Lab 3: Nucleophilic Substitution

2-Chloro-2-Methylbutane
(*t*-amyl chloride)
And Lucas Test

BIMOLECULAR (second order)

concerted

S_N

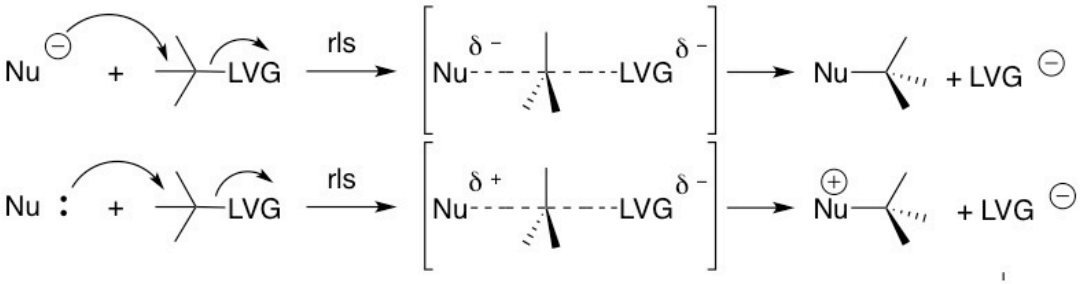
UNIMOLECULAR (first order)

stepwise

S_N2

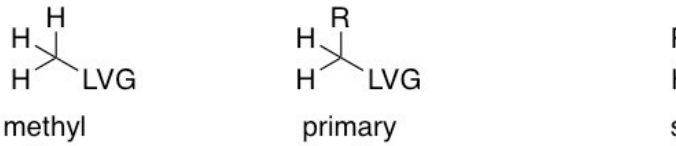
Nu: SOFT, NUCLEOPHILIC, POLARIZABLE, LARGE, LESS ELECTRONEGATIVE ATOM

S_N1



Inversion of configuration at carbon, optical activity is maintained

Racemization, loss of optical activity



SUBSTITUTION

ELIMINATION

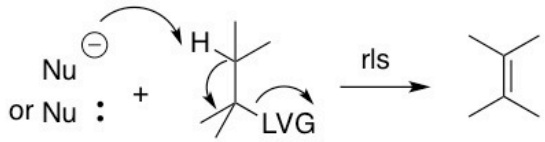
2 ⟷ **1**

bimolecular — unimolecular

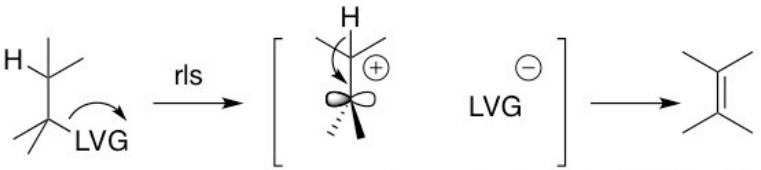
SUBSTITUTION

ELIMINATION

increased solvent polarity/protic solvents

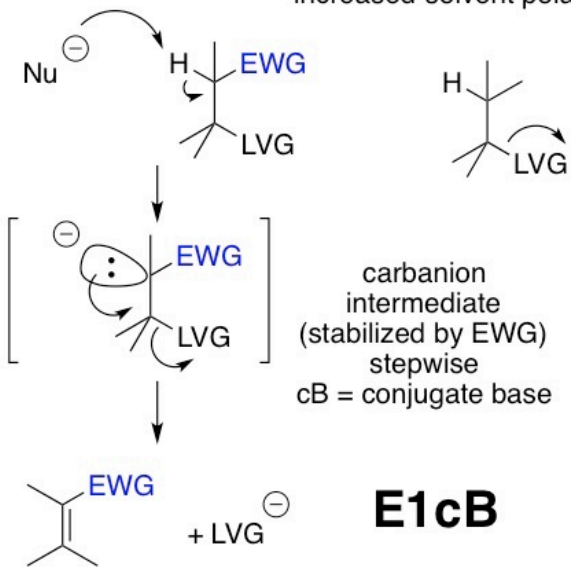


usually most substituted (Zaitsev)



usually most substituted (Zaitsev)

E2



carbanion intermediate (stabilized by EWG) stepwise

cB = conjugate base

E1

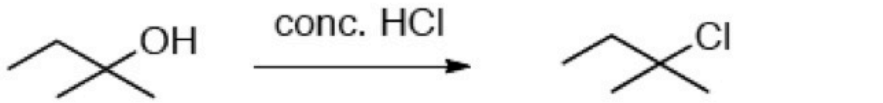
There is a continuum of mechanisms between E2 and E1cB

E1cB

E

Nu: HARD, BASIC, SMALL MORE ELECTRONEGATIVE ATOM

Lab 4: 2-Chloro-2-Methylbutane And Lucas Test

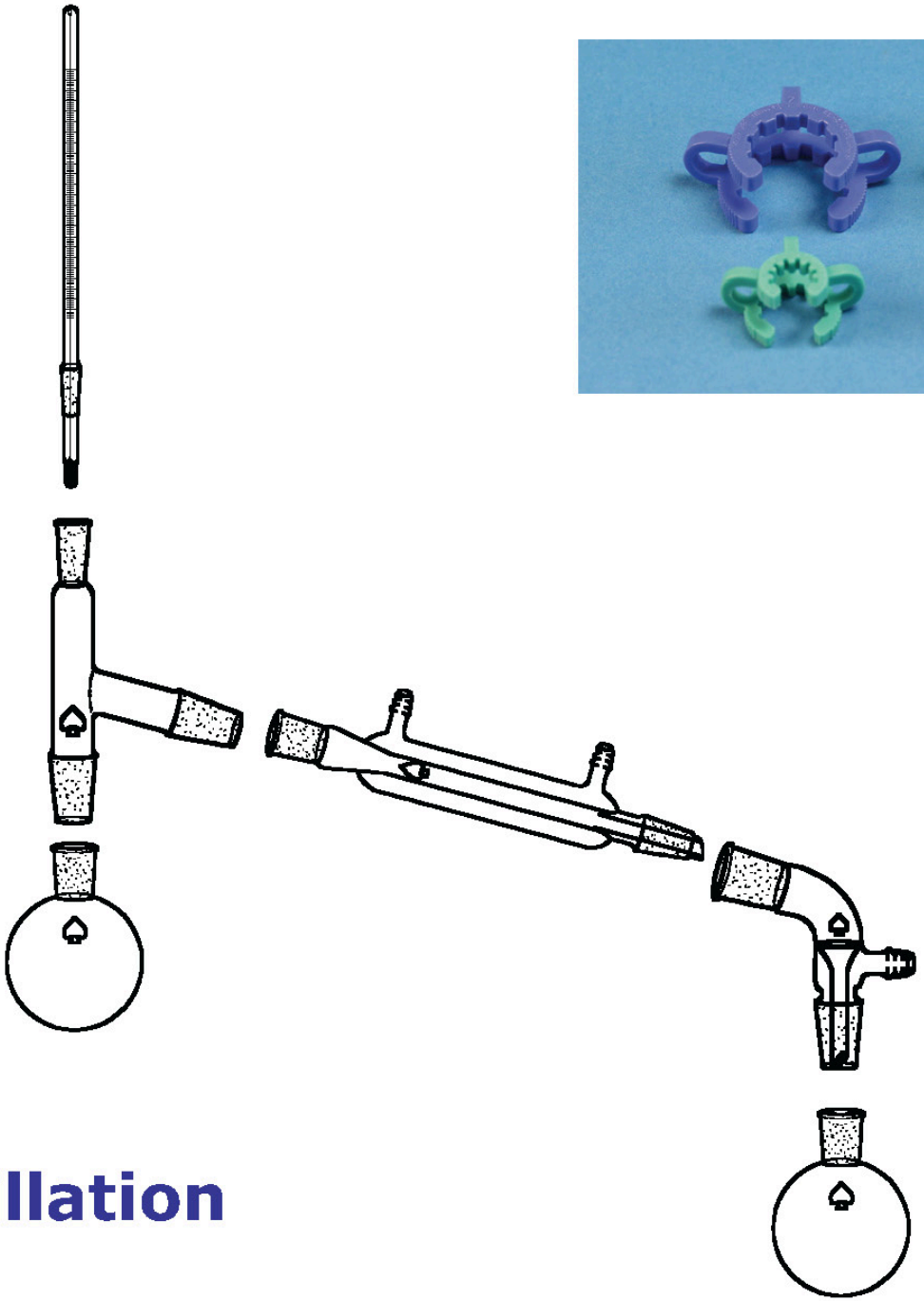


tert-amyl alcohol
(2-methyl-2-butanol)

