"Chemistry in Action" ~ Undergraduate Poster Session Experimental Chemistry II, CH 463 & 463H Wednesday, June 5, 2013 ~ Gilbert Addition Hall, 209 Department of Chemistry ~ Oregon State University

ATTEMPTED TWO STEP SYNTHESIS OF (4-BROMOPHENYL)PHENYL-METHANONE BY LIGAND FREE PD(II) SUZUKI COUPLING; Adam P Huntley, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331

Synthesis of (4-bromophenyl)phenyl-methanone was attempted, using a two step method;(1) 4-bromobenzoic anhydride, was synthesized using a novel grinding technique; (2) Suzuki coupling of the anhydride with phenyl boronic acid by PdCl2 catalyst. The adjusted yield of the anhydride was 19.6 % determined analytically by GCMS. The Suzuki reaction yielded (4-bromophenyl)phenyl-methanone at 3.1 % relative to injected sample; however the reaction favored a mixture of methyl 4-bromobenzoate at 31.5% and methyl 4-phenylbenzoate 14.5 %, relative to injected sample, suggesting a possible single pot synthesis of the esters.

2 COMPARISON OF PHOSPHORESCENCE OF 4- METHYLBENZOPHENONE IN A RIGID GLASS AND POLYMER MATRIX. **Michael Hughes**, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331

Usually the phosphorescence of 4- methylbenzophenone is only visible in a rigid glass at 77K. It is possible to immobilize the molecules in a polymer matrix and increase the lifetime enough to observe phosphorescence at room temperature. This was accomplished by using poly(methyl methacrylate) and curing over several days. Emission and excitation charts for both glass and polymer matrix will be presented as well as lifetime data.

FRIEDEL CRAFTS ACYLATION METHOD TO SYNTHESIS (4-ETHOXYPHENYL)PHENYLMETHANONE BY AlCl₃ CATALYST. **Xinran Tan**, Department of Chemistry, Oregon State University, Corvallis, Oregon 97333

The benzoyl chloride (0.098mol) reacted with ethoxylbenzene (0.1017mol) to form 10.5g (4-ethoxyphenyl)phenylmethanone (0.0464mol) via a Friedel-Crafts Acylation reaction with AlCl₃ catalyst. The whole reaction was reacted in the CH_2Cl_2 (DCM). The percent yield of the product was 47.36%.

4 FRIEDEL-CRAFTS SYNTHESIS AND CHARACTERIZATION OF 4-BROMO-4'-FLUOROBENZOPHENONE. **Jordan D.L. Reaksecker** Oregon State University Dept. of Chemistry 97330

Benzophenones are used as organic building blocks and UV absorbance in a wide array of applications. This study set out to synthesize 4-Bromo-4'-flurobenzophenone and characterize the compound both physically and photochemicaly. The compound was synthesized by Friedel-Crafts acylation. The melting point was determined to be 108-109 °C which is one degree higher compared to the literature value. The GCMS value was determined to be 278 amu which matches the literature value; showing that the compound synthesized was of exceptionally pure quality.

5 PHOTOCHEMICAL PROPERTIES OF 4-BROMO 4'-METHYLBENZOPHENONE. A. E. Mitschele. Department of Chemistry, Oregon State University, Corvallis, Oregon 97331.

Benzophenones, such as 4-bromo-4'-methylbenzophenone, are widely used as photoaffinity labeling in the study of cell cultures and living systems. Their distinct photoreactivity allows the chemical environment to be identified and characterized as the benzophenone ring reacts with its immediate environment in the cell membrane. These photochemical properties can be characterized using IR, quantitative UV measurements and the phosphorescence spectrum obtained experimentally.

- 6 SYNTHESIS OF 4-FLUOROBENZOPHENONE BY FRIEDEL-CRAFTS. **Ashley M. Moon**, Department of Chemistry, Oregon State University-Corvallis, OR 97333.
- 4-fluorobenzophenone was synthesized by Friedel-crafts method using fluorobenzene, benzoyl chloride, and aluminum trichloride catalyst. The reaction progress was monitored by TLC. 4-fluorobenzophenone was cleaned-up and purified by steam distillation, phase separation, and recrystallization. The percent yield after recrystallization was 12% and had a melting point of 47-48 °C.
- 7 SYNTHESIS OF 4,4'-DIFLUOROBENZOPHENONE. **Jared M. Harzan**, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331
- 4,4'-Difluorobenzophenone is important due to its use as a precursor to PEEK, a high performance polymer. Its synthesis using a Friedel-Crafts acylation is studied, as well as its NMR, which is made interesting due to the symmetry and presence of fluorine.
- 8. SYNTHESIS OF 4-FLUORO-4'-PROPYLBENZOPHENONE **A.C. Anderson**, E. Firpo, C. Pastorek. Department of Chemistry, Oregon State University-Corvallis, Oregon 97331.
- 4-fluoro-4'-propylbenzophenone was synthesized via Friedel-Crafts Acylation. Reaction product was characterized by proton, carbon, and fluorine nuclear magnetic resonance (NMR). Presented is a synthesis and purification method for this benzophenone that is not seen in prior art.
- 9. SYNTHESIS OF 4-METHYL-4'-PROPYLBENZOPHENONE. **Brian W. Eckelman**, Department of Chemistry, Oregon State University, Corvallis, Oregon 97331.

