

ADC(2)/cc-pVDZ/IEFPCM(S0)				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S1	1.0288	1.1896	-0.1608	0.0000
S2	0.9120	1.0232	-0.1112	0.0008
S3	1.3893	1.4976	-0.1083	0.0006
S4	1.6292	1.7696	-0.1404	0.0024
S5	1.5348	1.4194	0.1154	0.0002
S6	1.3952	1.4810	-0.0859	0.0004
S7	1.7489	1.8124	-0.0634	0.0006
S8	1.2911	1.3475	-0.0563	0.0023
S9	1.4392	1.5766	-0.1375	0.0003
S10	1.8151	1.7230	0.0921	0.0018
S11	1.5713	1.7078	-0.1365	0.0030
S12	1.8353	1.9848	-0.1495	0.0022
S13	1.9109	2.0261	-0.1152	0.0042
S14	2.0990	2.2529	-0.1539	0.0054
S15	1.5392	1.5566	-0.0174	0.0007
S16	1.8469	1.8757	-0.0288	0.0000
S17	1.6642	1.7391	-0.0749	0.0022
S18	1.8622	1.9809	-0.1187	0.0001
S19	1.3531	1.3419	0.0112	0.0024
S20	1.4155	1.4741	-0.0586	0.0080
S21	0.7976	0.8881	-0.0905	0.0007
S22	1.3064	1.2430	0.0634	0.0028
S23	1.6245	1.3540	0.2705	0.0003
S24	1.4649	1.3852	0.0796	0.0035
S25	1.6890	1.6552	0.0339	0.0042
S26	1.5195	1.5916	-0.0721	0.0043
S27	1.7669	1.8014	-0.0346	0.0105
S28	1.5660	1.3898	0.1761	0.0022
S29	1.8567	1.6886	0.1681	0.0032
S30	1.3076	1.3782	-0.0706	0.0004
S31	1.5428	1.5977	-0.0549	0.0048
S32	1.9289	1.7602	0.1688	0.0002
S33	1.7987	1.7719	0.0268	0.0054
S34	1.3627	1.4064	-0.0437	0.0009
S35	2.1388	1.8330	0.3058	0.0009
S36	2.0267	1.8611	0.1656	0.0010
S37	1.6022	1.6824	-0.0802	0.0042
S38	2.0031	1.9453	0.0579	0.0021
S39	1.9826	2.0093	-0.0266	0.0080
S40	1.2933	1.3775	-0.0842	0.0000
S41	1.5811	1.6542	-0.0731	0.0028
S42	1.8803	1.8385	0.0418	0.0039
S43	1.8588	1.9248	-0.0660	0.0001
S44	1.5433	1.7146	-0.1714	0.0003
S45	1.3945	1.4458	-0.0513	0.0028
S46	2.0846	2.1229	-0.0383	0.0000

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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]	$f_{12}(S_0-S_1)$
S47	1.8834	2.0428	-0.1594	0.0005
S48	1.6747	1.7299	-0.0552	0.0025
S49	1.8003	1.8849	-0.0846	0.0022
S50	1.7558	1.7956	-0.0398	0.0051
S51	2.1941	2.3297	-0.1356	0.0020
S52	2.1470	2.3098	-0.1628	0.0023
S53	2.3932	2.5955	-0.2023	0.0020
S54	2.2811	2.2555	0.0256	0.0006
S55	1.9066	1.9842	-0.0775	0.0028
S56	2.1662	2.2776	-0.1113	0.0017
S57	1.9424	1.6715	0.2708	0.0020
S58	1.1109	1.1419	-0.0310	0.0037
S59	1.4783	1.4451	0.0332	0.0073
S60	2.1888	2.0503	0.1385	0.0015
S61	2.1272	2.1128	0.0144	0.0085
S62	2.4179	2.1348	0.2831	0.0006
S63	1.7022	1.6493	0.0529	0.0031
S64	2.0209	1.9501	0.0708	0.0065
S65	1.7690	1.8727	-0.1037	0.0078
S66	1.6625	1.6728	-0.0103	0.0012
S67	1.6573	1.7199	-0.0626	0.0048
