

Molecule	ADC(2)/aug-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	1.0056	1.1497	-0.1440	0.0000
S2	0.8731	0.9778	-0.1047	0.0008
S3	1.3699	1.4588	-0.0889	0.0018
S4	1.5931	1.7241	-0.1310	0.0038
S5	1.4755	1.3756	0.0999	0.0000
S6	1.3523	1.4615	-0.1093	0.0000
S7	1.7286	1.7717	-0.0431	0.0013
S8	1.2675	1.3124	-0.0449	0.0022
S9	1.4043	1.5394	-0.1351	0.0002
S10	1.7859	1.7066	0.0793	0.0012
S11	1.5285	1.6575	-0.1290	0.0049
S12	1.8096	1.9386	-0.1290	0.0034
S13	1.8685	1.9785	-0.1100	0.0067
S14	2.0551	2.1963	-0.1412	0.0082
S15	1.4604	1.5025	-0.0420	0.0021
S16	1.7849	1.8384	-0.0535	0.0002
S17	1.6269	1.7316	-0.1047	0.0021
S18	1.8312	1.9766	-0.1454	0.0005
S19	1.3115	1.3021	0.0094	0.0032
S20	1.3738	1.4255	-0.0518	0.0106
S21	0.7441	0.8289	-0.0848	0.0006
S22	1.2714	1.1956	0.0758	0.0030
S23	1.5398	1.2989	0.2408	0.0010
S24	1.3728	1.3263	0.0466	0.0052
S25	1.6675	1.6206	0.0470	0.0047
S26	1.4730	1.5388	-0.0658	0.0057
S27	1.7271	1.7543	-0.0272	0.0125
S28	1.5002	1.3262	0.1740	0.0012
S29	1.8121	1.6488	0.1633	0.0031
S30	1.2399	1.3342	-0.0942	0.0004
S31	1.5142	1.5664	-0.0522	0.0061
S32	1.8555	1.7089	0.1466	0.0008
S33	1.7384	1.7353	0.0031	0.0073
S34	1.2993	1.3551	-0.0557	0.0012
S35	2.0502	1.7639	0.2863	0.0005
S36	1.9097	1.7754	0.1343	0.0020
S37	1.5616	1.6488	-0.0872	0.0060
S38	1.9043	1.8719	0.0324	0.0044
S39	1.9073	1.9544	-0.0471	0.0114
S40	1.1959	1.2946	-0.0988	0.0001
S41	1.5280	1.6078	-0.0798	0.0022
S42	1.8016	1.7693	0.0322	0.0018
S43	1.7608	1.8650	-0.1042	0.0010
S44	1.5234	1.6783	-0.1549	0.0002
S45	1.3536	1.4183	-0.0647	0.0030
S46	2.0674	2.0826	-0.0152	0.0000

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S47	1.8560	2.0099	-0.1539	0.0010
S48	1.6595	1.7259	-0.0664	0.0010
S49	1.7747	1.8423	-0.0676	0.0042
S50	1.7327	1.7857	-0.0530	0.0052
S51	2.1618	2.2883	-0.1265	0.0028
S52	2.1121	2.2598	-0.1477	0.0047
S53	2.3657	2.5540	-0.1883	0.0048
S54	2.2062	2.2018	0.0044	0.0014
S55	1.8665	1.9761	-0.1096	0.0030
S56	2.1390	2.2803	-0.1413	0.0007
S57	1.8766	1.6245	0.2522	0.0027
S58	1.0965	1.1489	-0.0524	0.0033
S59	1.4654	1.4471	0.0182	0.0084
S60	2.1539	2.0263	0.1275	0.0010
S61	2.0940	2.0897	0.0042	0.0117
S62	2.3441	2.0828	0.2613	0.0002
S63	1.6899	1.6460	0.0439	0.0015
S64	2.0239	1.9569	0.0670	0.0055
S65	1.7466	1.8795	-0.1330	0.0076