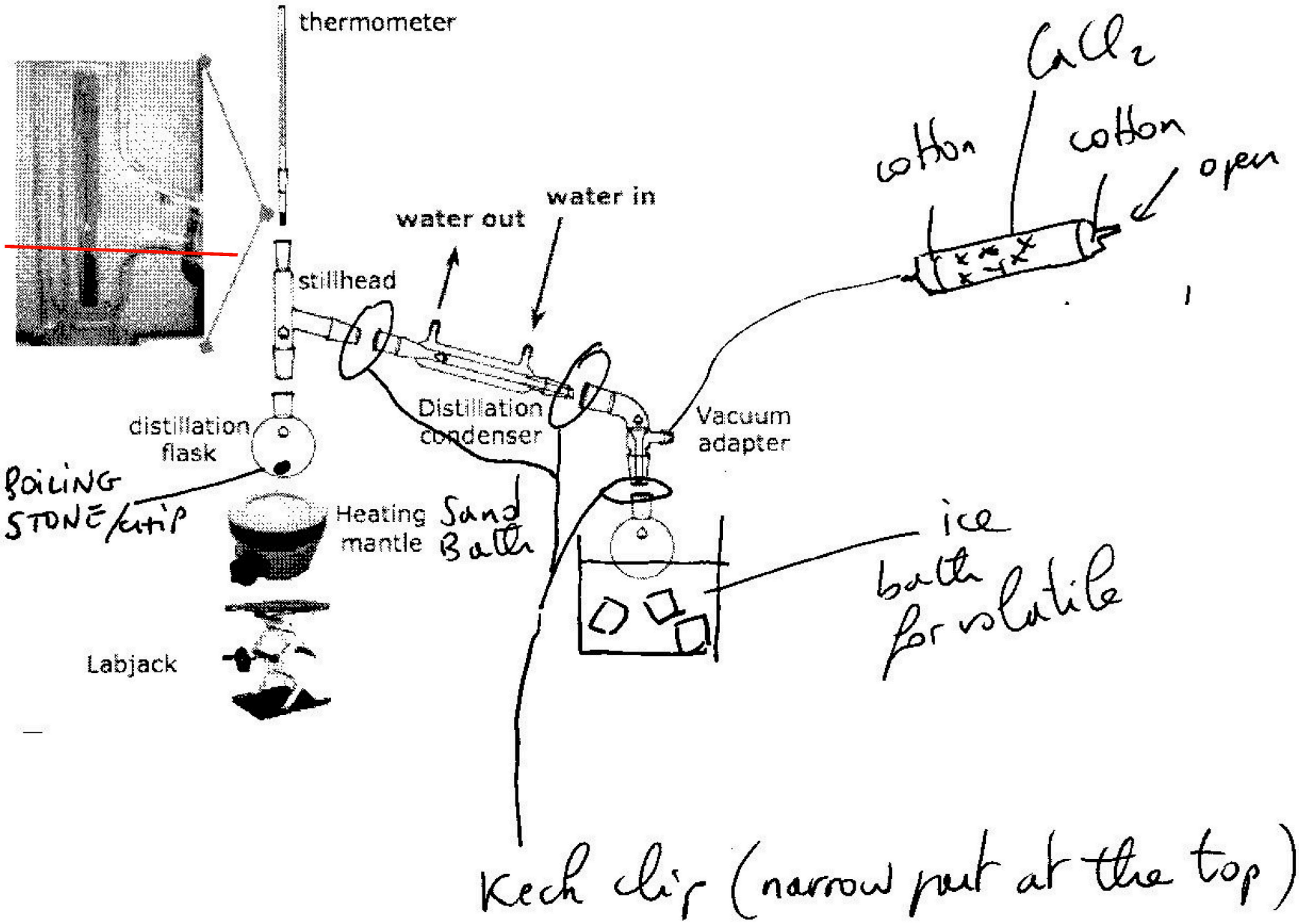
2-chloro-2-methyl-butane

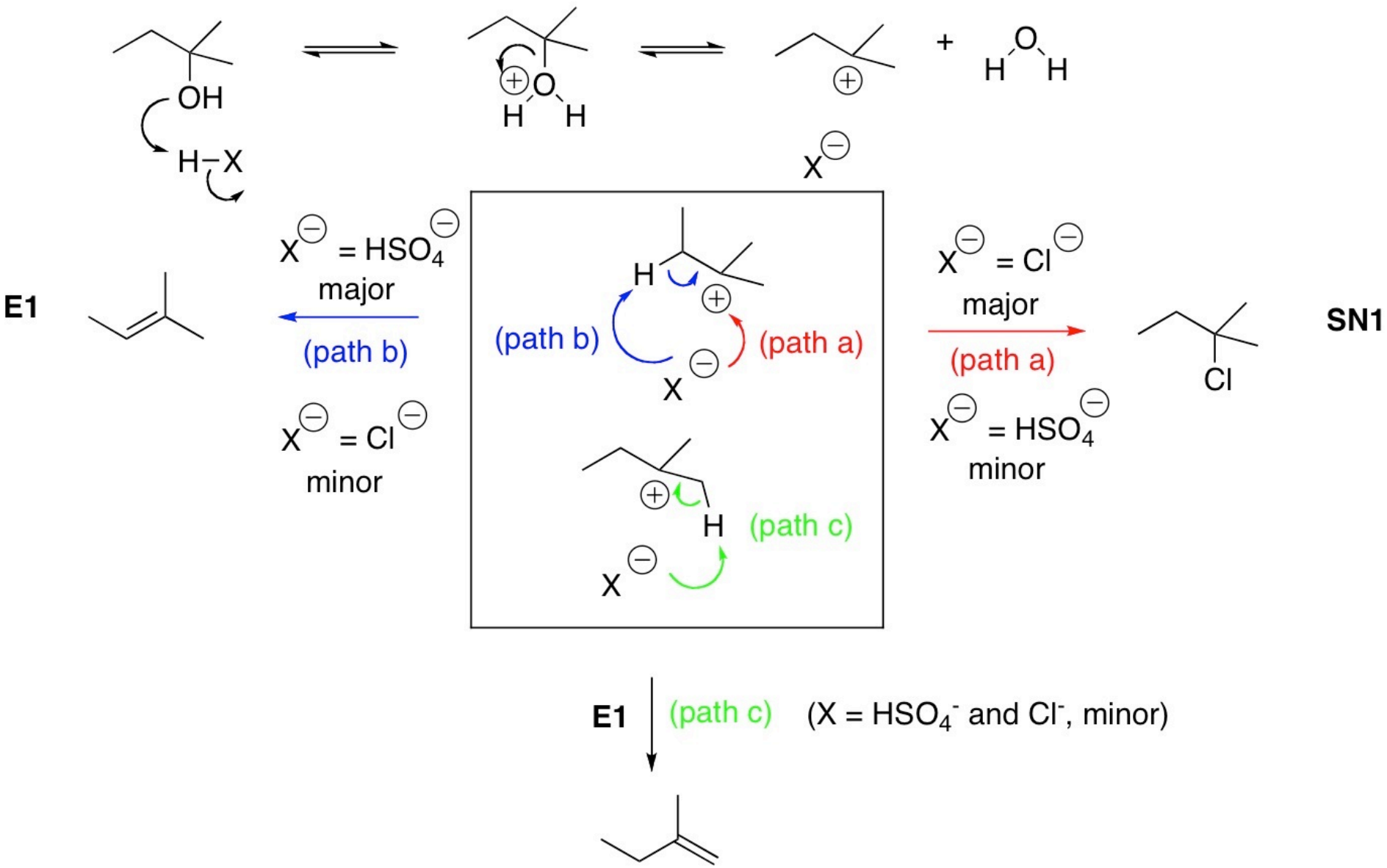
WARNING: wear gloves because of the strongly acidic solutions.

I. Synthesis of 2-Chloro-2-Methylbutane. Add 8 mL of *tert*-amyl alcohol and 20 mL of concentrated (~12 M) HCl to the separatory funnel. Swirl the contents gently without the stopper for about 1 min. Invert and vent to let the pressure equalize before shaking again. Repeat the shaking and venting for several minutes. Allow the mixture to separate into two distinct layers. (Which one is the organic layer?) The organic layer is washed with 10 mL of saturated aqueous NaCl. ["Wash" implies that the aqueous layer is removed before adding the next solution to the organic layer! Even though it is not written, the draining step still must be done.] Add a cold saturated aqueous solution of $NaHCO_3$ and swirl gently **without the stopper**. Once the effervescence ceases, stopper the separatory funnel, invert, vent. Wash with 10 mL of water, then with 10 mL of saturated aqueous NaCl. Dry the organic layer over anhydrous sodium or magnesium sulfate. Transfer to a 25 mL RBF and perform simple distillation (power controller on about 6, tare the receiver, cool the receiver in ice and use a drying tube). The product is collected around 80-85°C. Determine the percent yield. Purified 2-chloro-2-methylbutane will be collected in a specific waste container.

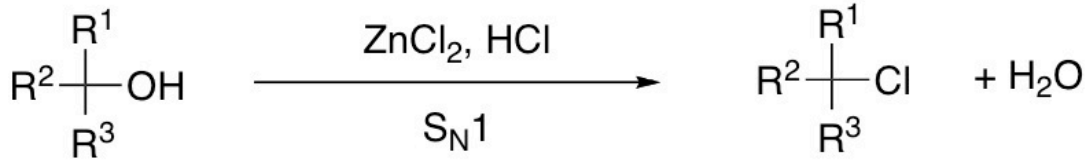


Simple distillation


thermometer
water out
water in
stillhead
distillation flask
Distillation condenser
Vacuum adapter
BOILING STONE/stir
Heating mantle
Sand Bath
Labjack
CaCl2
cotton
cotton
open
ice bath for volatile
Keck clip (narrow part at the top)


OH
H–X
O
H
H
+
O
H
H
X⊖
E1
X⊖ = HSO4⊖
major
(path b)
X⊖ = Cl⊖
minor
H
(path b)
(path a)
X
H
(path c)
X
X⊖ = Cl⊖
major
(path a)
X⊖ = HSO4⊖
minor
Cl
SN1
E1
(path c)
(X = HSO4- and Cl-, minor)

II. Lucas Test. You will run the test in 4 test tubes (3 known alcohols (1°, 2°, 3°), and one unknown alcohol you will need to classify). Use 5-10 drops of compound to be tested. Fill about 2/3 of a long pasteur pipette with the Lucas test solution (approx. 1.5 mL) and add to the test tubes.
The Lucas test proceeds via

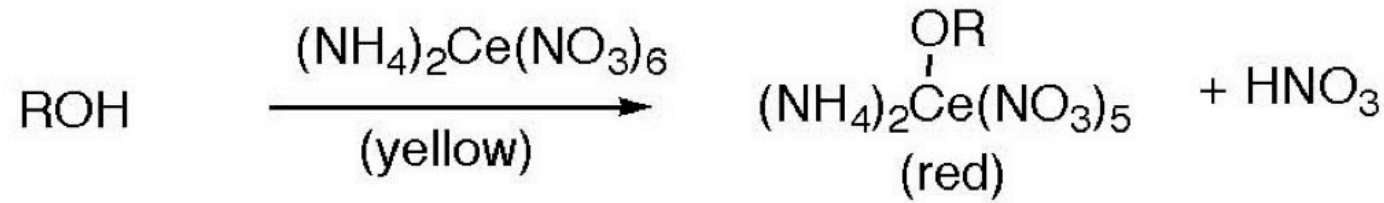


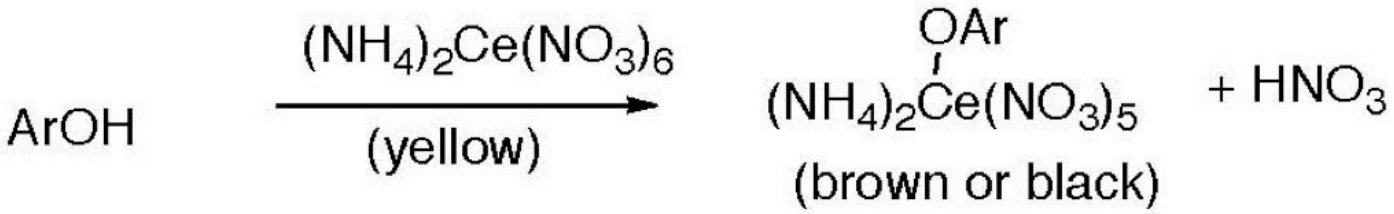
Notes on the Lucas Test: the reagent is made by dissolving 16 g of anhydrous $ZnCl_2$ in 10 ml of concentrated (12N) hydrochloric acid and cooling to avoid HCl loss (you will not need to prepare the reagent).
The Lucas test reagent is highly acidic: **WEAR GLOVES**. If the reagent comes into contact with the skin, was immediately and thoroughly with water, and 5% aqueous bicarbonate.
Tertiary alcohols form an emulsion that appears as two layers (due to the water-insoluble alkyl halide) almost immediately. Secondary alcohols form this emulsion after several minutes, while primary alcohols react after a very long time (if at all). Some secondary alcohols (e.g. isopropyl) may not *visually* form the layers because of the low-boiling alkyl halide, which may evaporate.

Positive Test (Alcohols (Secondary and Tertiary):
Appearance of a cloudy second layer or emulsion; 3° alcohols: immediate to ~2 minutes; 2° alcohols: 3 - 10 minutes; 1° alcohols: no reaction (or very slow > 10 min)
Complications
The test applies *only to those alcohols soluble in the reagent* (monofunctional alcohols lower than hexyl and some polyfunctional alcohols).

CERIC AMMONIUM NITRATE

Alcohols and Phenols:





Positive Test

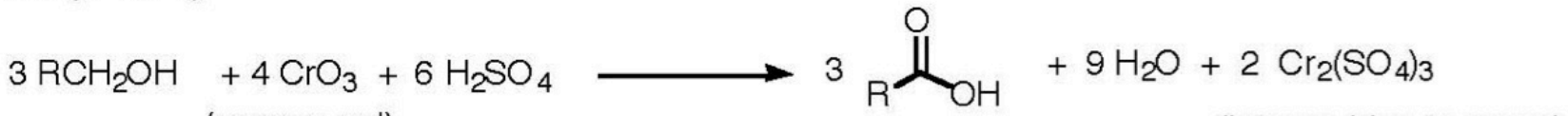
Formation of a red alkoxy cerium(IV) compound is a positive test.
Phenols give a brown color or precipitate as a positive test.

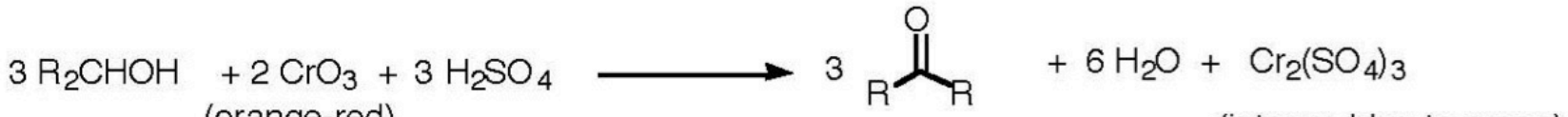
Complications

Hot solutions of Ce(IV) oxidize many organic compounds.

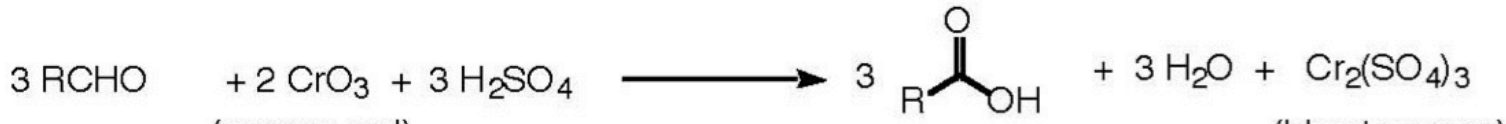
CHROMIC ANHYDRIDE (JONES OXIDATION)

Alcohols (1° & 2°):





Aldehydes:

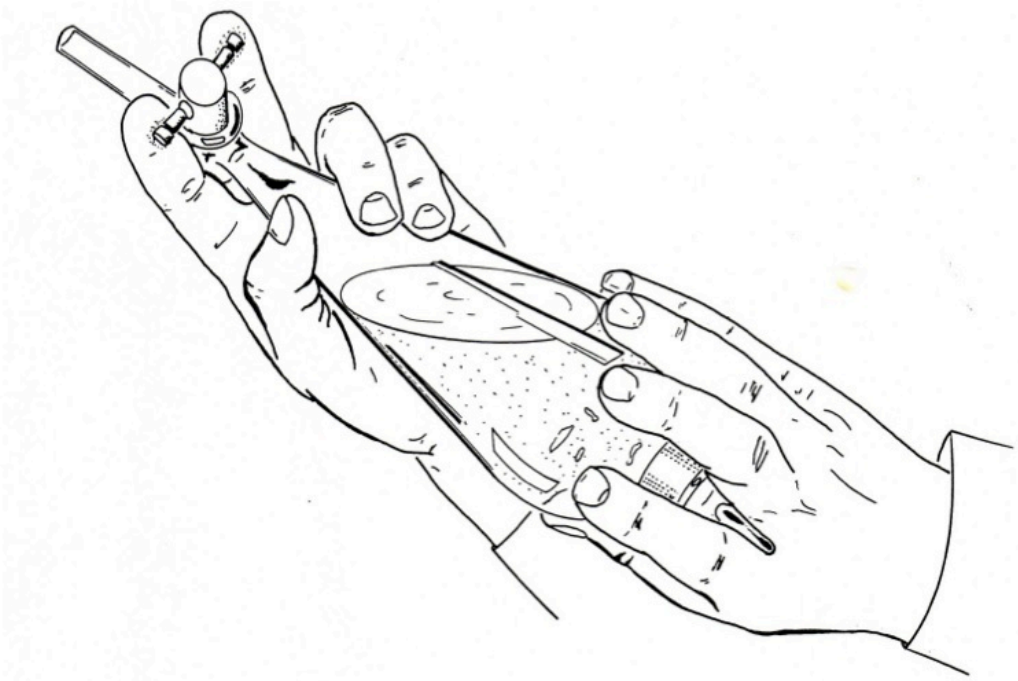


Positive Test

A positive test for primary or secondary alcohols consists in the production of an opaque suspension with a green to blue color. Tertiary alcohols give no visible reaction within 2 sec, the solution remaining orange in color. Disregard any changes after 2 sec.

