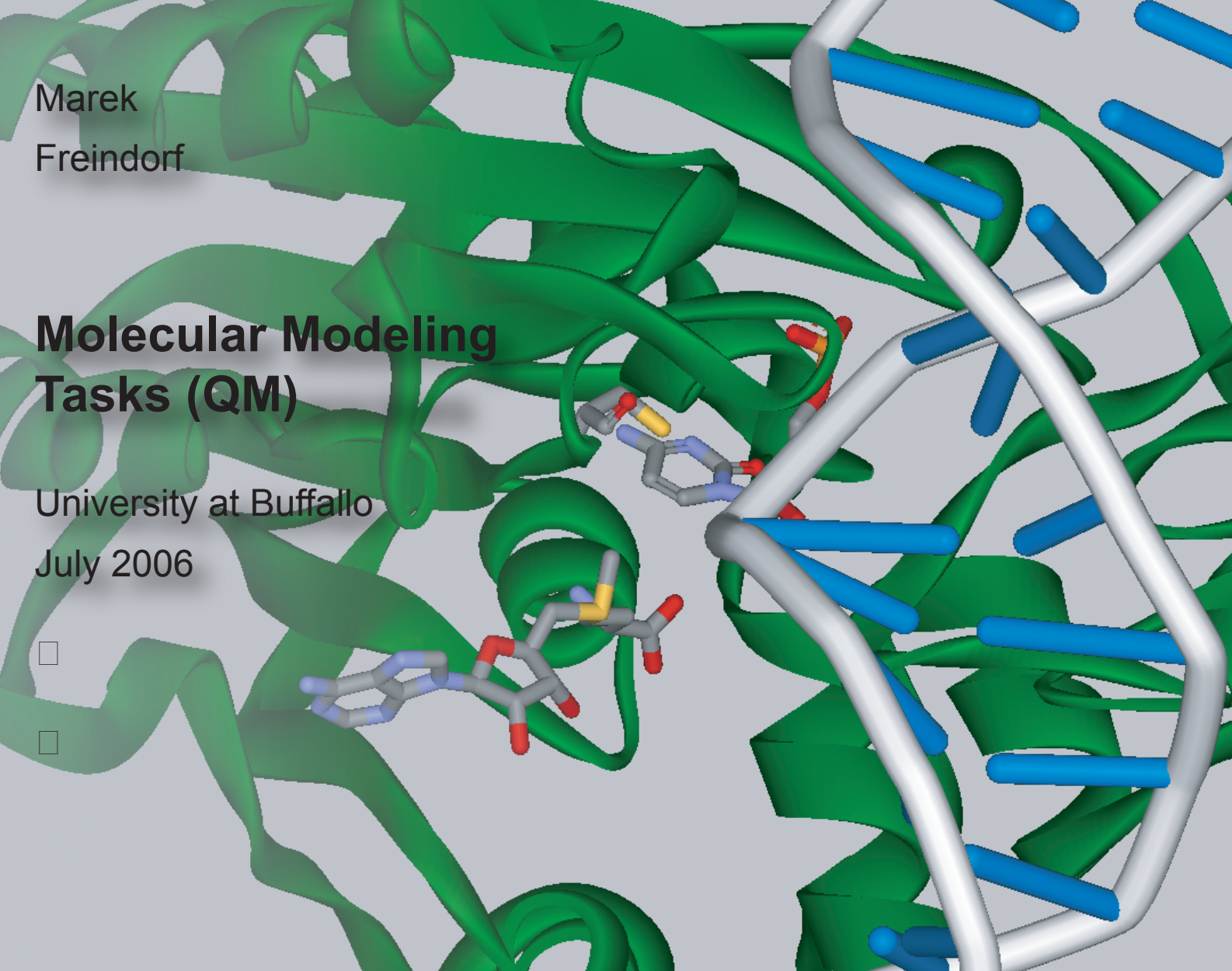
Marek
Freindorf

Molecular Modeling Tasks (QM)

University at Buffallo

July 2006



Introduction, first steps on your local desctop

1. Create your own drectory on your local desktop (if you want)

2. Create your own profile in the SSH program

3. For help open an internet browser, go into the course home page:

   http://www.ccr.buffalo.edu/display/~mfrein/Computer+Modeling+of+Biological+Systems

4. Open "Introduction"

Introduction, first steps on the server

1. Create your own directories (subdirectories) in your home directory (if you want)
2. Transfer a PDB file from your desktop into the server
3. Copy examples of the input file and PBS script into your home directory:

   > **cp** /tmp/marek/test.in .

   > **cp** /tmp/marek/test.pbs .

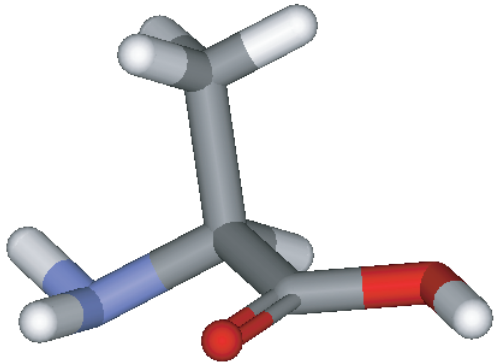
   > **cp** /tmp/marek/qchem2pdb.pl .

4. For help open an internet browser, go into the course home page:
   http://www.ccr.buffalo.edu/display/~mfrein/Computer+Modeling+of+Biological+Systems

5. Open "Introduction"

QM geometry optimization of amino acids (QM-1)

1. Calculate an optimal geometry of alanine using the B3LYP/6-31+G* level of theory



2. Report in a table atomic charges of all atoms

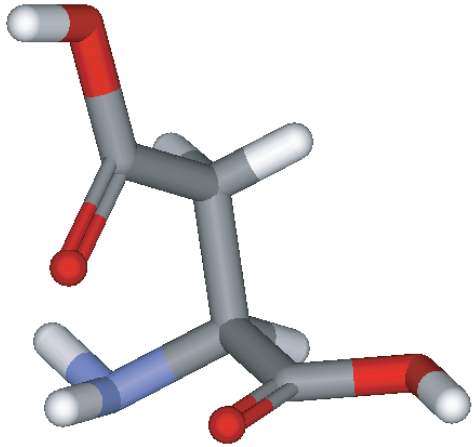
3. Report in a table interatomic distances and angles between bonds of the side chain

4. Report in a figure a value and an orientation of a molecular dipol moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-2)

1. Calculate an optimal geometry of aspartic acid (protonated) using the B3LYP/6-31+G* level of theory



2. Report in a table atomic charges of all atoms

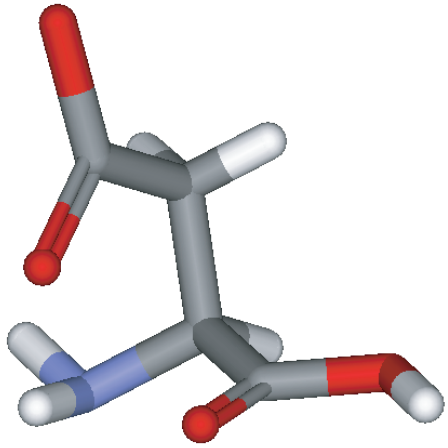
3. Report in a table interatomic distances and angles between bonds of the side chain

4. Report in a figure a value and an orientation of a molecular dipol moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-3)

1. Calculate an optimal geometry of aspartic acid (deprotonated) using the B3LYP/6-31+G* level of theory



2. Report in a table atomic charges of all atoms

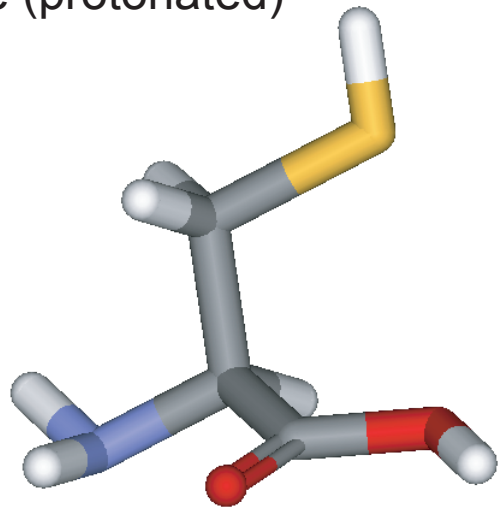
3. Report in a table interatomic distances and angles between bonds of the side chain

4. Report in a figure a value and an orientation of a molecular dipol moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-4)

1. Calculate an optimal geometry of cysteine (protonated) using the B3LYP/6-31+G* level of theory



2. Report in a table atomic charges of all atoms

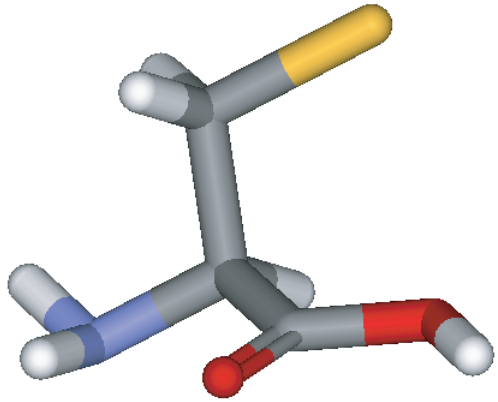
3. Report in a table interatomic distances and angles between bonds of the side chain

4. Report in a figure a value and an orientation of a molecular dipol moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-5)

1. Calculate an optimal geometry of cysteine (deprotonated) using the B3LYP/6-31+G* level of theory



2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the side chain

4. Report in a figure a value and an orientation of a molecular dipol moment

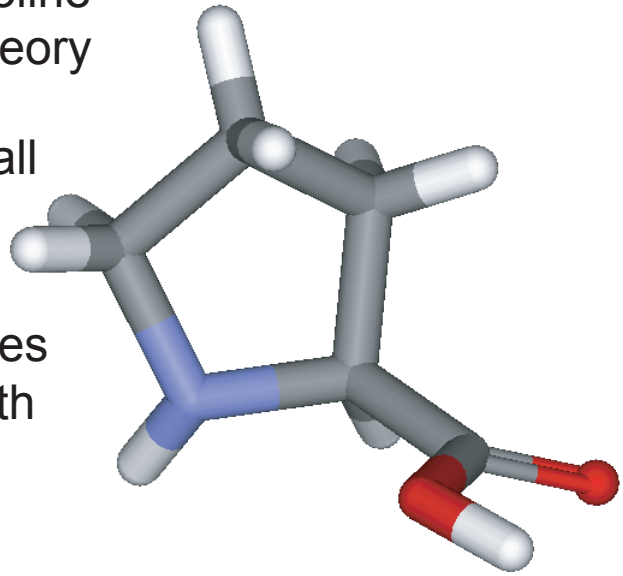
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-6)

