Honors Cup Group IV Section 231
Lauren Leader, Nikola Collins, Anuj Shah
1/25/08
Proposal

Honors Cup Proposal

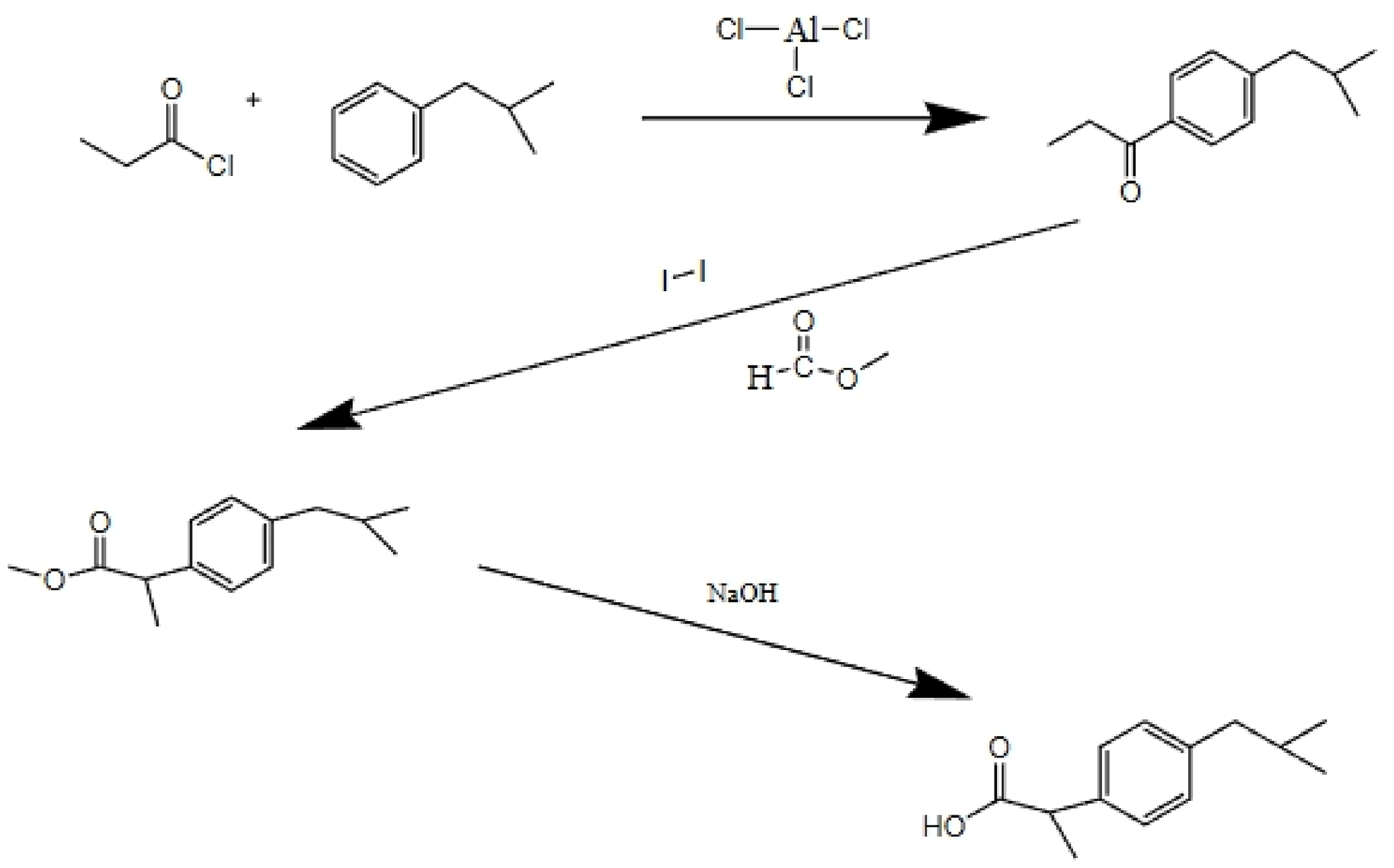
Title: Synthesis of Relief

Introduction: Ibuprofen is an over the counter pain reliever and is used as an alternative to Tylenol. It is an anti-inflammatory. It is used for relief of symptoms of arthritis, fever, and as a blood thinner.

History: Ibuprofen was discovered by the Boots Group, the dominant pharmacy chain in the UK, in the '60's. It was initially launched to heal rheumatoid arthritis.

Racemic mixtures do not affect the human body, in fact, most of ibuprofen is manufactured in racemic mixtures. However, the S-conformation in the one chiral carbon ibuprofen has is the active ingredient. Since that one conformation is very hard to produce, and its enantiomer has no negative effect on the body, it is acceptable to have a mixture.