S68	1.9616	2.0115	-0.0499	0.0058
S69	2.0771	2.1814	-0.1042	0.0111
S70	2.2012	2.1486	0.0526	0.0054
S71	1.6838	1.8028	-0.1190	0.0012
S72	1.9232	2.0503	-0.1270	0.0049
S73	2.0790	2.2841	-0.2050	0.0002
S74	1.9155	2.0209	-0.1054	0.0024
S75	1.3962	1.4427	-0.0465	0.0050
S76	1.9125	1.7783	0.1342	0.0069
S77	2.0180	2.0921	-0.0741	0.0079
S78	1.7621	1.7701	-0.0080	0.0033
S79	1.8005	1.8600	-0.0596	0.0036
S80	2.3756	2.2329	0.1427	0.0031
S81	2.3098	2.3658	-0.0560	0.0065
S82	1.7431	1.8921	-0.1490	0.0010
S83	2.2487	2.2995	-0.0508	0.0006
S84	2.6574	2.9385	-0.2810	0.0000
S85	2.3569	2.3952	-0.0383	0.0085
S86	1.6958	1.6936	0.0022	0.0123
S87	2.0499	2.0815	-0.0315	0.0101
S88	2.1132	2.1567	-0.0435	0.0060
S89	0.6805	0.7644	-0.0840	0.0000
S90	1.7014	1.3507	0.3507	0.0015
S91	1.1208	1.1576	-0.0368	0.0013
S92	2.2257	1.8129	0.4128	0.0022

ADC(2)/cc-pVDZ/IEFPCM(S0)				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S93	1.1786	1.2601	-0.0815	0.0000
S94	1.8351	1.6932	0.1419	0.0007
S95	1.8672	1.7361	0.1311	0.0065
S96	1.5668	1.6897	-0.1230	0.0000
S97	1.0320	1.0995	-0.0675	0.0011
S98	2.7362	2.3029	0.4333	0.0000
S99	1.8070	1.6154	0.1916	0.0056
S100	1.4280	1.5500	-0.1221	0.0013
S101	2.4261	2.2063	0.2198	0.0052
S102	1.5522	1.6448	-0.0926	0.0018
S103	2.1565	2.1456	0.0109	0.0036
S104	1.8871	2.0592	-0.1721	0.0000
S105	1.0729	1.2380	-0.1652	0.0000
S106	1.0841	1.2138	-0.1296	0.0000
S107	1.3146	1.4573	-0.1427	0.0029
S108	1.1242	1.1416	-0.0174	0.0006
S109	1.2616	1.4173	-0.1557	0.0018
S110	1.1182	1.1163	0.0019	0.0007
S111	1.1754	1.3445	-0.1691	0.0006
S112	1.0048	1.1071	-0.1023	0.0003
S113	1.1021	1.2697	-0.1676	0.0001
S114	0.9963	1.1271	-0.1308	0.0004
S115	1.0599	1.2206	-0.1607	0.0000
S116	0.9975	1.1544	-0.1569	0.0002
S117	1.0425	1.1989	-0.1564	0.0000
S118	1.0043	1.1631	-0.1588	0.0002
S119	1.3546	1.4824	-0.1278	0.0040
S120	1.0110	1.1345	-0.1235	0.0002
S121	0.9764	1.0970	-0.1205	0.0007
S122	1.0486	1.2022	-0.1536	0.0006
S123	0.8331	0.8761	-0.0430	0.0014
S124	1.3554	1.4709	-0.1155	0.0009
S125	0.9159	1.0431	-0.1272	0.0005
S126	1.1022	1.2493	-0.1471	0.0006
S127	0.9345	1.0638	-0.1293	0.0004
S128	1.1070	1.2585	-0.1515	0.0006
S129	0.8739	0.9540	-0.0801	0.0010
S130	1.2388	1.3585	-0.1197	0.0006
S131	1.3460	1.4783	-0.1323	0.0038
S132	0.9952	1.1515	-0.1563	0.0000
S133	0.8154	0.8923	-0.0769	0.0011
S134	1.3254	1.4398	-0.1144	0.0008
S135	0.9955	1.1266	-0.1311	0.0001
S136	1.0926	1.2522	-0.1597	0.0003
S137	0.8146	0.8428	-0.0282	0.0011
