

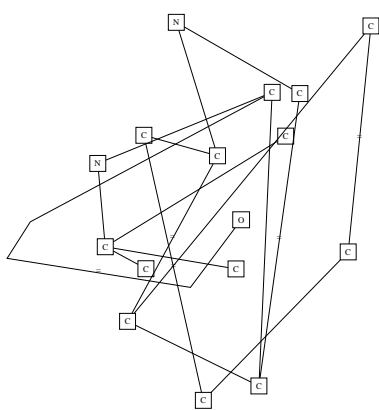
# Implementation of a Cheminformatics Library

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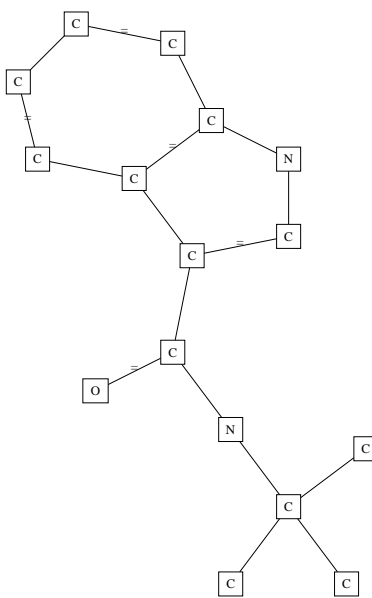
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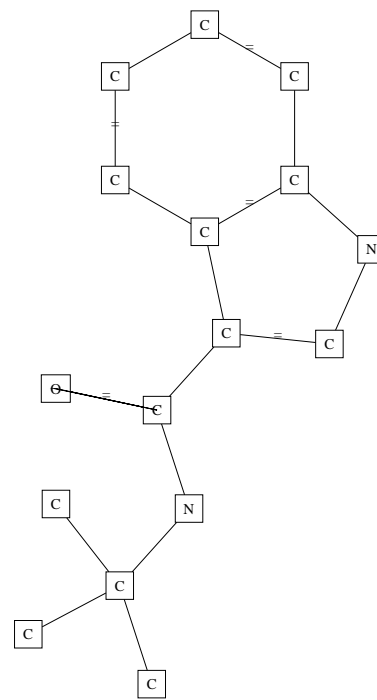
*Bled, 2002*



Random



Tunkelang



CDK

## Structure Diagram Generation with different algorithms

Schrödinger equation  
 $\hat{H}\Psi = E\Psi$

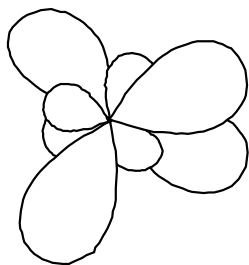


Born-Oppenheimer  
LCAO  
Extended Hückel  
Tight Binding  
VSEPR

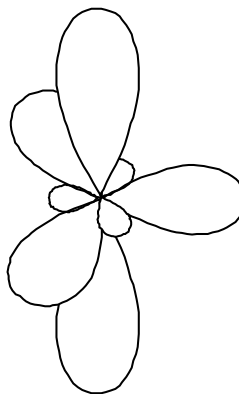
Generalized Eigenvalue Problem

$$\begin{pmatrix} \dots & & \\ & H_{AO_i-AO_j} & \\ & & \dots \end{pmatrix} \mathbf{C} = \begin{pmatrix} \dots & & \\ & S_{AO_i-AO_j} & \\ & & \dots \end{pmatrix} \mathbf{CE}$$

