

Chem 324 Spring 2008  
Keller  
Expt 5: Benzoin-Grignard Report

1. Experimental section. One paragraph for grignard rxn, and one for acetonide-forming rxn. Do not list NMR peaks.
2. TLC. Show scans or reproductions of your lab notebook, including solvent used. Identify the spots, origin, and solvent front. Measure or estimate the R<sub>f</sub> of the spots. Briefly tell what, if anything, you learned by running the TLC.
3. Print good quality (phased and integrated) <sup>1</sup>H, <sup>13</sup>C spectra of diol (if you took it) and acetonide. Assign peaks as best you can. Use a formula either careful hand-drawn or computer.
4. Show a nice graphic of the NOESY 2D spectrum. Paste graphics of the <sup>1</sup>H-1D spectra on x- and y-axes (or print out using the VNMR method that puts high resolution 1D spectra on x- and y-axes.) Put in hand- or computer-drawn lines with the cross peaks labeled (“A”, “B” etc). Then show which atoms are related by the cross peaks, using a formula of the acetonide, or a Hyperchem graphic.
5. Hyperchem molecular modeling. Show a graphic of the acetonide product you believe you or your partner isolated based on the NOESY cross-peaks. Using the MM+ molecular mechanics method, explore several conformations to make sure that the conformation you show is the most stable one. This is the one with the lowest energy. Put a copy of this .hin file in your Reports folder.
6. Answer the following questions using several complete sentences and mechanistic formulas (curved arrows etc) as needed. Please write out your answer by hand clearly.
  - a. Why did you settle on the structure shown in 4 or 5 above?
  - b. Mechanistically, why does this isomer form in preference to the other one?
  - c. Is your product chiral?
  - d. Is your product optically active?
  - e. What role or roles did the p-toluenesulfonic acid play in forming the acetonide?  
Be specific.
7. If you referred to any literature to answer these, give the reference in J. Org. Chem style.