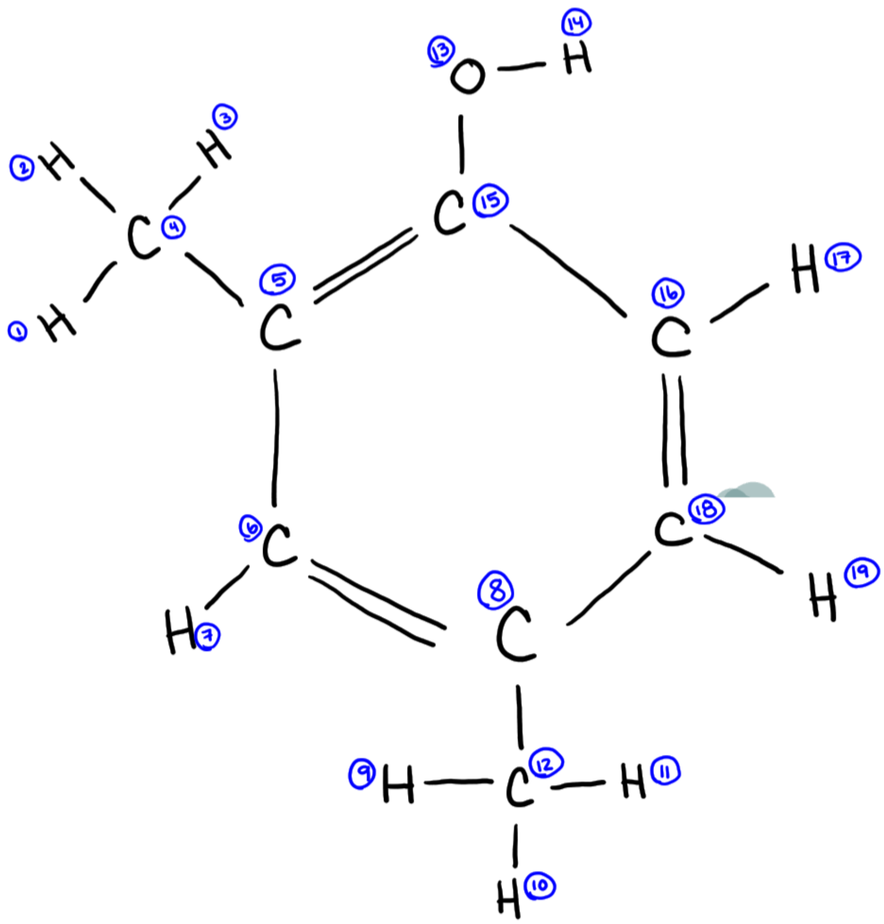
Molecule: 1,4-Dichlorobenzene

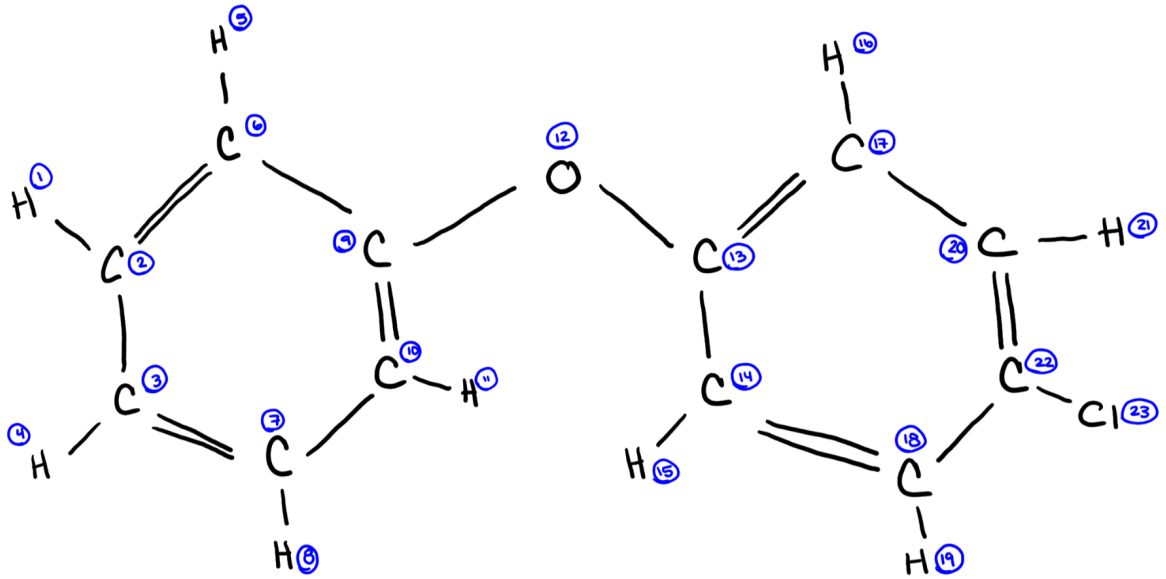
- No approximations made for bond, angle, or dihedral type