1. Calculate an optimal geometry of proline using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the 5-th member ring



4. Report in a figure a value and an orientation of a molecular dipol moment

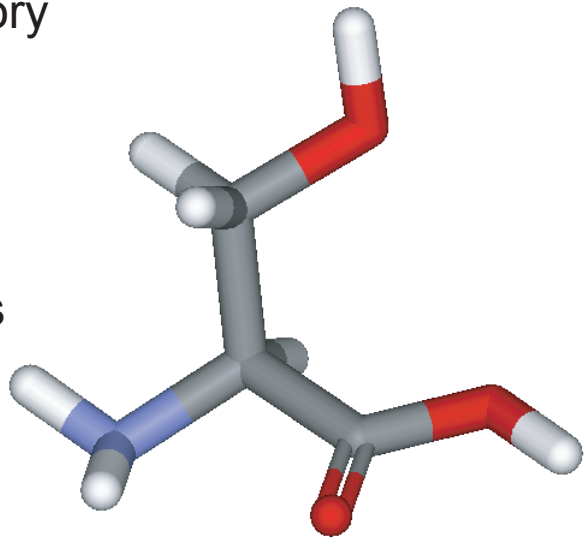
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-7)

1. Calculate an optimal geometry of serine (protonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the atoms of the side chain



4. Report in a figure a value and an orientation of a molecular dipol moment

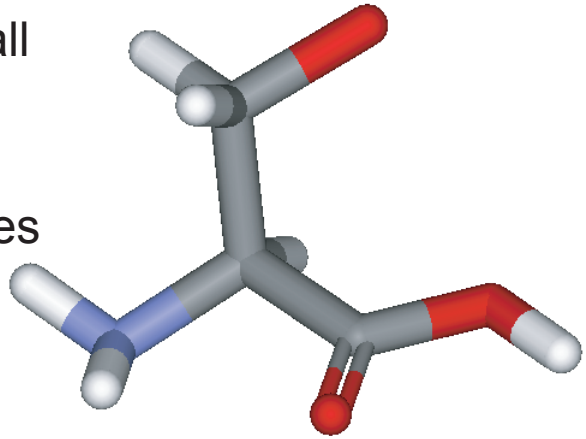
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-8)

1. Calculate an optimal geometry of serine (deprotonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the atoms of the side chain



4. Report in a figure a value and an orientation of a molecular dipol moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of amino acids (QM-9)

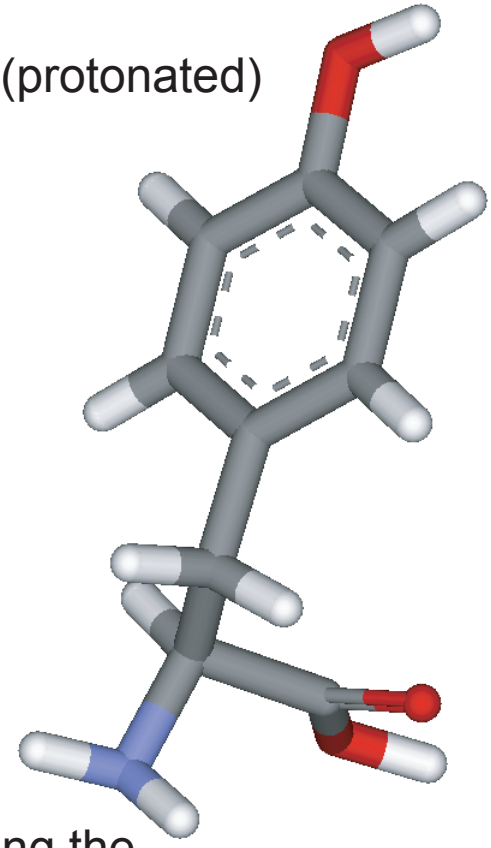
1. Calculate an optimal geometry of tyrosine (protonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the side chain atoms

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



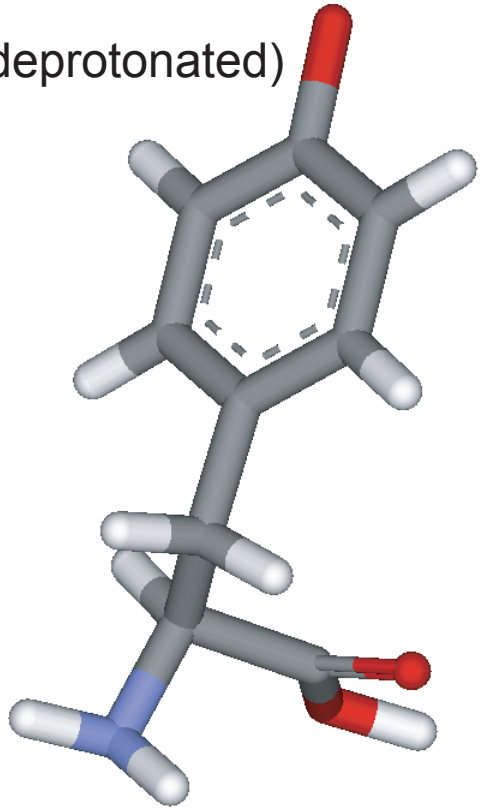
QM geometry optimization of amino acids (QM-10)

1. Calculate an optimal geometry of tyrosine (deprotonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the side chain atoms

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

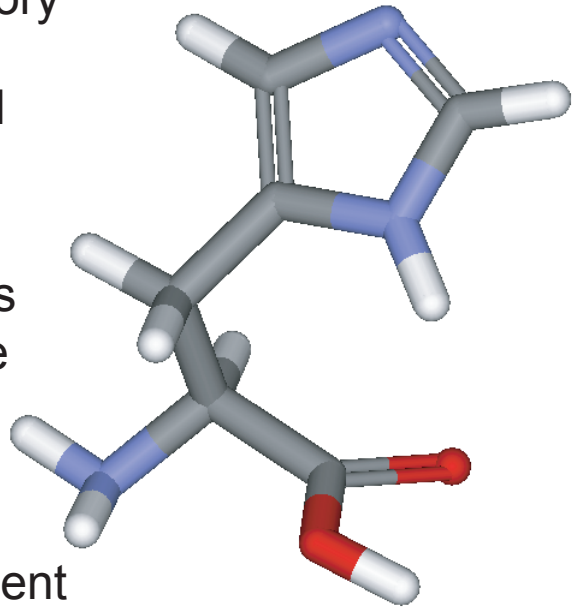
QM geometry optimization of amino acids (QM-11)

1. Calculate an optimal geometry of histidine (delta) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the side chain atoms

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

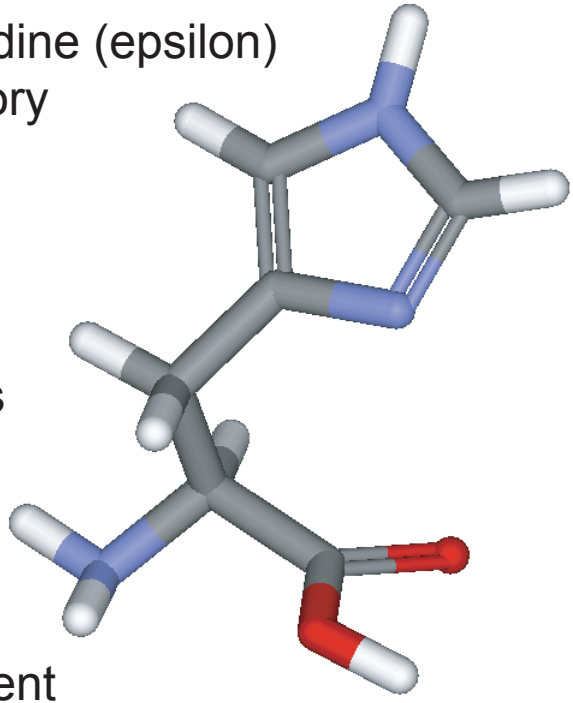
QM geometry optimization of amino acids (QM-12)

1. Calculate an optimal geometry of histidine (epsilon) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the side chain atoms

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

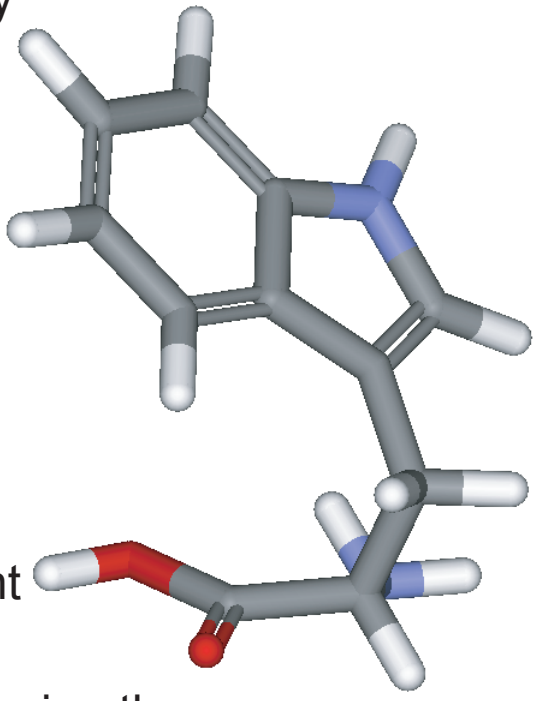
QM geometry optimization of amino acids (QM-13)

1. Calculate an optimal geometry of triptophan (protonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the 5-th member ring atoms

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

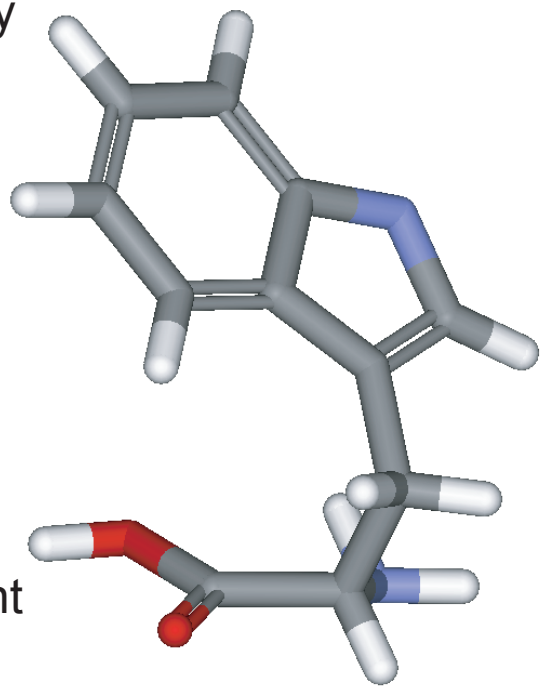
QM geometry optimization of amino acids (QM-14)

