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## DETERMINATION OF SPIN-SPIN RELAXATION IN 2-INDANONE BY DIFFERENTIAL SATURATION OF THE ODMR LINE

When 2-indanone is optically pumped into the phosphorescent triplet state the molecule becomes non-planar. Non-symmetrical deuteration of the a-carbons allows the detection of the two non-planar molecules. Cross-relaxation experiment showed that the barrier to inversion much higher than thermal energy allowed at the temperature with which the experiment was performed. In addition, the differential-saturation method was used to determine spin-spin relaxation times that are more accurate than by linewidths alone. Moreover, it revealed a second set of molecules in single crystals of 2-indanone that is postulated to be the crystallographically inequivalent set in the unit cell.

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## EXPLORATION OF GRAPHITE-CATALYZED ALKYLATION AND ACYLATION AT AN REU WORKSHOP

Reactivity of several organic halides in the graphite-catalyzed alkylation and acylation is compared. Surprisingly, 2-iodo-butane was unreactive as opposed to 2-bromobutane. A practical procedure for the synthesis of a photo initiator 2,5-dimethylbenzophenone is developed.

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## RING STRAIN EFFECTS IN CONJUGATED POLYENES

Ring strain is the energetic penalty paid by a cyclic molecule because ring geometry causes its bond angles differ from ideals predicted by valence shell electron pair repulsion theory (VSEPR). For example, if an atom has three bond partners and no lone pairs, VSEPR predicts that bond angles of 120º will be favored. If the molecule contains a ring, the ideal ring is a hexagon because a regular hexagon has interior angles of 120º. This project involves the use of theoretical models to calculate the effects caused by various rings compared to the more ideal hexagon. Trends of molecular stability versus ring size are calculated and discussed.

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## PYGMY SPERM WHALE (*KOGIA BREVICEPS*) AND BELUGA WHALE (*DELPHINAPTERUS LEUCAS*) LIVER TRACE ELEMENT ANALYSES BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY

The University of Maryland Eastern Shore was one of 24 institutions that participated in the 2003 Interlaboratory Comparison Exercise for the Determination of Trace Elements in Marine Mammals orchestrated by the National Institute of Standards and Technology (NIST) and the National Oceanographic and Atmospheric Administration (NOAA). This study involved the analysis of a control and an unknown whale liver sample. The element suite determined was As, Cd, Cu, Mn, Rb, Se, and V. The results obtained at our laboratory for the control material satisfactorily passed the established quality assurance goals. The data obtained by our laboratory for the unknown sample was used in the establishment of the consensus mean for this material.

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## QUANTITATIVE DETERMINATION OF ZnO NANO-PARTICLES IN HUMAN BRONCHOALVEOLAR CARCINOMA-DERIVED LUNG CANCER CELLS

The increasing uses of nanotechnology have caused public concerns on the health and environmental impacts of nanomaterials to living systems. Cytotoxicity of metal oxide nanoparticles has been studied by several different groups. However, the interaction of zinc oxide (ZnO) nanoparticles with cells, especially the amount of ZnO that attaches and penetrates in to the cells, has not been studied. In this paper, the interaction of 71 nm ZnO nanoparticles with human lung cancer cells has been studied, and the total amount of ZnO nanoparticles, including those attached to the cell surface and those penetrated into the cells at different exposure conditions, were quantitatively determined. The results demonstrated that the cell survival rate decreases as the doses of ZnO nanoparticles increase. However, the accumulation of ZnO nanoparticles on cell surface and within the cells increase dramatically, which may be one of the reasons that ZnO nanoparticles cause cell damage.

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## THERMAL STUDIES AND PHYSICAL STRUCTURE OF POLY(METHYL METHACRYLATE)/VAPOR GROWN CARBON NANOFIBERS COMPOSITES PREPARED THROUGH IN SITU BULK POLYMERIZATION

Poly(Methyl Methacrylate) (PMMA)/Vapor Grown Carbon Nanofibers (VGCNFs or CNFs) reinforced composites were obtained through free radical in situ bulk polymerization. Thermogravimetric analysis (TGA) indicated an increase of 15°C in the onset decomposition temperatures of the composites with CNFs concentrations as low as 3.2% weight/weight. Furthermore, composites containing 1.6% and 3.2% CNFs afforded materials that resembled a lightweight foam, but higher CNFs concentrations provided brittle materials. Scanning electron microscopy (SEM) revealed different regions of CNFs dispersion within the polymer matrix.