S66	1.6221	1.6448	-0.0227	0.0007
S67	1.6291	1.7107	-0.0816	0.0043
S68	1.9646	2.0216	-0.0570	0.0034
S69	2.0565	2.1774	-0.1209	0.0130
S70	2.1440	2.1043	0.0396	0.0022
S71	1.6277	1.7745	-0.1469	0.0004
S72	1.9058	2.0405	-0.1347	0.0039
S73	2.0503	2.2446	-0.1942	0.0001
S74	1.8830	2.0090	-0.1260	0.0020
S75	1.3493	1.3938	-0.0445	0.0051
S76	1.8306	1.7115	0.1191	0.0099
S77	1.9801	2.0390	-0.0590	0.0100
S78	1.7175	1.7233	-0.0057	0.0040
S79	1.7551	1.8245	-0.0693	0.0046
S80	2.2769	2.1560	0.1208	0.0051
S81	2.2525	2.3138	-0.0613	0.0082
S82	1.6999	1.8417	-0.1418	0.0013
S83	2.1790	2.2289	-0.0499	0.0011
S84	2.6143	2.8774	-0.2631	0.0000
S85	2.3248	2.3012	0.0236	0.0077
S86	1.6525	1.6641	-0.0116	0.0134
S87	2.0250	2.0654	-0.0404	0.0101
S88	2.0773	2.0490	0.0283	0.0056
S89	0.6145	0.6878	-0.0734	0.0000
S90	1.6123	1.2783	0.3340	0.0017
S91	1.0405	1.0887	-0.0482	0.0015
S92	2.1184	1.7322	0.3862	0.0027

Molecule	ADC(2)/aug-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	1.1092	1.1956	-0.0864	0.0002
S94	1.7819	1.6523	0.1296	0.0005
S95	1.8040	1.6597	0.1444	0.0054
S96	1.5109	1.6381	-0.1271	0.0000
S97	0.9997	1.0784	-0.0787	0.0010
S98	2.6061	2.2097	0.3964	0.0000
S99	1.7415	1.5666	0.1749	0.0065
S100	1.4075	1.5358	-0.1284	0.0010
S101	2.3522	2.1483	0.2038	0.0037
S102	1.4710	1.5653	-0.0942	0.0024
S103	2.1055	2.0838	0.0218	0.0050
S104	1.8477	1.9677	-0.1201	0.0000
S105	1.0523	1.1995	-0.1472	0.0000
S106	1.0641	1.1779	-0.1138	0.0001
S107	1.2571	1.3922	-0.1351	0.0023
S108	1.1064	1.1150	-0.0086	0.0008
S109	1.2344	1.3687	-0.1343	0.0031
S110	1.1056	1.0870	0.0187	0.0014
S111	1.1516	1.2986	-0.1469	0.0012
S112	0.9965	1.0848	-0.0883	0.0005
S113	1.0837	1.2379	-0.1542	0.0001
S114	0.9703	1.0835	-0.1133	0.0006
S115	1.0439	1.1942	-0.1503	0.0000
S116	0.9689	1.1068	-0.1379	0.0002
S117	1.0267	1.1736	-0.1468	0.0000
S118	0.9732	1.1137	-0.1405	0.0002
S119	1.3011	1.4217	-0.1206	0.0036
S120	0.9906	1.0958	-0.1052	0.0003
S121	0.9582	1.0643	-0.1061	0.0017
S122	1.0232	1.1643	-0.1411	0.0008
S123	0.8332	0.8900	-0.0568	0.0016
S124	1.3074	1.4202	-0.1128	0.0006
S125	0.9180	1.0349	-0.1169	0.0013
S126	1.0621	1.1966	-0.1345	0.0007
S127	0.9521	1.0793	-0.1272	0.0008
S128	1.0531	1.1905	-0.1374	0.0005
S129	0.8810	0.9784	-0.0973	0.0008
S130	1.1587	1.2769	-0.1182	0.0004
