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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The objective of the work was to extend our basic knowledge of nitration, the fundamental reaction producing high energy nitrogen compounds. Studies included exploration of new areas of aliphatic electrophilic nitration, improved preparative routes to known high energy compounds such as TNT and TNB (1,3,5-trinitrobenzene) and safe new methods to prepare O- and nitrogen compounds.		

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HIGH ENERGY NITROGEN COMPOUNDS

The objective of the work was to extend our basic knowledge of nitration, the fundamental reaction producing high energy nitrogen compounds. Studies included exploration of new areas of aliphatic electrophilic nitration, improved preparative routes to known high energy compounds such as TNT and TNB (1,3,5-trinitrobenzene) and safe new methods to prepare O- and nitrogen compounds.

All objectives of the research project were met. A new, efficient method for the trinitration of benzene to trinitrobenzene (TNB) was worked out using nitric-fluorosulfuric acid.

Mechanistic studies of the nitration of aromatics (both electrophilic, nucleophilic and free radical) were continued. The independence of substrate from regioselectivity in the nitration of reactive aromatics (toluene, anisole, o-xylene) was firmly established, clearly indicating the involvement of two separate reaction steps. No simple, linear relationship can thus exist. Free radical nitration and nitrolysis of aromatics, such as diarylhalonium ions, was also studied.

The use of pyridinium polyhydrogen fluoride as reaction medium for nitronium salt nitrations was found to be highly effective. This solvent has no oxidizing ability, is an excellent solvent for both organic substrates and nitronium salts alike, and thus shows promise in minimizing oxidative side reactions.

The nitration of aliphatic and cycloaliphatic hydrocarbons was continued under electrophilic conditions. Further preparative work for nitroaliphatic compounds, including nitroalkanes, nitroalkenes and nitroadamantane were developed. Work continued on the possible synthesis of tetranitroadamantane and hexanitrobenzene.

The following list of publications refers to published papers containing details of the work.

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