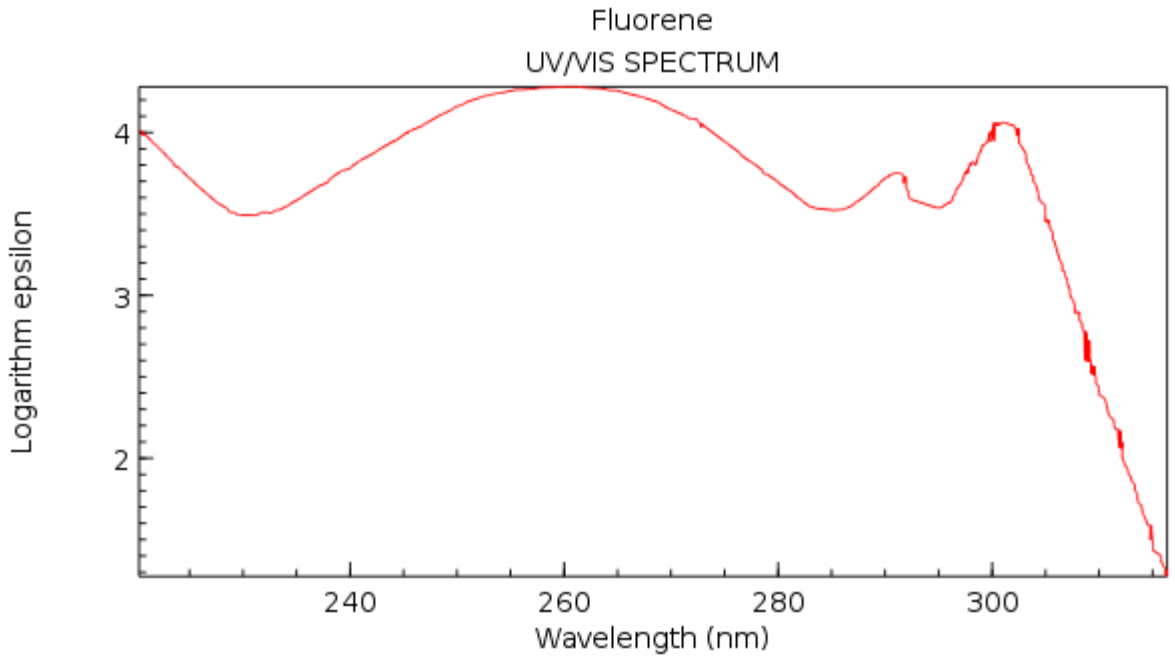
Conformation of organic molecules and biomolecules

Studying conformation of molecules ?
What for?

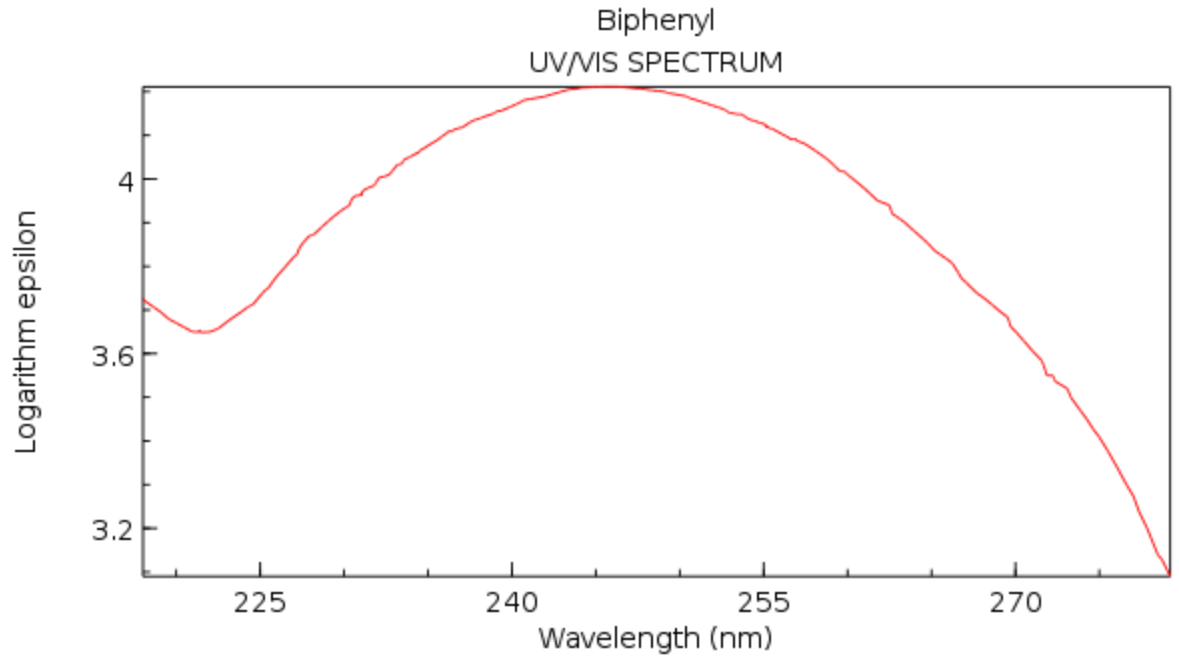
(Answer)
It is highly related to their functions, reactivities and selectivities.

