



Homework 2: Due April 13th

- Write a program that will compute the minimum rmsd between two molecules over all isomorphic projections
- Input: a list of pathnames to pairs of molecule files
- Output
 - Actual rmsd (atom number equivalence)
 - Min rmsd under isomorphism
 - Correspondence of atoms that gave rise to the min rmsd
- You should not check bond order equivalence, since it will cause trouble
- Instead, check atom equivalence
 - Atoms A and B are the same element
 - They have the same number of substituents
 - Their substituents are the same elements
- Only worry about the following elements: C N O S P F Cl Br I

What to turn in

- A listing of your program
- The output of your program on Pathlist (sensibly formatted)
- Brief discussion of the complexity of your algorithm
- Email 1 file to ajain@cc.ucsf.edu