

THE STABILITY AND REACTIVITY OF SOME TRIALKYL-TIN AND TRIALKYL-LEAD HYDROXYLATES. AN INVESTIGATION USING MOLECULAR QUANTUM MECHANICS METHODS

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The aim of this study was to determine the stability or reactivity of trimethyltin (TMT), trimethyllead (TML), triethyltin (TET) and triethyllead (TEL) hydroxylates, with respect to hydroxyl hydrogen abstraction, hydroxyl radical abstraction and protonation in water. The computations were performed with Gaussian94 and Gaussian98 by the *ab initio* Hartree-Fock method, followed by the non-local density functional method with B3LYP potential in the functional basis with pseudopotentials replacing the core of Pb, Sn, O and C (described in [1-3]). The studied compounds were optimized by the Berny algorithm, and Hessian was computed for the final structures. The abstraction studies were performed taking into account the basis set superposition error. The proton affinities of the hydroxylates' structures were studied taking into account the ZPE of the molecules. The results show that all the hydroxylates are stable with respect to hydroxyl hydrogen abstraction, and that TMT-OH and TET-OH are also stable with respect to hydroxyl group abstraction. The binding energies of the OH radical in TML-OH and TEL-OH are 71.8 and 73.6 kcal/mol, respectively. The binding of OH radical in the trialkyllead compounds seems to be very weak. The radical can be released in the presence of weakly-bound hydrogens (e.g. from antioxidants and unsaturated hydrocarbons) causing peroxydation of the lipid membrane medium and trialkyllead radical toxicity. However, the high proton affinities of TMT-OH (resultant value in water: 64.5 kcal/mol) and TML-OH (resultant value in water: 85.8 kcal/mol) show that dihydrated cationic forms of TMT and TML are much more stable in water in the presence of proton donors than in a non-polar medium.

REFERENCES

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