1. Calculate an optimal geometry of triptophan (deprotonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the 5-th member ring atoms

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

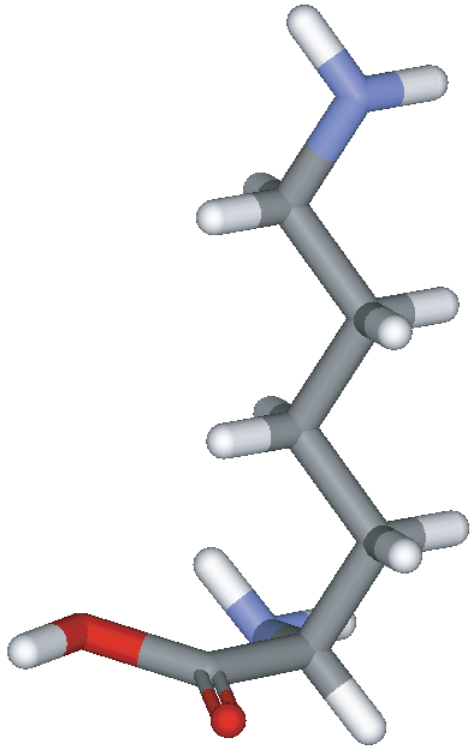
QM geometry optimization of amino acids (QM-15)

1. Calculate an optimal geometry of lysine using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the side chain atoms

4. Report in a figure a value and an orientation of a molecular dipole moment



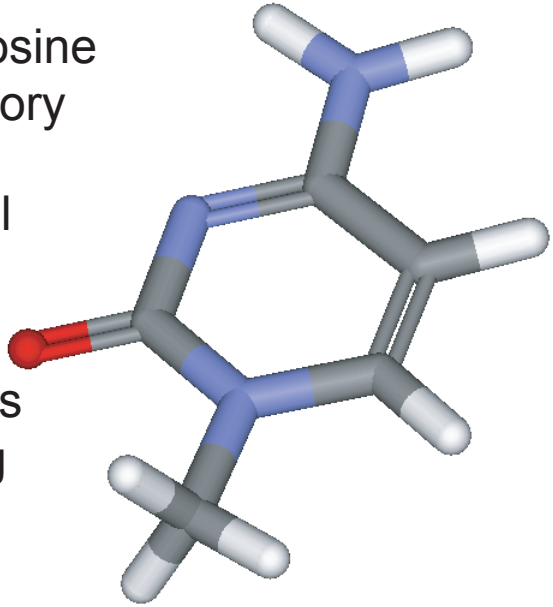
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of base pairs (QM-16)

1. Calculate an optimal geometry of cytosine using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

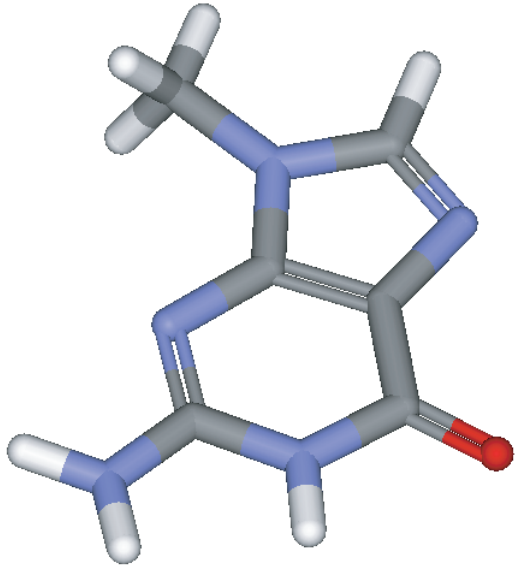


4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of base pairs (QM-17)

1. Calculate an optimal geometry of guanine (protonated) using the B3LYP/6-31+G* level of theory



2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the 5-th member ring

4. Report in a figure a value and an orientation of a molecular dipole moment

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

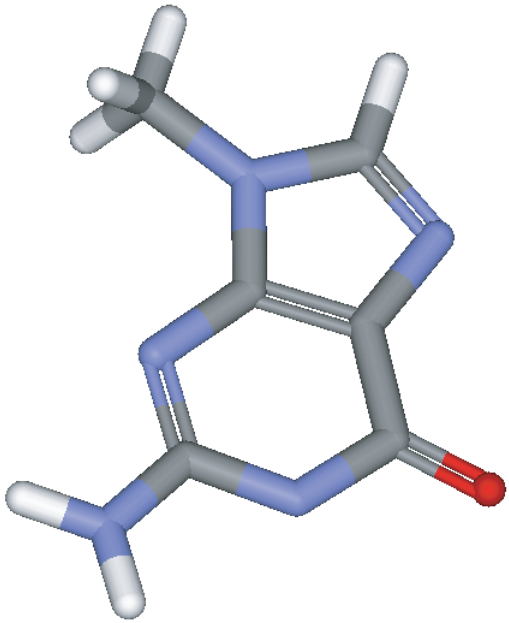
QM geometry optimization of base pairs (QM-18)

1. Calculate an optimal geometry of guanine (deprotonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the 5-th member ring

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

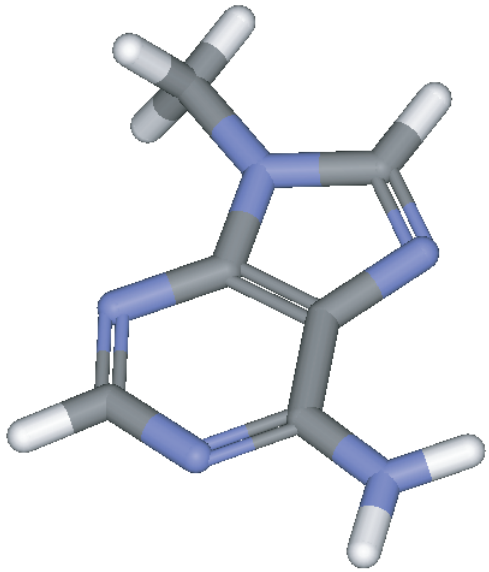
QM geometry optimization of base pairs (QM-19)

1. Calculate an optimal geometry of adenine using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the 5-th member ring

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

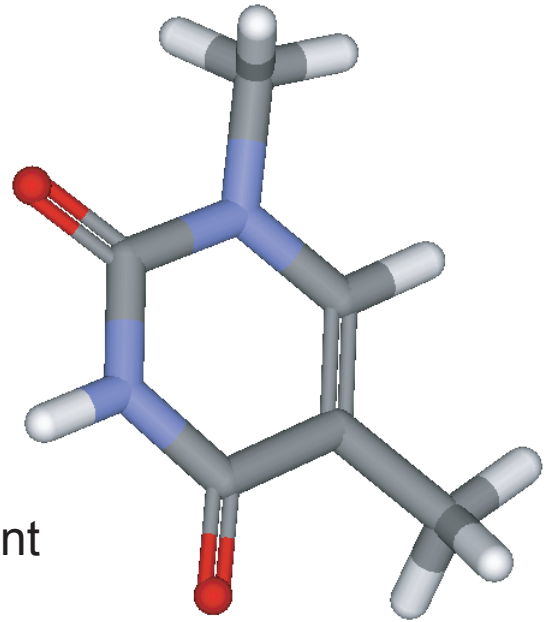
QM geometry optimization of base pairs (QM-20)

1. Calculate an optimal geometry of thymine (protonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

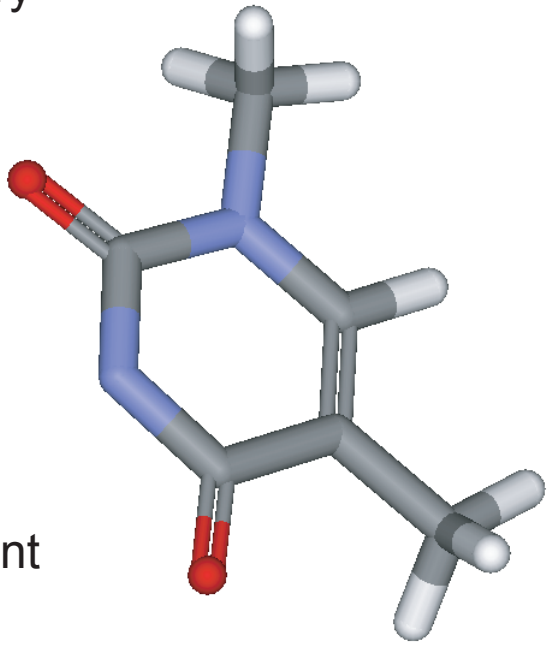
QM geometry optimization of base pairs (QM-21)

1. Calculate an optimal geometry of thymine (deprotonated) using the B3LYP/6-31+G* level of theory

2. Report in a table atomic charges of all atoms

3. Report in a table interatomic distances and angles between bonds of the ring

4. Report in a figure a value and an orientation of a molecular dipole moment



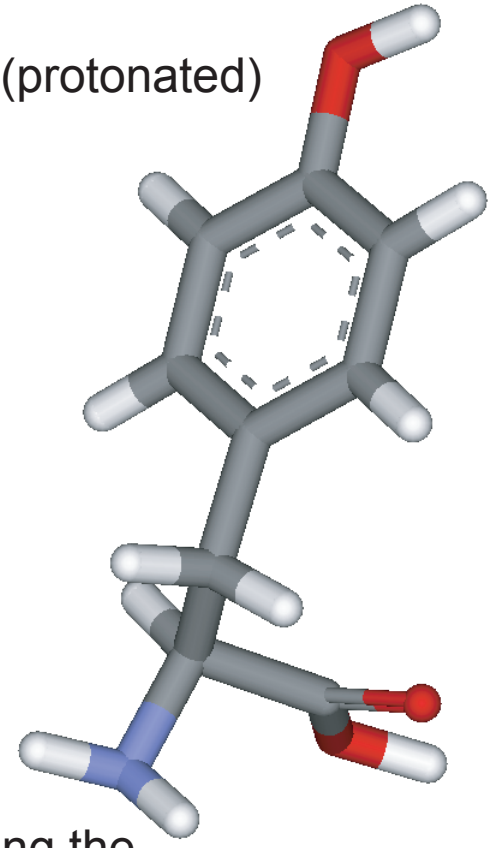
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of amino acids (QM-22)

