

## Chemistry Databases

- millions of different chemical compounds are known
- millions of studies of their properties, chemical reactions, and applications have been reported
- **about 20,000 new chemicals are reported each day**
- how can so much information be organized and searched?

# Chemical Abstract Service (CAS)

- largest available source of chemical information
- started by chemists in **1907**
- **provides summaries of research articles, technical reports, conference proceedings, and patents from about 8,000 sources in 50 different languages**
- run by volunteer chemists until 1994
- operated by the American Chemical Society (ACS)

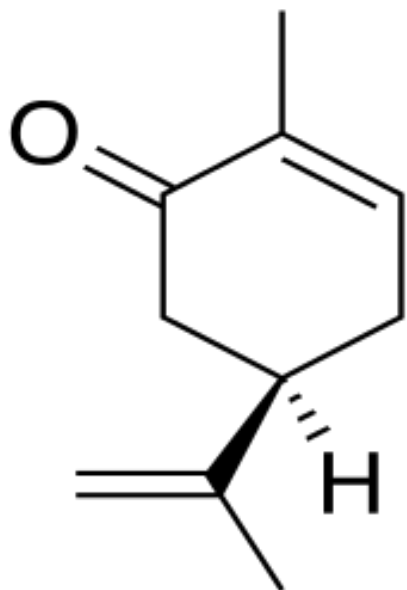
# Chemical Abstract Service (CAS)

- every known chemical substance is assigned a unique **chemical registry number** (CAS Number)
- approximately 70 million chemicals and 60 million protein sequences are registered
- CAS pioneered using computers to store information
- and access this information using search engines
- print version of CAS phased out in 2010
- CASSIE (Chemical Abstract Service Source Index) provides free bibliographic information online

Example:

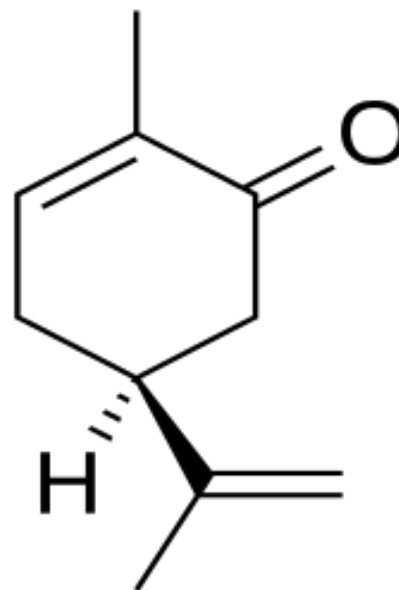
2-methyl-5-(1-methylethenyl)-2-cyclohexenone

“carvone”



**R-carvone**

CAS number 6485-40-1  
(spearmint taste)



**S-carvone**

2244-16-8  
(caraway taste)

racemic mixture 99-49-0

# CAS Commercial Products



**SCIFINDER**<sup>®</sup>

A CAS SOLUTION

## SciFinder

- online searchable database from CAS
- used by chemists worldwide to search for information about chemicals, reactions, ...
- standard issue in most chemistry departments

## STN

- **S**cientific and **T**echnical Information **N**etwork
- Scifinder plus many other databases

CAS, SciFinder, and STN are operated by the ACS

## American Chemical Society (ACS)

- founded in **1876**
- supports
  - chemical research
  - industrial chemistry
  - chemistry teaching
- largest scientific organization in the world (almost 200,000 members)
- *special student membership rates*



# American Chemical Society Publications

- *Journal of the American Chemical Society* (JACS)  
and ....
- *Journal of Physical Chemistry* (A, B and C)
- *Journal of Organic Chemistry*
- *Inorganic Chemistry*
- *Analytical Chemistry*
- *Biochemistry*
- *Chemical Reviews*
- *Journal of Chemical Education*

## Many other publications:

- *Catalysis*
- *Chemical Neuroscience*
- *Energy and Fuels*
- *Environmental Science and Technology*
- *Journal of Industrial Chemistry and Research*
- *Journal of Agricultural and Food Research*
- *Journal of Medicinal Chemistry*
- *Journal of Natural Products*
- *Journal of Theoretical and Computational Chemistry*
- ***Chemical and Engineering News (C&E News)***  
Weekly reports on **chemical research, industrial chemistry,**  
general chemistry, *job ads*, ... ***(pick up a sample copy)***



## Also covered by the ACS: Industrial Chemistry

The courses required for university chemistry degrees suggest the important chemistries are:

- physical
- analytical
- inorganic
- theoretical
- organic
- biochemical

But outside our world of university and academic chemistry, there is a **huge global chemical industry** worth exploring.

- different ways to do chemistry
- large scale and high production rates
- continuous flow processes preferred (not batch)
- **\$\$\$ business chemistry \$\$\$**

# What is Industrial Chemistry ?

**large-scale economical production of**

- basic chemicals (~ 20)
- chemical intermediates (~ 300)
- consumer products (~ 40,000)

from a few (~ 10) widely available and inexpensive naturally-occurring materials

**~ 70% of chemists work in the chemical industry**

# The Industrial Chemistry “Tree”

## Consumer Products (~ 40,000)

plastics, fibers, fertilizers, pharmaceuticals, paints, adhesives, detergents, solvents, ...



## Chemical Intermediates (~ 300)

acetic acid, formaldehyde, urea, ethylene oxide, acrylonitrile, acetaldehyde, styrene, ...



## Basic Industrial Commodity Chemicals (~ 20)

H<sub>2</sub>, CO, CO<sub>2</sub>, NH<sub>3</sub>, CH<sub>3</sub>OH, H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>, HNO<sub>3</sub>, Cl<sub>2</sub>, NaOH, ethylene, propylene, butylenes, benzene, liquid fuels (gasoline, diesel, kerosene)



## A Few Naturally-Occurring Raw Materials (~ 10)

air, water, petroleum, natural gas, coal, a few simple minerals (salt, limestone, sulfur...)

# BASF Headquarters, Ludwigshafen

- 10 km<sup>2</sup> site on the Rhine River
- 200 integrated chemical plants
- 40,000 employees
- 10 million tonnes of products per year

- BASF:**
- largest chemical producer in the world
  - production facilities on every continent (except Antarctica)



# **Chem 423 Industrial Chemistry**

prerequisites:

- Chem 231
- Chem 220 (completed or concurrent)