S138	1.4469	1.5255	-0.0785	0.0012

ADC(2)/cc-pVDZ/IEFPCM(S0)				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S139	0.9488	1.0738	-0.1250	0.0004
S140	1.1730	1.3245	-0.1515	0.0002
S141	2.7080	2.9886	-0.2806	0.0002
S142	3.0497	3.2296	-0.1799	0.0173
S143	2.9512	3.1951	-0.2439	0.0079
S144	2.8608	3.1431	-0.2823	0.0026
S145	2.7626	3.0457	-0.2832	0.0006
S146	2.7109	2.9912	-0.2803	0.0000
S147	2.6865	2.9619	-0.2754	0.0000
S148	3.0700	3.2373	-0.1673	0.0188
S149	2.6320	2.8970	-0.2651	0.0002
S150	2.4884	2.6861	-0.1977	0.0023
S151	2.5637	2.8086	-0.2449	0.0009
S152	2.6032	2.8514	-0.2482	0.0005
S153	2.5106	2.7007	-0.1900	0.0024
S154	3.0716	3.2374	-0.1658	0.0181
S155	2.4999	2.7132	-0.2133	0.0018
S156	2.6261	2.8755	-0.2494	0.0004
S157	2.6407	2.8803	-0.2396	0.0004
S158	2.5912	2.8345	-0.2432	0.0008
S159	1.6236	1.7691	-0.1455	0.0025
S160	1.6216	1.7551	-0.1334	0.0051
S161	1.5813	1.7022	-0.1209	0.0034
S162	1.5649	1.6877	-0.1228	0.0036
S163	1.9213	2.0676	-0.1463	0.0002
S164	1.8937	1.9415	-0.0478	0.0152
S165	1.4953	1.5371	-0.0418	0.0067
S166	1.4556	1.5309	-0.0753	0.0034
S167	1.8252	1.9904	-0.1652	0.0000
S168	1.8443	1.9179	-0.0736	0.0112
S169	1.4814	1.5590	-0.0776	0.0057
S170	1.4520	1.5128	-0.0608	0.0038
S171	1.7090	1.8833	-0.1743	0.0009
S172	1.7531	1.8678	-0.1147	0.0065
S173	1.4593	1.5655	-0.1062	0.0055
S174	1.4775	1.5841	-0.1066	0.0034
S175	1.6432	1.7999	-0.1567	0.0022
S176	1.6572	1.7852	-0.1281	0.0062
S177	1.5649	1.7116	-0.1466	0.0039
S178	1.6007	1.7393	-0.1387	0.0020
S179	1.5785	1.7256	-0.1471	0.0033
S180	1.6251	1.7525	-0.1275	0.0041
S181	1.4959	1.6332	-0.1373	0.0047
S182	1.5244	1.6580	-0.1336	0.0019
S183	1.5586	1.6986	-0.1400	0.0036
S184	1.6065	1.7322	-0.1256	0.0042

ADC(2)/cc-pVDZ/IEFPCM(S0)				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S185	1.5010	1.6411	-0.1401	0.0048
S186	1.5307	1.6666	-0.1359	0.0018
S187	1.9704	2.1028	-0.1325	0.0007
S188	1.9460	1.9576	-0.0116	0.0181
S189	1.5068	1.6064	-0.0996	0.0050
S190	1.4665	1.5184	-0.0519	0.0030
S191	1.4926	1.5967	-0.1041	0.0058
S192	1.5425	1.6573	-0.1149	0.0072
S193	1.5312	1.6601	-0.1290	0.0058
S194	1.5376	1.6726	-0.1349	0.0010
S195	1.3135	1.3399	-0.0264	0.0085
S196	1.4507	1.4907	-0.0400	0.0041
S197	1.6652	1.7960	-0.1308	0.0069
S198	1.7121	1.8447	-0.1326	0.0002
S199	1.4393	1.5335	-0.0942	0.0062
S200	1.4846	1.5910	-0.1064	0.0046
S201	1.5594	1.7008	-0.1413	0.0064
S202	1.5981	1.7366	-0.1385	0.0005
S203	1.4395	1.5424	-0.1029	0.0060
