

Chemistry 30A Exam 1 Solutions May 2, 2003

Statistics: High score = 94; Average score = 62.0; Low score = 17

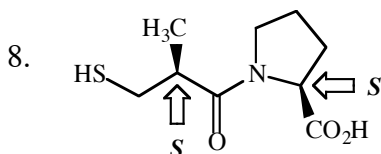
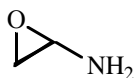
Standard Deviation = irrelevant as it does not control grade distribution in this class.

A note about exam keys: The answers presented here are usually significantly longer than expected from a student taking the exam. An exam key serves not only to reveal what was expected, but to instruct you as well.

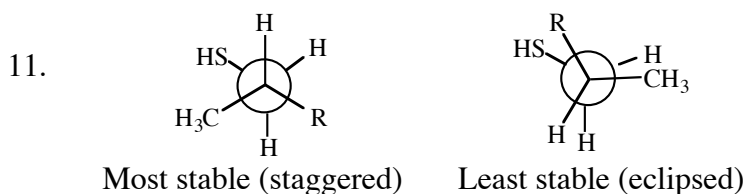
Exam key posted 10 AM, Friday May 2, 2003

To see the current course grade cutoffs, consult "If Grades Were Assigned Today" at the Chem 30A Home Page.

1. The number of sp^2 atoms in captopril is **4** (or 2 if you do not believe carbonyl oxygen atoms are sp^2 .)
2. **None** of the atoms in captopril have open octets.
3. There are **nine** lone pairs in captopril.
4. Influence #1: Lone pair repulsion influences molecular geometry.
Influence #2: Lone pairs may allow a species to be a base or nucleophile.
Influence #3: Lone pairs may play a role in determining formal charges.
5. **Carbon and sulfur** both have an electronegativity of 2.5.
6. From left to right: Thiol, amide, and carboxylic acid.
7. Captopril does not possess an amine group (NH_2).

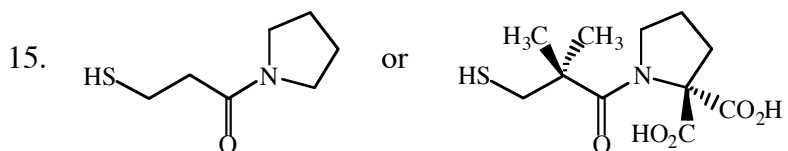
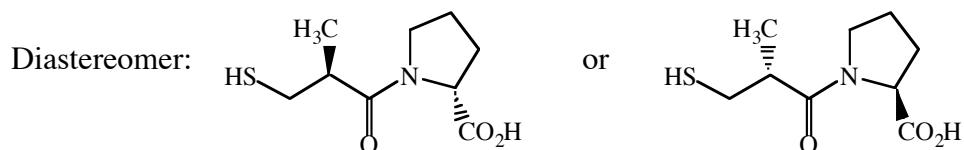
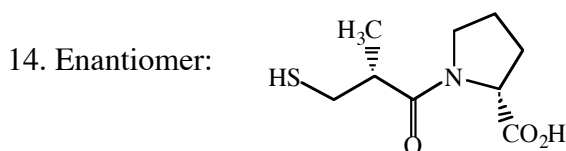
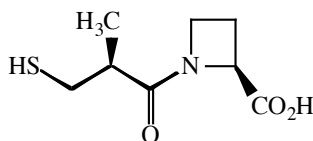


9. The single most important factor that drives any molecule into its lowest energy conformation or geometry is the **minimization of strain or electron repulsion**.
10. The S-C-C bond angle of captopril is **a bit more than 109.5°**.



12. Captopril **does not have** ring strain.

13. Shrinking the ring to four atoms causes the molecule to have significant ring strain.



16. The **enantiomer** and **diastereomer** are optically active.

17. Captopril has 2 stereocenters so it has **four** possible stereoisomers.

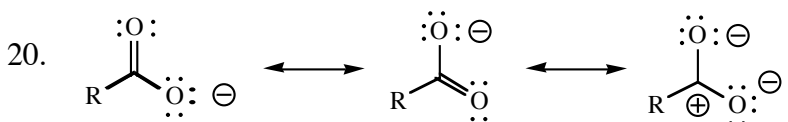
18. There is no direct relationship between absolute stereochemistry (R vs. S) and direction of rotation of plane polarized light, so we **cannot determine** if captopril is dextrorotatory or levorotatory.

19. (a) Resolution: Separation of enantiomers.

(b) Racemic mixture: A 1:1 mixture of enantiomers.

(c) Inductive effect: The electron-withdrawing or donating effect that one portion of the molecule has on another portion of the molecule.

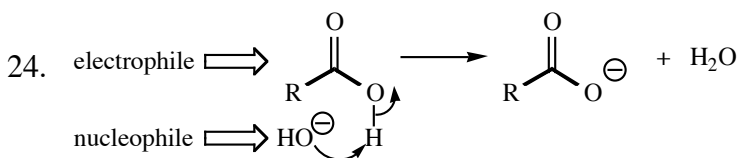
(d) Torsional strain: Increase in energy caused when two atoms or groups of atoms come too close, causing electron repulsion.



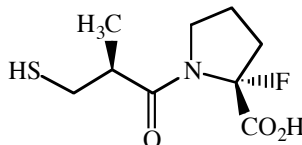
21. The single most important feature that influences the basicity of any base is its **ability to share an electron pair with a proton to form a new covalent bond.**

22. The most acidic hydrogen of captopril is **CO₂H**.

23. Deprotonation of RCO₂H leads to a conjugate base with resonance (question 20). The conjugate bases formed from RSH or RCH₃ do not enjoy this resonance and therefore their negative charges are not as effectively dispersed. Greater charge dispersal affords greater stability and reduced basicity. Thus RCO₂⁻ is a more stable (weaker) base than RS⁻ and RCH₂⁻. Recall that conjugate acid strength is inversely proportional to base strength, so the weakest base (RCO₂⁻) is derived from deprotonation of the strongest conjugate acid (RCO₂H).



25. Inclusion of a fluorine atom makes the RCO₂H more acidic due to the inductive effect.



26. Removing resonance causes a decrease in acidity.

