

**The American and English Railroad Cases A Collection of All Cases, Affecting Railroads of Every Kind, Decided by the Courts of Appellate Jurisdiction in the United States, England, and Canada 1894-1913. Volume 16**



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RareBooksClub. Paperback. Book Condition: New. This item is printed on demand. Paperback. 18 pages. Original publisher: Washington, D. C. : U. S. Dept. of Transportation, Federal Aviation Administration, Office of Aviation Research, 2005 OCLC Number: (OCoLC)62170039 Subject: Polymers -- Deterioration. Excerpt: . . . energy of 170 kJ mol, obtained for the 150-unit model. Based on the observation of these trends, it was concluded that the kinetics of the backbone scission reaction is affected by the density and by the degree of polymerization of the decomposing polymer. This means that the conventional approach to the kinetic modeling of polymer decomposition, in which the chain scission rate constants are assigned values obtained from the measurements performed on small gas-phase molecules, is not generally valid. This approach should be modified to account for the potential effects of the macromolecular environment on the rate of the scission reactions. For a complete description of the RMD simulations and comparison of the simulation results with experimental observations, see reference 6. Each of the computational approaches discussed in this report has its own advantages and limitations. The quantum chemical approach is an effective tool for mapping complex chemical transformations that are localized on a small segment of a polymer structure. The information obtained from the quantum chemical calculations can be used in combination with statistical reaction rate theories 17 to determine rate constants of the model reactions. However, it is not clear whether the calculated rate constants would represent the kinetics of the corresponding reactions in the polymer melt because the presence of the surrounding molecular structure ( the condensed-phase ) is ignored in the calculations. CONCLUDING REMARKS The application of reactive molecular dynamics ( RMD ) makes it possible to capture the effects of the condensed-phase environment. Unlike the case of the quantum chemical approach,...

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