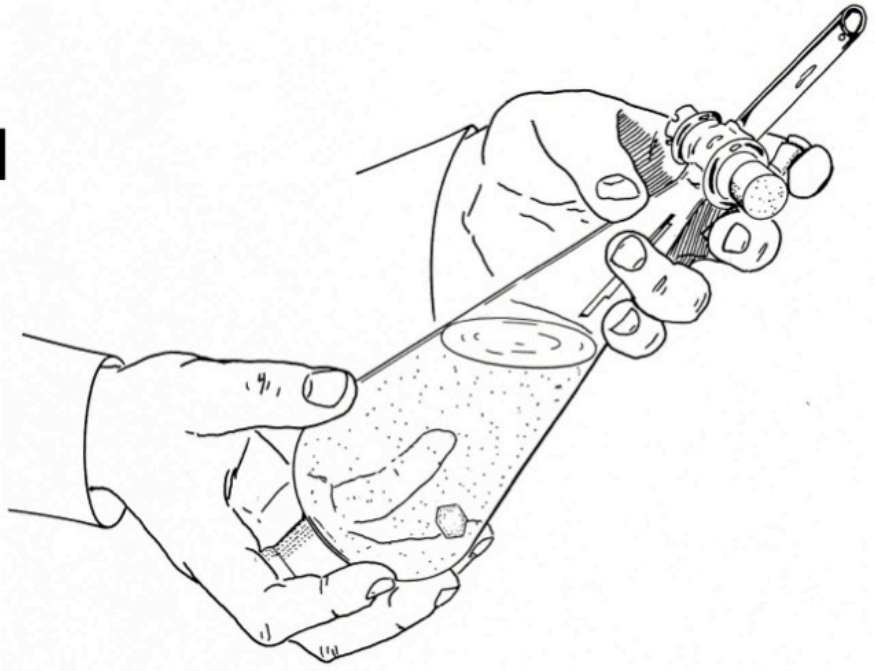
Complications

Aldehydes are better characterized in other ways. The color usually develops in 5 - 15 seconds. Enols may give a positive test. Phenols give a dark colored solution which is not blue-green like a positive test.

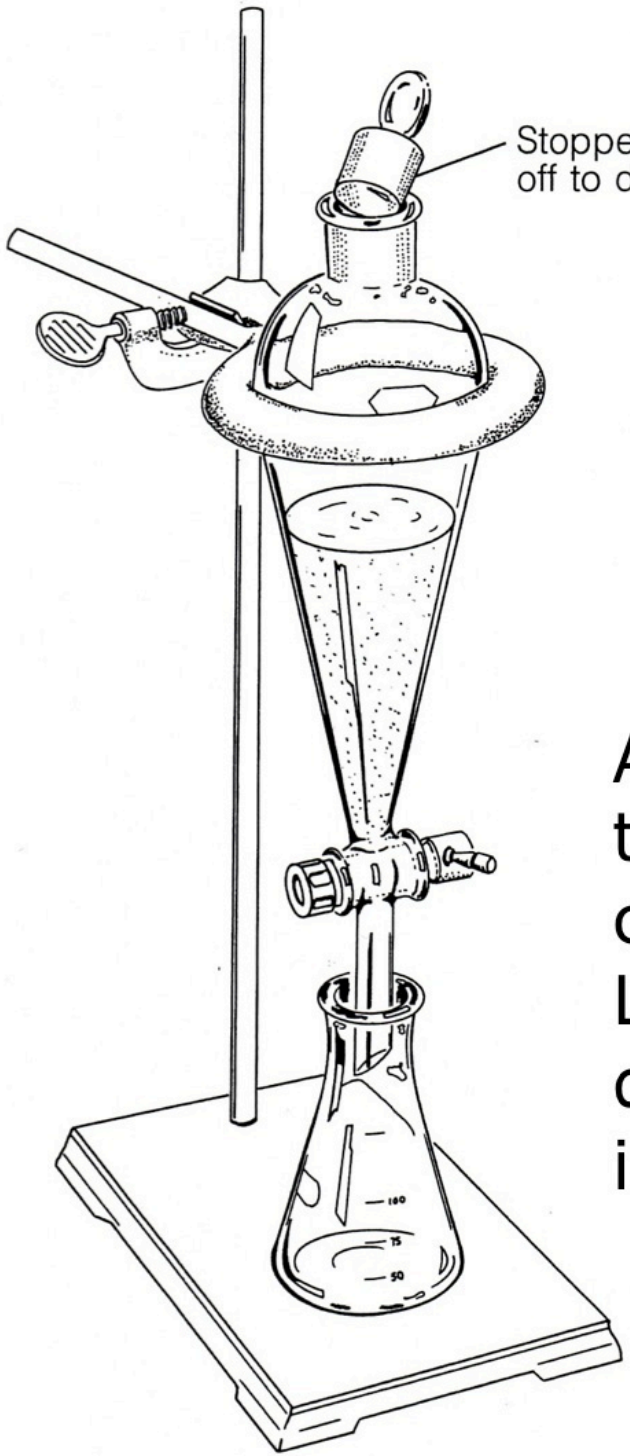


One hand holds the Stopper into place, The other controls the Stopcock.

Vent the separatory funnel Towards the back of the hood NOT YOUR NEIGHBOR!!!!



Vent often!!!



Make sure the stopcock is closed when you place the separatory funnel on the ring

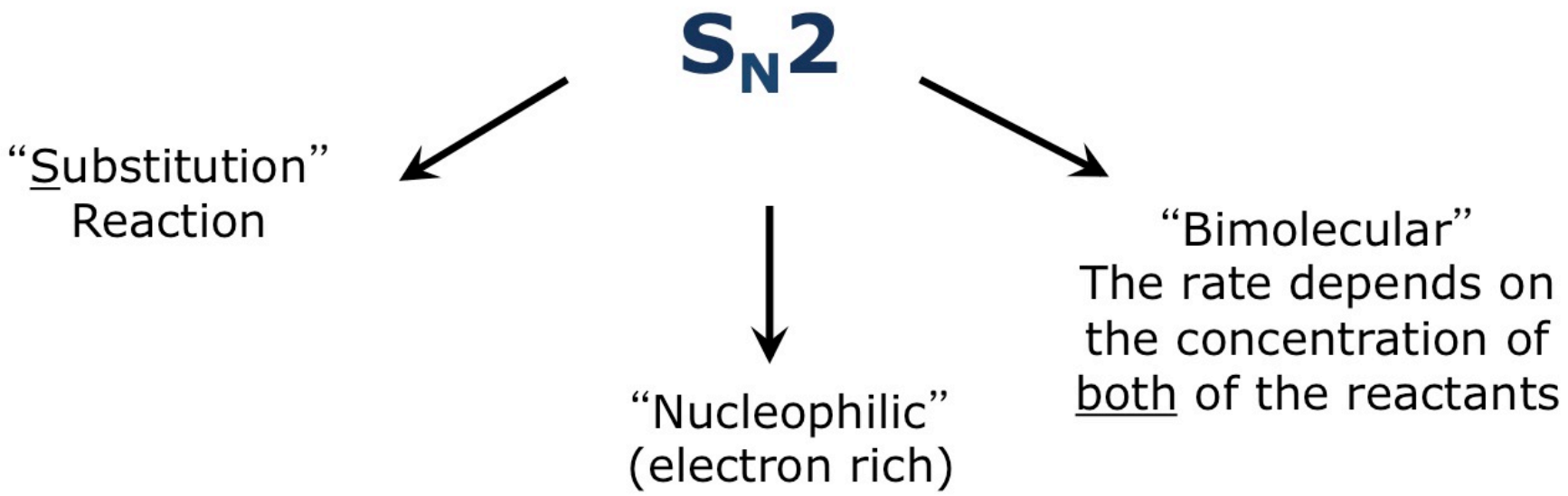
Always have a container under the separatory funnel, just in case.

Label all fractions and do not discard anything until you know it is okay to do so.

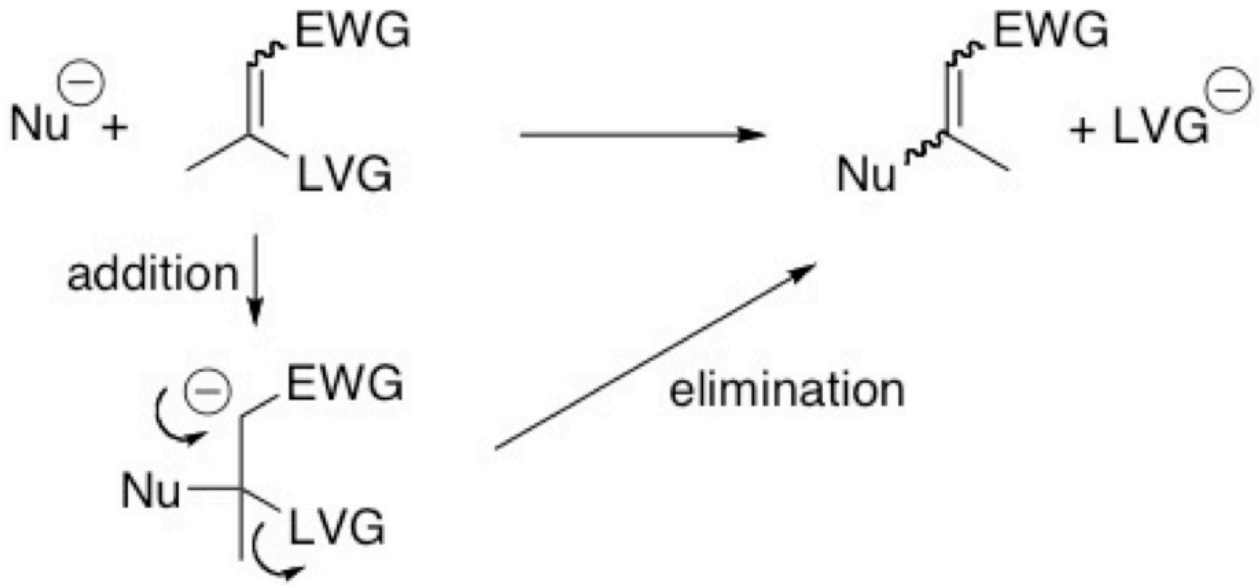
VENT OFTEN !!!!!

Using $NaHCO_3$ to neutralize acid leads to CO_2 gas. The pressure inside the separatory funnel can build up very quickly.

