

**Table 6. (9-MA)<sub>2</sub> S<sub>B</sub> state minimum. PCM/TD-PBE0/6-31G(d) partial geometry optimizations in solution**

Atomic number	Cartesian coordinates (in Å)		
7	1.682703	2.040620	-0.199402
6	0.880388	2.084832	-1.316844
7	0.672173	0.876259	-1.854637
6	1.450815	0.042998	-1.149274
6	2.112750	0.726586	-0.080148
6	1.504008	-1.403069	-1.057957
7	2.280021	-1.994018	-0.157391
6	3.039145	-1.210265	0.643884
7	2.812872	0.170668	0.863030
6	1.999003	3.107365	0.711635
1	0.480001	3.019852	-1.697903
7	0.789482	-2.136399	-1.927684
1	0.845980	-3.152949	-1.906211
1	0.226859	-1.687842	-2.647492
1	3.711406	-1.699218	1.342378
1	1.683021	2.830281	1.723727
1	3.075252	3.311955	0.718597
1	1.465365	4.008445	0.401913
7	-2.482152	1.283423	-0.051028
6	-3.126735	0.515752	-0.983368
7	-2.842766	-0.763609	-0.909258
6	-1.947335	-0.839730	0.134248
6	-1.707614	0.422052	0.680394
6	-1.253229	-1.912975	0.728278
7	-0.440911	-1.653122	1.768588
6	-0.297179	-0.384580	2.167723
7	-0.871079	0.715036	1.681586
6	-2.553084	2.718747	0.112603
1	-3.813822	0.963767	-1.697473
7	-1.396493	-3.189007	0.319574
1	-1.840491	-3.374725	-0.573976
1	-0.722062	-3.871407	0.653900
1	0.392782	-0.233857	2.998877
1	-2.093899	3.227733	-0.740171
1	-2.005887	2.978372	1.020448
1	-3.593572	3.039128	0.212871