

Table 7. (9-MA)₃ ground state minimum. PCM/PBE0/6-31G(d) partial geometry optimizations in solution

Atomic number	Cartesian coordinates (in Å)		
7	4.268228	1.130163	0.722409
6	4.710168	0.125409	1.540892
7	4.447523	-1.080296	1.094542
6	3.791138	-0.853003	-0.095313
6	3.667398	0.514554	-0.343672
6	3.259269	-1.709539	-1.080311
7	2.675485	-1.159104	-2.160128
6	2.603982	0.174524	-2.241316
7	3.059280	1.088888	-1.387203
6	4.382928	2.556973	0.931046
1	3.827001	2.862682	1.822175
1	3.962340	3.056198	0.056339
1	5.432253	2.844891	1.040136
1	5.231159	0.349220	2.468520
7	3.352402	-3.054086	-1.009487
1	3.554374	-3.474863	-0.107709
1	2.748931	-3.589262	-1.627558
1	2.098603	0.560310	-3.127612
7	0.164216	2.035737	0.206280
6	0.710737	1.762111	1.431413
7	0.813983	0.481593	1.698186
6	0.259716	-0.124382	0.592262
6	-0.154152	0.822713	-0.344054
6	0.048098	-1.474862	0.244778
7	-0.561170	-1.748741	-0.924002
6	-0.934899	-0.726282	-1.701186
7	-0.782002	0.581041	-1.500918
6	-0.029429	3.329439	-0.406161
1	-0.631734	3.186649	-1.305103
1	-0.553636	4.002283	0.277909
1	0.931629	3.768967	-0.689764
1	1.038837	2.565138	2.087511
7	0.434807	-2.491042	1.030728
1	0.217142	-3.444253	0.762484
1	0.860270	-2.316793	1.933497
1	-1.441453	-1.007279	-2.625711
7	-3.952095	1.485217	-0.523293
6	-3.471323	2.052666	0.627057
7	-3.095771	1.185984	1.536920
6	-3.383306	-0.031555	0.961206
6	-3.919953	0.131053	-0.316006
6	-3.250653	-1.359326	1.415732
7	-3.667151	-2.355779	0.613062
6	-4.168850	-2.040743	-0.586978
7	-4.331096	-0.840823	-1.140303
6	-4.376791	2.158510	-1.730057
1	-4.897927	1.431643	-2.355624
1	-5.056335	2.979332	-1.486921
1	-3.512458	2.545491	-2.278090
1	-3.407407	3.133432	0.729709
7	-2.762768	-1.663374	2.631732
1	-2.536734	-2.632711	2.831825
1	-2.287846	-0.947757	3.171672
1	-4.488581	-2.890526	-1.193348