Designing Matter:

Molecular Design and Synthesis

Molecular Design and Synthesis

> Links to Session 1: Light/Matter

> History of Making Things

> Structure and Reactivity 101

> Design Process/Matter Lifecycle

> Fraser Research: Polymeric Metal Complexes

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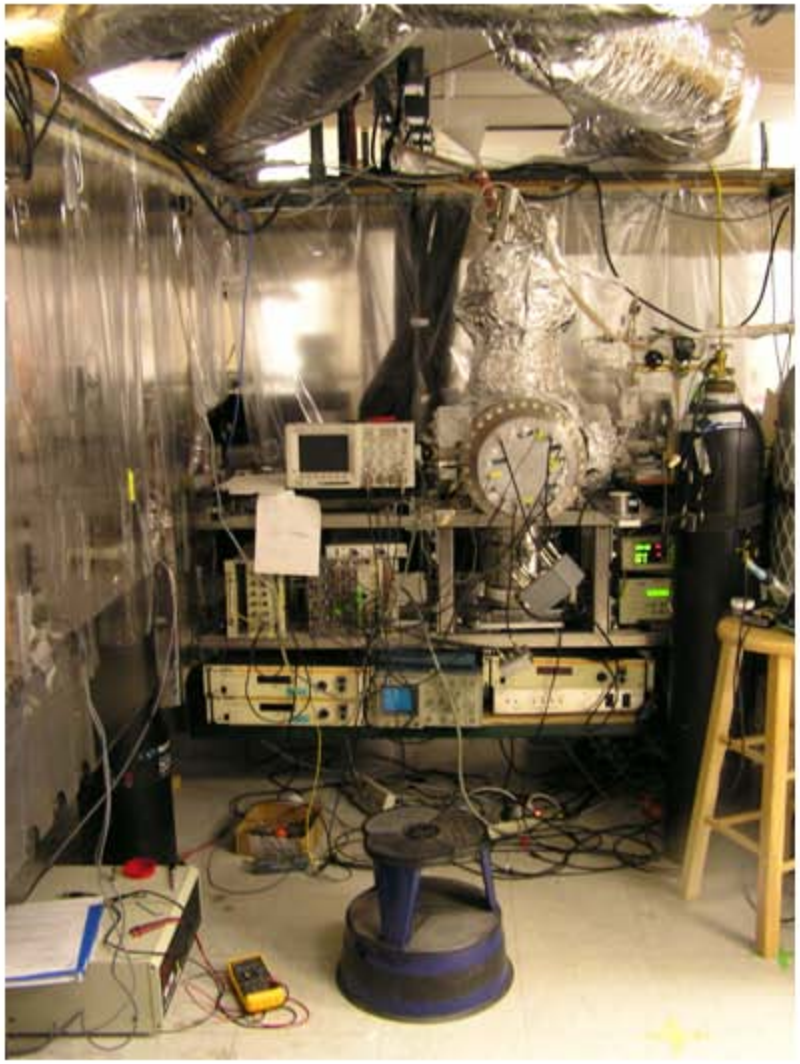
- Key points: Session 1 light and matter
- Kinds of chemistry: measurement, theory, synthesis

• Summary: Session 1 light and matter

- Light is a tool for understanding the structure of matter
- Matter is a source of specific kinds of light (i.e. laser)
- Lasers as tool for creating new behavior in matter and for understanding molecular dynamics

•Kinds of chemistry: measurement



•Kinds of chemistry: theory

•Kinds of chemistry: synthesis

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> History of Making Things

- Understanding nature: theories of matter, elements
- Copying nature
- Making brand new things (chance vs design)

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- Bacon, natural philosophers, 17th c

  old: vitalist notion: matter spirits; living matter special

  new: study natural laws separate from spiritual/magic
  experimental scientific communities
  knowledge shared not secret

  goals: "Nature to be commanded must be obeyed"
  dominate, improve upon nature
  wish list: Magnalia Naturae (natural wonders)

•Theories of matter: new

- Isolation, identification of fundamental particles

elements (vs compounds): 18th: e.g. Lavoisier, O

atoms: 19th: theory, wts, Dalton; 20th: experiment

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- Structure of matter

  molecular shape: 19th, valency, stereochemistry;
  (M's: 20th variable valency)

  subatomic particles: protons, neutrons, electrons

  quantum theory: orbitals, energies, spectroscopy
  (session 1)

