
S83	2.1816	2.2561	-0.0745	0.0005
S84	2.5780	2.8559	-0.2779	0.0000
S85	2.3000	2.2651	0.0349	0.0064
S86	1.6502	1.6907	-0.0405	0.0100
S87	2.0364	2.0534	-0.0171	0.0082
S88	2.0596	2.0124	0.0471	0.0046
S89	0.6932	0.7907	-0.0974	0.0000
S90	1.7001	1.3645	0.3356	0.0011
S91	1.0765	1.1510	-0.0746	0.0010
S92	2.2112	1.8077	0.4035	0.0018

Molecule	ADC(2)/cc-pVDZ			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S93	1.1436	1.2541	-0.1105	0.0001
S94	1.8463	1.7146	0.1317	0.0004
S95	1.8582	1.7243	0.1340	0.0045
S96	1.5176	1.6748	-0.1572	0.0000
S97	1.0368	1.1344	-0.0976	0.0008
S98	2.7007	2.2808	0.4199	0.0000
S99	1.8001	1.6257	0.1743	0.0038
S100	1.4161	1.5691	-0.1531	0.0010
S101	2.4308	2.2076	0.2232	0.0033
S102	1.4762	1.5971	-0.1209	0.0018
S103	2.1410	2.0564	0.0846	0.0026
S104	1.8341	1.9302	-0.0961	0.0000
S105	1.0793	1.2439	-0.1646	0.0000
S106	1.0972	1.2263	-0.1292	0.0000
S107	1.3134	1.4642	-0.1508	0.0026
S108	1.1412	1.1570	-0.0158	0.0006
S109	1.2731	1.4303	-0.1572	0.0018
S110	1.1333	1.1248	0.0085	0.0007
S111	1.1899	1.3584	-0.1686	0.0007
S112	1.0140	1.1125	-0.0985	0.0004
S113	1.1162	1.2841	-0.1679	0.0001
S114	1.0020	1.1295	-0.1275	0.0004
S115	1.0734	1.2366	-0.1632	0.0000
S116	0.9981	1.1544	-0.1563	0.0002
S117	1.0552	1.2146	-0.1594	0.0000
S118	1.0045	1.1633	-0.1588	0.0002
S119	1.3500	1.4877	-0.1377	0.0034
S120	1.0213	1.1431	-0.1218	0.0002
S121	0.9872	1.1107	-0.1236	0.0007
S122	1.0557	1.2090	-0.1533	0.0005
S123	0.8691	0.9394	-0.0703	0.0012
S124	1.3215	1.4436	-0.1222	0.0006
S125	0.9345	1.0715	-0.1369	0.0004
S126	1.0943	1.2431	-0.1488	0.0005
S127	0.9756	1.1201	-0.1445	0.0003
S128	1.0811	1.2357	-0.1546	0.0005
S129	0.9085	1.0176	-0.1091	0.0007
S130	1.1930	1.3237	-0.1307	0.0004
S131	1.3395	1.4817	-0.1422	0.0033
S132	1.0046	1.1596	-0.1550	0.0001
S133	0.8484	0.9452	-0.0968	0.0009
S134	1.3032	1.4215	-0.1183	0.0007
S135	1.0128	1.1453	-0.1326	0.0001
S136	1.1024	1.2635	-0.1611	0.0002
S137	0.8628	0.9383	-0.0755	0.0008
S138	1.3637	1.4659	-0.1022	0.0006

Molecule	ADC(2)/cc-pVDZ			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S139	0.9630	1.0968	-0.1338	0.0003
S140	1.1631	1.3178	-0.1547	0.0002
S141	2.6291	2.9075	-0.2784	0.0001
S142	2.9648	3.1741	-0.2093	0.0142
S143	2.8799	3.1287	-0.2487	0.0078
S144	2.7894	3.0666	-0.2773	0.0031
S145	2.6933	2.9736	-0.2803	0.0007
S146	2.6437	2.9239	-0.2802	0.0001
S147	2.6195	2.8962	-0.2767	0.0000
S148	2.9909	3.1876	-0.1967	0.0160
S149	2.5581	2.8238	-0.2657	0.0002
S150	2.4438	2.6696	-0.2258	0.0015
S151	2.4998	2.7560	-0.2562	0.0006
S152	2.5625	2.8273	-0.2648	0.0002
S153	2.4716	2.7011	-0.2295	0.0013
S154	2.9979	3.1921	-0.1942	0.0158