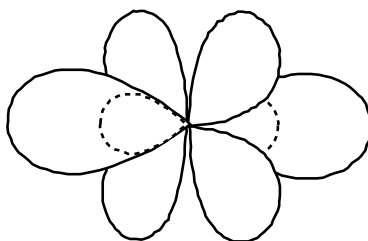
Electronic Energy Calculation



$sp^3$  hybridized

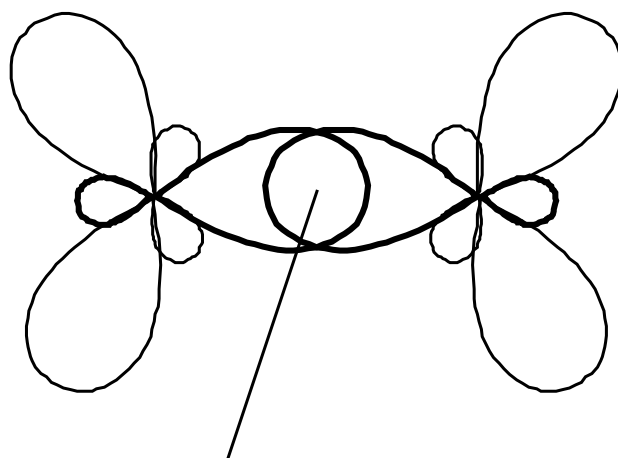


$sp^2$  hybridized + one p

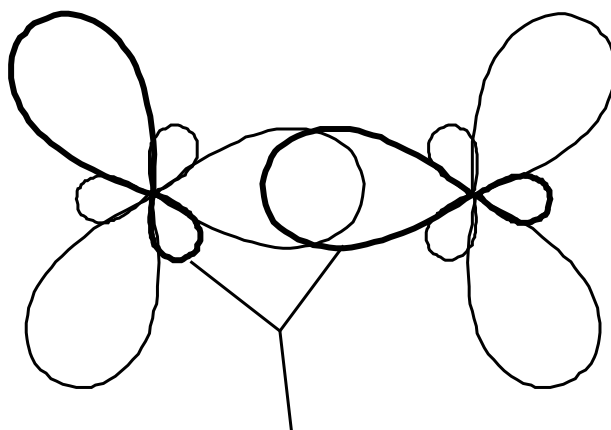


$sp$  hybridized + two p

## Atom Orbitals

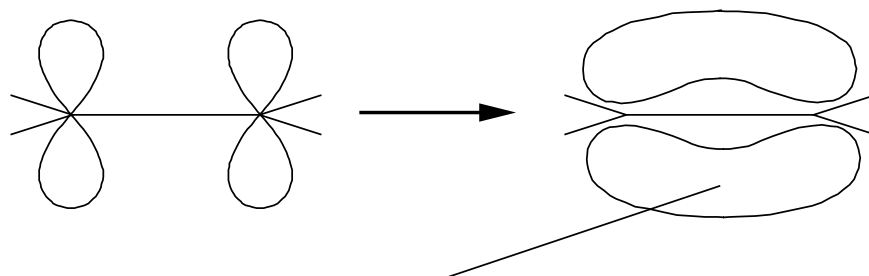


big  $\sigma$ -overlap between  $sp^2$  orbitals

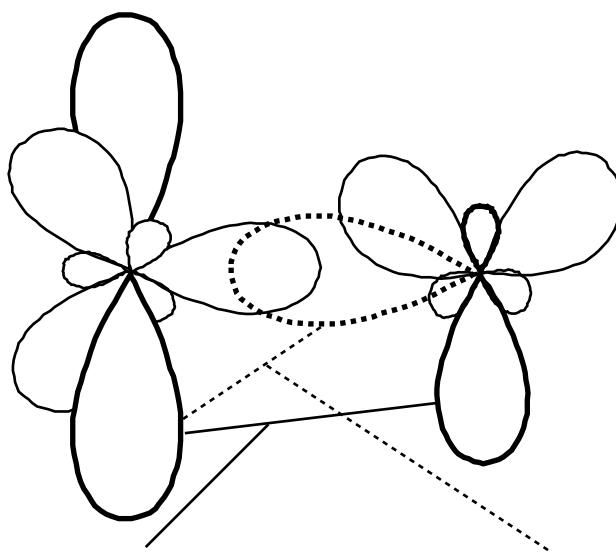