Molecule: 2,4-Dimethylphenol



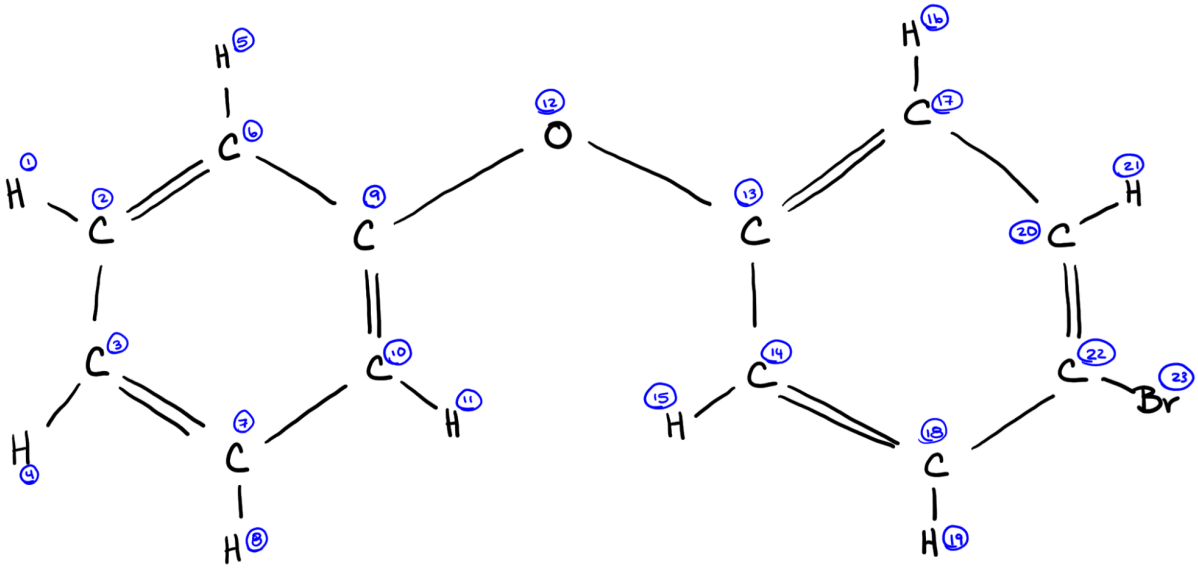
- No approximations made for bond or angle type
- Dihedral type approximations
  - OPLS dihedral type 5-48-48-48 (ex. atoms 13-15-5-6) approximated as OPLS dihedral type 0-48-48-48
  - OPLS dihedral type 5-48-48-13 (ex. atoms 13-15-5-4) approximated as OPLS dihedral type 0-48-48-13

Molecule: 4-Chlorodiphenyl ether



- No approximations made for bond type or angle type
- Dihedral approximations
    - OPLS dihedral type 20-48-48-48 (ex. atoms 2-6-9-12) approximated as OPLS dihedral type 0-48-48-48
    - OPLS dihedral type 20-48-48-49 (ex. atoms 5-6-9-12) approximated as OPLS dihedral type 0-48-48-49
    - OPLS dihedral type 48-20-48-48 (ex. atoms 9-12-13-17) approximated as OPLS dihedral type 3-20-48-48