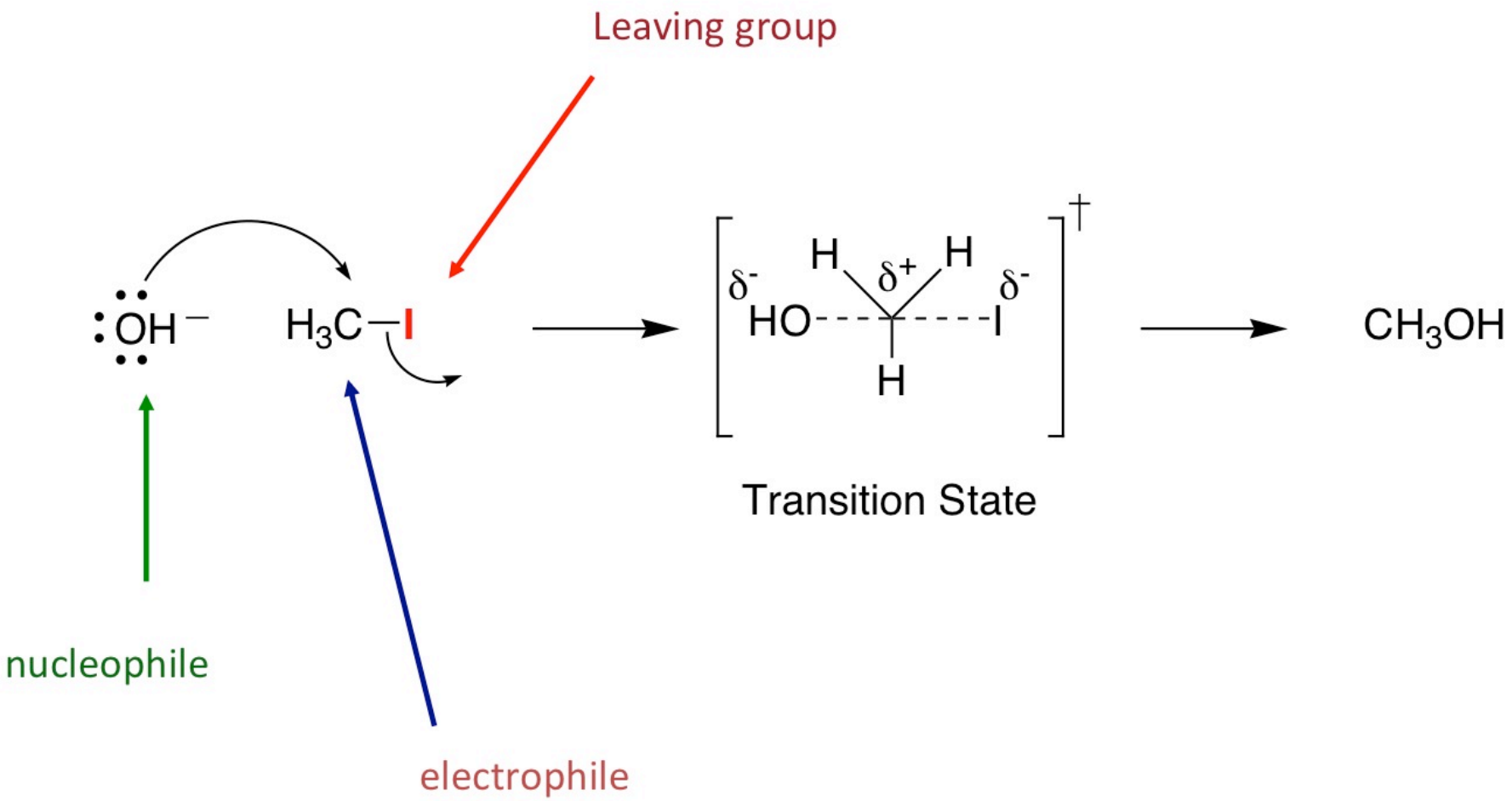
S_N2 Reaction



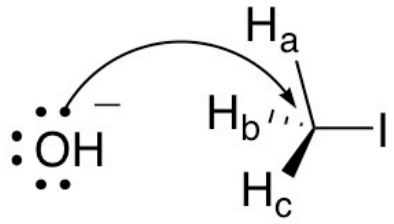
NO S_N2 on Csp^2 carbons



S_N2 Reaction Mechanism

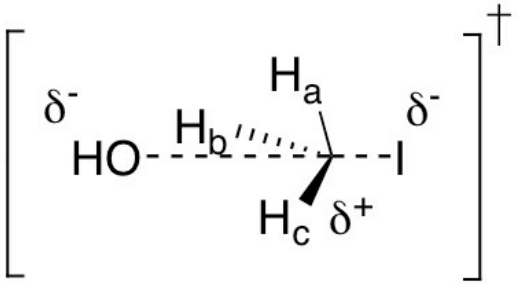


S_N2 Reaction

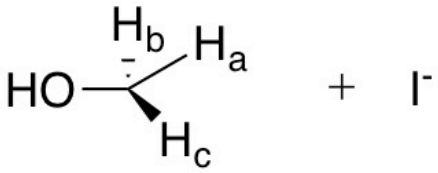


"Backside" attack of the nucleophile

Transition State



The partial negative charges are as far apart as possible

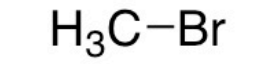


Product has "inverted" stereochemistry

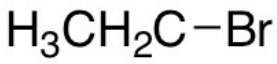
S_N2 Reaction

- There are a number of factors which determine the **rate** of the S_N2 reaction:
- 1) The nature of the substrate undergoing substitution:

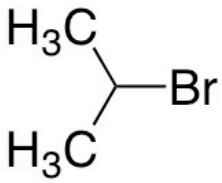
Reaction Rate



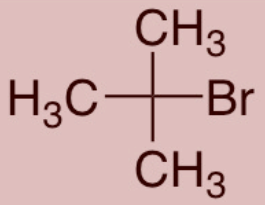
fast



intermediate



slow

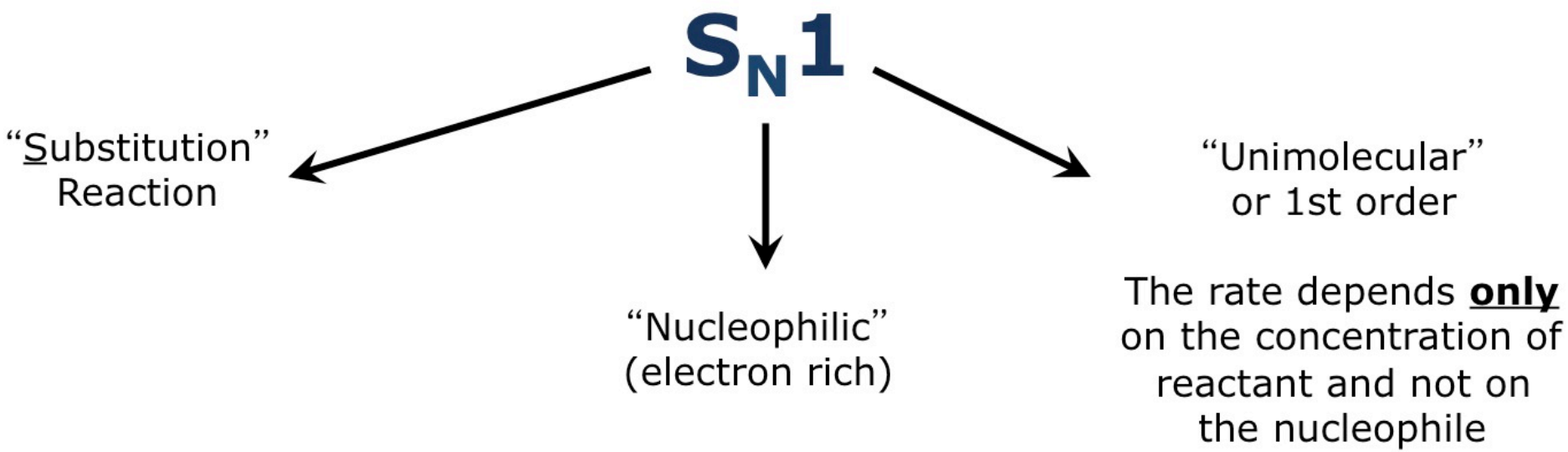


no S_N2 reaction

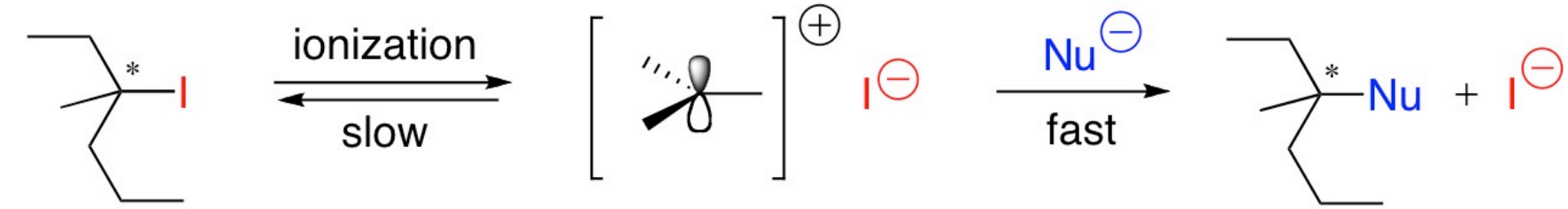
the bulkier the substituents around the reactive carbon atom the slower the reaction

"**Steric Effect**"

S_N1 Reaction



S_N1 Reaction - Mechanism



(+) or (-) or (±)

(±)

S_N1 Reaction - Reactivity

- In the S_N1 reaction the order of reactivity is the reverse to that of the S_N2 reaction

S_N1 Reaction - Reactivity

- The rate of the S_N1 reaction is highly dependent on the stability of the cation formed during the reaction

- The more substituted cation is the more stable it is

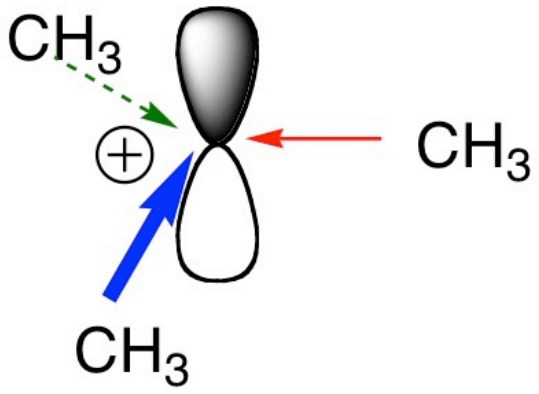
CH_3^+ $CH_3CH_2^+$ $(CH_3)_2CH^+$ $(CH_3)_3C^+$

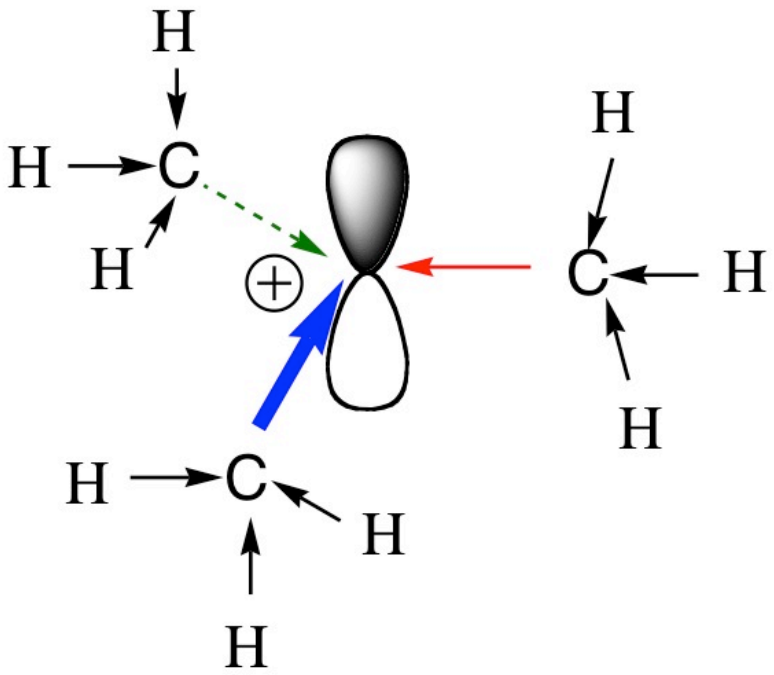
Stability of Carbocation

Inductive effect: the polarization of the bond by a nearby electronegative or electropositive atoms or groups

Carbocation: carbon is positively charged and electron density of the σ bonds should be shifted towards the carbon

The more stable carbocation - the faster/easier ionization of alkyl halide


CH3
CH3
CH3

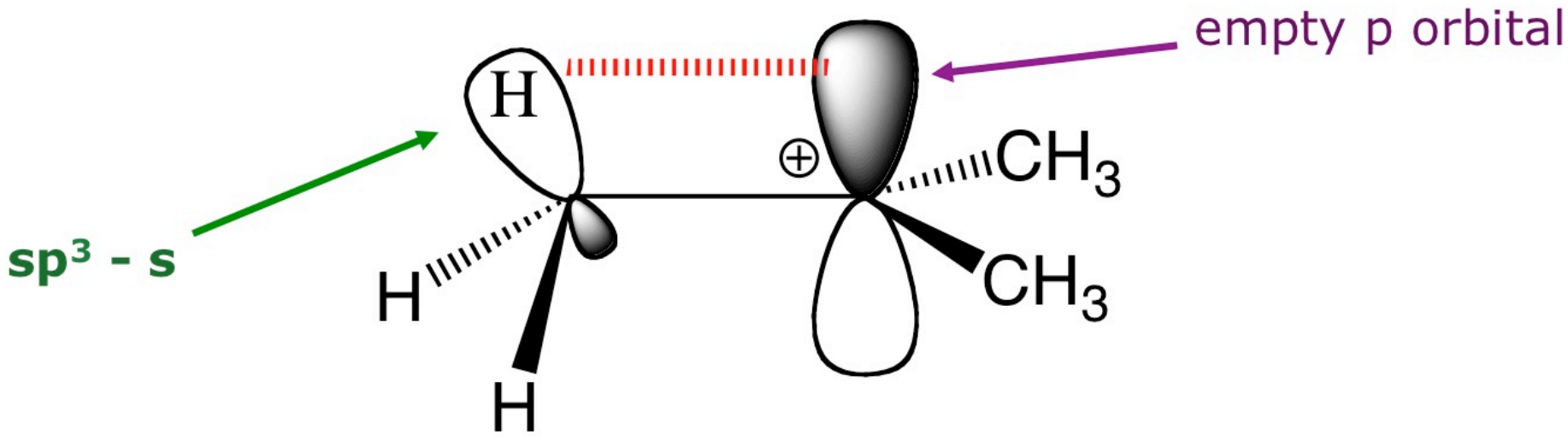


CH_3^+ $CH_3CH_2^+$ $(CH_3)_2CH^+$ $(CH_3)_3C^+$

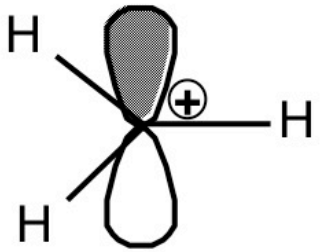
Increasing carbocation stability - increasing S_N1 rate

