Potential Surfaces for O Atom-Polymer Reactions

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Ab Initio quantum chemistry methods are used to study the energetics of interactions of O atoms with organic compounds. Polyethylene $(CH_2)_n$ has been chosen as model system to study the interactions of $O(^3P)$ and $O(^1D)$ atoms with polymers. Initially we are looking at H abstraction and represent polyethylene by a C3 (Propane) oligomeric model.

The gradient method, as implemented in the GRADSCF package of programs, is used to determine the geometries and energies of products and reactants. The saddle point, barrier, geometry is determined by minimizing the squares of the gradients of the potential with respect to the internal coordinates.

To correctly describe the change in bonding during the reaction at least a two configuration MCSCF or GVB wavefunction has to be used.

Basis sets include standard Pople and Dunning sets, however, increased with polarization functions and diffuse p functions on both the C and O atoms. The latter is important due to the O^- character of the wavefunction at the saddle point and products.

Normal modes and vibrational energy levels are given for the reactants, saddle point and products.

Finally, quantitative energetics are obtained by implementing a small CAS approach followed by limited CI calculations. Comparisons are made with limited available experimental data.

In future work we will be looking at reactions leading to carbon-carbon bond rupture in larger oligomers.

C-3