Reaction Scheme:



Journal of Organic Chemistry, 53(20), 4858-9; 1988□

Chemical & Pharmaceutical Bulletin, 31(9), 3139-48; 1983

Synthesis, (12), 1044-5; 1986

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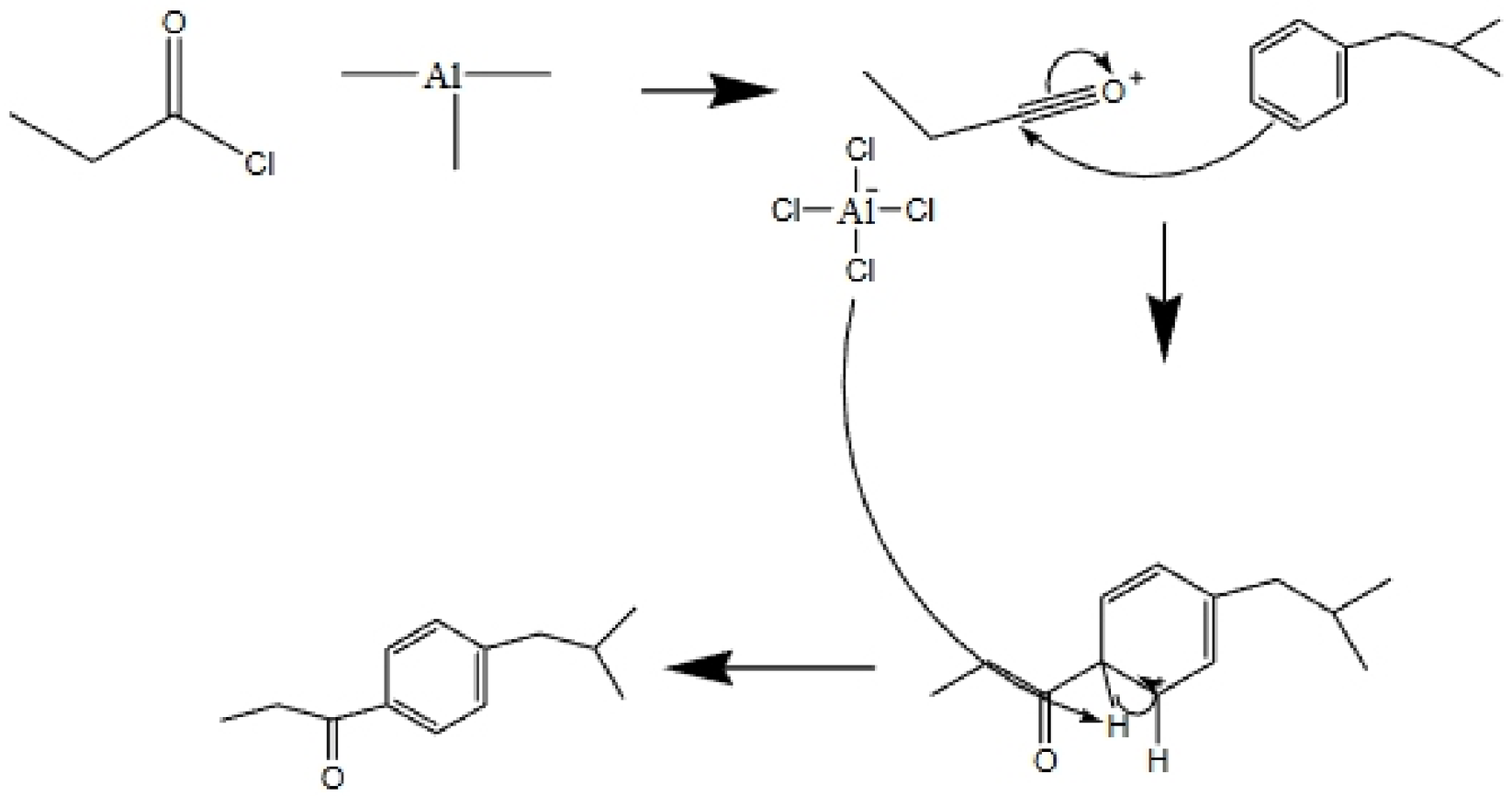
STEP 1



In step one, Electrophilic Aromatic Substitution occurs in which pi electrons from the double bonds of the benzene react with a good electrophile (EtC(=O)Cl). This reaction is very similar to the one done in experiment one (Friedel-Crafts Acylation reaction). First, Anhydrous aluminum chloride and propanoyl chloride should be mixed and flushed with nitrogen in a flask. Then cool temperature to zero degrees Celsius. Then the aromatic compound is added in the same manner. After stirring for an additional 15 minutes at room temperature, the reaction mixture was poured carefully and slowly, with stirring, into ice and HCl in a beaker. Separatory funnel was used to separate the organic layer from the aqueous. Separation through differing boiling points and additional seperatory methods were used to separate the reactants and solution from the products.

Expected Yield: 0.52744 grams

Safety, disposal and green issues 1:

Acetyl Chloride:

Safety: Flammable liquid and vapor. Corrosive. May cause central nervous system depression. Causes eye and skin burns. May cause severe respiratory tract irritation with possible burns. May cause severe digestive tract irritation with possible burns. Water-reactive.

Disposal: **RCRA P-Series:** None listed. **RCRA U-Series:** CAS# 75-36-5: waste number U006 (Corrosive waste, Reactive waste, Toxic waste).

Green Issues: None

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Isobutylbenzene:

Safety: Flammable liquid and vapor. Causes eye, skin, and respiratory tract irritation. Aspiration hazard if swallowed. Can enter lungs and cause damage. May cause central nervous system depression. Marine pollutant.
Target Organs: Central nervous system, lungs.

Disposal: Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

Green issues: Ecotoxicity: Algae: 35 mg/l; 96 hr; LC50 Sheepshead minnow: > 200 mg/l; 96 hr; LC50

Propanoyl Chloride:

Safety: Corrosive. Causes eye and skin burns. Water-reactive. Reacts violently and/or explosively with water, steam or moisture. Flammable liquid and vapor. May ignite or explode on contact with moist air. Lachrymator (substance which increases the flow of tears). May cause severe respiratory tract irritation with possible burns. May cause severe digestive tract irritation with possible burns.

Disposal: Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

Green Issues: No information is available