

Table 5. (9-MA)₂ S_{DEL} state minimum. PCM/TD-PBE0/6-31G(d) partial geometry optimizations in solution

| Atomic number | Cartesian coordinates (in Å) | | |
|---------------|------------------------------|-----------|-----------|
| 7 | -2.482696 | 1.272057 | -0.084298 |
| 6 | -3.106257 | 0.510188 | -1.033826 |
| 7 | -2.807608 | -0.794091 | -0.939084 |
| 6 | -1.956103 | -0.863624 | 0.103796 |
| 6 | -1.720635 | 0.411461 | 0.669460 |
| 6 | -1.256502 | -1.946200 | 0.729440 |
| 7 | -0.467440 | -1.685065 | 1.787419 |
| 6 | -0.320908 | -0.430189 | 2.187702 |
| 7 | -0.905640 | 0.700591 | 1.665439 |
| 6 | -2.570390 | 2.703594 | 0.092683 |
| 1 | -2.165951 | 3.224988 | -0.779838 |
| 1 | -1.982003 | 2.967433 | 0.973308 |
| 1 | -3.610719 | 3.004814 | 0.248023 |
| 1 | -3.780411 | 0.944926 | -1.765396 |
| 7 | -1.398352 | -3.217033 | 0.304985 |
| 1 | -1.856850 | -3.403807 | -0.582669 |
| 1 | -0.777717 | -3.930715 | 0.680096 |
| 1 | 0.340084 | -0.263984 | 3.036254 |
| 7 | 1.656751 | 2.048859 | -0.187511 |
| 6 | 0.865844 | 2.093520 | -1.308728 |
| 7 | 0.667014 | 0.884100 | -1.857010 |
| 6 | 1.358222 | 0.043252 | -1.059651 |
| 6 | 1.993817 | 0.731557 | 0.000438 |
| 6 | 1.582701 | -1.369207 | -1.092456 |
| 7 | 2.387819 | -1.921114 | -0.162316 |
| 6 | 2.915751 | -1.145389 | 0.771210 |
| 7 | 2.765134 | 0.209082 | 0.941119 |
| 6 | 2.012286 | 3.147092 | 0.677909 |
| 1 | 2.797766 | 2.804183 | 1.354106 |
| 1 | 2.384270 | 3.989000 | 0.087398 |
| 1 | 1.148065 | 3.467785 | 1.268763 |
| 1 | 0.472662 | 3.028693 | -1.692764 |
| 7 | 1.026400 | -2.153573 | -2.038408 |
| 1 | 1.193315 | -3.155359 | -2.031006 |
| 1 | 0.405123 | -1.763089 | -2.739250 |
| 1 | 3.555747 | -1.637871 | 1.502770 |