Example of conformational effect on function

Biphenyl vs. Fluorene (UV spectra)



NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)



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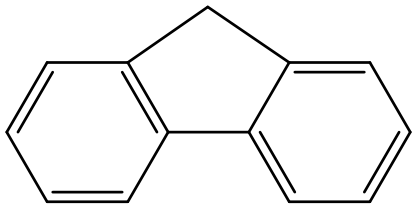
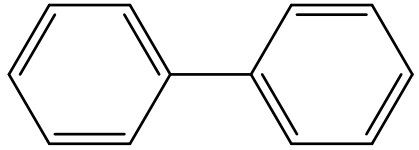




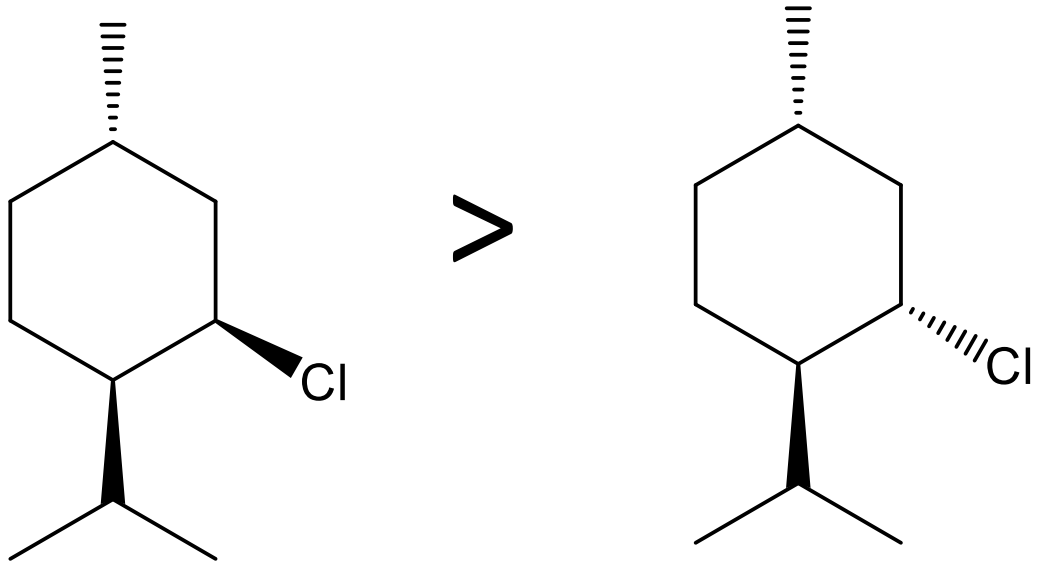
Example of conformational effect on reactivity

NaOH hydrolysis rate

19.8 : 1

Example of conformational effect on reactivity (2)

E2 elimination rate



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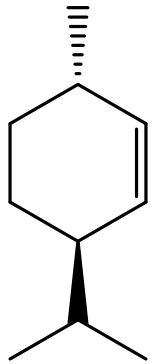
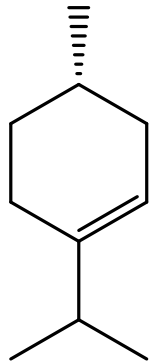
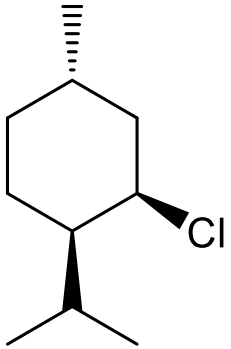
Example of conformational effect on selectivity

E2 elimination product







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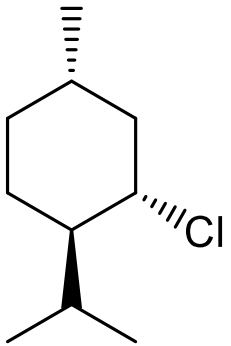

