APPLICATIONS OF COMPUTATIONAL CHEMISTRY TO THE REACTIONS OF LIGNIN

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Recent political and economic issues concerning petroleum supply and availability have renewed interest in the use of biomass as a secure source from which fuels and bioproducts can be developed. While not without difficulties, the carbohydrate constituents are at least somewhat amenable to chemical processing. The lignin fraction however, with its variety of interunit linkages, can be more intransigent in this regard. Both chemical and physical methods are currently being applied to the lignin polymer as routes to useful products. Given the capabilities of computer hardware and software in addressing structures of the size and complexity of lignin models, this paper is concerned with the use of contemporary computational methods to aid in interpreting and guiding experimental results. Results are reported on catalytic oxidation of lignin models and thermochemical reactions.