S131	1.3001	1.4270	-0.1269	0.0038
S132	0.9708	1.1107	-0.1399	0.0001
S133	0.8055	0.8873	-0.0818	0.0011
S134	1.2877	1.3966	-0.1090	0.0008
S135	0.9891	1.1019	-0.1127	0.0003
S136	1.0676	1.2118	-0.1441	0.0002
S137	0.8135	0.8671	-0.0536	0.0006
S138	1.3535	1.4439	-0.0904	0.0009

Molecule	ADC(2)/aug-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	0.9320	1.0539	-0.1219	0.0003
S140	1.1279	1.2689	-0.1410	0.0001
S141	2.6680	2.9228	-0.2548	0.0002
S142	2.9657	3.1582	-0.1925	0.0182
S143	2.8897	3.1236	-0.2339	0.0105
S144	2.8054	3.0644	-0.2590	0.0043
S145	2.7242	2.9812	-0.2570	0.0010
S146	2.6748	2.9389	-0.2640	0.0002
S147	2.6524	2.9124	-0.2600	0.0001
S148	2.9968	3.1750	-0.1783	0.0231
S149	2.5865	2.8322	-0.2456	0.0001
S150	2.4648	2.6616	-0.1969	0.0019
S151	2.5322	2.7709	-0.2387	0.0006
S152	2.5885	2.8358	-0.2473	0.0001
S153	2.5008	2.7091	-0.2082	0.0014
S154	3.0083	3.1800	-0.1717	0.0217
S155	2.4734	2.6159	-0.1425	0.0013
S156	2.5955	2.7615	-0.1660	0.0001
S157	2.6031	2.8445	-0.2414	0.0001
S158	2.5561	2.7922	-0.2361	0.0005
S159	1.5809	1.7247	-0.1438	0.0045
S160	1.5818	1.7009	-0.1191	0.0082
S161	1.5425	1.6574	-0.1150	0.0063
S162	1.5250	1.6377	-0.1127	0.0064
S163	1.8256	1.9853	-0.1598	0.0000
S164	1.8210	1.8772	-0.0562	0.0195
S165	1.4634	1.5073	-0.0439	0.0084
S166	1.4296	1.4975	-0.0679	0.0058
S167	1.7664	1.9313	-0.1649	0.0004
S168	1.7884	1.8544	-0.0660	0.0160
S169	1.4604	1.5340	-0.0736	0.0087
S170	1.4227	1.4735	-0.0508	0.0063
S171	1.6711	1.8415	-0.1704	0.0016
S172	1.6983	1.8080	-0.1097	0.0093
S173	1.4409	1.5309	-0.0901	0.0087
S174	1.4497	1.5407	-0.0910	0.0073
S175	1.6047	1.7532	-0.1484	0.0043
S176	1.6207	1.7450	-0.1243	0.0088
S177	1.5282	1.6651	-0.1369	0.0065
S178	1.5608	1.6864	-0.1256	0.0047
S179	1.5551	1.6990	-0.1439	0.0051
S180	1.5852	1.7141	-0.1290	0.0061
S181	1.4565	1.5804	-0.1239	0.0076
S182	1.4783	1.5968	-0.1185	0.0044
S183	1.5338	1.6717	-0.1379	0.0054
S184	1.5766	1.6964	-0.1197	0.0071

Molecule	ADC(2)/aug-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	1.4673	1.5883	-0.1210	0.0078
S186	1.4835	1.5990	-0.1155	0.0039
S187	1.8876	2.0273	-0.1398	0.0005
S188	1.8827	1.9034	-0.0207	0.0229
S189	1.4664	1.5546	-0.0881	0.0072
S190	1.4503	1.5020	-0.0517	0.0058
S191	1.4407	1.5323	-0.0917	0.0098
S192	1.5021	1.6163	-0.1142	0.0096