1. Calculate an optimal geometry of tyrosine (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the electrostatic potential around the molecule

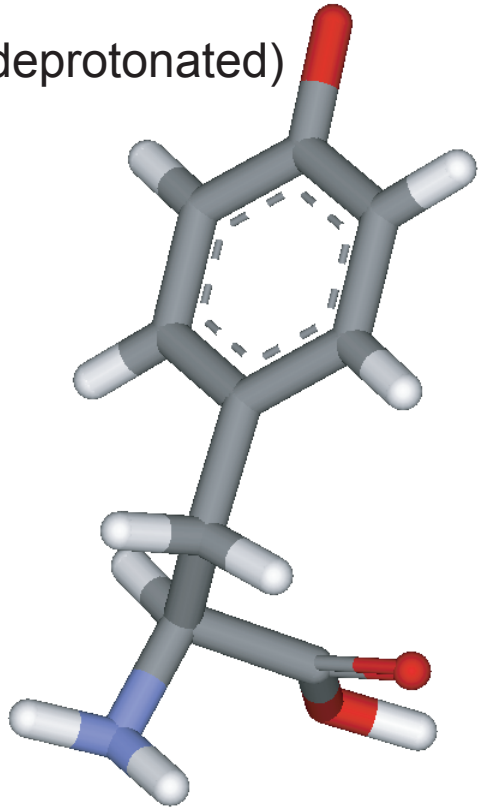
3. Report in a figure the electrostatic potential in the plane of the side chain



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of amino acids (QM-23)

1. Calculate an optimal geometry of tyrisone (deprotonated) using the B3LYP/6-31+G* level of theory



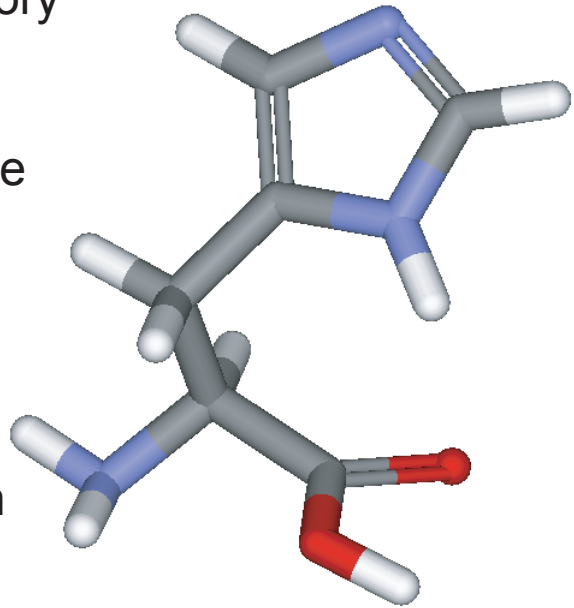
2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the side chain

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of amino acids (QM-24)

1. Calculate an optimal geometry of histidine (delta) using the B3LYP/6-31+G* level of theory



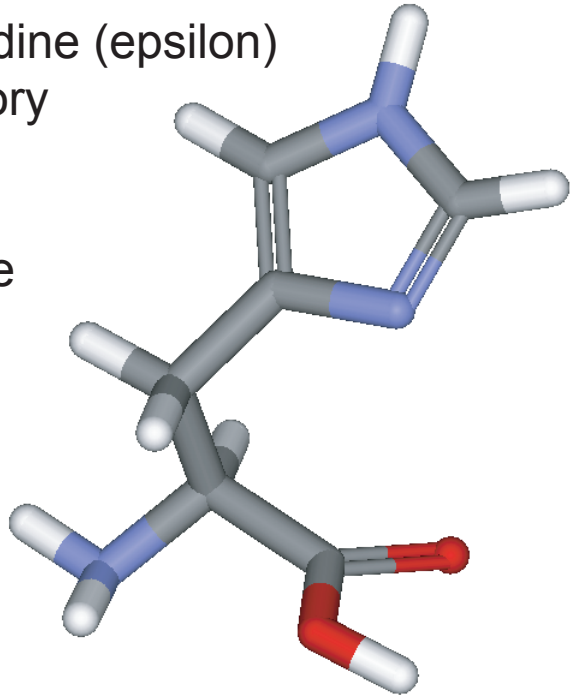
2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the side chain

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of amino acids (QM-25)

1. Calculate an optimal geometry of histidine (epsilon) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the side chain

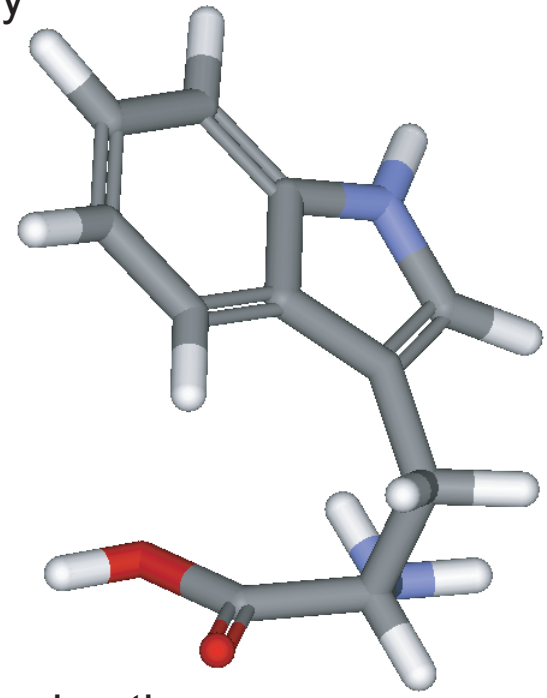
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of amino acids (QM-26)

1. Calculate an optimal geometry of triptophan (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the electrostatic potential around the molecule

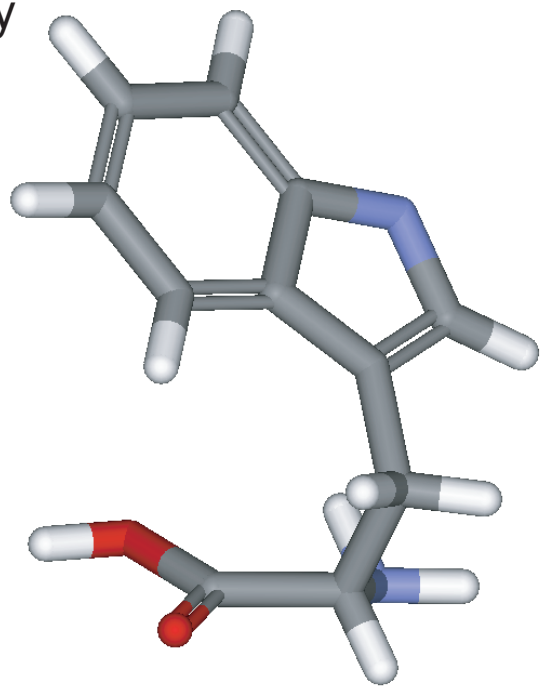
3. Report in a figure the electrostatic potential in the plane of the side chain



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of amino acids (QM-27)

1. Calculate an optimal geometry of triptophan (deprotonated) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the side chain

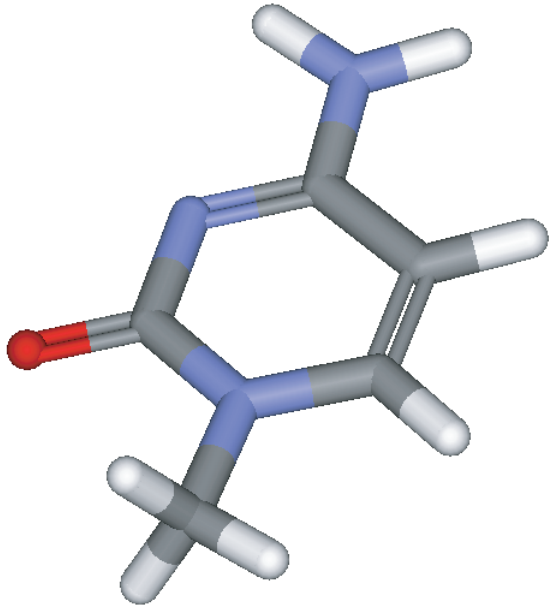
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of base pairs (QM-28)

1. Calculate an optimal geometry of cytosine using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the electrostatic potential around the molecule

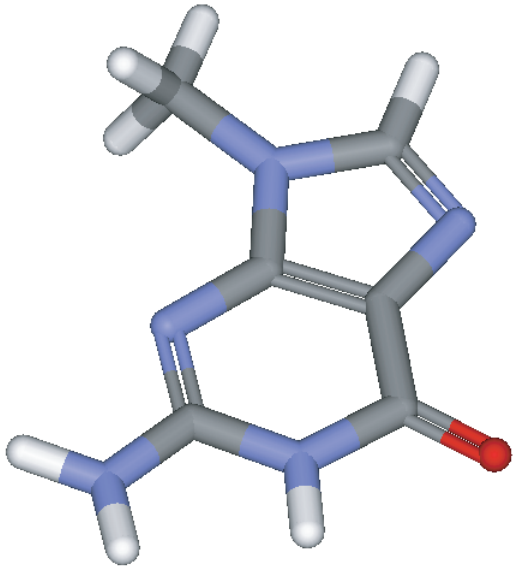
3. Report in a figure the electrostatic potential in the plane of the molecule



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of base pairs (QM-29)

1. Calculate an optimal geometry of guanine (protonated) using the B3LYP/6-31+G* level of theory



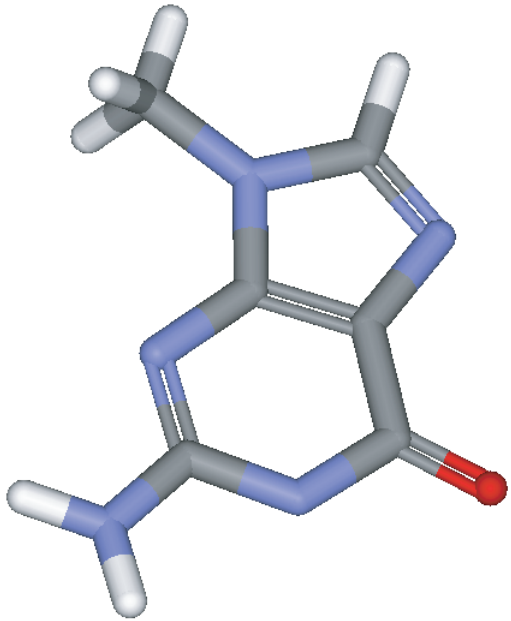
2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the molecule