S204	1.5181	1.6256	-0.1075	0.0042
S205	1.5652	1.7093	-0.1441	0.0057
S206	1.6116	1.7515	-0.1399	0.0006
S207	1.3600	1.4073	-0.0473	0.0079
S208	1.4709	1.5251	-0.0542	0.0029
S209	1.6382	1.7800	-0.1418	0.0057
S210	1.7189	1.8524	-0.1335	0.0003
S211	1.9531	2.0887	-0.1355	0.0004
S212	1.9187	1.9548	-0.0361	0.0195
S213	1.5127	1.6117	-0.0990	0.0050
S214	1.5030	1.6122	-0.1092	0.0026
S215	1.3334	1.3751	-0.0417	0.0077
S216	1.4136	1.4796	-0.0660	0.0041
S217	1.6846	1.8242	-0.1397	0.0062
S218	1.7916	1.9163	-0.1247	0.0002
S219	1.4948	1.6086	-0.1138	0.0046
S220	1.5756	1.6838	-0.1082	0.0044
S221	1.5801	1.7307	-0.1506	0.0042
S222	1.5990	1.7453	-0.1463	0.0014
S223	1.3039	1.3083	-0.0044	0.0077
S224	1.4670	1.5013	-0.0343	0.0031
S225	1.7473	1.8725	-0.1252	0.0060
S226	1.8521	1.9699	-0.1178	0.0002
S227	1.4485	1.5444	-0.0959	0.0060
S228	1.5486	1.6428	-0.0942	0.0024
S229	1.6279	1.7849	-0.1570	0.0035
S230	1.7036	1.8430	-0.1394	0.0017

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S231	1.9574	2.0826	-0.1252	0.0035
S232	1.9627	2.0789	-0.1162	0.0077
S233	1.9443	2.0582	-0.1138	0.0054
S234	1.8742	1.9837	-0.1095	0.0047
S235	1.9339	2.0169	-0.0829	0.0047
S236	1.9299	2.0199	-0.0900	0.0052
S237	2.2504	2.3554	-0.1050	0.0008
S238	2.1705	2.2156	-0.0451	0.0194
S239	2.2555	2.2556	-0.0001	0.0268
S240	1.7158	1.7540	-0.0383	0.0083
S241	1.8119	1.7536	0.0582	0.0097
S242	1.8296	1.8444	-0.0149	0.0065
S243	2.1604	2.2882	-0.1278	0.0006
S244	2.0865	2.1859	-0.0995	0.0111
S245	2.1992	2.2388	-0.0396	0.0184
S246	1.7039	1.7467	-0.0427	0.0095
S247	1.8613	1.8427	0.0186	0.0084
S248	1.8495	1.8517	-0.0021	0.0071
S249	2.0392	2.1894	-0.1502	0.0018
S250	2.0150	2.1493	-0.1343	0.0056
S251	2.1327	2.2048	-0.0721	0.0120
S252	1.7578	1.8521	-0.0943	0.0077
S253	1.8707	1.9247	-0.0540	0.0058
S254	1.8149	1.8924	-0.0775	0.0065
S255	1.9851	2.1217	-0.1366	0.0033
S256	1.9429	2.0666	-0.1236	0.0099
S257	2.0047	2.1054	-0.1007	0.0071
S258	1.7636	1.8568	-0.0932	0.0073
S259	1.8257	1.8805	-0.0548	0.0091
S260	1.9226	2.0435	-0.1209	0.0023
S261	1.9181	2.0478	-0.1297	0.0047
S262	1.9161	2.0366	-0.1205	0.0054
S263	1.8142	1.9333	-0.1191	0.0062
S264	1.8343	1.9425	-0.1082	0.0073
S265	1.8729	1.9720	-0.0991	0.0029
S266	1.9836	2.0823	-0.0987	0.0054
S267	1.8643	1.9997	-0.1354	0.0041
S268	1.8987	2.0152	-0.1165	0.0058
S269	1.9627	2.0612	-0.0985	0.0049
S270	1.8216	1.9426	-0.1210	0.0061
S271	1.8357	1.9475	-0.1118	0.0078
S272	1.8706	1.9760	-0.1054	0.0026