Hyperconjugation

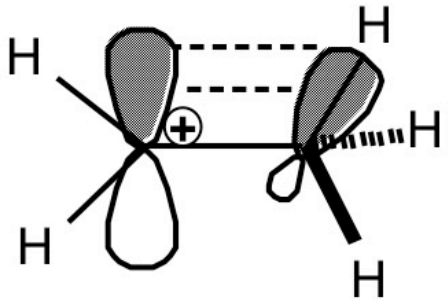
Partial overlap of an sp^3-s orbital of an C-H with the empty orbital of the positively charged carbon



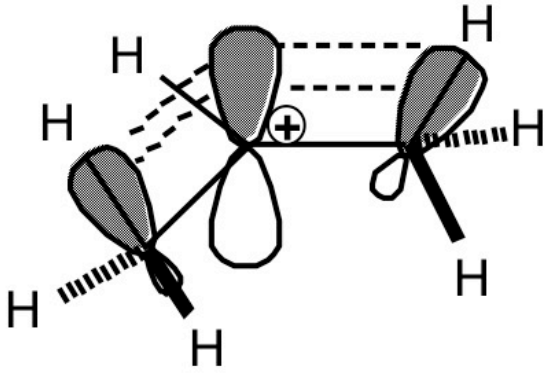
Hyperconjugation



No hyperconjugation (not stable)



Hyperconjugation from one bond
Primary cation (1°)

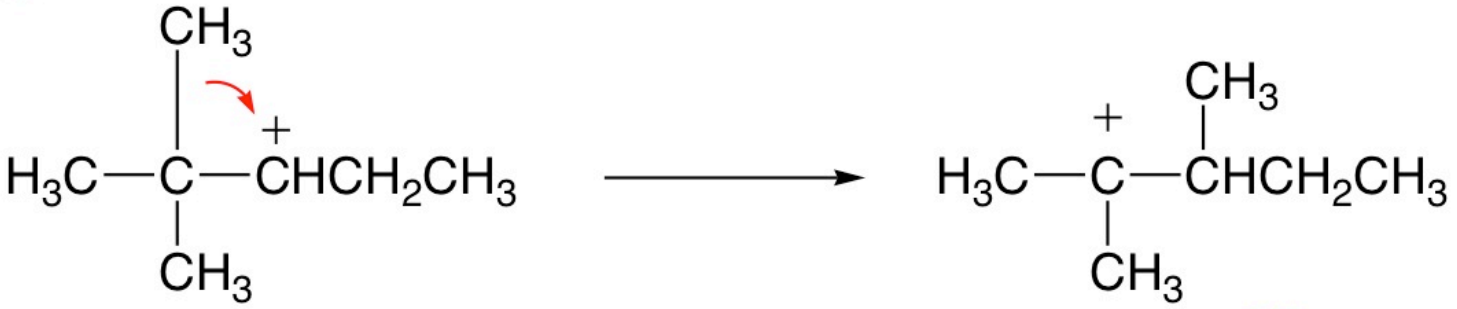


Hyperconjugation from two bonds
Secondary cation (2°)

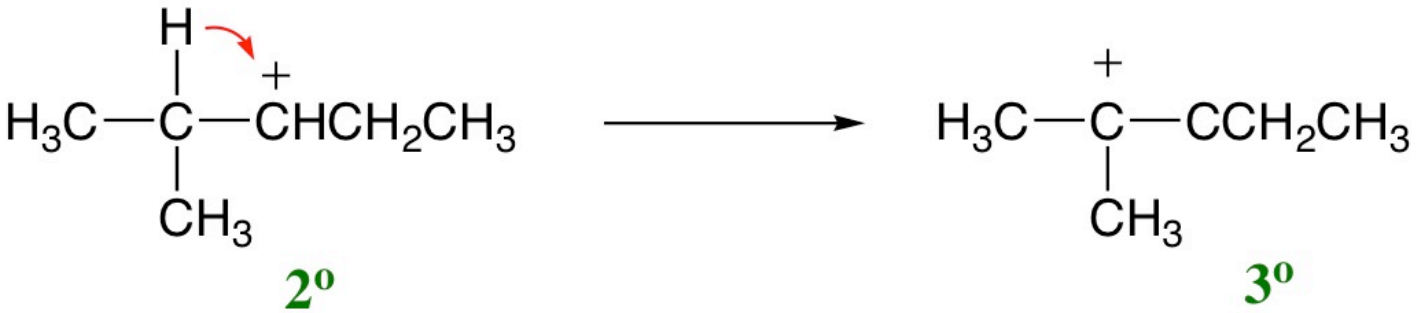
The most stable cation is tertiary (3°)

Rearrangement occurs if an alkyl group, aryl group or hydrogen shift would lead to a more stable cation