S193	1.4938	1.6111	-0.1173	0.0077
S194	1.4958	1.6280	-0.1322	0.0028
S195	1.2968	1.3163	-0.0195	0.0118
S196	1.4287	1.4819	-0.0532	0.0067
S197	1.6252	1.7353	-0.1101	0.0112
S198	1.6506	1.7802	-0.1296	0.0008
S199	1.4104	1.5055	-0.0951	0.0074
S200	1.4482	1.5655	-0.1173	0.0060
S201	1.5317	1.6533	-0.1216	0.0107
S202	1.5538	1.6863	-0.1325	0.0019
S203	1.4374	1.5429	-0.1054	0.0072
S204	1.4981	1.6203	-0.1222	0.0057
S205	1.5256	1.6481	-0.1224	0.0096
S206	1.5539	1.6867	-0.1328	0.0025
S207	1.3596	1.4233	-0.0637	0.0089
S208	1.4508	1.5399	-0.0891	0.0045
S209	1.5888	1.7134	-0.1246	0.0085
S210	1.6470	1.7668	-0.1198	0.0017
S211	1.8704	2.0220	-0.1516	0.0001
S212	1.8612	1.9010	-0.0398	0.0211
S213	1.4740	1.5723	-0.0983	0.0068
S214	1.4626	1.5632	-0.1006	0.0037
S215	1.3092	1.3438	-0.0346	0.0090
S216	1.3862	1.4615	-0.0754	0.0057
S217	1.6743	1.7894	-0.1151	0.0098
S218	1.7644	1.8844	-0.1200	0.0023
S219	1.4710	1.5732	-0.1022	0.0071
S220	1.5322	1.6427	-0.1105	0.0080
S221	1.5678	1.6989	-0.1311	0.0087
S222	1.5569	1.6945	-0.1375	0.0043
S223	1.2844	1.3060	-0.0216	0.0100
S224	1.4210	1.4917	-0.0707	0.0040
S225	1.7046	1.8252	-0.1206	0.0076
S226	1.7929	1.9201	-0.1272	0.0023
S227	1.4263	1.5211	-0.0948	0.0079
S228	1.5055	1.6077	-0.1022	0.0046
S229	1.5962	1.7334	-0.1372	0.0057
S230	1.6535	1.7835	-0.1300	0.0041

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S231	1.9141	2.0378	-0.1238	0.0051
S232	1.9228	2.0262	-0.1034	0.0112
S233	1.9077	2.0078	-0.1001	0.0098
S234	1.8351	1.9364	-0.1014	0.0091
S235	1.8938	1.9748	-0.0810	0.0078
S236	1.8936	1.9713	-0.0777	0.0101
S237	2.1548	2.2859	-0.1311	0.0008
S238	2.1038	2.1787	-0.0749	0.0240
S239	2.1733	2.1812	-0.0079	0.0330
S240	1.6885	1.7313	-0.0428	0.0131
S241	1.8023	1.7579	0.0444	0.0121
S242	1.8099	1.8156	-0.0057	0.0086
S243	2.1018	2.2462	-0.1444	0.0020
S244	2.0409	2.1437	-0.1028	0.0166
S245	2.1371	2.1665	-0.0294	0.0269
S246	1.6697	1.7081	-0.0384	0.0158
S247	1.8547	1.8393	0.0154	0.0124
S248	1.8252	1.8165	0.0087	0.0122
S249	2.0008	2.1437	-0.1429	0.0027
S250	1.9686	2.1041	-0.1355	0.0085
S251	2.0654	2.1306	-0.0652	0.0177
S252	1.7265	1.8099	-0.0834	0.0115
S253	1.8334	1.8778	-0.0444	0.0097
S254	1.7931	1.8609	-0.0678	0.0086
S255	1.9442	2.0807	-0.1365	0.0054
S256	1.9098	2.0329	-0.1231	0.0152