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of base pairs (QM-30)

1. Calculate an optimal geometry of guanine (deprotonated) using the B3LYP/6-31+G* level of theory



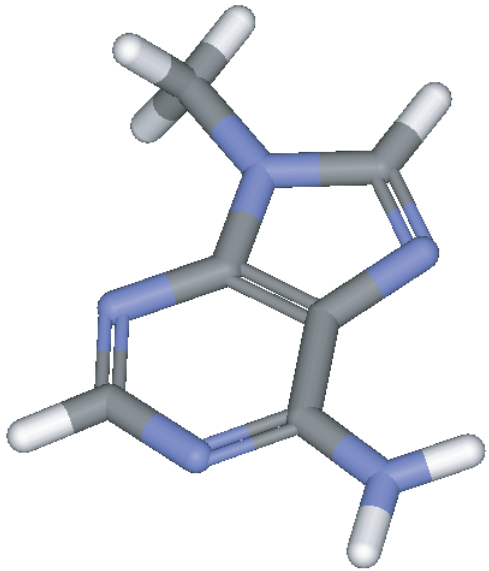
2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the molecule

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of base pairs (QM-31)

1. Calculate an optimal geometry of adenine using the B3LYP/6-31+G* level of theory



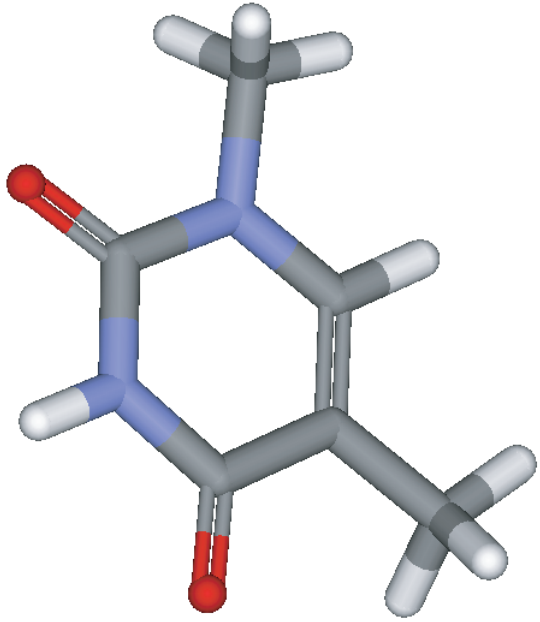
2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the molecule

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of base pairs (QM-32)

1. Calculate an optimal geometry of thymine (protonated) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the molecule

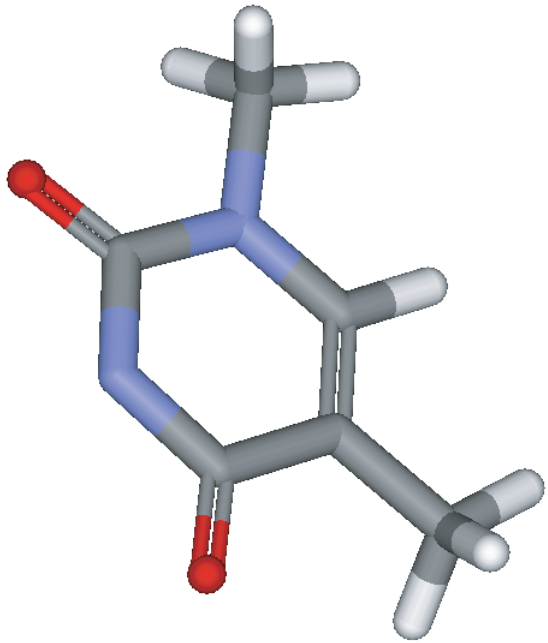
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of base pairs (QM-33)

1. Calculate an optimal geometry of thymine (deprotonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the molecule



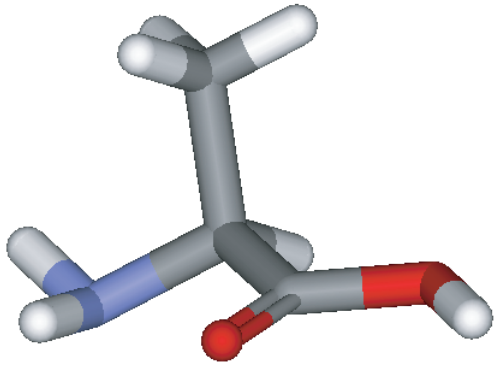
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-34)

1. Calculate an optimal geometry of alanine using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving atoms of the methyl side chain

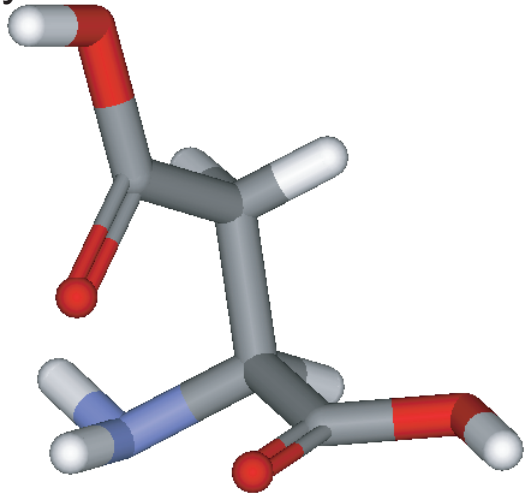


4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the methyl side chain

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-35)

1. Calculate an optimal geometry of aspartic acid (protonated) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the molecular vibrations

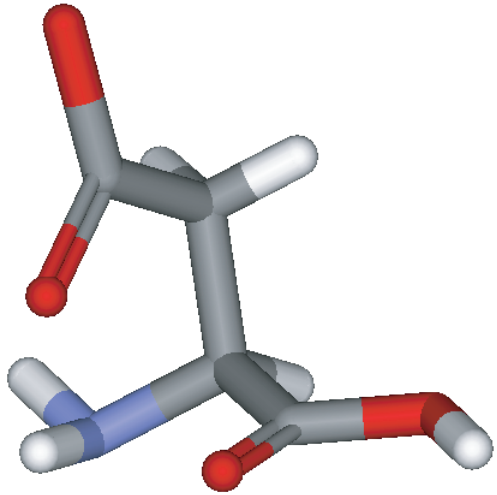
3. Report in a table frequencies and IR intensities of vibrations involving atoms of the side chain

4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-36)

1. Calculate an optimal geometry of aspartic acid (deprotonated) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving atoms of the side chain

4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

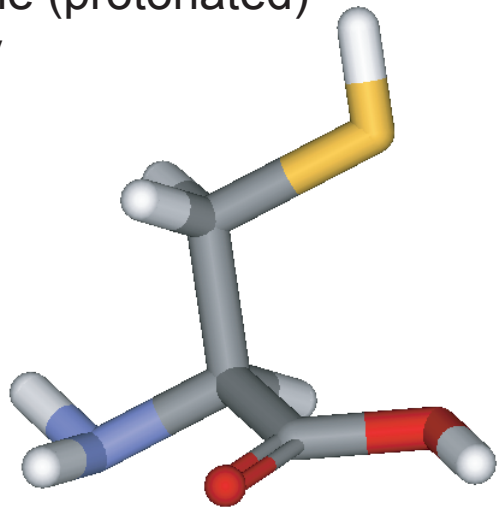
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-37)

1. Calculate an optimal geometry of cysteine (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving atoms of the side chain



4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

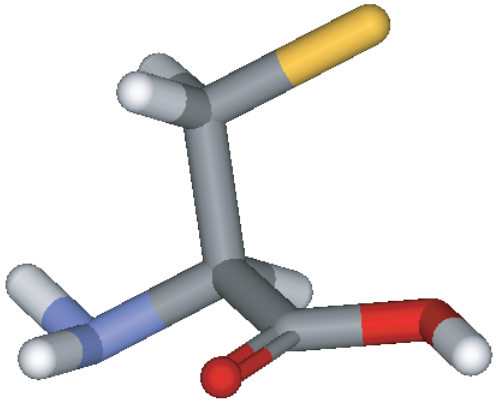
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-38)

1. Calculate an optimal geometry of cysteine (deprotonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving atoms of the side chain



4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

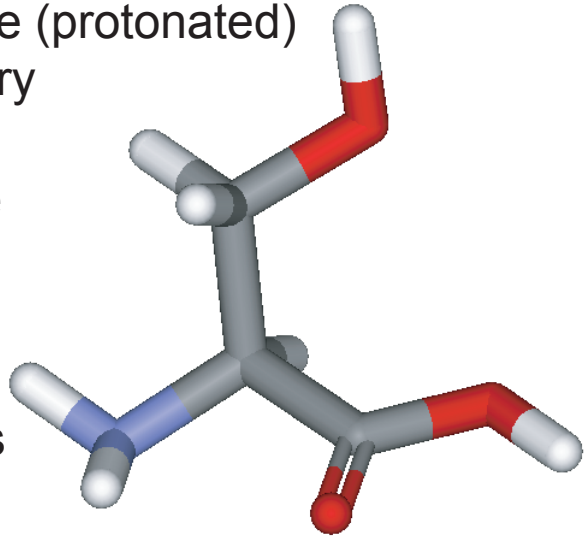
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-39)

1. Calculate an optimal geometry of serine (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving atoms of the side chain



4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

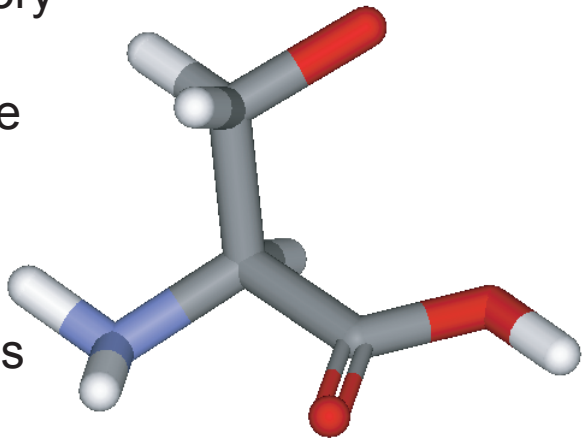
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-40)

