

Table 3. (9-MA)₂ ground-state minimum. PCM/PBE0/6-31G(d) partial geometry optimizations in solution

Atomic number	Cartesian coordinates (in Å)		
7	-2.536903	1.198700	-0.120730
6	-3.140583	0.401405	-1.055895
7	-2.820466	-0.867774	-0.961887
6	-1.944017	-0.904863	0.100365
6	-1.752951	0.368822	0.636788
6	-1.253213	-1.955030	0.738097
7	-0.463319	-1.660302	1.786946
6	-0.356931	-0.381805	2.167484
7	-0.950170	0.694876	1.656106
6	-2.668285	2.631118	0.032745
1	-2.219807	3.155030	-0.816550
1	-2.147425	2.918726	0.947696
1	-3.722492	2.908754	0.115458
1	-3.825832	0.820779	-1.789130
7	-1.385183	-3.243263	0.366115
1	-1.807317	-3.455799	-0.532231
1	-0.721057	-3.916175	0.738357
1	0.312281	-0.201112	3.009885
7	1.615346	2.068104	-0.174053
6	0.845122	2.078886	-1.306331
7	0.668475	0.897474	-1.847728
6	1.408489	0.059317	-1.043479
6	2.002097	0.765629	0.004310
6	1.682794	-1.322914	-1.095116
7	2.487748	-1.849545	-0.154021
6	2.979280	-1.043421	0.794117
7	2.796587	0.265194	0.959206
6	1.886651	3.174114	0.716774
1	2.887355	3.057230	1.137886
1	1.836276	4.109997	0.156288
1	1.154060	3.192141	1.529648
1	0.418181	3.007486	-1.678717
7	1.208161	-2.127428	-2.066390
1	1.282912	-3.131706	-1.928522
1	0.457481	-1.794765	-2.663782
1	3.622739	-1.530402	1.529613