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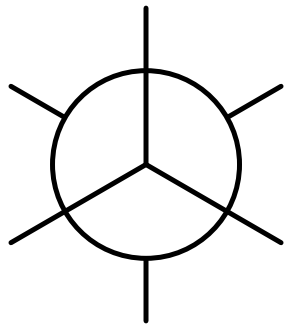
Our fundamental knowledge on energetically preferred structure

1)



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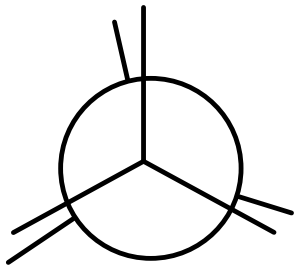

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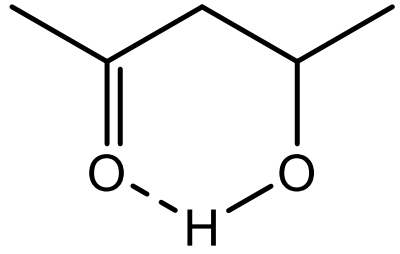
2)



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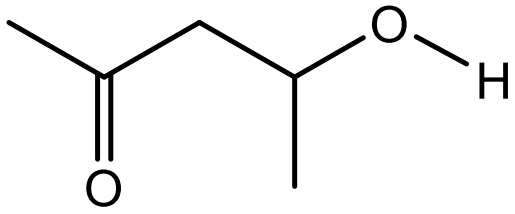

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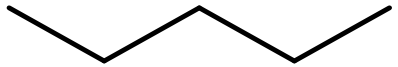

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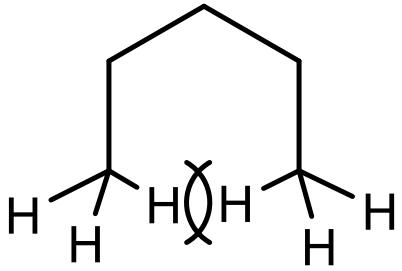

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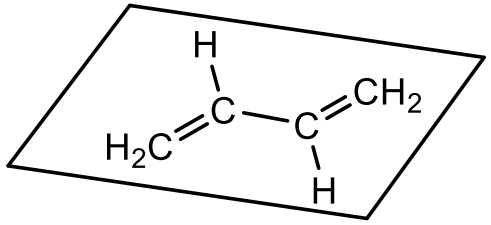

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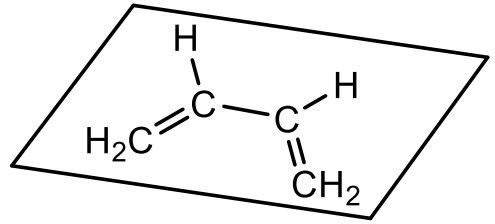
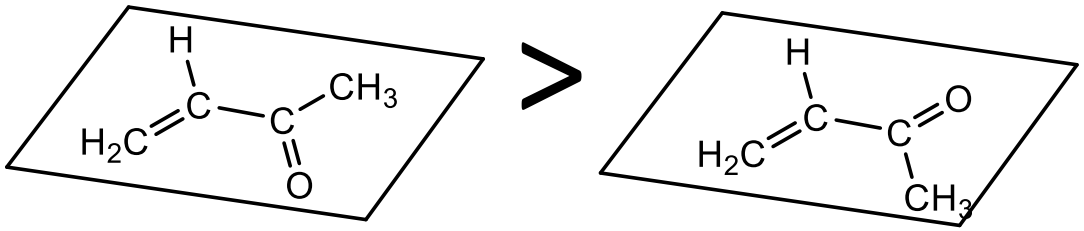


Our fundamental knowledge on energetically preferred structure

5)