Benzophenones are used as UV blockers with commercial applications in sunscreen and packaging. Synthesis by Friedel-Crafts acylation has been followed from literature found for 4,4'-dimethylbenzophenone, with the substitution of propylbenzene instead of toluene, in order to determine suitability of proposed method.

10. SYNTHESIS OF DISUBSTITUTED BENZOPHENONE, (4-BROMOPHENYL)-(4-METHOXYPHENYL)METHANONE. **D.J. Hawes.** Department of Chemistry, Oregon State University-Corvallis, Oregon 97331.

Synthesis of disubstituted benzophenone, (4-bromophenyl)-(4-methoxyphenyl)methanone, via a Friedel-Crafts Acylation developed by Beecham Corp is currently being validated. Thin layer chromatography shows the creation of new product between known carboxylic acid Rf and anisol Rf. Purification via crystallization yielded small white crystals with melting point of 160.5 °C. GC/MS data show high abundance of parent ions at 290 and 292m/z at retention time 14.34 minutes. NMR data also indicate synthesis of benzophenone.

11. FRIEDEL-CRAFTS SYNTHESIS OF 4-CHLORO-4'-FLUOROBENZOPHENONE. **D.Q. Gumaer**. Department of Chemistry, Oregon State University-Corvallis, Oregon 97331.

Benzophenones have a wide variety of applications such as preventing UV light from damaging sensitive materials and in mapping peptide-protein interactions. In this report is a detailed Friedel-Crafts acylation synthesis for 4-chloro-4'-fluorobenzophenone using fluorobenzene and 4-chlorobenzoyl chloride in the presence of an aluminum chloride catalyst.

12. QUANTITATIVE UV SOLVENT STUDY OF 4-FLUOROBENZOPHENONE. **Nicolas H. Abayare**. Gilbert Addition, Oregon State University, Corvallis, Oregon, 97331.

Using a palladium-catalyzed cross-coupling reaction, 4-fluorobenzophenone was synthesized from 4-fluorophenylboronic acid and benzoic anhydride. After characterization was done to confirm the successful synthesis of the benzophenone, a quantitative UV study was done using both polar (EPA) and non-polar (methylcyclohexane) solvents. Data was collected from solutions with both a high and low concentration of the benzophenone dissolved in each solvent through spectroscopic instruments. Analysis of the data was done using GRAMSAI software.

13. SYNTHESIS AND CHARACTERIZATION OF 4-FLUORO-4'-METHYLBENZOPHENONE. M. Fargher, Department of Chemistry, Oregon State University- Corvallis, Oregon 97331

The synthesis of 4-fluoro-4'methylbenzophenone required a Friedel-Crafts acylation of 4-toluoyl chloride and fluorobenzene in the presence of carbon disulfide and an aluminum chloride catalyst. NMR, gas chromatography, and IR spectroscopy were used to characterize the compound, determine the purity and the percent yield of the synthesis.

15. SYNTHESIS AND CHARACTERIZATION OF 4-CHLORO-4'-METHYLBENZOPHENONE. **Clark W Peterson**, Department of Chemistry, Oregon State University, Corvallis OR 97331

4-chloro-4'-methylbenzophenone was synthesized from 4-chlorobenzoyl chloride and an excess of toluene by the process of Friedel-Crafts acylation. The benzophenone was purified by recyrstallization with ethanol to produce a 35.97% yield. Through melting point determination, IR spectroscopy, and HNMR and CNMR spectra analysis the identity of the compound was confirmed to be 4-chloro-4'-methylbenzophenone.

16. SYNTHESIS OF 2-CHLORO-4'-ETHOXYBENZOPHENONE. **Bret Hartsfield**, Department of Chemistry, Oregon State University-Corvallis, Oregon 97330.

The synthesis of 4-Chloro-4'-Ethoxybenzophenone via Friedel Crafts Acylation using phenetole and 4-Chlorobenzoic Acid. After quenching, vacuum distilling and recrystallization from ethanol, the desired product was obtained. Yield was determined to be 24%. IR, NMR, and GC/MS will be presented to demonstrate evidence of the formation of the benzophenone.

17. SYNTHESIS, PURIFICATION, AND CHARACTERIZATIONOF 4-BROMO-4'-PROPYLBENZOPHENONE. **William Ping**, Department of Chemistry, Oregon State University, Corvallis 97331.