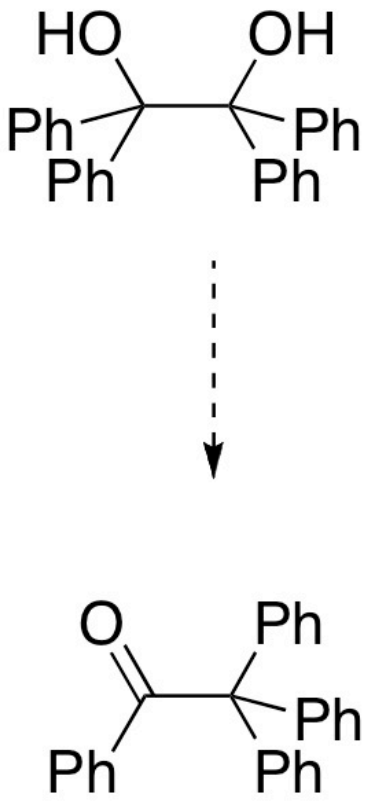
A methide shift



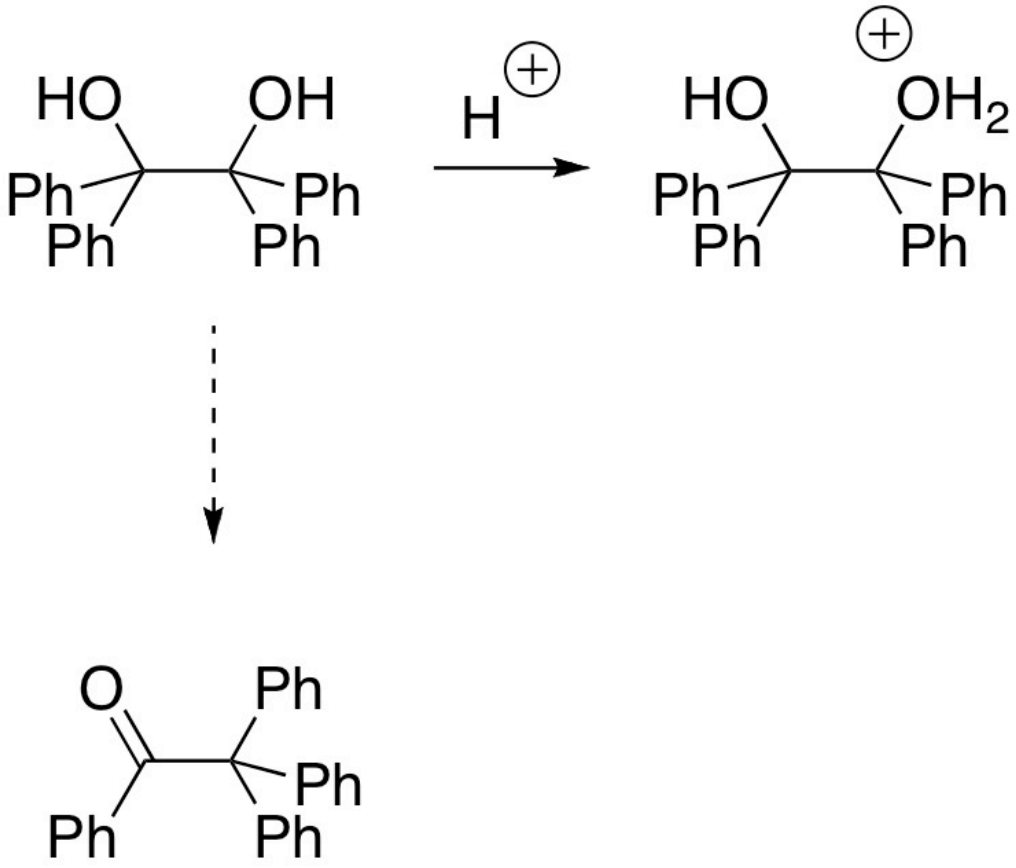
A hydride shift



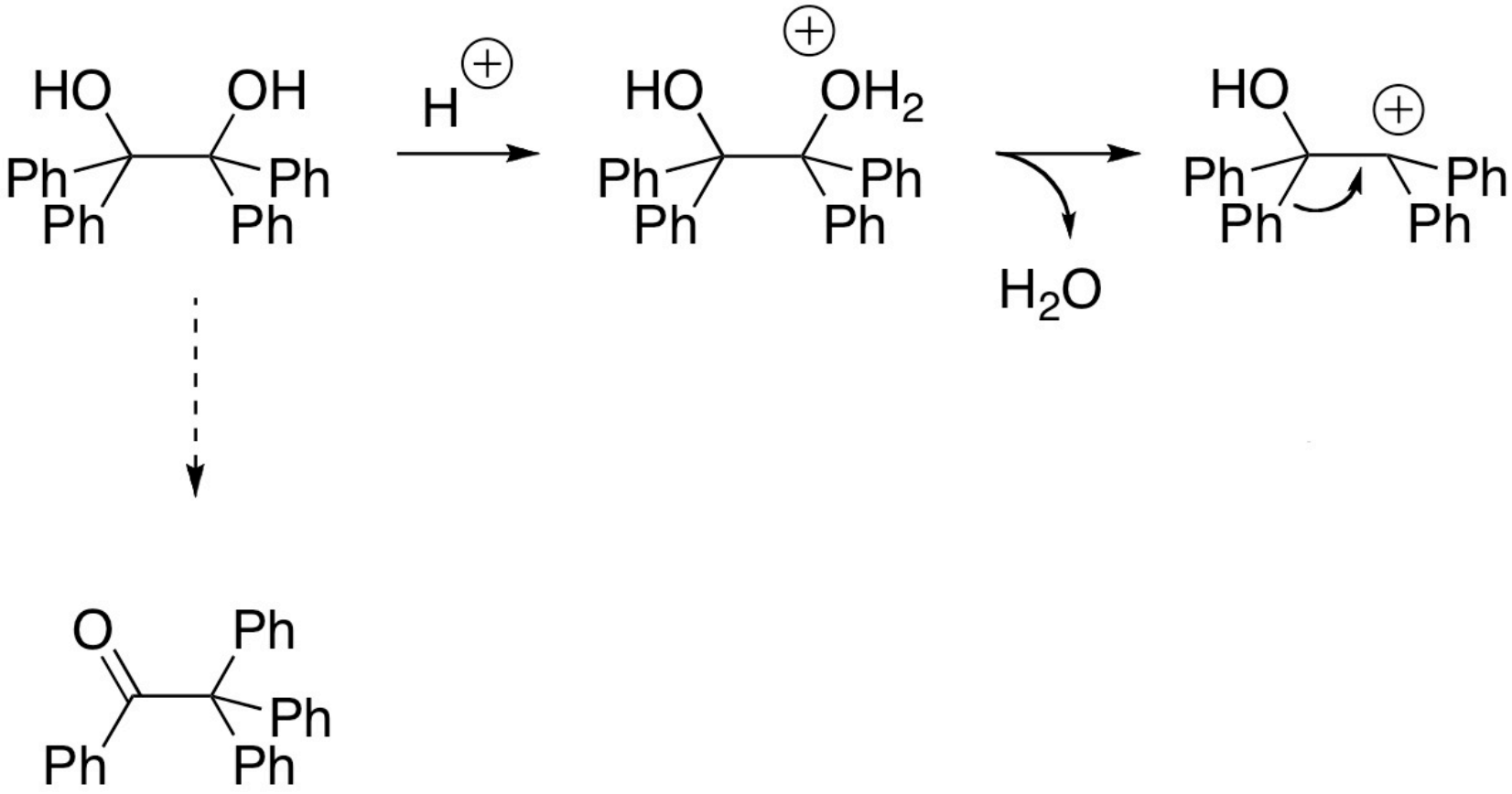
Pinacol-Pinacolone Rearrangement



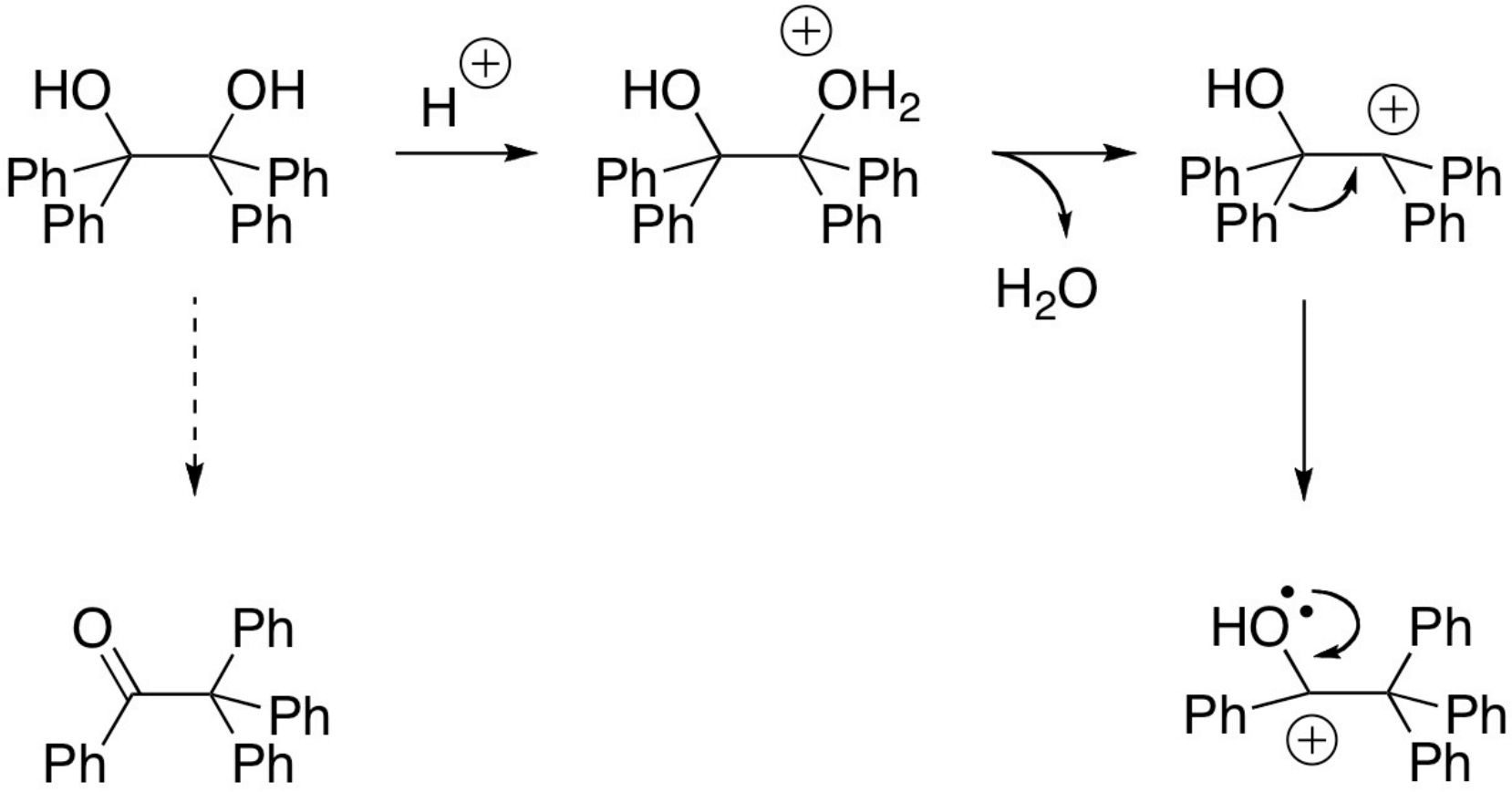
Pinacol-Pinacolone Rearrangement



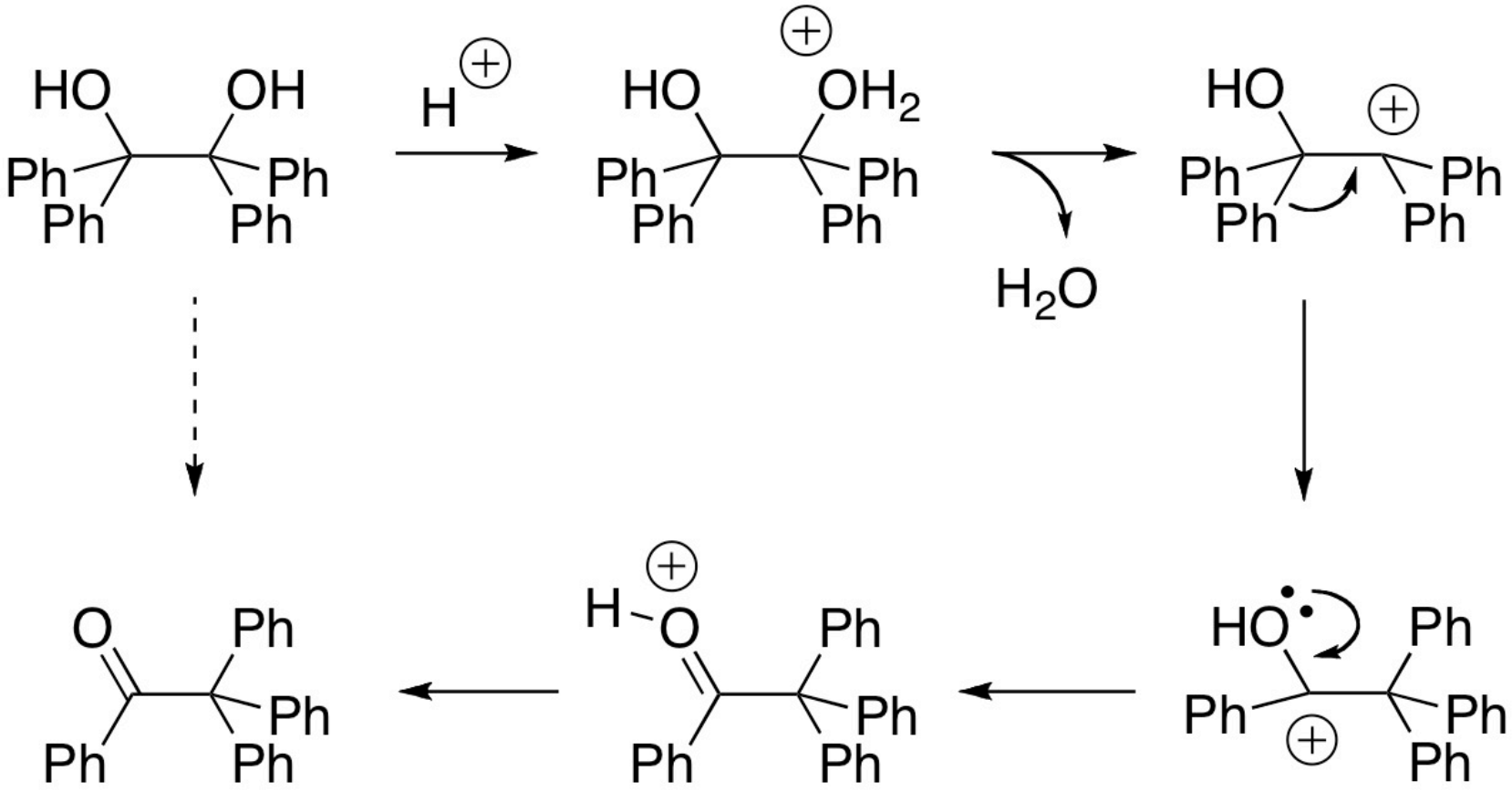
Pinacol-Pinacolone Rearrangement



Pinacol-Pinacolone Rearrangement



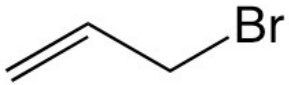
Pinacol-Pinacolone Rearrangement

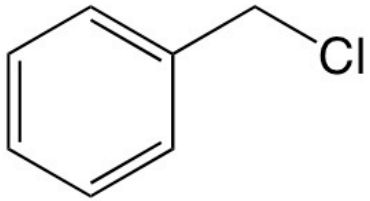


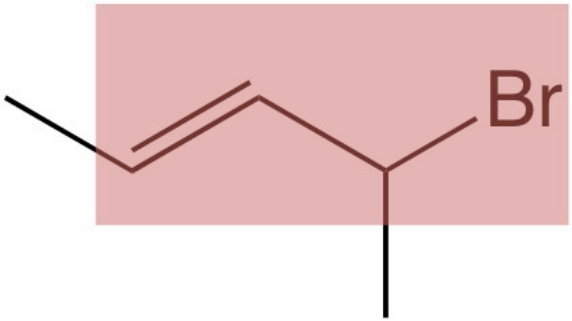
S_N2 and S_N1 - comparison

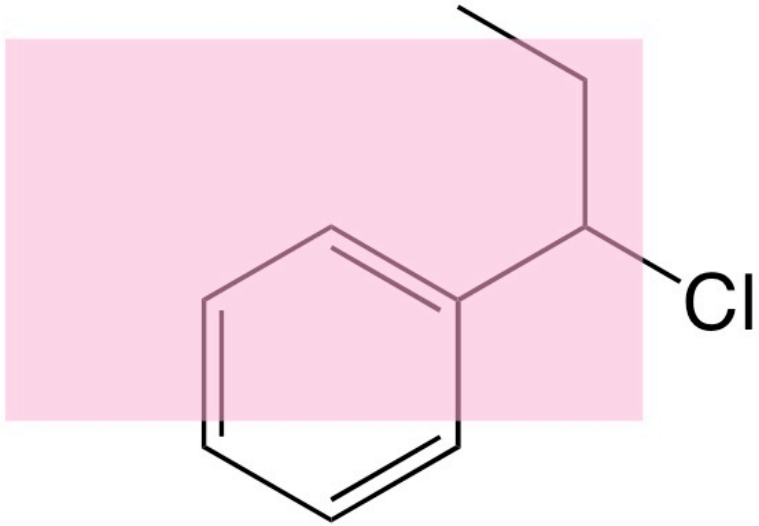
	S_N2	S_N1
Rate:	$CH_3 > 1° > 2° > 3°$ depends on steric effects (can nucleophile get close?)	$3° > 2° > 1° > CH_3$ depends on electronic effects (how stable is the cation?)
Rearrangement:	No: direct replacement	Yes: to form more stable cations
Stereochemistry:	concerted reaction "backside" attack inversion of configuration	stepwise reaction planar cation intermediate racemization

Substitution reactions of allylic and benzylic halides

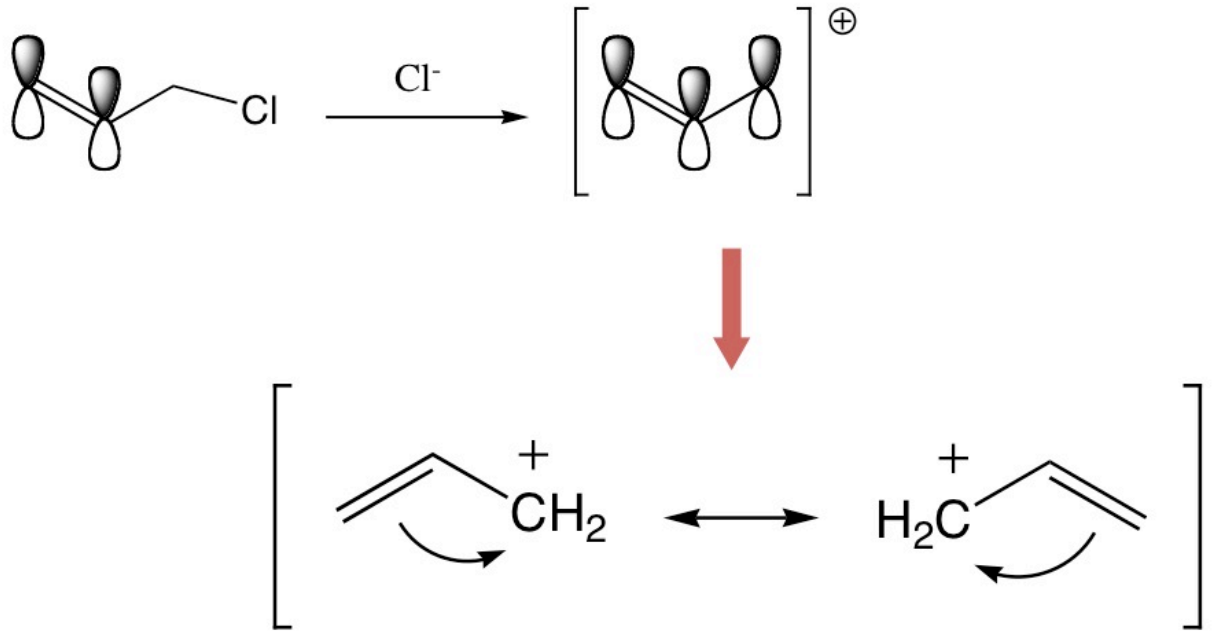






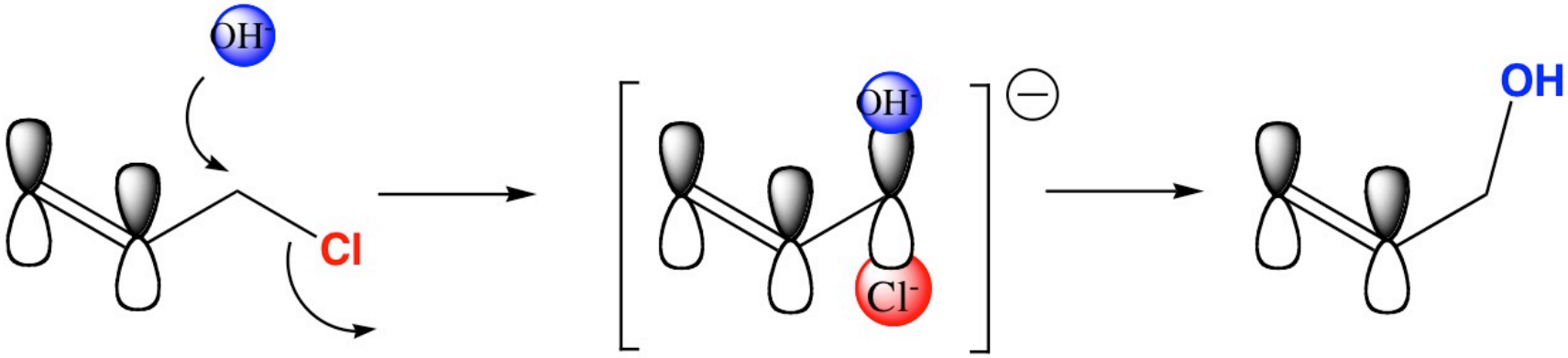


Allylic chloride in S_N1 reaction

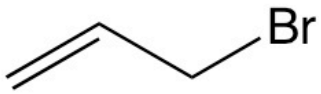


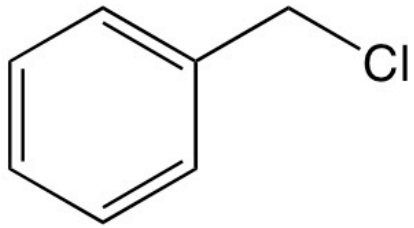
Resonance structures - structures differing only in the position of π electrons

