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APPLICATION OF NEGATIVE CHEMICAL IONIZATION MASS SPECTROMETRY TO THE STRUCTURE ELUCIDATION OF PERFLUOROCHEMICALS AND RELATED COMPOUNDS

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The negative chemical ionization mass spectra of representative perfluorinated alkanes, cycloalkanes, ethers and tertiary amines have been examined, using Ar at about 0.5 torr as the reagent gas. The compounds chosen are typical of those under study as components of fluorochemical emulsion blood substitutes. Many such PFC's, particularly those with cyclic or branched structures, give intense molecular ions; most give simple spectra with a few major fragment ions at high mass, in marked contrast to the EI spectra which are dominated by m/e 69 (CF_3+) and 131 (C_3F_5+) of no value for structure elucidation. NCI-GC/MS is more sensitive than conventional EI-GC/MS and promises to be more generally useful for structure determination. Specific examples from the various classes will be presented, and their NCI and EI mass spectra compared.

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ELECTROCHEMICAL FLUORINATION OF CYCLIC AMINES USEFUL AS BLOOD SUBSTITUTE COMPONENTS

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Fluosol-DA, a PFC emulsion has been developed by The Green Cross Corp. of Japan as the first practical artificial blood substitute. From basic and clinical studies, this preparation has been proven to be safe and effective.

In many cases with massive hemorrhage, this preparation significantly improved hemodynamics and blood gas state. A major inconvenience of this preparation, however, is that it must be kept under frozen state for long-term storage due to its instability at room temperature. To improve this point, we have continued to study new PFCs from the aspects of toxicity and emulsion stability. As a main part of this project, a number of compounds were synthesized by electrochemical fluorination, purified , characterized, and used for screening test.

Among these are: F-N-alkylperhydroisoindoles, F-octahydroquinolidines, F-N-methylperhydroquinoline, and F-N-cycloalkylpyrrolidines.

There has been a little known about electrochemical fluorination on cyclic amines. Our findings concerning the effects of molecular structure, reaction conditions on the fluorination of these cyclic amines will be reported in detail.