

Table 4. (9-MA)₂ S_{CT} state minimum. PCM/TD-PBE0/6-31G(d) partial geometry optimizations in solution

Atomic number	Cartesian coordinates (in Å)		
7	7.884208	-0.244544	1.237906
6	8.026405	-1.597313	1.495491
7	7.608725	-2.339279	0.466617
6	7.173686	-1.439058	-0.464231
6	7.327628	-0.121880	-0.006931
6	6.598866	-1.577835	-1.767709
7	6.271369	-0.457965	-2.441128
6	6.459373	0.730828	-1.881571
7	6.977461	1.020525	-0.632390
6	8.240562	0.847676	2.105763
1	7.648058	0.832585	3.028077
1	8.043292	1.778839	1.569934
1	9.302015	0.807060	2.372717
1	8.471280	-1.960860	2.412958
7	6.479027	-2.834044	-2.405000
1	6.216210	-3.560693	-1.739099
1	5.766416	-2.789369	-3.132512
1	6.164103	1.595876	-2.474437
7	4.120143	1.690986	1.157399
6	4.432863	0.752971	2.068983
7	4.261021	-0.513230	1.649737
6	3.815598	-0.371844	0.401328
6	3.694269	1.002919	0.040839
6	3.407515	-1.303990	-0.605736
7	2.921512	-0.824154	-1.778458
6	2.868742	0.476218	-1.949161
7	3.228298	1.473652	-1.079782
6	4.325102	3.124080	1.242924
1	3.516645	3.627352	0.710345
1	4.318748	3.422778	2.292263
1	5.285614	3.370524	0.782218
1	4.795285	1.017439	3.061242
7	3.478040	-2.603716	-0.429935
1	3.177988	-3.234272	-1.179072
1	3.844637	-3.008637	0.435197
1	2.477496	0.823342	-2.905253