

On the Nature of Lead(II) “Lone Pair”

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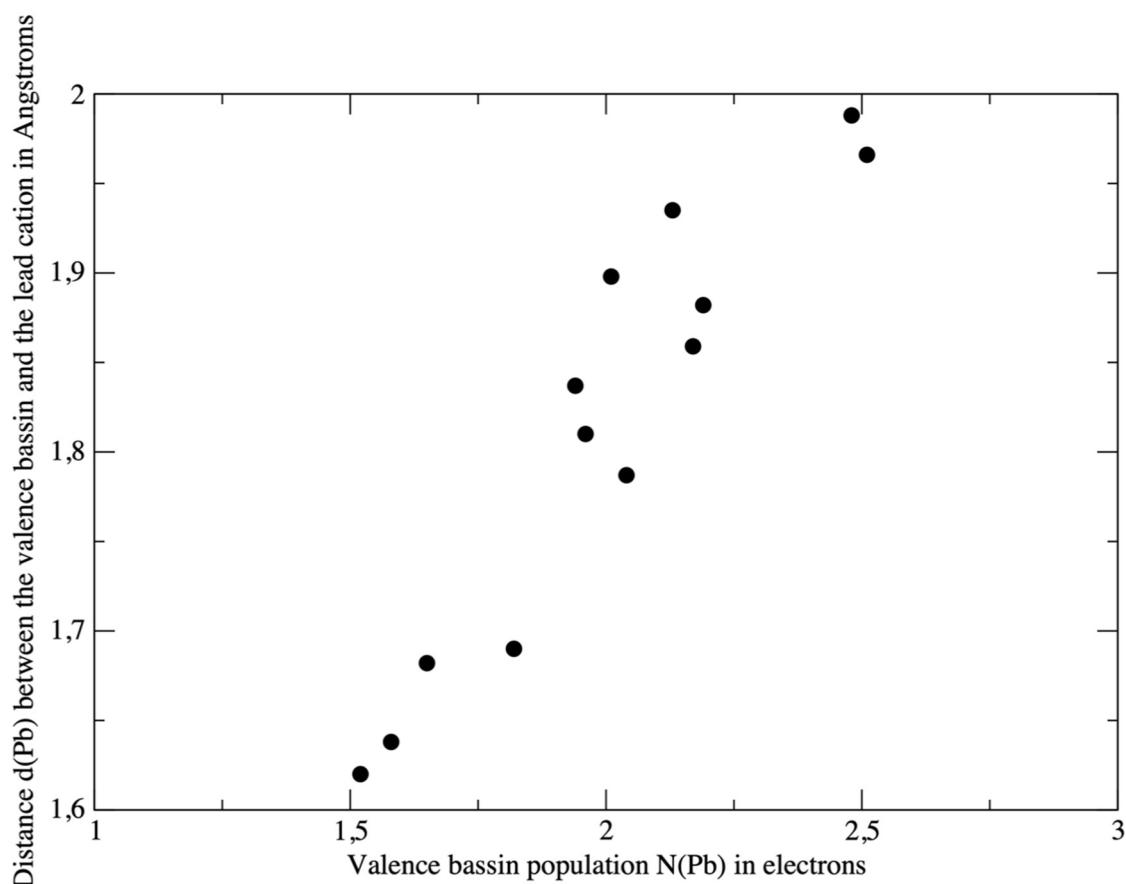


Figure S1. Distance between the ELF attractor of the lead valence basin in function of the population of V(Pb), data extracted from Table 3.

Table S1. Pb-L distances in Angströms and L-Pb-L angles in degrees of the complexes optimized with the different methods.

| | Turbomole | | GAUSSIAN | | | |
|--|-----------|--------|----------|--------|--------|--------|
| | MP2 | | B3LYP | | wB97XD | |
| | Pb-L | L-Pb-L | Pb-L | L-Pb-L | Pb-L | L-Pb-L |
| [Pb(H) ₃] ⁻ | 1.848 | 91.2 | 1.894 | 91.8 | 1.881 | 91.9 |
| [Pb(Me) ₃] ⁻ | 2.328 | 90.8 | 2.386 | 93.1 | 2.348 | 92.1 |
| [Pb(F) ₃] ⁻ | 2.115 | 97.1 | 2.142 | 97.7 | 2.125 | 96.9 |
| [Pb(Cl) ₃] ⁻ | 2.560 | 99.8 | 2.613 | 100.8 | 2.587 | 99.5 |
| [Pb(Br) ₃] ⁻ | 2.719 | 100.6 | 2.776 | 102.2 | 2.742 | 100.5 |
| [Pb(I) ₃] ⁻ | 2.911 | 100.8 | 2.991 | 103.2 | 2.956 | 101.2 |
| [Pb(CN) ₃] ⁻ | 2.306 | 91.9 | 2.358 | 93.6 | 2.337 | 92.7 |
| [Pb(OH) ₃] ⁻ | 2.176 | 91.8 | 2.207 | 93.4 | 2.188 | 92.6 |
| [Pb(SH) ₃] ⁻ | 2.619 | 94.6 | 2.690 | 97.2 | 2.652 | 96.0 |
| [Pb(HCN) ₃] ²⁺ | 2.415 | 84.7 | 2.457 | 89.0 | 2.447 | 87.0 |
| [Pb(CO) ₃] ²⁺ | 2.635 | 81.9 | 2.702 | 86.7 | 2.683 | 83.3 |
| [Pb(OH ₂) ₃] ²⁺ | 2.374 | 83.8 | 2.406 | 88.2 | 2.400 | 85.4 |
| [Pb(NH ₃) ₃] ²⁺ | 2.451 | 90.0 | 2.503 | 92.3 | 2.480 | 90.3 |