

## Supplementary.

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

Molecular ion	$E_{\text{tot}}$ (a.u.)
PbO <sup>+</sup>	-267.940878
Pb <sub>2</sub> O <sub>2</sub> <sup>+</sup>	-536.381295
As <sub>4</sub> O <sub>6</sub> <sup>+</sup>	-9396.109026
Sb <sub>4</sub> O <sub>6</sub> <sup>+</sup>	-1413.122828
AsO <sup>+</sup>	-2311.074637
PbAs <sub>2</sub> O <sub>4</sub> <sup>+</sup>	-4966.247324
PbAsO <sub>2</sub> <sup>+</sup>	-2579.542825
Pb <sub>3</sub> As <sub>2</sub> O <sub>6</sub> (I) <sup>+</sup>	-5503.083897
PbSb <sub>2</sub> O <sub>4</sub> <sup>+</sup>	-974.753730