S257	1.9672	2.0533	-0.0861	0.0114
S258	1.7211	1.8065	-0.0854	0.0114
S259	1.7914	1.8375	-0.0460	0.0143
S260	1.8806	1.9874	-0.1068	0.0036
S261	1.8919	2.0144	-0.1225	0.0063
S262	1.8769	2.0041	-0.1272	0.0083
S263	1.7725	1.8798	-0.1073	0.0094
S264	1.7932	1.8914	-0.0982	0.0109
S265	1.8258	1.9150	-0.0892	0.0064
S266	1.9401	2.0397	-0.0995	0.0088
S267	1.8723	1.9949	-0.1226	0.0065
S268	1.8598	1.9836	-0.1239	0.0091
S269	1.9211	2.0176	-0.0965	0.0080
S270	1.7793	1.8887	-0.1093	0.0091
S271	1.7911	1.8871	-0.0960	0.0114
S272	1.8233	1.9115	-0.0882	0.0057
S273	2.2126	2.3363	-0.1237	0.0005
S274	2.1166	2.1728	-0.0562	0.0258
S275	2.2144	2.1973	0.0170	0.0367
S276	1.6761	1.7118	-0.0356	0.0116

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S277	1.8309	1.7426	0.0883	0.0145
S278	1.8282	1.8823	-0.0541	0.0078
S279	1.8073	1.8887	-0.0813	0.0095
S280	1.8628	1.9262	-0.0634	0.0213
S281	1.7924	1.9118	-0.1194	0.0061
S282	1.8130	1.9118	-0.0987	0.0096
S283	1.7499	1.8229	-0.0730	0.0175
S284	1.8207	1.9226	-0.1019	0.0028
S285	1.6277	1.6494	-0.0218	0.0151
S286	1.8131	1.8003	0.0128	0.0134
S287	1.6929	1.7958	-0.1029	0.0032
S288	1.9403	2.0574	-0.1170	0.0073
S289	1.8536	2.0130	-0.1594	0.0005
S290	1.9124	2.0294	-0.1171	0.0147
S291	1.7602	1.8388	-0.0786	0.0108
S292	1.8022	1.8680	-0.0658	0.0140
S293	1.7737	1.8866	-0.1130	0.0038
S294	1.8425	1.9577	-0.1152	0.0103
S295	1.8079	1.9092	-0.1013	0.0169
S296	1.8399	1.9611	-0.1212	0.0026
S297	1.7822	1.8789	-0.0967	0.0098
S298	1.8257	1.9159	-0.0902	0.0107
S299	1.8497	1.9530	-0.1033	0.0052
S300	1.8323	1.9536	-0.1214	0.0086
S301	1.8236	1.9193	-0.0958	0.0142
S302	1.8607	1.9735	-0.1128	0.0027
S303	1.7071	1.7553	-0.0482	0.0123
S304	1.8078	1.8312	-0.0234	0.0087
S305	1.7697	1.8650	-0.0952	0.0032
S306	1.9000	2.0282	-0.1282	0.0076
S307	1.8483	1.9603	-0.1120	0.0159
S308	1.9063	2.0311	-0.1248	0.0023
S309	2.1958	2.3178	-0.1220	0.0021
S310	2.1316	2.1803	-0.0487	0.0379
S311	2.2074	2.1972	0.0102	0.0383
S312	1.7614	1.8388	-0.0775	0.0112
S313	1.7844	1.7785	0.0059	0.0175
S314	1.8346	1.8847	-0.0500	0.0092
S315	1.6531	1.6802	-0.0271	0.0122
S316	1.7422	1.7592	-0.0170	0.0119
S317	1.7014	1.8116	-0.1103	0.0028
S318	1.9653	2.1042	-0.1389	0.0086
S319	2.0006	2.1300	-0.1294	0.0011
S320	1.8822	1.9916	-0.1094	0.0163
S321	1.7951	1.8839	-0.0888	0.0105