• Copying nature

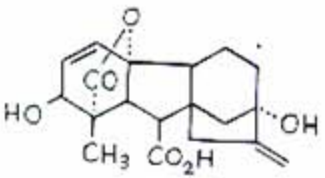
- Isolation, characterization of natural products

  determine active agents

- Duplicating in laboratory:

  by synthetic pathways:

  E.J. Corey, Nobel Prize in Chemistry 1990



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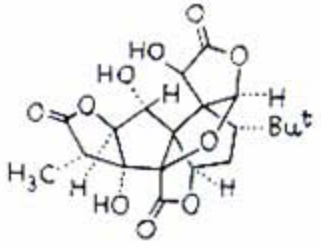

2

gibberillic acid
plant hormone

ginkgolide
chinese medicine: circulation

by natural pathway: molecular biology, protein engineering

*structures from www.nobel.se.

• Making brand new things

- Elaboration, improvement, optimization of nature

  sweeteners: sucrose vs saccharin, nutrasweet

  fats/oils: natural vs olestra

  soaps: fatty acids vs detergents

  drugs: natural products vs synthetic drugs; SARs

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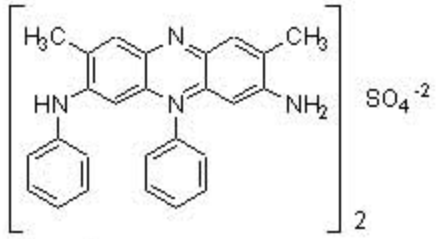

  dyes: 1856, Perkins mauve, aniline dye
  trying to make quinine, first synthetic dye
  start of chemical industry, retired age 36

  polymers: plastics, molecular biology (DNA, peptides)

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- Elements and their compounds have tendencies depending on where they are in the periodic table (structure, reactivity)
- Orbitals are important for understanding molecular shape (s, p, d orbitals; single, double, triple bonds).
- The spatial distribution of charge density in a molecule is helpful in predicting reactivity (ions, electronegativity, polarized bonds).
- Chemists represent molecular structure in all kinds of different ways.

- Position in periodic table

S.E. Van Bramer 9/11/97

Periodic Table of the Elements

1 H																1 H	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110	111	112		114		116		118

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

- Position in periodic table

American Chemical Society Periodic Table

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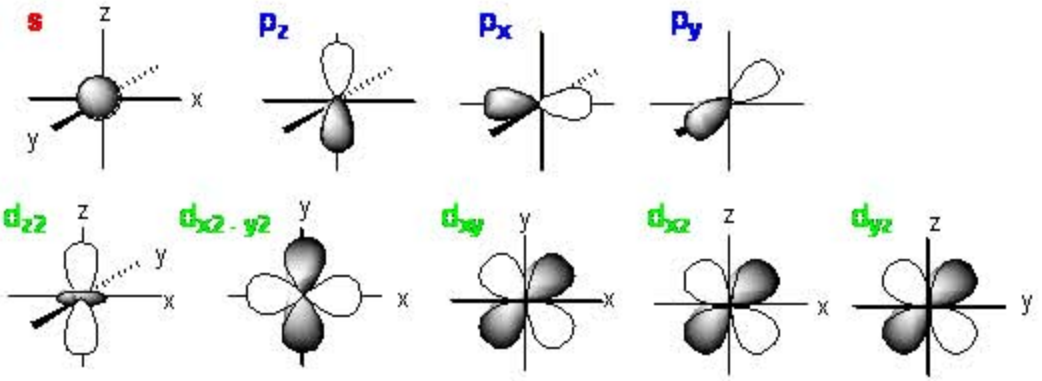
m_l = magnetic quantum #; 2l + 1 (m_l = l, l-1, l-2, ….-l)
boundary surfaces (shapes) of orbitals
(90% probability of finding an electron there)