1. Calculate an optimal geometry of serine (deprotonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

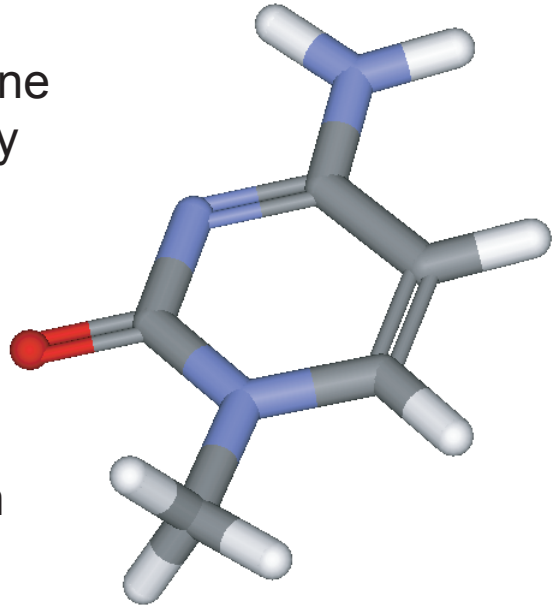
3. Report in a table frequencies and IR intensities of vibrations involving atoms of the side chain



4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of base pairs (QM-41)



1. Calculate an optimal geometry of cytosine using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving carbon atoms of the six-memeber ring

4. Report in a figure the theoretical IR spectrum of vibrations involving carbon atoms of the six-memeber ring

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of base pairs (QM-42)

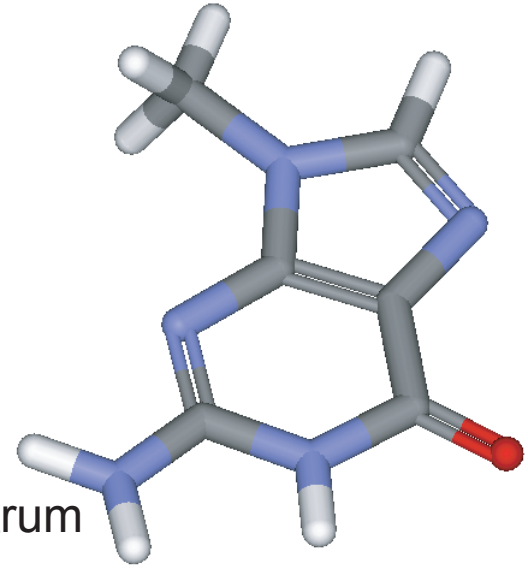
1. Calculate an optimal geometry of guanine (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving carbon atoms of the six-memeber ring

4. Report in a figure the theoretical IR spectrum of vibrations involving carbon atoms of the six-memeber ring

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



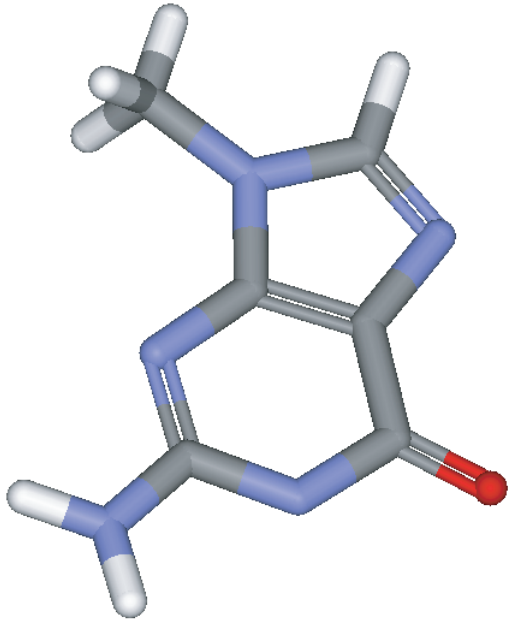
QM molecular vibrations of base pairs (QM-43)

1. Calculate an optimal geometry of guanine (deprotonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving carbon atoms of the six-memeber ring

4. Report in a figure the theoretical IR spectrum of vibrations involving carbon atoms of the six-memeber ring



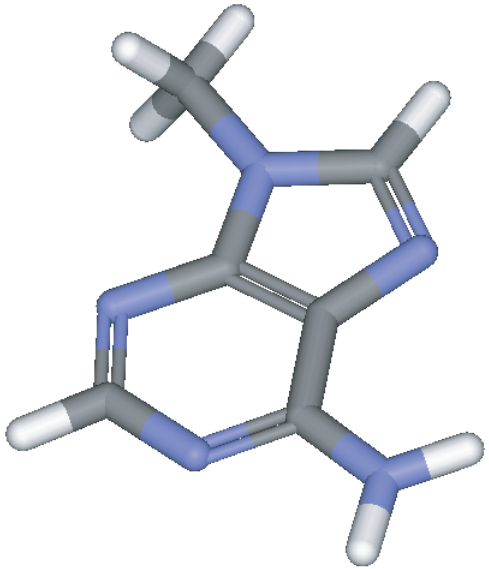
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of base pairs (QM-44)

1. Calculate an optimal geometry of adenine using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving carbon atoms of the six-memeber ring

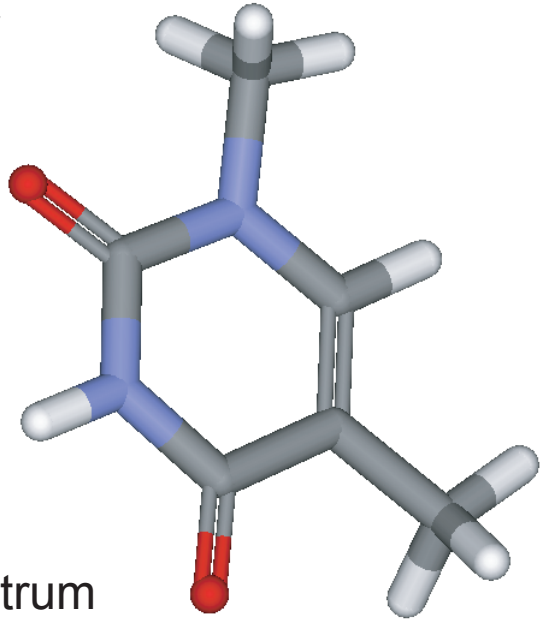


4. Report in a figure the theoretical IR spectrum of vibrations involving carbon atoms of the six-memeber ring

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of base pairs (QM-45)

1. Calculate an optimal geometry of thymine (protonated) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving carbon atoms of the six-memeber ring

4. Report in a figure the theoretical IR spectrum of vibrations involving carbon atoms of the six-memeber ring

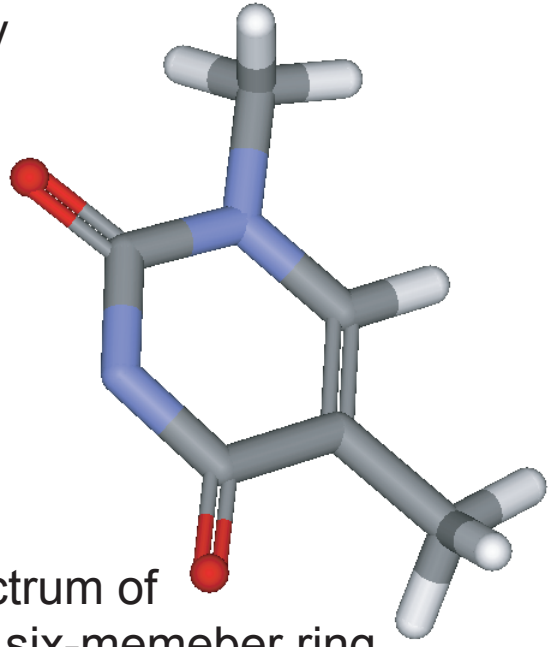
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of base pairs (QM-46)

1. Calculate an optimal geometry of thymine (deprotonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations

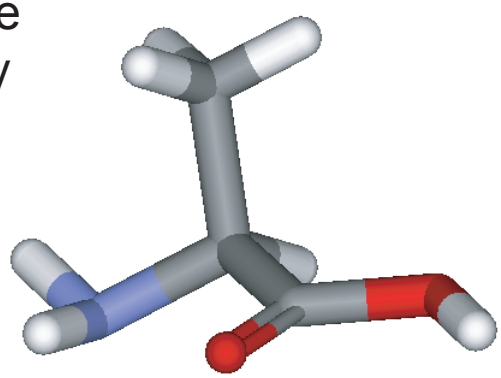
3. Report in a table frequencies and IR intensities of vibrations involving carbon atoms of the six-memeber ring



4. Report in a figure the theoretical IR spectrum of vibrations involving carbon atoms of the six-memeber ring

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

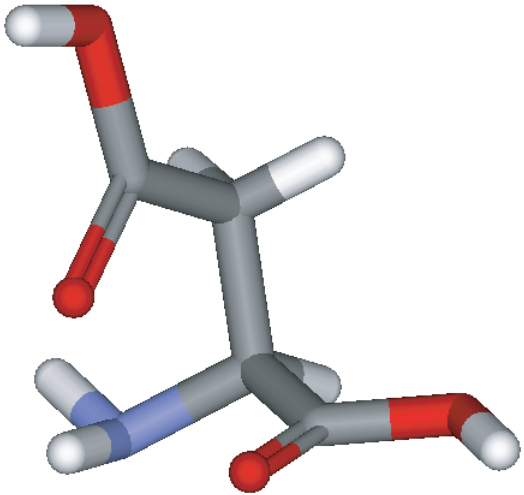
QM molecular vibrations of amino acids (QM-47)



1. Calculate an optimal geometry of alanine using the B3LYP/6-31+G* level of theory
2. For the optimal geometry, calculate the molecular vibrations and anharmonic frequencies
3. Report in a table harmonic frequencies, anharmonic frequencies, and IR intensities of vibrations involving atoms of the methyl side chain
4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the methyl side chain
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-48)