S155	2.4547	2.6846	-0.2299	0.0011
S156	2.5620	2.6955	-0.1335	0.0014
S157	2.5848	2.8451	-0.2602	0.0001
S158	2.5297	2.7863	-0.2566	0.0004
S159	1.5825	1.7423	-0.1597	0.0021
S160	1.5868	1.7322	-0.1453	0.0042
S161	1.5513	1.6869	-0.1357	0.0028
S162	1.5358	1.6702	-0.1344	0.0030
S163	1.8604	2.0408	-0.1804	0.0001
S164	1.8589	1.9358	-0.0768	0.0131
S165	1.4709	1.5304	-0.0595	0.0057
S166	1.4390	1.5253	-0.0863	0.0031
S167	1.7908	1.9783	-0.1875	0.0000
S168	1.8206	1.9074	-0.0869	0.0106
S169	1.4559	1.5486	-0.0927	0.0048
S170	1.4276	1.4952	-0.0676	0.0035
S171	1.6908	1.8803	-0.1895	0.0004
S172	1.7254	1.8512	-0.1258	0.0063
S173	1.4260	1.5399	-0.1139	0.0048
S174	1.4346	1.5528	-0.1182	0.0031
S175	1.6141	1.7852	-0.1711	0.0016
S176	1.6352	1.7748	-0.1397	0.0053
S177	1.5410	1.6979	-0.1569	0.0033
S178	1.5655	1.7162	-0.1507	0.0017
S179	1.5596	1.7206	-0.1610	0.0023
S180	1.5964	1.7398	-0.1434	0.0036
S181	1.4636	1.6089	-0.1453	0.0041
S182	1.4803	1.6261	-0.1458	0.0018
S183	1.5389	1.6926	-0.1537	0.0027
S184	1.5774	1.7198	-0.1424	0.0036

Molecule	ADC(2)/cc-pVDZ			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S185	1.4698	1.6182	-0.1483	0.0042
S186	1.4878	1.6359	-0.1481	0.0016
S187	1.9031	2.0739	-0.1708	0.0005
S188	1.9151	1.9609	-0.0459	0.0158
S189	1.4717	1.5852	-0.1135	0.0044
S190	1.4571	1.5190	-0.0619	0.0029
S191	1.4520	1.5665	-0.1146	0.0053
S192	1.5156	1.6496	-0.1339	0.0059
S193	1.5057	1.6463	-0.1406	0.0051
S194	1.5077	1.6555	-0.1477	0.0009
S195	1.3098	1.3604	-0.0506	0.0072
S196	1.4317	1.5206	-0.0888	0.0031
S197	1.6412	1.7847	-0.1435	0.0053
S198	1.6657	1.8132	-0.1474	0.0006
S199	1.4171	1.5275	-0.1104	0.0052
S200	1.4560	1.5908	-0.1349	0.0036
S201	1.5322	1.6814	-0.1493	0.0057
S202	1.5564	1.7075	-0.1511	0.0006
S203	1.4470	1.5735	-0.1265	0.0047
S204	1.5100	1.6495	-0.1395	0.0033
S205	1.5228	1.6729	-0.1501	0.0051
S206	1.5525	1.7051	-0.1526	0.0007
S207	1.3669	1.4456	-0.0788	0.0062
S208	1.4490	1.5555	-0.1064	0.0024
S209	1.5949	1.7447	-0.1498	0.0050
S210	1.6506	1.8004	-0.1498	0.0005
S211	1.8849	2.0562	-0.1714	0.0003
S212	1.8870	1.9526	-0.0656	0.0167
S213	1.4825	1.5969	-0.1144	0.0043
S214	1.4750	1.5967	-0.1216	0.0023
S215	1.3235	1.3851	-0.0615	0.0065
S216	1.3986	1.5029	-0.1042	0.0035
S217	1.6652	1.8059	-0.1407	0.0060
S218	1.7483	1.8861	-0.1378	0.0003
S219	1.4776	1.6004	-0.1228	0.0037
S220	1.5403	1.6661	-0.1258	0.0040
S221	1.5661	1.7283	-0.1622	0.0033
S222	1.5674	1.7244	-0.1571	0.0015
S223	1.3214	1.3645	-0.0432	0.0061
S224	1.4512	1.5470	-0.0958	0.0023
S225	1.7024	1.8421	-0.1397	0.0048
S226	1.7790	1.9177	-0.1387	0.0004
S227	1.4335	1.5444	-0.1109	0.0048
S228	1.5085	1.6311	-0.1226	0.0021