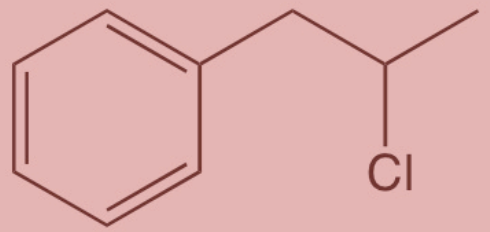
Allylic chloride in S_N2 reaction



For increased stabilization to occur either in S_N1 or S_N2 reactions, the π system MUST be adjacent to the reacting carbon







F2019 LITERATURE REPORT

Literature Assignment
Due Date:
Before 8:00 am Tuesday, December 3, 2019
(50 points)

CHEM 30121 – Literature Assignment
Due Date: Before 8 am Tuesday, December 3, 2019
(50 points)

For this year's literature assignment, you have been assigned a drug (prescription or over the counter = OTC). **Do not wait until the end of the semester to get going on your literature problem.** I will not answer last minute questions unless I see that you have been trying to work on your own already.
On the other hand, you can email me or stop by my office (if possible let me know in advance) if you need help with specific questions.
That being said, **here are a few tips about your literature problem**:

The purpose of this exercise is multi-fold. 1) Familiarization with literature search tools and TCU Library resources. This will be critical during the second semester organic lab at TCU. 2) Make a connection between organic chemistry and actual real life cases, and the way compounds are synthesized. 3) Give you a chance to research a particular compound. 4) Prescription and OTC drugs are used everyday and many of you might end up recommending them some day as a physician. 5) Students interested in health professions should be familiar with the chemistry, structure, and mode of action of compounds that go into your own body or someone else's.

Drawing Software: To draw molecules, you should be able to use the TCU site license for ChemDraw (standard version for Windows or Mac format) for anyone with an @tcu.edu e-mail account.
To download ChemDraw Std 16.0 and/or renew your one year subscription, go to:
http://sitelicense.cambridgesoft.com/sitelicense.cfm?sid=2405

You should run a SciFinder search
Registration to SciFinder is free, but you will need your own login and password.

You can access the SciFinder database through the TCU library:
http://library.tcu.edu/research/databases/SciFinderScholar/SciFinder_main.html
Tutorials and How To Guides are available at: http://www.cas.org/training/scifinder

Other resources are (but not limited to):
NIH information portal: http://druginfo.nlm.nih.gov/drugportal/drugportal.jsp

FDA Orange Book: http://www.accessdata.fda.gov/scripts/cder/ob/default.cfm

http://library.tcu.edu/research/databases/SciFinderScholar/SciFinder_main.html

I. Going through Scifinder. There are several scenarios:
1) your molecule can be found using Scifinder, and there are just a few hits for a given structure, and not too much info but yet all data IR , NMR...etc... is referenced there. If that's so, then you are in luck.

2) Your molecule may be found in Scifinder but there are many hits and/or references to choose from.
First, the hit that you want is usually at the beginning. The rest are either isotopically labeled versions, or they are salts which vary in the counterion. Try to find the "normal" compound (most abundant isotopes of CHNOPS... only). For salts, either try to find the fully protonated form (ie. COOH instead of COONa) or else pick a common salt (ie. Na better than Cs). Other than that, it is likely that you are in good shape.

3) Your molecule is unknown in Scifinder (this is HIGHLY UNLIKELY). **Make sure you drew it correctly. If you are sure it's not in Scifinder, you must check the Chemical Abstract volumes in the library. Use the molecular formula to search, and then the name of the compound. Go back as far as you can to check if your compound is there.** Make sure you write on your report how far back you checked.
If it is still not there, it is quite likely that your molecule has not been described previously. Obviously you are done with the data part of the assignment (mp, bp, IR, NMR, ..etc...). However see **III. Synthesis problem** below.

References for spectral data, etc. CANNOT be straight from SciFinder which uses simulations. Instead, a primary literature reference must be listed with actual spectral data. Primary literature is a journal article, or actual data from a handbook, a database of EXPERIMENTAL data, etc. It CANNOT BE COMPUTED DATA.

II. Selecting the references.

In general, you should try to pick 1) a journal the library has!, and 2) the most recent articles. (For example, NMR data will likely be of better quality in 1990 than in 1960). Also it allows you to search backwards from the most recent paper. This way you may even find references that were not cited in Scifinder.

Also, you can select what Scifinder displays. This is done in several ways. One which may be most useful for reactions is: once you have displayed the hits, go to "View" . Under "Reaction View", select "substance as product". The reactions displayed will now be only related to the preparation of your compound.

Be aware that sometimes Scifinder does not link articles properly. It means that you should always check journal through http://qz4xh7bf6f.search.serialssolutions.com/ and http://library.tcu.edu/catalog regardless of the outcome on SciFinder.

For additional resources: http://libguides.tcu.edu/chemistry

III. Synthesis Problem.

For people who found references in Scifinder, this is fairly easy. But you should select the paper that seems to provide the best yield, or that uses the simplest chemicals (Aldrich chemicals. Ask yourself, "Could I do this experiment in the lab? If I had to make this compound, which method would be best?"). See also II. If the molecule is known but there are no preparations, check a reference, which talks about that compound. By definition, all the compounds in this assignment will be known.

EXAMPLES OF SPECTRAL DATA:

Example of spectral data and the information you need to look for concerning your literature compound: note that in a particular paper, one might find only a subset of these details. You might need to look for additional papers to try to get as much data as possible. You can cut and paste on the form, or attach a copy of the relevant section, or copy by hand. **Simulated or calculated spectra are NOT acceptable.**

Physical state (for a solid, the melting point would be listed)

pale yellow oil

Proton NMR. The solvent and frequency are usually listed, and then a listing describing the spectrum is provided

^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.88 (3H, t, J = 6.8 Hz), 1.24-1.32 (10H, m), 1.41-1.47 (2H, m), 1.76 (6H, d, J = 12.4 Hz), 1.90 (3H, d, J = 13.2 Hz), 2.18 (2H, qd, J = 7.6, 2.8 Hz), 6.57 (1H, dtd, J = 24.0, 7.6, 1.6 Hz)

Carbon NMR

^{13}C-NMR (100 MHz, $CDCl_3$) δ 12.6 (d, J = 12.8 Hz), 14.2, 20.0, 20.5, 22.7, 28.5, 28.6, 29.0 (d, J = 15.2 Hz), 29.2, 29.4, 31.9, 128.1 (d, J = 75.0 Hz), 144.1 (d, J = 9.9 Hz).

Phosphorus NMR

^{31}P-NMR (162 MHz, $CDCl_3$) δ 35.5.

Infrared

IR (neat) 2924, 2854, 1634, 1464, 1416, 942, 914, 732 cm^{-1}.

Mass spectrometry (MS = low resolution, HRMS = high resolution)

MS (EI) m/z 246 (**M**$^+$, 11%), 94 (**M**$^+$-152, 100%).
HRMS Calcd for $C_{13}H_{27}PS$: 246.1571. Found: 246.1577.

In the experimental section of an article, you might find something like this:

Full characterization of the product was as follows: m.p.= 85 °C; ^{1}H NMR (300 MHz,$CDCl_3$) δ: 2.77 (dd, J_{HP} = 19.3 Hz, J = 7.0 Hz, 2H), 6.02 – 6.18 (m, 1H), 6.53 (dd, J = 15.8 Hz, J = 5.3 Hz, 1H), 7.04 (d, J_{HP} = 558.2 Hz, 1H), 7.18 – 7.42 (m, 5H), 10.45 (bs, 1H); ^{13}C NMR (75.45 MHz, $CDCl_3$) δ: 34.7 (d, J_{PC} = 91.0 Hz, CH_2), 117.0 (d, J_{PCC} = 10.1 Hz, CH), 126.6 (2xCH), 128.1 (CH), 128.8 (2xCH), 136.3 (d, J_{PCCC} = 14.7 Hz, CH), 136.7 (d, J_{PCCCC} = 4.0 Hz, C); ^{31}P NMR (121.47 MHz, $CDCl_3$) δ: 35.32 (dm, J_{PH} = 557.7 Hz); IR (thin film, KBr), cm^{-1}: 2621 and 1688 (P-O-H); 2422, 2292 and 2181 (P-H); and 1241 (P=O); UV (EtOH, C≈8μM) λ_{max} = 274 nm; HRMS (EI) *m/z* Calcd for $C_9H_{11}O_2P$: 182.0495. Found: 182.0497. Anal. Calcd. for $C_9H_{11}O_2P$: C, 59.34; H, 6.09. Found: C, 59.04; H, 6.02.

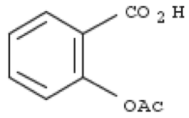
It is also possible that you will find some of the information in one paper, and other information in other papers.

CAS Registry Number: 50-78-2

$C_9H_8O_4$

Benzoic acid, 2-(acetyloxy)-

Rhodine (7CI); Salicylic acid acetate (8CI); 2-(Acetyloxy)benzoic acid; 2-Acetoxybenzoic acid; 2-Carboxyphenyl acetate; A.S.A. Empirin; AC 5230; ASA; Acenterine; Acesal; Acesan; Acetard; Aceticyl; Acetilum acidulatum; Acetisal; Acetol; Acetonyl; Acetophen; Acetosal; Acetosalic acid; Acetosalin; Acetylin; Acetylsal; Acetylsalicylic acid; Acetyonyl; Acetysal; Acidum acetylsalicylicum; Acimetten; Acisal; Acylpyrin; Adiro; Albyl E; Angettes 75; Anopyrin; Asaflow; Asagran; Asatard; Ascoden 30; Ascolong; Ascriptin; Aspalon; Aspergum; Aspirdrops; Aspirin; Aspirin Protect 100; Aspirin Protect 300; Aspirin-Direkt; Aspirina 03; Aspirine; Aspro; Aspro Clear; Aspropharm; Asteric; Astrix; Bayaspirin; Benaspir; Bialpirina; Bialpirinia; Caprin; Cardioaspirin; Cardioaspirina; Cardiomagnyl; Claradin; Colfarit; Colsprin; Contrheuma Retard; Coraspin; Coricidin; Coricidin D; Crystar; Darvon Compound; Dolean pH 8; Dominal; Duramax; ECM; Easprin; Ecopirin; Ecosprin; Ecotrin; Empirin; Endosprin;



