

Table 8. (9-MA)₃ S_{CT} state minimum. PCM/TD-PBE0/6-31G(d) partial geometry optimizations in solution

Atomic number	Cartesian coordinates (in Å)		
7	4.223970	1.156009	0.737272
6	4.661071	0.167445	1.603361
7	4.409104	-1.052811	1.121883
6	3.779566	-0.838354	-0.071245
6	3.645359	0.533103	-0.335999
6	3.239243	-1.714636	-1.065023
7	2.664532	-1.167534	-2.153585
6	2.587585	0.152762	-2.268225
7	3.042652	1.118472	-1.390034
6	4.335602	2.579605	0.920304
1	3.778445	2.911682	1.804179
1	3.921535	3.065027	0.033621
1	5.382495	2.880636	1.035162
1	5.183666	0.403054	2.521260
7	3.390086	-3.118896	-0.989559
1	3.351384	-3.436432	-0.021503
1	2.644489	-3.579664	-1.509456
1	2.100202	0.532517	-3.165591
7	0.133207	2.057453	0.181756
6	0.658846	1.781178	1.389063
7	0.766124	0.471154	1.666154
6	0.276551	-0.119146	0.575242
6	-0.159798	0.837276	-0.387704
6	0.062448	-1.488849	0.218076
7	-0.544049	-1.767599	-0.962932
6	-0.910289	-0.765846	-1.728669
7	-0.775045	0.579497	-1.506008
6	-0.032188	3.355564	-0.444985
1	-0.655208	3.223421	-1.330305
1	-0.517562	4.042769	0.250572
1	0.944351	3.740632	-0.747326
1	0.969903	2.570116	2.071536
7	0.417283	-2.478141	1.005130
1	0.237557	-3.444725	0.719399
1	0.879844	-2.308757	1.901528
1	-1.399972	-1.025962	-2.666011
7	-3.948739	1.462893	-0.521097
6	-3.466984	2.051912	0.618169
7	-3.076569	1.199694	1.537021
6	-3.347463	-0.029565	0.976761
6	-3.891055	0.111353	-0.300893
6	-3.195147	-1.352903	1.446008
7	-3.587193	-2.362881	0.645307
6	-4.087674	-2.068054	-0.559872
7	-4.272409	-0.874541	-1.122698
6	-4.426190	2.117225	-1.720946
1	-4.933941	1.369178	-2.332145
1	-5.129685	2.911900	-1.460932
1	-3.592000	2.537015	-2.290929
1	-3.425913	3.134985	0.711491
7	-2.679252	-1.642077	2.648535
1	-2.547335	-2.612451	2.917093
1	-2.329816	-0.911572	3.259663
1	-4.385271	-2.928618	-1.161848