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## OLIGOSACCHARIDES LABELED WITH NEW SMALL MOLECULE TAGS

Several monosaccharides, higher molecular weight sugars, and high-mannose *N*-glycans released from RNase B, were labeled with newly synthesized tags [cpd. 2 + 3] by reductive amination. The estimated efficiency of oligosaccharide labeling was high for monosaccharides (90-100%) and low molecular weight sugars (80-95%) but decreased for high molecular weight sugars (<70%). In the latter context, compound [3] with an extended spacer was found to be more successful than compound [2]. The decrease in labeling efficiency is attributed to structural differences in the tags as well as the sugars.

Olga Goltvyanitsa\*, Nandkishor Chindarkar, Andreas H. Franz†  
Department of Chemistry, University of the Pacific, Stockton, CA 95211,  
email: afranz@pacific.edu

## MIXED LIGAND COMPLEXES OF OSMIUM(II) WITH STERICALLY HINDERING POLYPYRIDINE LIGANDS

Ten new Os(II) mixed ligand complexes were synthesized and characterized by UV-visible spectrophotometry. The general formula of the complexes is  $[\text{Os}(\text{II})(\text{N-N})_2\text{LL}]^{n+}$ , where N-N is either 6-methyl-2,2'-bipyridine (6-mbpy) or 2-(2'-pyridyl)quinoline (pq), and LL = *cis*-bis(1,2-diphenylphosphino)ethylene (dppene), ethylenediamine (en), acetylacetonate (acac), oxalate (ox), or  $\text{Cl}_2$ , and  $n = 0, 1, \text{ or } 2$ . The absorption spectra of the complexes exhibit characteristic ligand centered (LC)  $\pi$ - $\pi^*$  bands in the UV and metal-to-ligand charge-transfer (MLCT) transitions in the visible region, whose energy and relative intensity depend on the N-N and LL ligands. For a given N-N ligand, the absorption maxima of the major  $^1\text{MLCT}$  band and the  $^3\text{MLCT}$  band are related to the  $\sigma$ -donor,  $\pi$ -donor, or  $\pi$ -acceptor ability of the LL ligand. The luminescence at room temperature of the two complexes with dppene is assigned to a  $^3\text{MLCT}$  phosphorescence.

Russell T. Sliter\* and David M. Klassen†  
Department of Chemistry and Biochemistry, McMurry University,  
Abilene, Texas 79697, dklassen@mcm.edu.

## ENHANCEMENT EFFECTS OF SURFACTANTS ON THE DC PLASMA ANALYSIS OF COPPER

Investigation of the enhancement effects of several surfactants on the emission lines of copper using a three electrode Direct Current Plasma, DCP, is reported. Of the six different micellar systems (LDS, lithium dodecyl sulfate, SDS, sodium dodecyl sulfate, KDS, potassium dodecyl sulfate, CPB, cetylpyridinium bromide, CTAB, cetyltrimethyl ammonium bromide; Triton X-100) studied the greatest enhancement occurred in the presence of SDS. Because of this sodium sulfate was also studied and it was found not to have as great an enhancement effect as SDS. This effect can be explained by a combination of earlier observed phenomena: effects of easily ionized elements, increased Penning ionization, thermal pinch and increased residence time in the plasma.

Aaron Hickman\* and Daniel Y. Pharr†  
Chemistry Department VMI, Lexington, VA 24450, pharryd@vmi.edu

## SUBSTITUENT EFFECTS ON THE RELATIVE ELECTRONIC ENERGIES OF PYRROLE AND THE IMINE TAUTOMERS OF PYRROLE

Using Hartree-Fock computational methods, the structures and properties of twenty-three tetra-substituted pyrroles have been calculated in order to determine the effect of ring substituents on the relative energies of the pyrroles and the tautomeric cyclic azadienes derived from the pyrroles through the shift of the N-H proton to either  $\text{C}^2$  or  $\text{C}^3$  in the ring. Calculations were carried out at the RHF/3-21G(\*) and RHF/6-31G\* levels of theory with generally similar results. Seven tetra-substituted systems, those with either fluoro, hydroxy, methoxy, amino, dimethylamino, nitro, or vinyl substituents, changed the order of stability, indicating that the pyrrole tautomer will be less stable than one of the two azadiene tautomers. Further, all three tautomers in the tetramethyl-, tetramethoxy-, tetrakismonofluoroamino-, tetranitro-, and tetravinyl-substituted systems, and the two azadiene tautomers in the tetrakisdimethylamino-substituted system, are predicted to exist in equilibrium at relative abundances high enough to potentially allow for the detection of the tautomers simultaneously. Although experimental structural data are limited to pyrrole, the calculated bond distances and angles appear to be consistent with experiment and with other computational data.

Wilton R. Wilson,\* Marshall R. Ligare,\* Sara J. Coddling,\* Jason M. Berumen,\* and Robert W. Zoellner†  
Department of Chemistry, Humboldt State University, One Harpst  
Street, Arcata, California 95521-8299, (707) 826-3244,  
rwz7001@humboldt.edu

### **G2, G3, AND COMPLETE BASIS SET CALCULATIONS OF THE THERMODYNAMIC PROPERTIES OF SMALL BERYLLIUM MOLECULES**

Following our recent studies on new high-energy materials, we perform high accuracy energy calculations on small beryllium molecules. For this study, a small molecule is defined as a molecule that contains one to three beryllium atoms. We present data on optimized geometries, enthalpies of formation, enthalpies of combustion, ring strain energy, and spectroscopic data. Of all the beryllium compounds studied, diberyllium dihydride,  $\text{Be}_2\text{H}_2$ , has the highest specific enthalpy of combustion at approximately 94 kJ/g, making it one of the highest high energy materials we have studied to date.

Ryan M. Richard\*, David W. Ball†

Department of Chemistry, Cleveland State University, 2121 Euclid Avenue, Cleveland OH 44115, d.ball@csuohio.edu

### **PYROLYSIS REACTIONS OF 2-PENTADECYL PYRIDINE AND SURFACE EFFECTS: STAINLESS STEEL COMPARED TO GOLD**

Middle distillate fuels contain short-chain alkyl pyridines as the most common organo-nitrogen species. Petroleum, tar-sands, coal, and oil-shale crude sources have been found to contain long-chain alkyl substituted, but not short-chain alkyl pyridines. When these crude oils are refined under what is termed delayed coking conditions, the short-chain alkyl pyridines may be produced by thermal cracking reactions. This research will investigate the thermal cracking reactions and the effect of stainless steel and gold metal surfaces on these cracking reactions.

Jae J. Kwak\*, Gerald L. R. Weatherspoon\*, and George W. Mushrush†  
Chemistry Department, George Mason University, 4400 University Drive, Fairfax, VA

### **ANALYSIS OF VOLATILE CONSTITUENTS OF PERFUMES BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY**

This paper describes the results of an undergraduate research project in which (a) selected perfumes were analyzed by gas chromatography-mass spectrometry (GCMS); (b) the constituents were compared to one of the most successful perfumes of the twentieth century, *L'Air du Temps* (Nina Ricci); (c) the odoriferous properties of the perfumes and their constituents are described and compared; and (d) "his" and "her" perfume products of the same brand and name are compared.

Jennifer Foret,\* and Massimo D. Bezoari†

\*Huntingdon College, Montgomery, AL 36106,

†Northwestern State University, LA Scholars' College, Morrison Hall, Natchitoches, LA 71497, bezoarim@nsula.edu

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