S273	2.3005	2.3837	-0.0832	0.0010
S274	2.1737	2.1978	-0.0242	0.0216
S275	2.2816	2.2630	0.0185	0.0282
S276	1.6896	1.7089	-0.0194	0.0088

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S277	1.8192	1.7068	0.1124	0.0118
S278	1.8607	1.9222	-0.0615	0.0047
S279	1.8596	1.9504	-0.0908	0.0064
S280	1.9069	1.9682	-0.0613	0.0155
S281	1.8223	1.9519	-0.1296	0.0036
S282	1.8463	1.9532	-0.1069	0.0060
S283	1.8009	1.8849	-0.0840	0.0128
S284	1.8611	1.9655	-0.1043	0.0016
S285	1.6595	1.6811	-0.0216	0.0115
S286	1.8527	1.8212	0.0315	0.0091
S287	1.7042	1.7871	-0.0829	0.0022
S288	1.9768	2.1065	-0.1297	0.0053
S289	1.9102	2.0638	-0.1536	0.0008
S290	1.9437	2.0710	-0.1274	0.0100
S291	1.7927	1.8747	-0.0820	0.0083
S292	1.8463	1.8949	-0.0486	0.0101
S293	1.7937	1.9032	-0.1095	0.0024
S294	1.8755	2.0010	-0.1256	0.0065
S295	1.8529	1.9654	-0.1125	0.0111
S296	1.8820	2.0038	-0.1218	0.0011
S297	1.7888	1.8793	-0.0905	0.0083
S298	1.8513	1.9166	-0.0653	0.0077
S299	1.8603	1.9583	-0.0980	0.0030
S300	1.8793	2.0114	-0.1321	0.0058
S301	1.8754	1.9899	-0.1145	0.0101
S302	1.9116	2.0320	-0.1204	0.0009
S303	1.7129	1.7459	-0.0330	0.0109
S304	1.8447	1.8321	0.0127	0.0060
S305	1.7745	1.8407	-0.0662	0.0021
S306	1.9500	2.0869	-0.1369	0.0052
S307	1.9127	2.0372	-0.1245	0.0117
S308	1.9540	2.0987	-0.1447	0.0005
S309	2.2741	2.3682	-0.0941	0.0011
S310	2.1753	2.2119	-0.0366	0.0271
S311	2.2640	2.2600	0.0040	0.0269
S312	1.7961	1.8781	-0.0820	0.0067
S313	1.7996	1.7891	0.0106	0.0105
S314	1.8645	1.9218	-0.0572	0.0043
S315	1.6891	1.7224	-0.0333	0.0099
S316	1.7891	1.7844	0.0047	0.0088
S317	1.7187	1.8145	-0.0958	0.0016
S318	1.9804	2.1185	-0.1381	0.0054
S319	2.0186	2.1546	-0.1360	0.0007
S320	1.9128	2.0409	-0.1281	0.0103
S321	1.8255	1.9270	-0.1016	0.0069
S322	1.9192	2.0005	-0.0813	0.0068

ADC(2)/cc-pVDZ/IEFPCM(S0)				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
S323	1.9123	2.0052	-0.0929	0.0043
S324	1.8892	2.0255	-0.1362	0.0043
S325	1.9115	2.0459	-0.1344	0.0015
S326	1.9277	2.0434	-0.1157	0.0085
S327	1.6663	1.6595	0.0068	0.0107
S328	1.8241	1.7987	0.0253	0.0056
S329	1.9063	1.9763	-0.0700	0.0031
S330	2.0226	2.1601	-0.1375	0.0043
S331	2.0223	2.1720	-0.1497	0.0028
S332	1.9373	2.0683	-0.1309	0.0116
S333	1.7995	1.8782	-0.0787	0.0082
S334	1.9207	1.9696	-0.0489	0.0039
S335	1.8737	1.9613	-0.0876	0.0027
S336	1.9478	2.0935	-0.1457	0.0041
S337	1.9412	2.0749	-0.1338	0.0066
S338	1.9968	2.1383	-0.1416	0.0011
S339	2.1967	2.3666	-0.1699	0.0017