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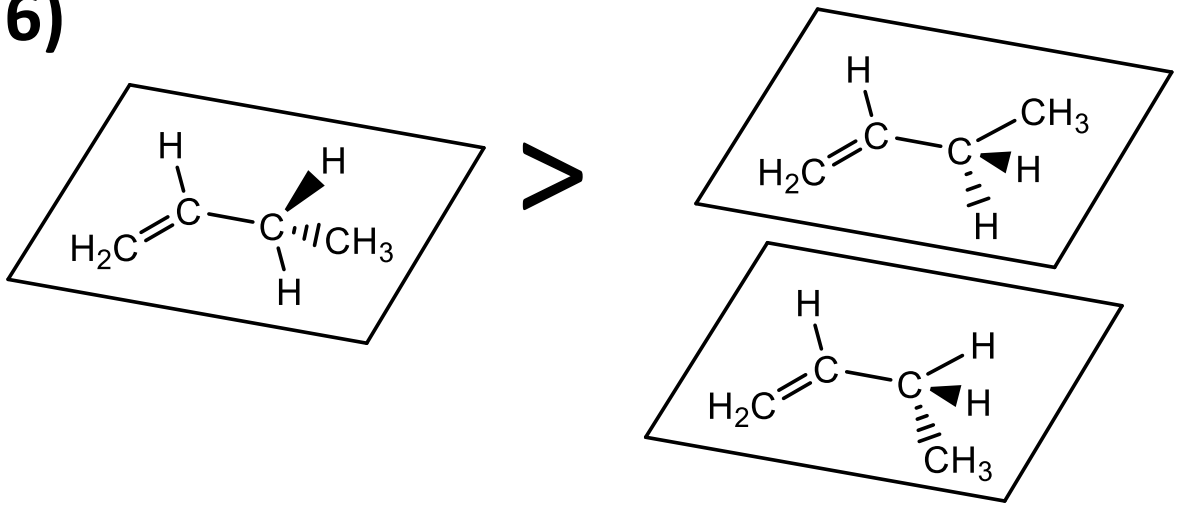

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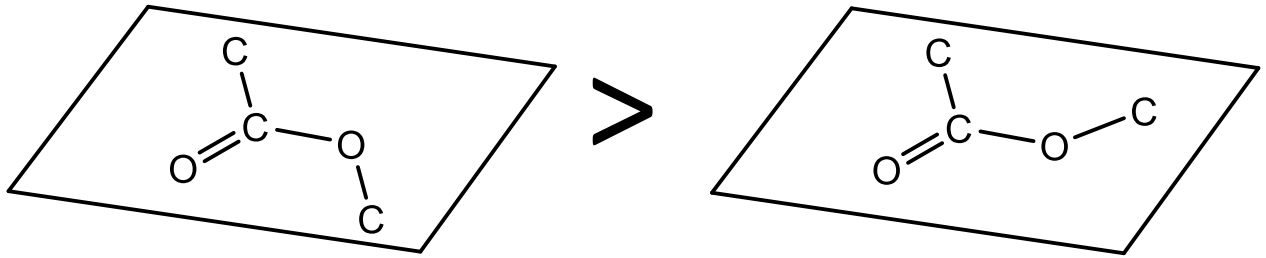
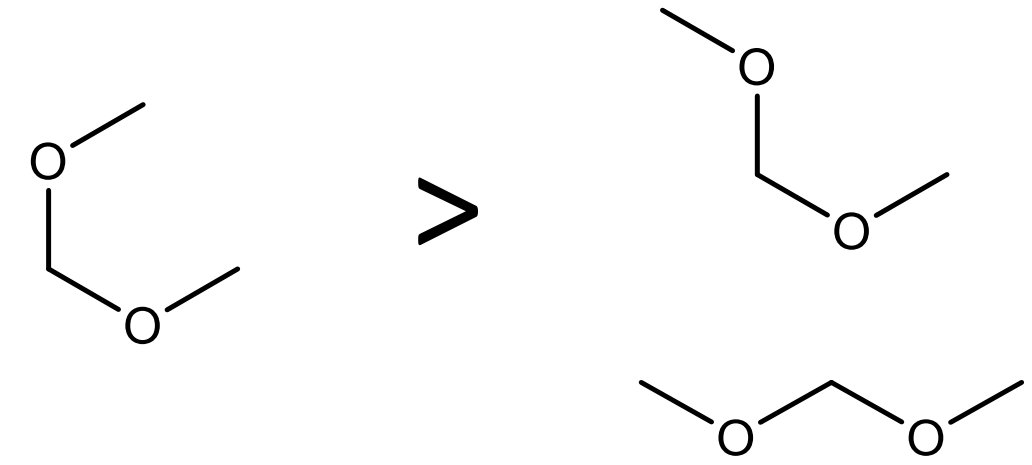


8) (a little bit difficult)



However, we are not able to know conformation of a given molecule because contribution of each factor cannot be estimated in a *quantitative* manner.

Possible solutions are …

1) Direct observation of molecular structure
   - X-ray crystallography
   - 2D NMR
2) Predict structure by calculation
   - Mainly MM-based methods