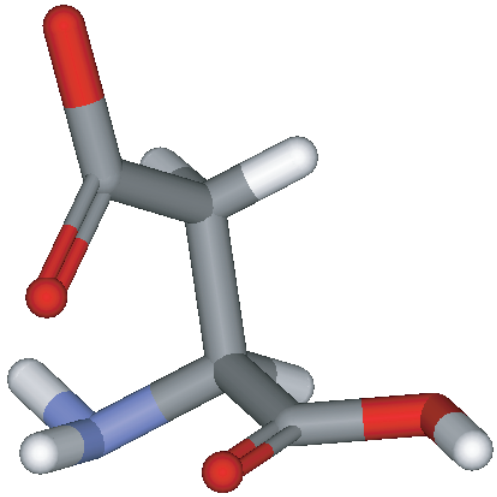
1. Calculate an optimal geometry of aspartic acid (protonated) using the B3LYP/6-31+G* level of theory
2. For the optimal geometry, calculate the molecular vibrations and anharmonic frequencies
3. Report in a table harmonic frequencies, anharmonic frequencies, and IR intensities of vibrations involving atoms of the side chain



4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-49)

1. Calculate an optimal geometry of aspartic acid (deprotonated) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the molecular vibrations and anharmonic frequencies

3. Report in a table harmonic frequencies, anharmonic frequencies, and IR intensities of vibrations involving atoms of the side chain

4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

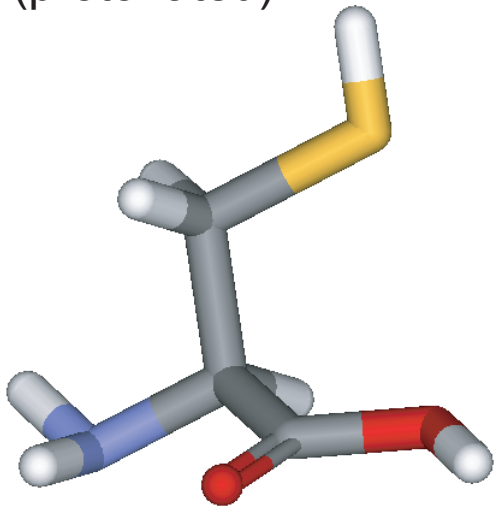
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-50)

1. Calculate an optimal geometry of cysteine (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations and anharmonic frequencies

3. Report in a table harmonic frequencies, anharmonic frequencies, and IR intensities of vibrations involving atoms of the side chain



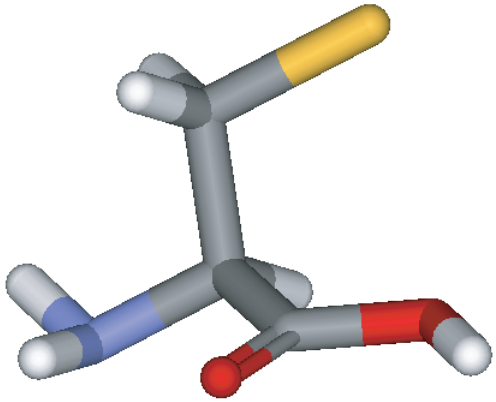
4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-51)

1. Calculate an optimal geometry of cysteine (deprotonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the molecular vibrations and anharmonic frequencies

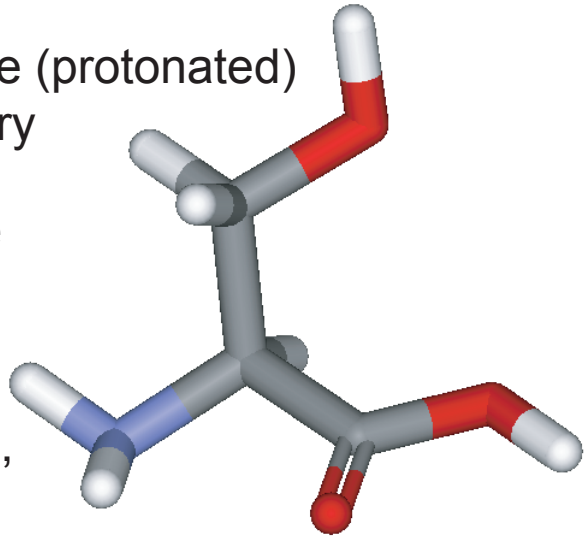


3. Report in a table harmonic frequencies, anharmonic frequencies, and IR intensities of vibrations involving atoms of the side chain

4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

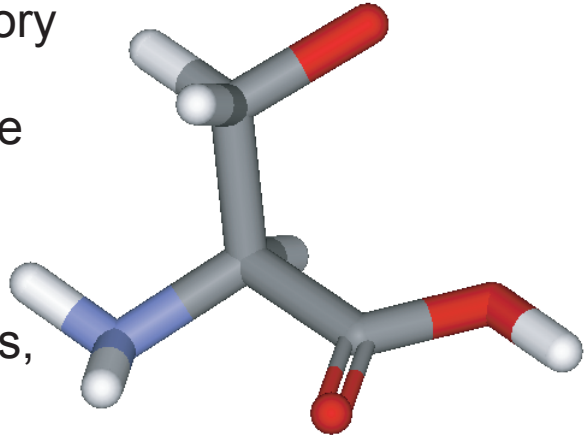
QM molecular vibrations of amino acids (QM-52)



1. Calculate an optimal geometry of serine (protonated) using the B3LYP/6-31+G* level of theory
2. For the optimal geometry, calculate the molecular vibrations and anharmonic frequencies
3. Report in a table harmonic frequencies, anharmonic frequencies, and IR intensities of vibrations involving atoms of the side chain
4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of amino acids (QM-53)

1. Calculate an optimal geometry of serine (deprotonated) using the B3LYP/6-31+G* level of theory



2. For the optimal geometry, calculate the molecular vibrations and anharmonic frequencies

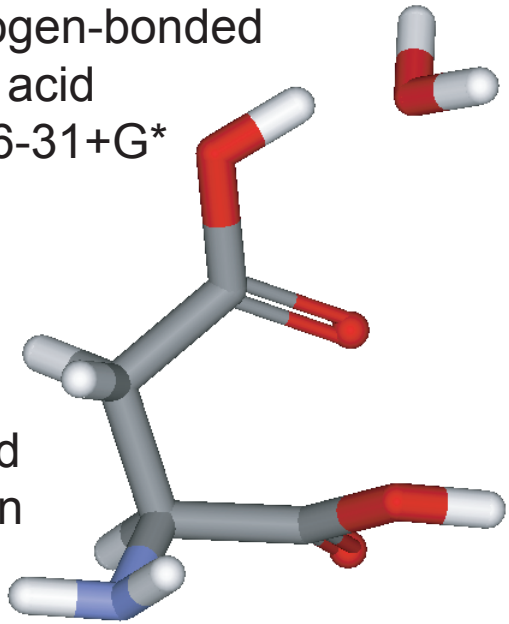
3. Report in a table harmonic frequencies, anharmonic frequencies, and IR intensities of vibrations involving atoms of the side chain

4. Report in a figure the theoretical IR spectrum of vibrations involving atoms of the side chain

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-54)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of aspartic acid (protonated) and water, using the B3LYP/6-31+G* level of theory



2. Report in a table hydrogen bond energies of all calculated dimers

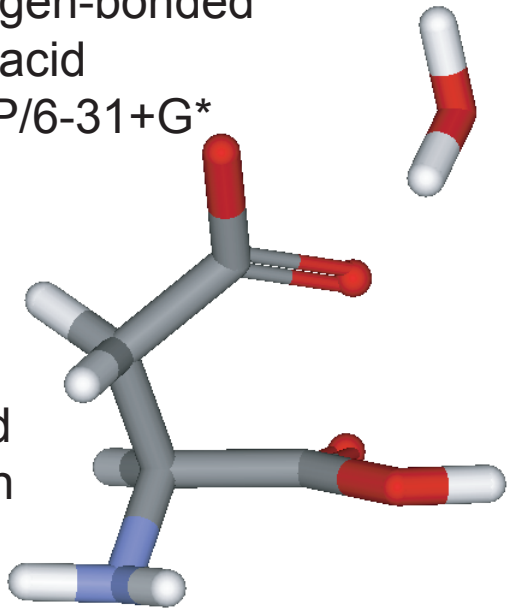
3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-55)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of aspartic acid (deprotonated) and water, using the B3LYP/6-31+G* level of theory



2. Report in a table hydrogen bond energies of all calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

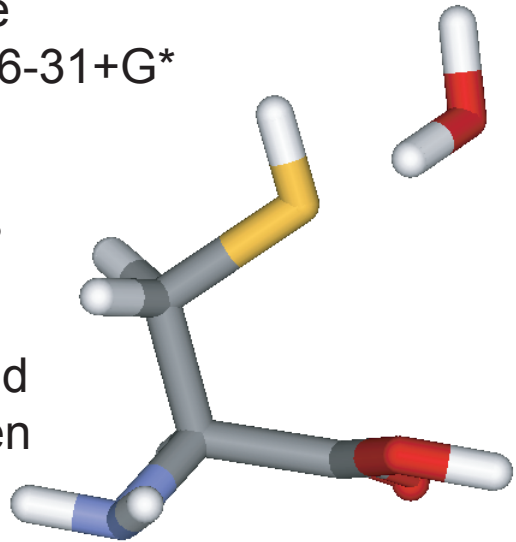
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-56)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of cysteine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of all calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

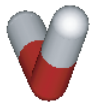


4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

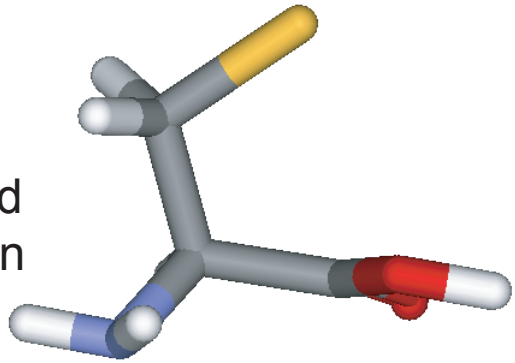
QM geometry optimization of hydrogen bonds (QM-57)

1. Calculate an optimal geometry of a hydrogen-bonded dimer between the side chain of cysteine (deprotonated) and water, using the B3LYP/6-31+G* level of theory



2. Report in a table hydrogen bond energy of a calculated dimer

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

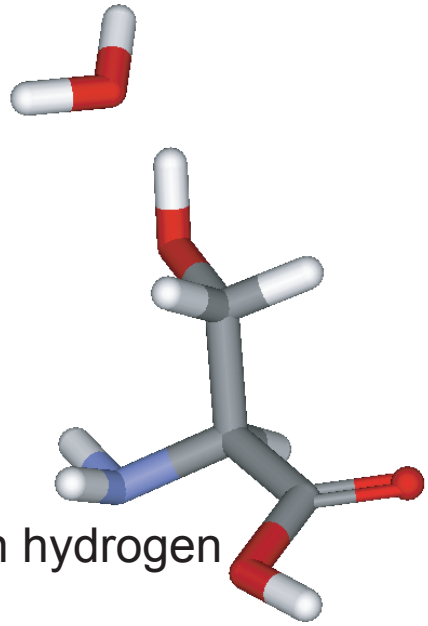


4. Report in a table charges of atoms involved in hydrogen bonds for a dimer and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-58)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of serine (protonated) and water, using the B3LYP/6-31+G* level of theory