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## A COMPUTATIONAL INVESTIGATION OF CYCLIC KNOTTED ALKANES: *cyclo*-$C_{27}H_{54}$ IS A STABLE TREFOIL KNOT

Cyclic alkanes, each containing a single trefoil knot, were constructed and investigated using the *PC Spartan Pro* molecular modeling software package. The semiempirical PM3 method was first used to delineate a potential size range in which stable alkane knots might exist. Following this determination, the RHF/3-21G(*) *ab initio* Hartree-Fock method was used to determine energy minima, structures, properties, and complete vibrational analyses of these alkane knots. The $C_{27}H_{54}$ cyclic alkane trefoil knot was found to be the smallest stable alkane knot; calculations indicated that knots smaller than this size either exhibited imaginary vibrational frequencies or unreasonably long carbon-carbon bonds. Some of these smaller knots also rearranged during the computational process to eliminate the knotted portion from the optimized final structure.

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## A THERMOGRAVIMETRIC ANALYSIS STUDY OF THE THERMAL DECOMPOSITION OF SOME TRIS(DIORGANO-DITHIOCARBAMATO)INDIUM(III) AND -GALLIUM(III) COMPLEXES[1]

Seven tris(diorganodithiocarbamato)indium(III) and -gallium(III) complexes, $In(S_2CNR_2)_3$ and $Ga(S_2CNR_2)_3$ respectively, (where R = organic substituent) have been examined for their suitability as precursors for sulfides for the fabrication of photovoltaic materials. Each complex was decomposed thermally and the products analyzed by TGA and, in some cases, by GC/MS and FTIR.

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## FREE AND POLYMER β-CYCLODEXTRINS IMPART UNIQUE SEPARATION EFFECTS WHEN USED AS BUFFER MODIFIERS IN CAPILLARY ZONE ELECTROPHORESIS

A comparison of free (monomer) and polymer β-cyclodextrins as separation buffer modifiers in capillary electrophoresis was performed. Selectivity, migration time modification, and fluorescence detection signal enhancement were the separation parameters evaluated. Fluorescein, 2'7'-difluorofluorescein (Oregon Green ®488), and 5-(bromomethyl)fluorescein were the test analytes. Oregon Green ® 488 phalloidin was used as an electroosmotic flow marker. Separations carried out with polymer β-CD produced a different elution order that those using free β-CD or borate buffer. Both the free and polymer β-CD produced a concentration-dependent decrease in migration time for the test analytes. Free β-CD addition to the separation buffer produced a concentration-dependent fluorescence signal enhancement while the polymer β-CD produced little or no enhancement. These changes in separation characteristics can be attributed to unique complexation interactions between the β-CDs and the individual test analytes. The use of free and polymer β-CDs as buffer modifiers in CZE provides a unique strategy to improve separations of structurally similar molecules.

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## SYNTHESIS OF A SERIES OF DIHYDRO-4,4-DIMETHYL-2,3-FURANDIONE THIOSEMICARBAZONE AND SEMI-CARBAZONE COMPOUNDS

This work will present the synthesis of a new series of dihydro-4,4-dimethyl-2,3-furandione (DDF) thiosemicarbazone and semicarbazone compounds. Dihydro-4,4-dimethyl-2,3-furandione was reacted with eight different thiosemicarbazides and semicarbazides to give a series of eight compounds. The eight compounds are: DDF-thiosemicarbazone, DDF-methylthiosemicarbazone, DDF-ethylthiosemicarbazone, DDF-benzylthiosemicarbazone, DDF-phenylthiosemicarbazone, DDF-dimethylthiosemicarbazone, DDF-semicarbazone, and DDF-phenyl-semicarbazone.

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