S229	1.6000	1.7642	-0.1642	0.0029
S230	1.6547	1.8073	-0.1527	0.0016

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S231	1.9030	2.0436	-0.1406	0.0033
S232	1.9168	2.0439	-0.1271	0.0068
S233	1.8983	2.0235	-0.1252	0.0048
S234	1.8273	1.9538	-0.1265	0.0042
S235	1.8937	1.9900	-0.0963	0.0042
S236	1.8894	1.9891	-0.0997	0.0048
S237	2.1773	2.3290	-0.1517	0.0007
S238	2.1351	2.2214	-0.0863	0.0168
S239	2.2005	2.2253	-0.0248	0.0235
S240	1.6725	1.7388	-0.0663	0.0077
S241	1.7907	1.7498	0.0410	0.0090
S242	1.8097	1.8327	-0.0230	0.0064
S243	2.1147	2.2710	-0.1562	0.0007
S244	2.0591	2.1756	-0.1165	0.0109
S245	2.1544	2.2043	-0.0499	0.0176
S246	1.6488	1.7090	-0.0602	0.0092
S247	1.8328	1.8218	0.0109	0.0076
S248	1.8199	1.8224	-0.0025	0.0070
S249	2.0063	2.1730	-0.1668	0.0013
S250	1.9822	2.1307	-0.1485	0.0058
S251	2.0781	2.1628	-0.0847	0.0119
S252	1.7038	1.8069	-0.1031	0.0073
S253	1.8174	1.8772	-0.0597	0.0058
S254	1.7737	1.8563	-0.0826	0.0057
S255	1.9413	2.0931	-0.1518	0.0028
S256	1.9093	2.0493	-0.1400	0.0088
S257	1.9690	2.0798	-0.1107	0.0068
S258	1.7176	1.8239	-0.1063	0.0069
S259	1.7861	1.8465	-0.0603	0.0086
S260	1.8786	2.0110	-0.1324	0.0022
S261	1.8840	2.0265	-0.1425	0.0037
S262	1.8744	2.0160	-0.1416	0.0051
S263	1.7681	1.8943	-0.1262	0.0057
S264	1.7883	1.9026	-0.1143	0.0067
S265	1.8205	1.9288	-0.1083	0.0030
S266	1.9399	2.0554	-0.1155	0.0054
S267	1.8643	1.9997	-0.1354	0.0041
S268	1.8556	1.9939	-0.1383	0.0054
S269	1.9193	2.0360	-0.1167	0.0049
S270	1.7776	1.9055	-0.1280	0.0056
S271	1.7899	1.9086	-0.1187	0.0072
S272	1.8196	1.9346	-0.1150	0.0027
S273	2.2265	2.3624	-0.1359	0.0007
S274	2.1449	2.2144	-0.0695	0.0189
S275	2.2338	2.2392	-0.0054	0.0253
S276	1.6584	1.7105	-0.0520	0.0080

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S277	1.8219	1.7318	0.0900	0.0108
S278	1.8233	1.8949	-0.0715	0.0044
S279	1.8070	1.9055	-0.0985	0.0061
S280	1.8624	1.9461	-0.0837	0.0134
S281	1.7951	1.9397	-0.1446	0.0031
S282	1.8118	1.9332	-0.1214	0.0052
S283	1.7570	1.8496	-0.0927	0.0122
S284	1.8211	1.9413	-0.1202	0.0015
S285	1.6348	1.6776	-0.0428	0.0096
S286	1.8091	1.8263	-0.0173	0.0076
S287	1.7039	1.8300	-0.1261	0.0017
S288	1.9519	2.0900	-0.1382	0.0037
S289	1.8704	2.0456	-0.1752	0.0003
S290	1.9003	2.0339	-0.1336	0.0096
S291	1.7540	1.8496	-0.0956	0.0071
S292	1.7966	1.8784	-0.0818	0.0087
S293	1.7719	1.9064	-0.1346	0.0020
S294	1.8404	1.9744	-0.1340	0.0058
S295	1.8054	1.9237	-0.1183	0.0105
S296	1.8360	1.9743	-0.1383	0.0011
S297	1.7786	1.8907	-0.1120	0.0067
S298	1.8234	1.9287	-0.1053	0.0066
S299	1.8536	1.9784	-0.1248	0.0030
S300	1.8271	1.9632	-0.1361	0.0053
S301	1.8170	1.9359	-0.1189	0.0092