lesser overlap between  $sp^2$  orbitals

Implemented Overlaps

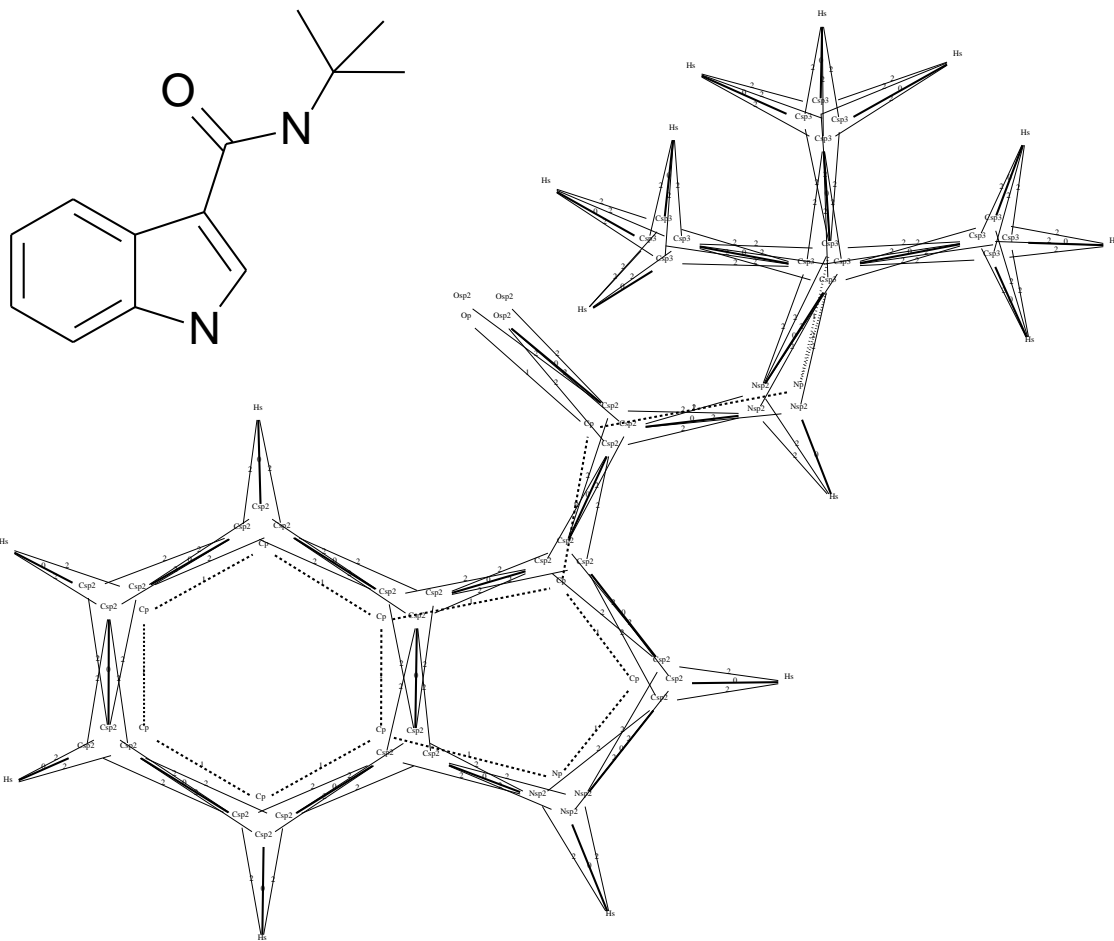


$\pi$ -overlap between p orbitals

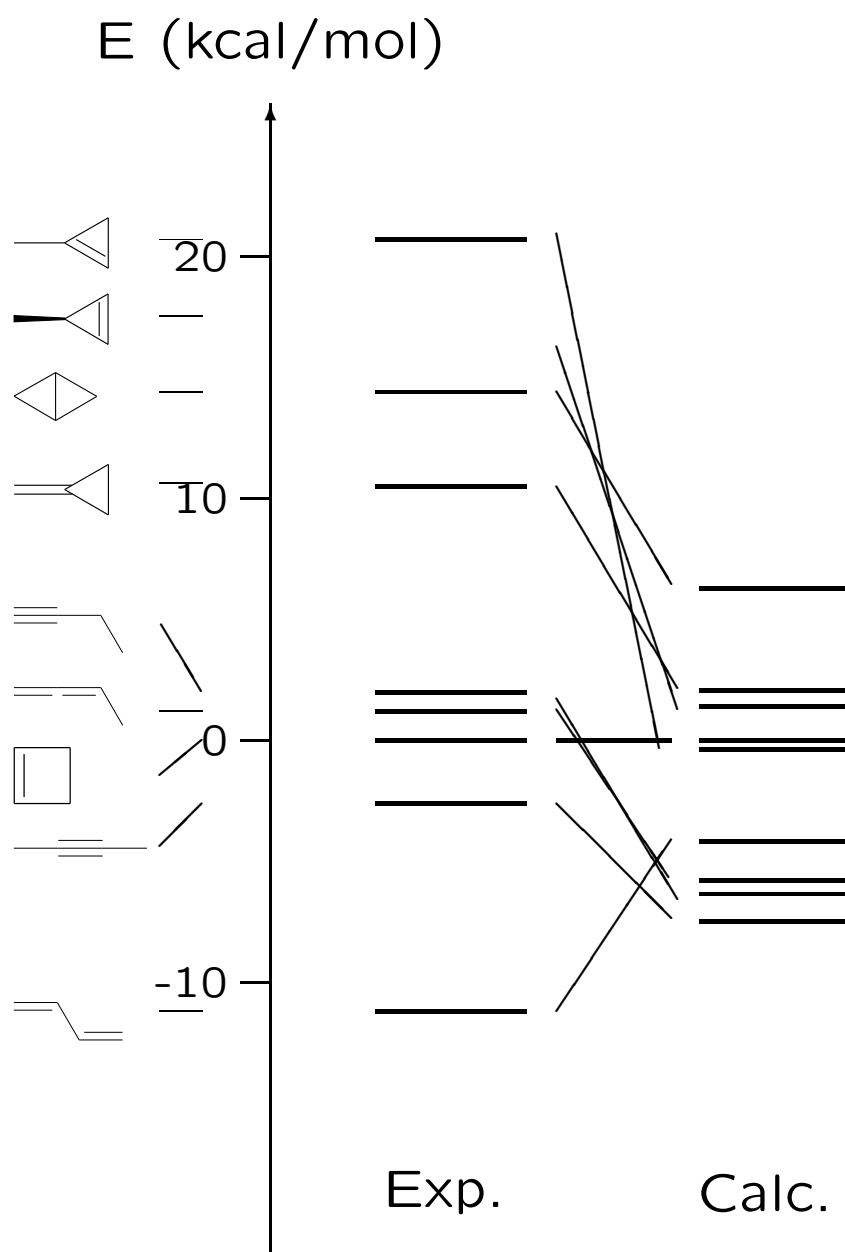


hyperconjugation and artificial  
overlap between p and  $sp^3$  orbitals

Implemented Overlaps



Graph of Implemented Overlaps



Relative energy of C<sub>4</sub>H<sub>6</sub> isomers



1

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