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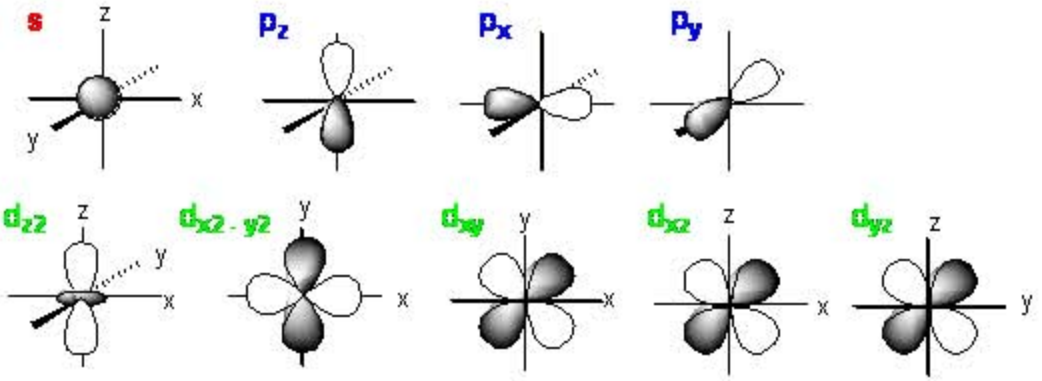
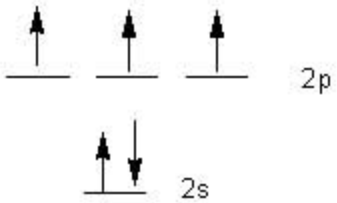




m_s = spin quantum #; +1/2, -1/2 (spin up; spin down)
an orbital can have only two electrons in it

• Important principles

- Filled shells are a good thing
  (octet rule: s, p filled; 18 e- rule: s, p, d filled)

- Elements have different tendencies to give up or accept e-
  (ionization, electron affinity, electronegativity)

- Group # relates to valency (# atoms attached) and
  molecular shape (VSEPR)

• Bonding and shape

Ionic Bonding:

Na has one valence electron ($3s^1$). Na •

Cl has 7valence electrons ($3s^2\ 3p^5$) :Cl•

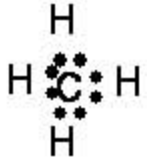
Na wants 0, not 1. (if gives up 1,has 8)
Cl wants 8 not 1. (if accepts 1, has 8)
So Na gives electron to Cl.

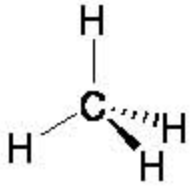
Covalent Bonding:

H has one valence electron ($1s^1$). H•

C has 4 valence electrons ($2s^2$ and $2p^2$) •C•

C wants 8, not 4. (all 2s and 2p filled)
H wants 2 not 1. (all 1s filled)
So C teams up with 4 H





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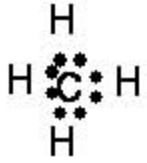
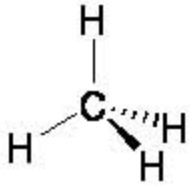


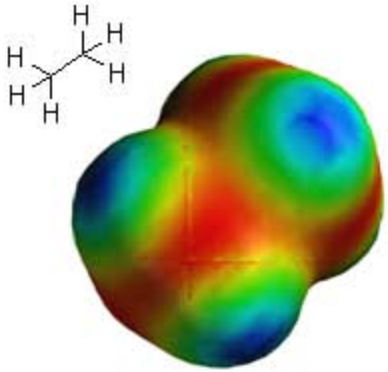
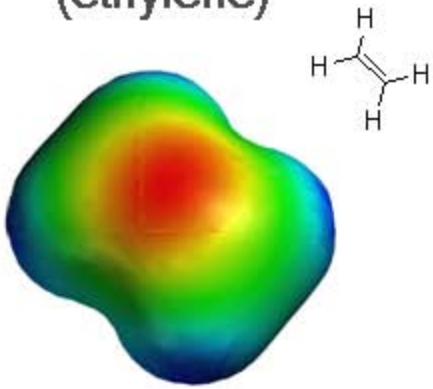
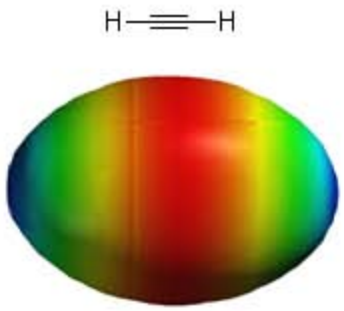
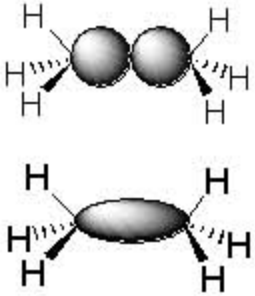
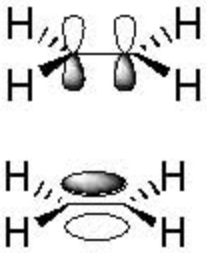
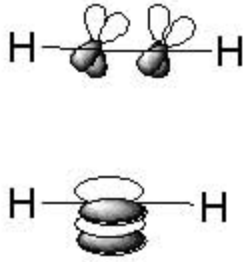