S302	1.8523	1.9830	-0.1307	0.0011
S303	1.7019	1.7647	-0.0628	0.0087
S304	1.7999	1.8430	-0.0431	0.0053
S305	1.7703	1.8847	-0.1144	0.0020
S306	1.9023	2.0426	-0.1402	0.0047
S307	1.8490	1.9828	-0.1338	0.0104
S308	1.8941	2.0528	-0.1587	0.0005
S309	2.1959	2.3386	-0.1427	0.0008
S310	2.1452	2.2224	-0.0772	0.0232
S311	2.2204	2.2382	-0.0178	0.0242
S312	1.7523	1.8545	-0.1022	0.0061
S313	1.7833	1.7910	-0.0077	0.0097
S314	1.8316	1.9004	-0.0688	0.0042
S315	1.6619	1.7114	-0.0494	0.0082
S316	1.7497	1.7851	-0.0354	0.0078
S317	1.7164	1.8479	-0.1315	0.0013
S318	1.9534	2.0928	-0.1394	0.0053
S319	1.9797	2.1296	-0.1499	0.0006
S320	1.8728	2.0059	-0.1330	0.0098
S321	1.7869	1.8970	-0.1101	0.0062
S322	1.8727	1.9690	-0.0963	0.0066

Molecule	ADC(2)/cc-pVDZ			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S323	1.8831	1.9957	-0.1126	0.0043
S324	1.8624	2.0076	-0.1452	0.0033
S325	1.8720	2.0172	-0.1451	0.0016
S326	1.8979	2.0251	-0.1272	0.0076
S327	1.6637	1.6923	-0.0286	0.0085
S328	1.7874	1.8251	-0.0377	0.0045
S329	1.8779	1.9873	-0.1094	0.0034
S330	1.9837	2.1261	-0.1424	0.0035
S331	1.9705	2.1414	-0.1709	0.0008
S332	1.8822	2.0290	-0.1468	0.0096
S333	1.7696	1.8617	-0.0922	0.0067
S334	1.8651	1.9413	-0.0761	0.0038
S335	1.8430	1.9576	-0.1146	0.0027
S336	1.9078	2.0572	-0.1495	0.0036
S337	1.8971	2.0414	-0.1443	0.0059
S338	1.9440	2.0943	-0.1503	0.0012
S339	2.1396	2.3239	-0.1843	0.0018
S340	2.1455	2.3128	-0.1672	0.0042
S341	2.0751	2.2267	-0.1516	0.0028
S342	2.4126	2.6099	-0.1973	0.0008
S343	2.4502	2.5198	-0.0696	0.0210
S344	1.8791	1.8959	-0.0168	0.0073
S345	2.3253	2.5373	-0.2121	0.0001
S346	2.3882	2.4933	-0.1050	0.0141
S347	1.9002	1.9666	-0.0665	0.0073
S348	2.2302	2.4487	-0.2186	0.0002
S349	2.3084	2.4520	-0.1436	0.0079
S350	1.9526	2.0858	-0.1332	0.0051
S351	2.1736	2.3741	-0.2006	0.0013
S352	2.1950	2.3554	-0.1604	0.0060
S353	1.9501	2.0633	-0.1132	0.0066
S354	2.1176	2.3077	-0.1901	0.0021
S355	1.9922	2.1517	-0.1595	0.0046
S356	2.1629	2.3284	-0.1655	0.0036
S357	2.0987	2.2809	-0.1822	0.0025
S358	2.1402	2.3055	-0.1653	0.0033
S359	1.9976	2.1596	-0.1620	0.0048
S360	2.4370	2.6254	-0.1883	0.0014
S361	2.4734	2.5354	-0.0620	0.0240
S362	1.8559	1.9010	-0.0451	0.0077
S363	2.0401	2.1848	-0.1447	0.0050
S364	2.0290	2.2008	-0.1718	0.0028
S365	2.0249	2.1718	-0.1469	0.0048
S366	1.9140	1.9854	-0.0714	0.0080
S367	1.9381	2.0754	-0.1373	0.0024
S368	2.1175	2.2991	-0.1816	0.0056

Molecule	ADC(2)/cc-pVDZ			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S369	2.0056	2.1412	-0.1356	0.0054
S370	1.9997	2.1618	-0.1621	0.0032
S371	2.0251	2.1905	-0.1654	0.0061
S372	2.0263	2.1806	-0.1543	0.0049