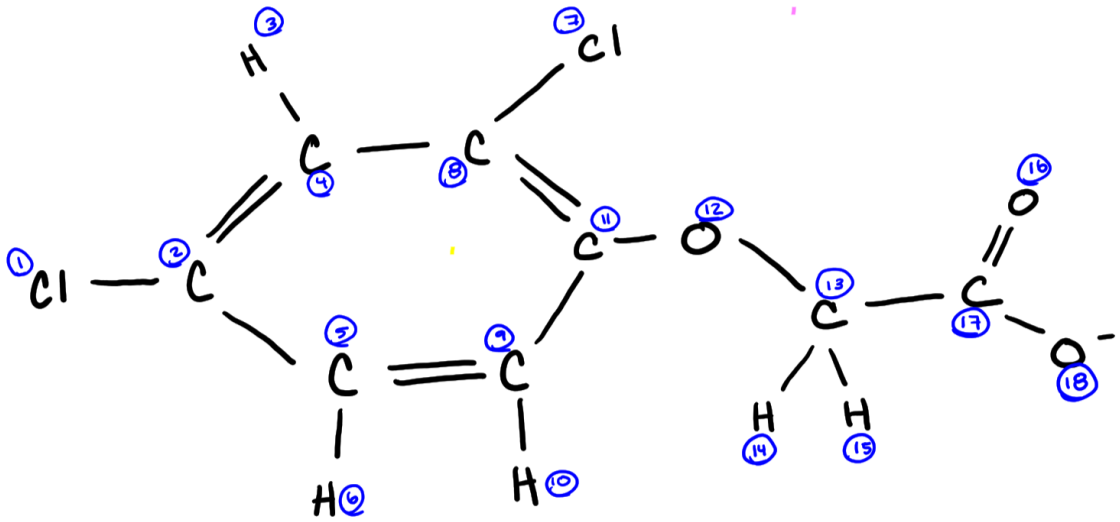
Molecule: 4-Bromophenyl phenyl ether



- No approximations made for bond type or angle type

- Dihedral approximations
    - OPLS dihedral type 20-48-48-48 (ex. atoms 2-6-9-12) approximated as OPLS dihedral type 0-48-48-48
    - OPLS dihedral type 20-48-48-49 (ex. atoms 5-6-9-12) approximated as OPLS dihedral type 0-48-48-49
    - OPLS dihedral type 48-20-48-48 (ex. atoms 6-9-12-13) approximated as OPLS dihedral type 3-20-48-48

Molecule: 2.4-Dichlorophenoxyacetic acid



- Atoms
    - 2.4-Dichlorophenoxyacetic acid has a pka of 2.73 so this molecule is modeled as deprotonated resulting in an overall charge of -1.0. The carboxylate group has a cumulative charge of -0.9. As a result the C-O-CH2 chain needs an overall charge of -0.1. The carbon in the benzene ring is modelled as OPLS atom type 141/48, anisole, and the oxygen is modelled as OPLS atom type 121/20, the oxygen in anisole. The hydrogens are modeled as alkane hydrogens which are OPLS atom type 127/46. The carbon connected to the carboxylate group and oxygen is modelled as OPLS atom type 216/13 which is a CH2 group connected to an oxygen atom. The charge on this atom was adjusted from -0.22 to 0.04 to achieve a cumulative charge of -1.0. In the OPLS model, a carbon in alkane CH2, OPLS type 81/13, has a charge of -0.12. An ether CH2, OPLS atom type 43/2, has a charge of 0.25. The difference between these charges is 0.37. The atom charge for OPLS type 216/13 is -0.22, so adding this offset results in -0.22+0.37 = 0.15. If

half of the charge from OPLS atom type 216/13 can be attributed to the oxygen atom then 0.15 - 0.11 = 0.04, the new charge on the carbon atom.

- No approximations made for bond or angle type
- Dihedral approximations
    - OPLS dihedral type 20-48-48-48 (ex. atoms 4-8-11-12) approximated as OPLS dihedral type 0-48-48-48
    - OPLS dihedral type 20-48-48-21 (ex. atoms 7-8-11-12) approximated as OPLS dihedral type 0-48-48-0
    - OPLS dihedral type 3-13-20-48 (ex. atoms 11-12-13-17) approximated as OPLS dihedral type 0-13-20-13
    - OPLS dihedral type 20-48-48-49 (ex. atoms 10-9-11-12) approximated as OPLS dihedral type 0-48-48-49
    - OPLS dihedral type 20-13-3-52 (ex. atoms 12-13-17-18) approximated as OPLS dihedral type 52-3-13-13