

Supplementary.

Table 15. Total energies of the molecular ions in the geometries of the neutral molecule.

Molecular ion	E_{tot} (a.u.)
PbO^+	-267.940878
Pb_2O_2^+	-536.381295
As_4O_6^+	-9396.109026
Sb_4O_6^+	-1413.122828
AsO^+	-2311.074637
$\text{PbAs}_2\text{O}_4^+$	-4966.247324
PbAsO_2^+	-2579.542825
$\text{Pb}_3\text{As}_2\text{O}_6(\text{I})^+$	-5503.083897
$\text{PbSb}_2\text{O}_4^+$	-974.753730