S340	2.2003	2.3591	-0.1588	0.0043
S341	2.1237	2.2610	-0.1374	0.0028
S342	2.4780	2.6218	-0.1438	0.0016
S343	2.5089	2.5493	-0.0404	0.0237
S344	1.9019	1.8907	0.0112	0.0074
S345	2.3724	2.5529	-0.1806	0.0001
S346	2.4358	2.5323	-0.0965	0.0138
S347	1.9441	1.9982	-0.0542	0.0070
S348	2.2696	2.4717	-0.2021	0.0004
S349	2.3594	2.4957	-0.1363	0.0070
S350	2.0097	2.1382	-0.1285	0.0050
S351	2.2250	2.4120	-0.1870	0.0013
S352	2.2345	2.3856	-0.1511	0.0058
S353	1.9501	2.0633	-0.1132	0.0066
S354	2.1176	2.3077	-0.1901	0.0021
S355	2.0485	2.2034	-0.1549	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	2.5037	2.6357	-0.1320	0.0023
S361	2.5285	2.5614	-0.0330	0.0272
S362	1.8798	1.8977	-0.0179	0.0077
S363	2.1082	2.2490	-0.1408	0.0047
S364	2.0624	2.2141	-0.1517	0.0034
S365	2.0669	2.2023	-0.1353	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

ADC(2)/cc-pVDZ/IEFPCM(S0)				
Molecule	$\Delta E(S_0-S_1)$ [eV]	$\Delta E(S_0-T_1)$ [eV]	$\Delta E(S_1-T_1)$ [eV]	$f_{12}(S_0-S_1)$
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	2.4935	2.6269	-0.1333	0.0020
S379	2.5190	2.5448	-0.0257	0.0271
S380	1.8940	1.9089	-0.0149	0.0082
S381	1.9755	2.0428	-0.0673	0.0078
S382	1.9646	2.0679	-0.1033	0.0034
S383	2.1711	2.3536	-0.1825	0.0044
S384	2.0864	2.2339	-0.1475	0.0040
S385	2.1468	2.2809	-0.1341	0.0027
S386	2.1346	2.3018	-0.1672	0.0041
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	2.0554	2.1801	-0.1247	0.0058
S391	2.1032	2.2286	-0.1254	0.0017
S392	2.1776	2.3669	-0.1892	0.0030
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	2.1829	2.3382	-0.1553	0.0095
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	2.5157	2.5548	-0.0391	0.0134

ADC(2)/cc-pVDZ/IEFPCM(S0)				
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	2.4347	2.4531	-0.0185	0.0364
S416	1.9838	2.0714	-0.0877	0.0078
S417	2.0735	2.1871	-0.1136	0.0168
S418	2.0490	2.2104	-0.1614	0.0031
S419	2.0179	2.1523	-0.1344	0.0049
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	2.5028	2.5558	-0.0530	0.0176
S433	2.4316	2.4523	-0.0207	0.0349
S434	1.9704	2.0459	-0.0755	0.0076
S435	1.9226	1.9789	-0.0564	0.0127
S436	1.9467	2.0829	-0.1362	0.0007
S437	2.1935	2.3717	-0.1783	0.0037
S438	2.0729	2.1987	-0.1258	0.0097
S439	2.0921	2.2292	-0.1371	0.0037
S440	2.0777	2.2515	-0.1738	0.0042
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	2.0380	2.1432	-0.1052	0.0083
S445	2.0606	2.1954	-0.1348	0.0022
S446	2.1659	2.3539	-0.1880	0.0037