Table1: DFT-Derived Electronic and Reactivity Parameters of Lead Compounds

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| File | Energy (au) | EHOMO (eV) | ELUMO (eV) | Eg (eV) | I (eV) | A (eV) | η (eV) | δ (eV⁻¹) | μ (eV) | χ (eV) |
| A1 | -1240.3467 | -4.977 | 6.158 | 11.1349 | 4.977 | -6.158 | 5.5675 | 0.1796 | 0.5905 | -0.5905 |
| B1 | -1797.6756 | -4.83 | 3.5212 | 8.3512 | 4.83 | -3.5212 | 4.1756 | 0.2395 | -0.6544 | 0.6544 |
| C1 | -2701.9419 | -5.0967 | 6.626 | 11.7227 | 5.0967 | -6.626 | 5.8613 | 0.1706 | 0.7646 | -0.7646 |
| D1t | -1134.7697 | -4.3702 | 3.4477 | 7.8178 | 4.3702 | -3.4477 | 3.9089 | 0.2558 | -0.4612 | 0.4612 |

**Legend:** **EHOMO**; highest occupied molecular orbital energy, **ELUMO**; lowest unoccupied molecular orbital energy, **Eg**; energy band gaps, **I**; ionisation energy, **A**; electron affinity, **η**; chemical hardness, **δ**; chemical softness, **μ**; chemical potential, **χ**; electronegativity