S373	2.0745	2.2358	-0.1614	0.0028
S374	2.0306	2.2006	-0.1699	0.0051
S375	1.9545	2.0547	-0.1002	0.0070
S376	1.9885	2.1264	-0.1379	0.0023
S377	2.0853	2.2679	-0.1826	0.0054
S378	2.4255	2.6128	-0.1874	0.0012
S379	2.4719	2.5272	-0.0552	0.0243
S380	1.8839	1.9314	-0.0475	0.0079
S381	1.9302	2.0119	-0.0818	0.0071
S382	1.9549	2.0970	-0.1421	0.0031
S383	2.1284	2.3188	-0.1904	0.0035
S384	2.0420	2.1939	-0.1519	0.0037
S385	2.1097	2.2617	-0.1520	0.0028
S386	2.0953	2.2703	-0.1750	0.0036
S387	1.9236	1.9890	-0.0654	0.0067
S388	2.0933	2.2413	-0.1480	0.0020
S389	2.1194	2.3125	-0.1931	0.0044
S390	2.0096	2.1448	-0.1352	0.0050
S391	2.0612	2.2150	-0.1537	0.0018
S392	2.1244	2.3185	-0.1941	0.0029
S393	2.0986	2.2708	-0.1722	0.0063
S394	2.0805	2.2434	-0.1629	0.0059
S395	2.0254	2.1752	-0.1498	0.0056
S396	2.4303	2.5581	-0.1278	0.0097
S397	2.3661	2.4211	-0.0550	0.0292
S398	1.8763	1.9412	-0.0649	0.0093
S399	2.3376	2.4915	-0.1539	0.0065
S400	2.3073	2.3975	-0.0902	0.0214
S401	1.8684	1.9219	-0.0535	0.0104
S402	2.2268	2.4141	-0.1873	0.0039
S403	2.2418	2.3640	-0.1221	0.0143
S404	1.9055	2.0234	-0.1179	0.0086
S405	2.1403	2.3165	-0.1762	0.0074
S406	2.1423	2.2929	-0.1506	0.0081
S407	2.0375	2.2144	-0.1769	0.0041
S408	2.0863	2.2639	-0.1776	0.0055
S409	1.9507	2.1067	-0.1560	0.0059
S410	2.1127	2.2698	-0.1570	0.0062
S411	2.0644	2.2371	-0.1727	0.0062
S412	2.0916	2.2509	-0.1593	0.0053
S413	1.9561	2.1162	-0.1602	0.0056
S414	2.4583	2.5654	-0.1070	0.0114

Molecule	ADC(2)/cc-pVDZ			
	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S415	2.3862	2.4304	-0.0442	0.0311
S416	1.9367	2.0488	-0.1120	0.0068
S417	2.0163	2.1542	-0.1379	0.0133
S418	2.0121	2.1892	-0.1771	0.0028
S419	1.9750	2.1311	-0.1561	0.0040
S420	1.8981	1.9854	-0.0873	0.0108
S421	1.9251	2.0920	-0.1669	0.0007
S422	2.0981	2.3012	-0.2031	0.0020
S423	1.9479	2.0816	-0.1337	0.0101
S424	1.9694	2.1483	-0.1789	0.0017
S425	2.0084	2.1815	-0.1731	0.0045
S426	1.9912	2.1419	-0.1507	0.0086
S427	2.0425	2.2101	-0.1676	0.0030
S428	2.0070	2.1810	-0.1740	0.0043
S429	1.9166	2.0186	-0.1020	0.0090
S430	1.9659	2.1274	-0.1615	0.0011
S431	2.0814	2.2752	-0.1938	0.0033
S432	2.4413	2.5582	-0.1169	0.0142
S433	2.3891	2.4334	-0.0442	0.0305
S434	1.9335	2.0389	-0.1054	0.0067
S435	1.8837	1.9744	-0.0907	0.0104
S436	1.9314	2.1037	-0.1722	0.0010
S437	2.1512	2.3362	-0.1850	0.0032
S438	2.0243	2.1654	-0.1412	0.0081
S439	2.0498	2.2104	-0.1605	0.0037
S440	2.0379	2.2233	-0.1854	0.0032
S441	1.9189	2.0105	-0.0916	0.0079
S442	2.0722	2.2270	-0.1548	0.0035
S443	2.1641	2.3662	-0.2022	0.0024
S444	1.9852	2.1169	-0.1317	0.0067
S445	2.0153	2.1822	-0.1669	0.0023
S446	2.1097	2.3034	-0.1937	0.0031