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NEW POTENTIAL HIGH-ENERGY MATERIALS: 1,3-DIOXA-2,4-DIAZETIDINE, $N_2H_2O_2$, HIGH-LEVEL CALCULATIONS.

As a follow-up to a study of oxadiaziridine, N_2H_2O, as a potential high energy density material, we determine the enthalpies of formation and combustion of a very similar compound with an oxygen-nitrogen four-membered ring, 1,3-dioxa-2,4-diazetidine, which also would exist as *cis* and *trans* isomers. As a fundamental measure of the reactivity of $N_2H_2O_2$, the proton affinities of both isomers were also determined. Gaussian-2, Gaussian-3, and two complete basis set methods were used.

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SYNTHESIS OF A SERIES OF POTENTIAL ANTITUMOR METAL-COMPLEXING LIGANDS: ALLOXAN THIOSEMI-CARBAZONE AND ALLOXAN SEMICARBAZONE COMPOUNDS

This work will present the synthesis of a new series of alloxan-based thiosemicarbazone and semicarbazone compounds. The alloxan substrate was reacted with thiosemicarbazide, 4-methyl-3-thiosemicarbazide, 4-ethyl-3-thiosemicarbazide, 4-phenyl-3-thiosemicarbazide, 4-benzyl-3-thiosemicarbazide, 4,4-dimethyl-3-thiosemicarbazide, semicarbazide, and phenylsemicarbazide, to give a dual series of eight compounds. The eight compounds are: alloxan-thiosemicarbazone, alloxanmethylthiosemicarbazone, alloxan-benzylthiosemicarbazone, alloxanphenylthiosemicarbazone, alloxan-dimethylthiosemicarbazone, alloxan-semicarbazone, and alloxan-phenylsemicarbazone. The data supports an assignment for the structure of the products to include a stable and strongly hydrogen-bonded hydrazinic proton that forms a portion of a uniquely characteristic six-membered ring. The far-downfield resonance (12-15 ppm) in the proton NMR spectrum for this unique hydrogen-bonded proton makes it very easy to identify.

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GREEN PHOTOCHEMISTRY: SUN-INDUCED AROMATIC NUCLEOPHILIC SUBSTITUTION OF ALKOXY GROUPS BY ALKYLAMINES

Solar photochemistry was proved to be efficient for the nucleophilic substitution of alkoxy groups by amines in alkoxynitrobenzenes. The results of the sun-induced photochemical substitution were comparable to the outcome of the same reaction under irradiation by a low-pressure mercury lamp. Using 4'-nitrobenzo-15-crown-5 as a starting material we obtained a polyether amino alcohol - a precursor for the regioselective synthesis of benzoazacrown ethers.

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EXTRACTION OF POLLUTANTS FROM FISH TISSUE FOR ANALYSIS USING MICROEMULSION

A technique for extraction of persistent organic pollutants from fish tissue for analysis is described. 4,4'-dichlorobiphenyl (4,4'-DCB) spiked on fish tissue is extracted using a microemulsion instead of organic solvents. Microemulsions are clear, visually homogeneous fluids prepared by mixing water, oil and a surfactant. They are environmentally friendly replacements for toxic organic solvents. Gas chromatography-electron capture detector (GC-ECD) results show quantitative recovery of 4,4'-DCB from the fish tissue.

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HYBRID DENSITY FUNCTIONAL THEORY INVESTIGATION OF THE HYDROGEN ABSTRACTION REACTION OF FLUOROMETHANE BY THE HYDROXYL RADICAL

A number of hybrid density functional theory methods have been used to calculate energetic and geometric parameters for the hydrogen abstraction reaction of fluoromethane by the hydroxyl radical, an important atmospheric reaction. The results show that some of the theoretical methods investigated here give calculated classical barrier heights for the abstraction reaction that are very small while other methods overestimate the recommended value. The determining factor is the contribution of the Hartree-Fock exchange. We propose three new hybrid density functional theory methods that give classical barrier heights in the range of the best estimate proposed in the literature of 2.8-3.1 kcal/mol.

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ANALYSIS OF SHIITAKE MUSHROOMS BY ICP-OES

In May 2003, the Chattanooga area was subject to a series of heavy rains resulting in the flooding of several local businesses including Crabtree Farms. Crabtree Farms is an organic farm located near the banks of the Chattanooga Creek which is an EPA Superfund Site. Due to the rains, the creek overflowed its banks and submerged Crabtree Farms for several days. This caused the question to be raised as to whether future crops of the farm, especially that of Shiitake mushrooms, would be contaminated by the pollution rich creek. The first four crops of Shiitake mushrooms were harvested, dried, and digested using a variation of EPA 200.3 method. After digestion and dilution, the samples were analyzed by ICP-OES. Contamination levels when compared to reference sample mushrooms were found to be elevated especially in the first crop with each successive crop containing less contaminates than the previous.

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EFFECTS OF MICROWAVE IRRADIATION ON THE POLYMERIZATION OF STYRENE AND METHYL METHACRYLATE IN MICROEMULSIONS

Samples of polystyrene (PS) and poly(methyl methacrylate) (PMMA) were prepared in microemulsions using stearyl trimethylammonium chloride (STAC) as the surfactant (surfactant/monomer = 0.5) via free radical polymerization using a constant (1.0% wt/wt) ratio of initiator (potassium persulfate, KPS) to monomer. Comparisons were drawn among the yields and molecular weights of the polymers produced using microwave irradiation and those produced using a conventional conductive heating method as the respective thermal energy sources for the polymerizations, each conducted at 60°C. Percent recoveries were measured at 5, 15, 30, and 60 minutes after the addition of the initiator. Microwave irradiation produced greater yields of PS at longer reaction times but no significant difference was found in the early stages of polymerization. For PMMA, the effects were more significant and microwave irradiation produced greater yields of PMMA at all reaction times. Molecular weights were higher for the polymers produced using microwave irradiation with PMMA again showing a more significant effect. Branching likely occurs for the polymer samples prepared using microwave irradiation.

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ANALYSIS OF SEMI-VOLATILE ORGANIC COMPOUNDS FROM PARKING LOT RUNOFF IN NEARBY WETLANDS USING GAS CHROMATOGRAPHY/MASS SPECTROMETRY

The presence of semi-volatile organic compounds in soil as a result of parking lot runoff was investigated. Soil samples were collected from the drainage area of the largest parking lot on the university's campus and then dried. The organics were extracted with a Soxhlet extractor and analyzed by GC-MS. Three polycyclic aromatic hydrocarbons (PAHs) known to be environmental hazards were detected, pyrene, phenanthrene, and fluoranthene. The abundance of these pollutants were found to decrease as the sites of collection progressed further from the parking lot, strongly suggesting that the samples originated from the parking lot. Previous reports suggest that these PAHs can be found in asphalt tar and may also originate from the incomplete combustion of gasoline. In either case, this research suggests that runoff water from asphalt parking lots may carry and concentrate toxic PAHs into parking lot drainage areas.

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SYNTHESIS, CHARACTERIZATION, AND ANTIMICROBIAL ACTIVITY OF ORGANOMETALLIC RUTHENIUM(II) COMPLEXES[1]

Six new organometallic ruthenium(II) complexes have been synthesized and characterized by elemental analyses and spectroscopic methods. They have been tested for their antimicrobial activity against various Gram(+) and Gram(-) bacteria. All the complexes are active against *bacillus cereus* and *Salmonella typhimurium* with complex [6], $[(\eta^6\text{-}p\text{-cymene})Ru(3\text{-nb-TSC})Cl]PF_6$, being the most active.

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