Try ammonia (NH_3), water (H_2O), and BF_3. (show # valence electrons and shape)

• Bonding and charge density

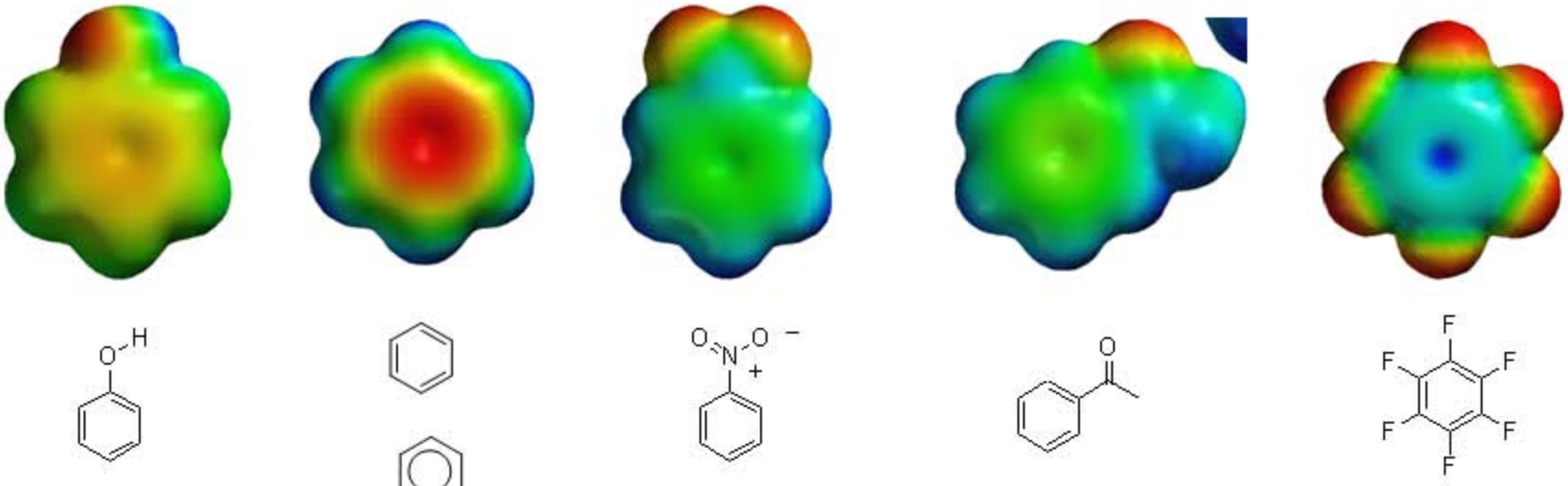
Electrostatic Potential Plots — red = highest electron density in molecule

blue = lowest electron density in molecule

ethane	ethene (ethylene)	ethyne (acetylene)
		
single bond	double bond	triple bond
		

•Spatial arrangement of charge density

phenol | benzene | nitrobenzene | acetophenone | perfluorobenzene



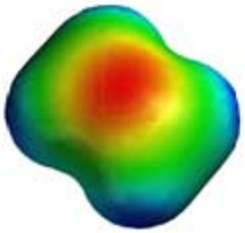
Electron donating

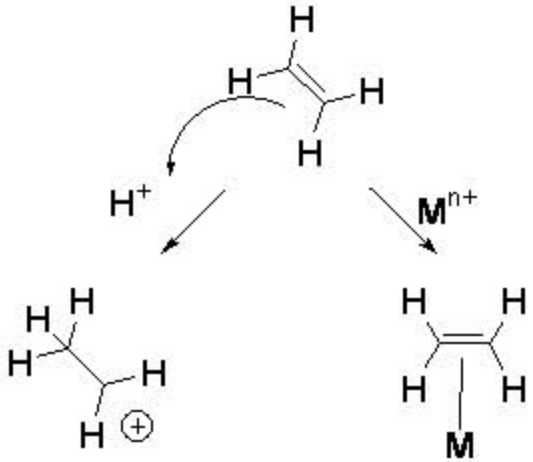
Electron withdrawing groups

*Spartan structures here and on following pages courtesy of Hill Harman, former Chem 281 TA.

