**Chem 342 Lab: Allylation of Carvone**

**Overview of the 2020 project**

This year we will aim to find conditions for alkylation of R(–)-carvone (**1**) with an allyl halide (or similar) to produce (*2S,3S*)-3-allylcarvone (**2**), using commercially available solvents and catalysts. Likely by-products include the stereoisomer (**3**), and the 5-allyl isomer (**4**), but we aim to maximize our yield of compound **2**.



The goal of this project is to find a suitable method for making compound **2** using the starting materials given (carvone and an allyl halide). “Suitable” in this case means appropriate for undergraduates working with standard lab equipment and affordable chemicals, preferably within a normal laboratory period (3 hours). We also prefer to use materials which are non–toxic and safe for the environment. This type of reaction is usually referred to as (in general) an enolate alkylation or (more specifically) an alpha-allylation, so if you need to narrow your search these are useful keywords to use. If the exact reaction cannot be found, then similar reactions using related compounds (for example, the enantiomer (S)‑carvone) are also of interest. Since (S)‑carvone is chemically identical to (R)‑carvone, the method for allylation of either enantiomer can be applied to the other enantiomer.

**Search strategy**

There is a good chance you will find an exact match for the target product, especially if you are using STN Easy/SciFinder or Reaxys. However if you’re unable to find an exact match, you will need to broaden the search terms enough to get useful hits, but not so much that you get too much, or things that are only tangentially useful. Since the *para*-methyl derivatives of the common reactants are commercially available, you can also search for these.

To understand the idea of broadening the search: Consider a geographical search; some maps cover the whole world, whereas some are just for the US, and some may be just for New York State. If you are looking for SUNY Potsdam on a map – if you don’t find it, you may decide to look for Potsdam. If you can’t find Potsdam, you may look for St. Lawrence County. If you can’t find the county, you may have to settle for New York State as the closest “hit”. The same will apply to your chemical search – and you will have to judge what searches are a good match.

Here are some suggested search methods:

***Using search terms***

*Level 1: Exact – chemical reactants or products*

For the (2S,3S)-3-allylcarvone we know the target product, but this is a semi–trivial name. Note that chemists often use trivial names, formulae or abbreviations in place of chemical names, even in the titles of papers. The full IUPAC name is (*5R,6S*)-6-allyl-5-isopropenyl-2-methylcyclohex-2-en-1-one.

We can also search for the reactants *R*-carvone and an allyl halide such as allyl chloride or allyl bromide.

*Level 2: Broader search*

If this fails, try a broader search:

Strip away the numbers and prefixes and search for the word part of the name (such as just “carvone” or even “ carvone “ with spaces around it) – that will help you find simple derivatives and related structures. However, the term “carvone” alone may show up as a fragment in many carvone derivatives that are quite different from carvone itself.

***Using chemical identifiers*** *(InChIKeys and CAS Nos.)*

*Level 1: Exact*

Most useful with Google Web, ChemSpider, or similar. CAS numbers are commonly used, but may not be known for your product, so they may not be found. InChIKeys are less common, but will give exact “hits” where they occur. Use combinations of InChIKeys if you have many hits. You may need to limit your no. of hits by searching with AND “Suzuki”

(*R*)‑Carvone *(reactant, compound* ***1****)*

* Common name: (*R*)‑carvone or (–)-carvone
* IUPAC name: (*5R,6S*)-6-allyl-5-isopropenyl-2-methylcyclohex-2-en-1-one
* CAS No: [6485-40-1]
* InChI: InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9H,1,5-6H2,2-3H3/t9-/m1/s1
* InChIKey: ULDHMXUKGWMISQ-SECBINFHSA-N

(S)–Carvone *(enantiomer of reactant)*

* Common name: (*S*)‑carvone or (+)-carvone
* IUPAC name: (*5S,6R*)-6-allyl-5-isopropenyl-2-methylcyclohex-2-en-1-one
* CAS No: [2244-16-8]
* InChI: InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9H,1,5-6H2,2-3H3/t9-/m0/s1
* InChIKey: ULDHMXUKGWMISQ-VIFPVBQESA-N

Racemic carvone *(racemate of reactant)*

* Common name: (R/*S*)‑carvone or (+/–)-carvone or DL–carvone
* IUPAC name: 6-allyl-5-isopropenyl-2-methylcyclohex-2-en-1-one
* CAS No: [99-49-0]
* InChI: InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9H,1,5-6H2,2-3H3
* InChIKey: ULDHMXUKGWMISQ-UHFFFAOYSA-N

(2S,3S)-3-Allylcarvone (*product,* *compound* ***2****)*

* Common name: (2S,3S)-3-Allylcarvone
* IUPAC name: (5R,6S)-6-Allyl-5-isopropenyl-2-methylcyclohex-2-en-1-one
* CAS No: 98-80-6
* InChI: InChI=1S/C13H18O/c1-5-6-12-11(9(2)3)8-7-10(4)13(12)14/h5,7,11-12H,1-2,6,8H2,3-4H3/t11-,12-/m0/s1
* InChIKey: MYUWADSPUFOHQQ-RYUDHWBXSA-N