The synthesis of 4-bromo-4'-propylbenzophenone was obtained via a Friedel-Crafts acylation reaction of 4-bromobenzoyl chloride, n-propylbenzene, and aluminum chloride. The product was recovered with a 51% yield following recrystallization in ethanol. The product was characterized by; NMR, mass spectrometry, IR, and melting point. These techniques confirmed the compound obtained was both pure and the desired benzophenone.

- **18.** SYNTHESIS OF 4, 4'-DIBROMOBENZOPHENONE. **Brittany Johnston.** Department of Chemistry, Oregon State University, Corvallis 97331.
- 4, 4'-dibromobenzophenone was synthesized from 4-bromobenzoyl chloride and bromobenzene catalyzed by aluminum trichloride. 4-bromobenzoyl chloride, the limiting reagent, formed a carboxylic acid byproduct. Through the synthesis, due to difficulties of solubility, only a portion of the product was fully purified. The crude product was recrystallized in ethanol. The final yield was 3.9%. The pure crystal was analyzed by various methods such as the melting point, GCMS, Proton NMR and Carbon NMR. The melting point was 177.5 °C, and the molecular weight was 339.9 g/mol.
- **19.** QUALITATIVE PHOTOCHEMISTRY OF 4-CHLORO-4'-N-PROPYLBENZOPHENONE. **Tsz Pang Lui.** Department of Chemistry, Oregon State University, Gilbert Addition, Corvallis, OR 97331.

A 5% 4-chloro-4'-n-propylbenzophenone solution in isopropyl alcohol was exposed to UV light for 7 days. A color change of the solution from colorless to yellow is observed. The solution was then transferred to a sample vial that was lightly capped. Some solid was crystallized from the solution. The melting point of the crystal is higher than the original benzophenone. Also the IR and NMR of the crystal shows no carbonyl group vibration. These information shows that the benzophenone has turned into benzopinacol after exposed to UV light.

20. CHARACTERIZATION OF 4-BROMOBENZOPHENONE. **Brandon D. Roses**. Oregon State University Corvallis, Oregon 97333.

The physical and chemical properties of 4-bromobenzophenone make it relatively easy to be characterized using MP, GC-MS, IR and NMR technology.

21. RECRYSTALLIZATION OF 4-BROMO-4'-CHLOROBENZOPHENONE. **Denise S. Williams.** Department of Chemistry, Oregon State University, Gilbert Addition, Corvallis, OR 97331

After crystallizing the product, a filtration was done to extract the crystals. There were two filtrations. One produced pink crystals and the second one produced white crystals. Both of these crystals were tested for purity with melting temp, NMR, GCMS and IR. The pink crystals were found to be 7.081% less pure than the white crystals from a GCMS. But both crystals still had impurities. In comparing the data, the 7.081% difference in purity can be seen in the physical data collected.

22. SOLVENT STUDY OF 4-CHLORO-4-METHOXYBENZOPHENONE TO DETERMINE PHOTOPHYSICAL PARAMETERS: ABSORPTION, EXCITTION AND EMISSION: **Erica Nuth**, Department of Chemistry, Oregon State University, Corvallis, OR 97331

4-chloro-4'-methoxybenzophenone was synthesized via the Friedel-Crafts acylation with chlorobenzene and 4-methoxybenzoyl chloride. The characterization of the compound was done by MS, IR, NMR, melting point. After the characterization, a quantitative solvent study was done using UV spectrometry, to determine the photophysical parameters for the electronic transition state. A concentrated and a dilute solution of a nonpolar solvent, methylcyclohexane, was made with 4-Chloro-4-methoxybenzophenone. The same was done in a polar solvent, ether-isopentane-ethanol, EPA. The UV absorbance was measured for each of the four mixtures and GRAMSAI software was used for curve-fitting. The lifetime was found from studying the UV excitation and emission state.

23. SYNTHESIS AND CHARACTERIZATION OF 4-CHLORO-4'-METHYLBENZOPHENONE. **Arsalan Zolfaghari**, Department of Chemistry, Oregon State University, Corvallis, OR 97331.

Our class employed two different routes, a Friedel-Crafts acylation and a Suzuki-Miyaura coupling. The Suzuki coupling was a 2 step synthesis from a benzoic acid derivative (1) to anhydride (3). 3 was then converted to 4 via Suzuki coupling. The characterization of 4-chloro-4'-methylbenzophenone will also be discussed.

24. CONFIRMATION OF MOLECULAR STRUCTURE BY NMR **Jacquellyn Helm** Oregon State University, Department of Chemistry, Corvallis, OR 97331

Nuclear magnetic resonance spectroscopy (NMR) is a powerful tool in determining the molecular structure of organic compounds. In this study, NMR was used to confirm the successful synthesis of 4-methoxybenzophenone (4-MBP) via Friedel-Crafts acylation from anisole and benzoyl chloride.