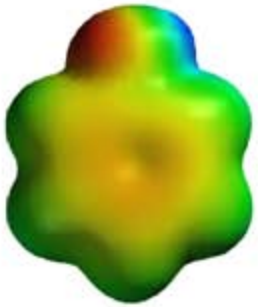
• Predicting reactivity

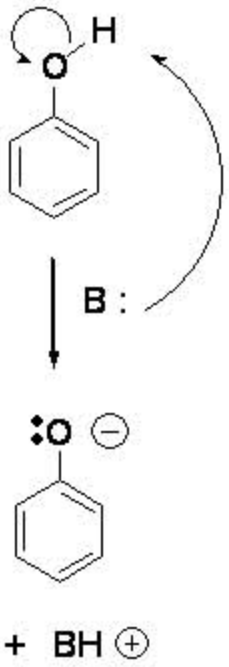
ethene



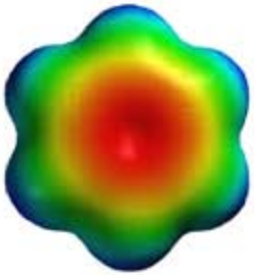


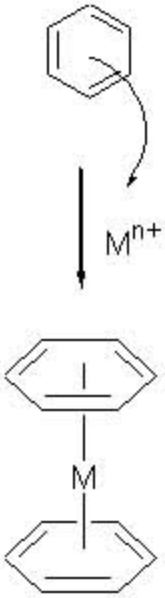
phenol



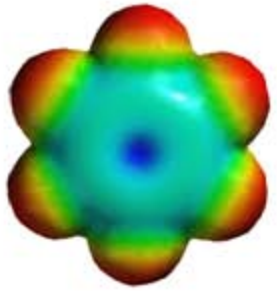


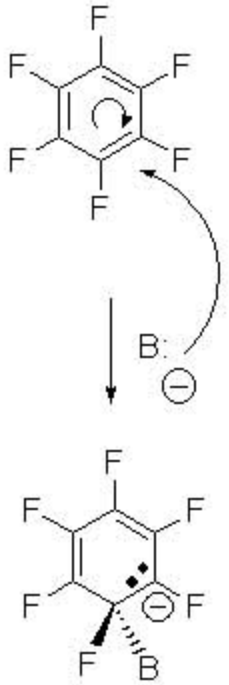
benzene



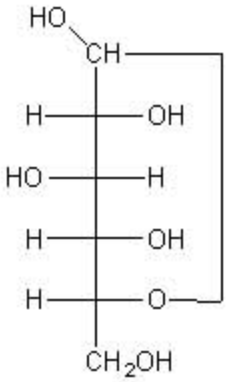


perfluorobenzene

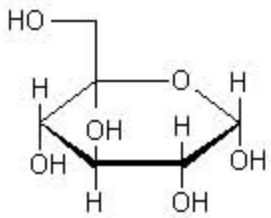




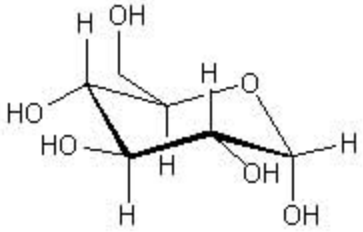
•More Representations: Glucose



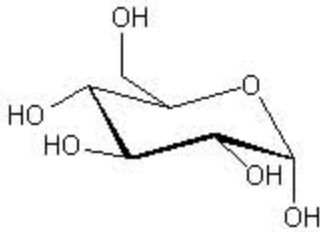
FISCHER



HAWORTH

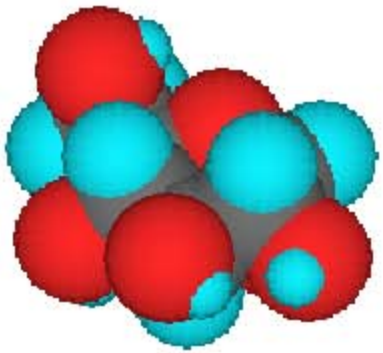


CHAIR



CHAIR (NO H)

SPACE FILLING



BALL AND STICK