S322	1.8794	1.9606	-0.0811	0.0119

Molecule	ADC(2)/aug-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	1.8779	1.9780	-0.1001	0.0074
S324	1.8665	1.9931	-0.1266	0.0062
S325	1.8766	2.0035	-0.1268	0.0046
S326	1.8998	2.0045	-0.1047	0.0133
S327	1.6444	1.6455	-0.0011	0.0114
S328	1.7751	1.7833	-0.0083	0.0080
S329	1.8625	1.9526	-0.0901	0.0055
S330	1.9959	2.1218	-0.1259	0.0057
S331	1.9809	2.1299	-0.1490	0.0029
S332	1.8911	2.0255	-0.1345	0.0157
S333	1.7764	1.8545	-0.0781	0.0102
S334	1.8682	1.9268	-0.0585	0.0064
S335	1.8370	1.9374	-0.1005	0.0041
S336	1.9199	2.0383	-0.1184	0.0088
S337	1.8985	2.0195	-0.1210	0.0096
S338	1.9510	2.0865	-0.1354	0.0034
S339	2.1627	2.3246	-0.1619	0.0039
S340	2.1658	2.3073	-0.1415	0.0076
S341	2.0901	2.2154	-0.1253	0.0055
S342	2.3973	2.5744	-0.1771	0.0004
S343	2.4328	2.4988	-0.0660	0.0298
S344	1.9124	1.9157	-0.0033	0.0081
S345	2.3247	2.5190	-0.1943	0.0001
S346	2.3806	2.4796	-0.0990	0.0143
S347	1.9295	1.9856	-0.0562	0.0118
S348	2.2357	2.4285	-0.1929	0.0008
S349	2.3067	2.4270	-0.1203	0.0115
S350	1.9876	2.0997	-0.1121	0.0077
S351	2.1897	2.3776	-0.1879	0.0032
S352	2.2065	2.3416	-0.1351	0.0110
S353	1.9634	2.0484	-0.0850	0.0117
S354	2.1378	2.3068	-0.1690	0.0022
S355	2.0102	2.1433	-0.1330	0.0080
S356	2.1752	2.3170	-0.1419	0.0062
S357	2.1198	2.2887	-0.1689	0.0042
S358	2.1542	2.2956	-0.1414	0.0061
S359	2.0110	2.1501	-0.1391	0.0053
S360	2.4294	2.6036	-0.1742	0.0008
S361	2.4633	2.5133	-0.0500	0.0312
S362	1.8785	1.9005	-0.0220	0.0135
S363	2.0557	2.1760	-0.1203	0.0088
S364	2.0348	2.1814	-0.1465	0.0057
S365	2.0449	2.1666	-0.1217	0.0083
S366	1.9224	1.9651	-0.0427	0.0124
S367	1.9341	2.0458	-0.1117	0.0033
S368	2.1225	2.2753	-0.1528	0.0116

Molecule	ADC(2)/aug-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	2.0273	2.1417	-0.1145	0.0092
S370	2.0138	2.1521	-0.1383	0.0058
S371	2.0405	2.1802	-0.1398	0.0109
S372	2.0444	2.1834	-0.1390	0.0075
S373	2.0821	2.2200	-0.1379	0.0053
S374	2.0504	2.1951	-0.1446	0.0085
S375	1.9755	2.0706	-0.0951	0.0103
S376	2.0004	2.1159	-0.1155	0.0037
S377	2.0992	2.2565	-0.1573	0.0095
S378	2.4268	2.6000	-0.1732	0.0015
S379	2.4687	2.4984	-0.0297	0.0392
S380	1.8999	1.9234	-0.0235	0.0133
S381	1.9394	1.9966	-0.0572	0.0114
S382	1.9514	2.0678	-0.1163	0.0054