Partition Coefficient	See full text	1 of 6	(81)CAS
Potential of Electrode Reaction	See full text	1 of 2	(28)CAS
Solubility	See full text	1 of 19	(89)CAS
Density Properties	**Value**	**Condition**	**Note**
Density	1.430 g/cm3		(14)CAS
Density	1.40 g/cm3		(15)APC
Density	1.40 g/cm3		(16)NLM
Density	1.4 g/cm3		(17)NIOSH
Density	1.396 g/cm3	Temp: 30 °C	(18)CAS
Density	See full text		(19)CAS
Flow and Diffusion Properties	**Value**	**Condition**	**Note**
Diffusion Coefficient	See full text		(20)CAS
Interface Properties	**Value**	**Condition**	**Note**
Contact Angle	See full text	1 of 2	(12)CAS
Lipinski and Related Properties	**Value**	**Condition**	**Note**
logP	See full text	1 of 13	(34)CAS
Optical and Scattering Properties	**Value**	**Condition**	**Note**
Refractive Index	1.652	Wavlen: 589.3 nm	(88)CAS
Refractive Index	1.640	Wavlen: 589.3 nm	(88)CAS
Refractive Index	1.502	Wavlen: 589.3 nm	(88)CAS
Refractive Index	1.4842-1.4936	Wavlen: 589.3 nm; Temp: 25 °C	(16)NLM
Spectra Properties	**Value**	**Condition**	**Note**
Carbon-13 NMR Spectrum	See spectrum		(5)AIST
Carbon-13 NMR Spectrum	See spectrum		(6)BIORAD
Carbon-13 NMR Spectrum	See spectrum		(7)ACD
Carbon-13 NMR Spectrum	See spectrum		(8)WSS
Carbon-13 NMR Spectrum	See spectrum		(8)WSS
Carbon-13 NMR Spectrum	See spectrum		(9)WSS
Carbon-13 NMR Spectrum	See spectrum		(9)WSS
Carbon-13 NMR Spectrum	See full text	1 of 4	(10)CAS
Circular Dichroism Spectrum	See full text		(11)IC
Emission/Luminescence Spectrum	See full text		(22)CAS
IR Absorption Spectrum	See spectrum		(8)WSS
IR Absorption Spectrum	See spectrum		(8)WSS
IR Absorption Spectrum	See spectrum		(5)AIST
IR Absorption Spectrum	See spectrum		(5)AIST
IR Absorption Spectrum	See spectrum		(29)BIORAD
IR Absorption Spectrum	See spectrum		(29)BIORAD
IR Absorption Spectrum	See spectrum		(29)BIORAD
IR Absorption Spectrum	See spectrum		(29)BIORAD
IR Absorption Spectrum	See spectrum		(29)BIORAD
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IR Absorption Spectrum	See spectrum		(29)BIORAD
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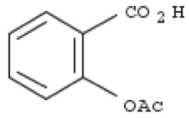
IR Absorption Spectrum	See full text	1 of 16	(10)CAS
IR Reflectance Spectrum	See full text		(30)CAS
IR Spectrum	See full text	1 of 3	(31)CAS
Mass Spectrum	See spectrum		(35)BIORAD

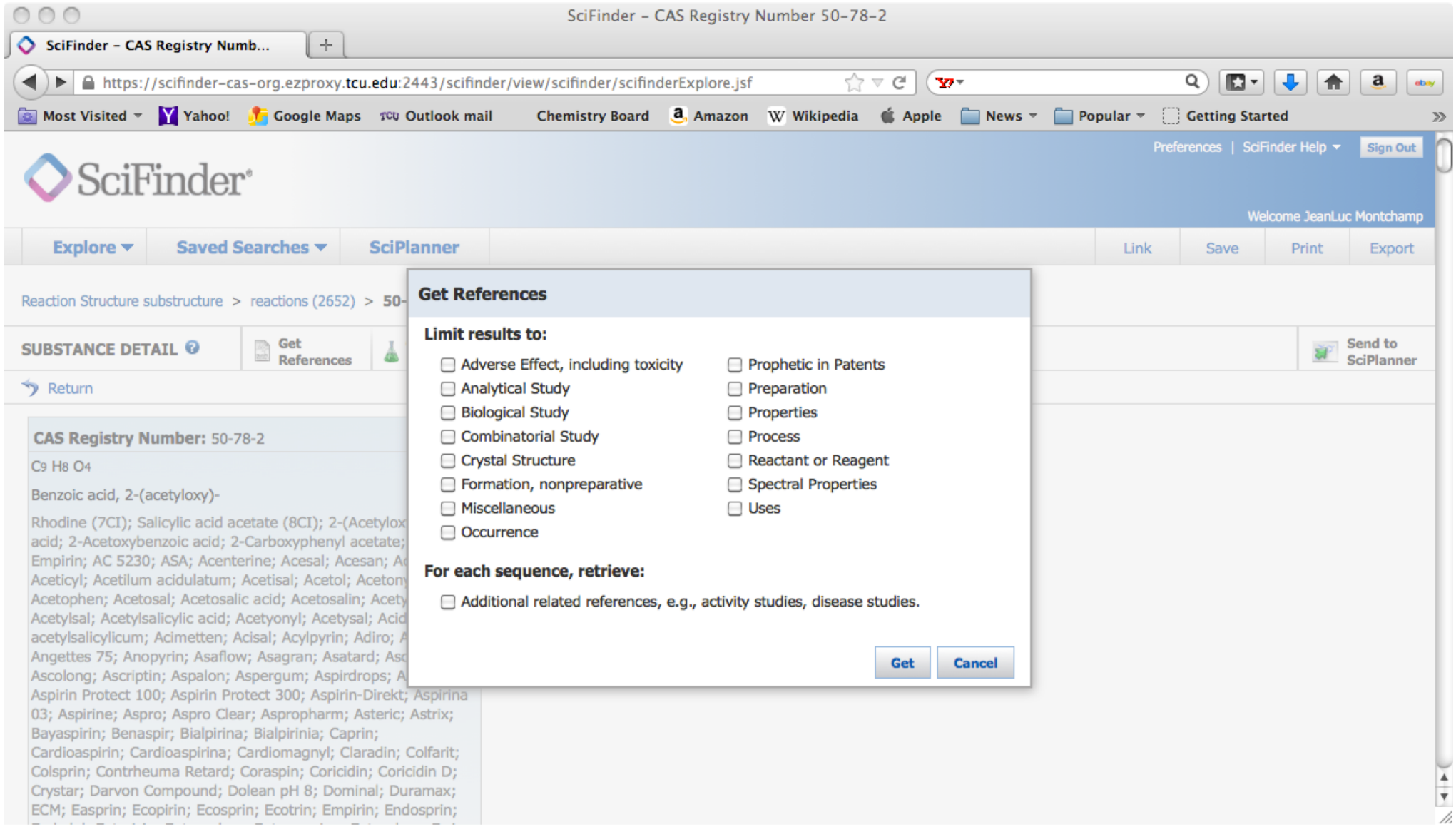
CAS Registry Number: 50-78-2

$C_9H_8O_4$

Benzoic acid, 2-(acetyloxy)-

Rhodine (7CI); Salicylic acid acetate (8CI); 2-(Acetyloxy)benzoic acid; 2-Acetoxybenzoic acid; 2-Carboxyphenyl acetate; A.S.A. Empirin; AC 5230; ASA; Acenterine; Acesal; Acesan; Acetard; Aceticyl; Acetilum acidulatum; Acetisal; Acetol; Acetonyl; Acetophen; Acetosal; Acetosalic acid; Acetosalin; Acetylin; Acetylsal; Acetylsalicylic acid; Acetyonyl; Acetysal; Acidum acetylsalicylicum; Acimetten; Acisal; Acylpyrin; Adiro; Albyl E; Angettes 75; Anopyrin; Asaflow; Asagran; Asatard; Ascoden 30; Ascolong; Ascriptin; Aspalon; Aspergum; Aspirdrops; Aspirin; Aspirin Protect 100; Aspirin Protect 300; Aspirin-Direkt; Aspirina 03; Aspirine; Aspro; Aspro Clear; Aspropharm; Asteric; Astrix; Bayaspirin; Benaspir; Bialpirina; Bialpirinia; Caprin; Cardioaspirin; Cardioaspirina; Cardiomagnyl; Claradin; Colfarit; Colsprin; Contrheuma Retard; Coraspin; Coricidin; Coricidin D; Crystar; Darvon Compound; Dolean pH 8; Dominal; Duramax; ECM; Easprin; Ecopirin; Ecosprin; Ecotrin; Empirin; Endosprin;




SciFinder – CAS Registry Number 50-78-2
SciFinder – CAS Registry Numb...
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Most Visited
Yahoo!
Google Maps
Outlook mail
Chemistry Board
Amazon
Wikipedia
Apple
News
Popular
Getting Started
SciFinder
Preferences | SciFinder Help
Sign Out
Welcome JeanLuc Montchamp
Explore
Saved Searches
SciPlanner
Link
Save
Print
Export
Reaction Structure substructure > reactions (2652) > 50-
SUBSTANCE DETAIL
Get References
Send to SciPlanner
Return
CAS Registry Number: 50-78-2
C9 H8 O4
Benzoic acid, 2-(acetyloxy)-
Rhodine (7CI); Salicylic acid acetate (8CI); 2-(Acetylox
acid; 2-Acetoxybenzoic acid; 2-Carboxyphenyl acetate;
Empirin; AC 5230; ASA; Acenterine; Acesal; Acesan; A
Aceticyl; Acetilum acidulatum; Acetisal; Acetol; Aceton
Acetophen; Acetosal; Acetosalic acid; Acetosalin; Acety
Acetylsal; Acetylsalicylic acid; Acetyonyl; Acetysal; Acid
acetylsalicylicum; Acimetten; Acisal; Acylpyrin; Adiro;
Angettes 75; Anopyrin; Asaflow; Asagran; Asatard; Asc
Ascolong; Ascriptin; Aspalon; Aspergum; Aspirdrops;
Aspirin Protect 100; Aspirin Protect 300; Aspirin-Direkt; Aspirina
03; Aspirine; Aspro; Aspro Clear; Aspropharm; Asteric; Astrix;
Bayaspirin; Benaspir; Bialpirina; Bialpirinia; Caprin;
Cardioaspirin; Cardioaspirina; Cardiomagnyl; Claradin; Colfarit;
Colsprin; Contrheuma Retard; Coraspin; Coricidin; Coricidin D;
Crystar; Darvon Compound; Dolean pH 8; Dominal; Duramax;
ECM; Easprin; Ecopirin; Ecosprin; Ecotrin; Empirin; Endosprin;
Get References
Limit results to:
Adverse Effect, including toxicity
Analytical Study
Biological Study
Combinatorial Study
Crystal Structure
Formation, nonpreparative
Miscellaneous
Occurrence
Prophetic in Patents
Preparation
Properties
Process
Reactant or Reagent
Spectral Properties
Uses
For each sequence, retrieve:
Additional related references, e.g., activity studies, disease studies.
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- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Document Type(s)

- [ ] Biography
- [ ] Book
- [ ] Clinical Trial
- [ ] Commentary
- [ ] Conference
- [ ] Dissertation
- [ ] Editorial
- [ ] Historical
- [x] Journal
- [ ] Letter
- [ ] Patent
- [ ] Preprint
- [ ] Report
- [x] Review

Refine

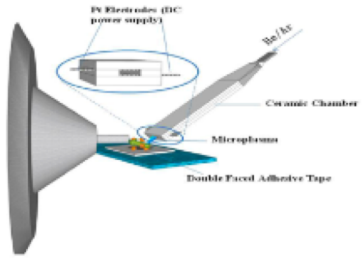
1. **An LC-MS assay for the screening of cardiovascular medications in human samples** Full Text

   By Dias, Eduardo; Hachey, Brian; McNaughton, Candace; Nian, Hui; Yu, Chang; Straka, Brittany; Brown, Nancy J.; Caprioli, Richard M.
   From Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 937, 44-53. | Language: English, Database: CAPLUS

   Cardiovascular drugs are the most commonly prescribed medications. Some prior assays successfully detect cardiovascular drugs among multiple classes using a single sample. Here, we develop an assay to detect a broad range of cardiovascular drug classes to include commonly used cardiovascular drugs and evaluate the assay's anal. and statistical properties in a clin. setting. We describe a protocol for drug detection that encompasses 34 commonly prescribed cardiovascular drugs or drug metabolites with a single LC-**MS**/**MS** method using 100 µL of serum or plasma. Drug classes monitored by this as...

2. **Microfabricated Glow Discharge Plasma (MFGDP) for Ambient Desorption/Ionization Mass Spectrometry** Full Text

   By Ding, Xuelu; Zhan, Xuefang; Yuan, Xin; Zhao, Zhongjun; Duan, Yixiang
   From Analytical Chemistry (Washington, DC, United States) (2013), 85(19), 9013-9020. | Language: English, Database: CAPLUS



   A novel ambient ionization technique for **mass** spectrometry, microfabricated glow discharge plasma (MFGDP), is reported. This device is made of a millimeter-sized ceramic cavity with two platinum electrodes positioned face-to-face. He or Ar plasma can be generated by a d.c. voltage of several hundreds of volts requiring a total power <4 W. The thermal plume temp. of the He plasma was measured and is 25-80° at a normal discharge current. Gaseous, liq., creamy, and solid samples with mol. wts. up to 1.5 kDa could be examd. in both pos. and neg. mode, giving limits of detection (LOD) at or bel...

3. **Transforming aspirin into novel molecular salts of salicylic acid** Full Text

   By Andre, Vania; Martins, Ines; Quaresma, Silvia; Martins, Marta; Duarte, M. Teresa
   From Structural Chemistry, Ahead of Print. | Language: English, Database: CAPLUS

   Abstr.: Aspirin is one of the most widely used analgesic, antipyretic, and anti-inflammatory drugs. Herein we disclose a way to **transform** aspirin into novel multicomponent crystal forms of salicylic acid, also a long-known analgesic with anti-inflammatory properties, among others, covering a broad spectrum of applications, including skin care products. A salicylic acid:salicylate ammonium salt and a salicylate:2-methyl-4-oxopentan-2-aminium mol.