S383	2.1393	2.3032	-0.1638	0.0081
S384	2.0632	2.2033	-0.1400	0.0067
S385	2.1209	2.2496	-0.1287	0.0063
S386	2.1111	2.2628	-0.1517	0.0067
S387	1.9327	1.9599	-0.0272	0.0114
S388	2.0882	2.2165	-0.1283	0.0021
S389	2.1406	2.3203	-0.1797	0.0079
S390	2.0286	2.1560	-0.1275	0.0064
S391	2.0713	2.2037	-0.1324	0.0037
S392	2.1418	2.3091	-0.1673	0.0060
S393	2.1154	2.2633	-0.1478	0.0102
S394	2.0954	2.2267	-0.1313	0.0120
S395	2.0354	2.1596	-0.1241	0.0081
S396	2.4089	2.5198	-0.1109	0.0149
S397	2.3442	2.3730	-0.0288	0.0436
S398	1.8907	1.9328	-0.0421	0.0169
S399	2.3257	2.4534	-0.1277	0.0104
S400	2.2957	2.3567	-0.0610	0.0330
S401	1.8865	1.9112	-0.0247	0.0178
S402	2.2223	2.3962	-0.1739	0.0067
S403	2.2364	2.3301	-0.0937	0.0228
S404	1.9314	2.0263	-0.0949	0.0142
S405	2.1475	2.3061	-0.1586	0.0141
S406	2.1488	2.2669	-0.1180	0.0141
S407	2.0433	2.1962	-0.1528	0.0084
S408	2.0971	2.2481	-0.1510	0.0099
S409	1.9596	2.0837	-0.1241	0.0104
S410	2.1212	2.2550	-0.1338	0.0107
S411	2.0762	2.2312	-0.1550	0.0112
S412	2.1020	2.2399	-0.1379	0.0094
S413	1.9627	2.0984	-0.1357	0.0099
S414	2.4451	2.5346	-0.0895	0.0167

ADC(2)/aug-cc-pVDZ				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S415	2.3675	2.3822	-0.0146	0.0460
S416	1.9510	2.0378	-0.0868	0.0132
S417	2.0238	2.1311	-0.1073	0.0235
S418	2.0189	2.1659	-0.1471	0.0065
S419	1.9824	2.1115	-0.1291	0.0081
S420	1.8999	1.9519	-0.0519	0.0184
S421	1.9270	2.0671	-0.1400	0.0005
S422	2.0919	2.2840	-0.1920	0.0038
S423	1.9601	2.0643	-0.1042	0.0165
S424	1.9812	2.1333	-0.1521	0.0041
S425	2.0170	2.1690	-0.1520	0.0084
S426	1.9985	2.1205	-0.1220	0.0139
S427	2.0487	2.1894	-0.1407	0.0059
S428	2.0195	2.1640	-0.1445	0.0081
S429	1.9284	2.0188	-0.0904	0.0142
S430	1.9832	2.1132	-0.1300	0.0039
S431	2.0882	2.2535	-0.1653	0.0064
S432	2.4419	2.5280	-0.0861	0.0143
S433	2.3759	2.3844	-0.0085	0.0491
S434	1.9413	2.0235	-0.0822	0.0099
S435	1.8823	1.9474	-0.0651	0.0154
S436	1.9301	2.0768	-0.1467	0.0020
S437	2.1840	2.3409	-0.1569	0.0088
S438	2.0367	2.1569	-0.1202	0.0150
S439	2.0554	2.1966	-0.1412	0.0072
S440	2.0481	2.2125	-0.1644	0.0073
S441	1.9093	1.9700	-0.0606	0.0122
S442	2.0694	2.1995	-0.1301	0.0065
S443	2.1892	2.3794	-0.1903	0.0056
S444	1.9959	2.1020	-0.1061	0.0114
S445	2.0206	2.1726	-0.1520	0.0044
S446	2.1206	2.2849	-0.1644	0.0067