2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

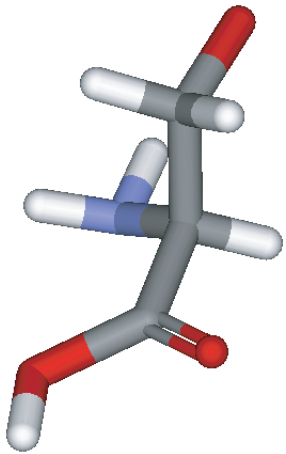
4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-59)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of serine (deprotonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers



3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

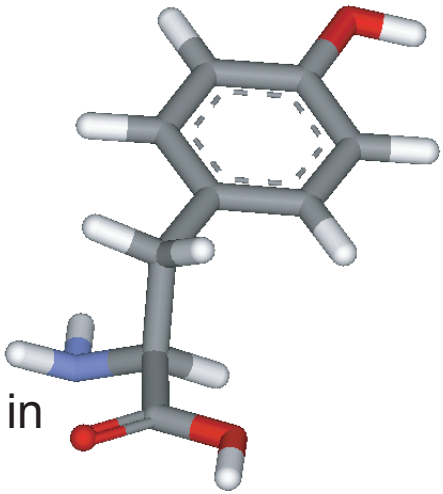
4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-60)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of tyrosine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers



3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-61)

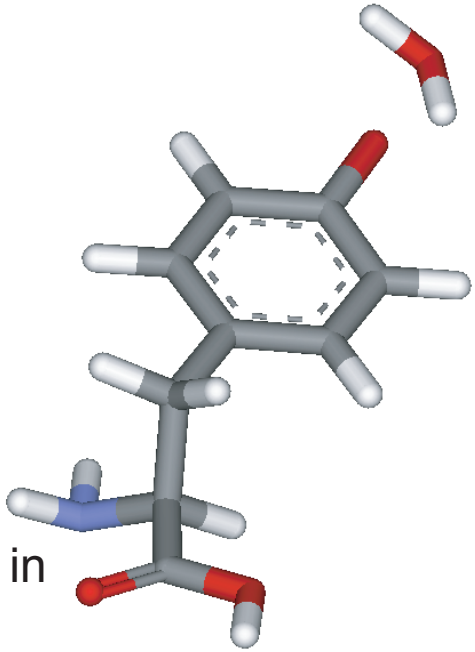
1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of tyrosine (deprotonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

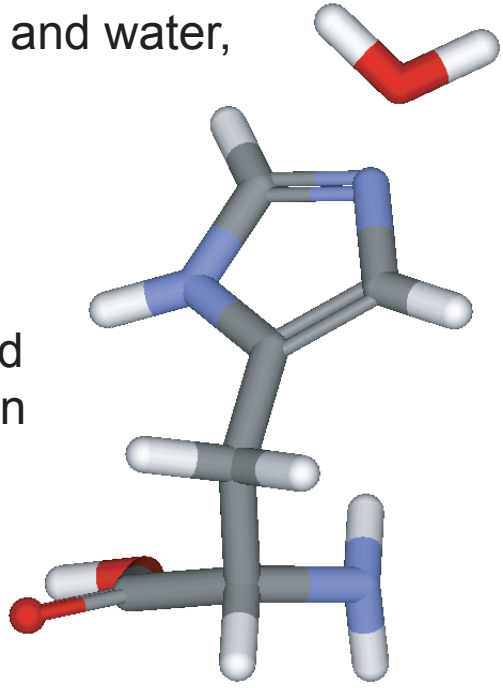
4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM geometry optimization of hydrogen bonds (QM-62)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of histidine (delta) and water, using the B3LYP/6-31+G* level of theory



2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

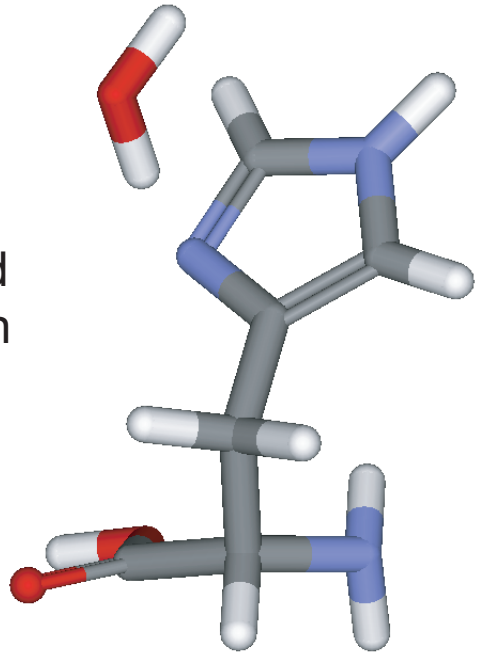
QM geometry optimization of hydrogen bonds (QM-63)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of histidine (epsilon) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM geometry optimization of hydrogen bonds (QM-64)

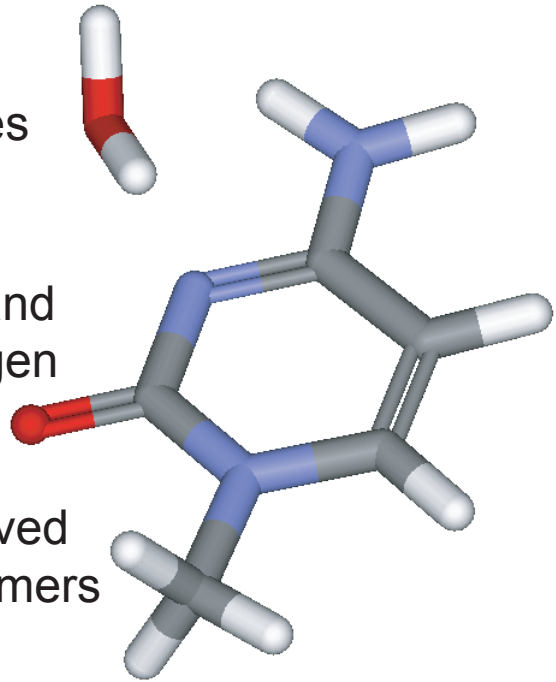
1. Calculate an optimal geometry of hydrogen-bonded dimers between cytosine and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM geometry optimization of hydrogen bonds (QM-65)

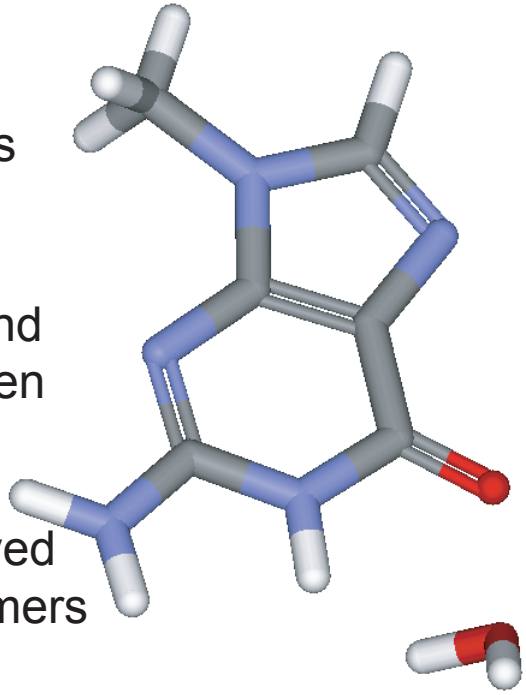
1. Calculate an optimal geometry of hydrogen-bonded dimers between guanine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM geometry optimization of hydrogen bonds (QM-66)

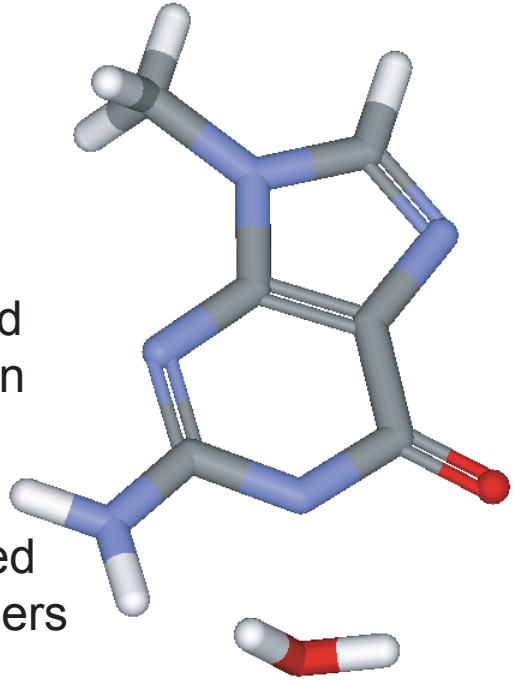
1. Calculate an optimal geometry of hydrogen-bonded dimers between guanine (deprotonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM geometry optimization of hydrogen bonds (QM-67)

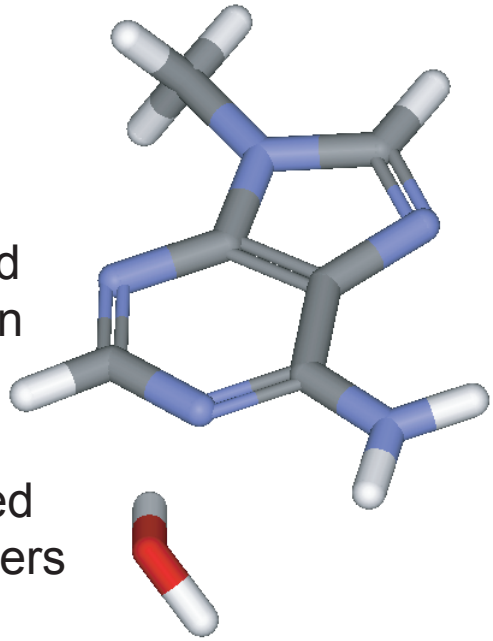
1. Calculate an optimal geometry of hydrogen-bonded dimers between adenine and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



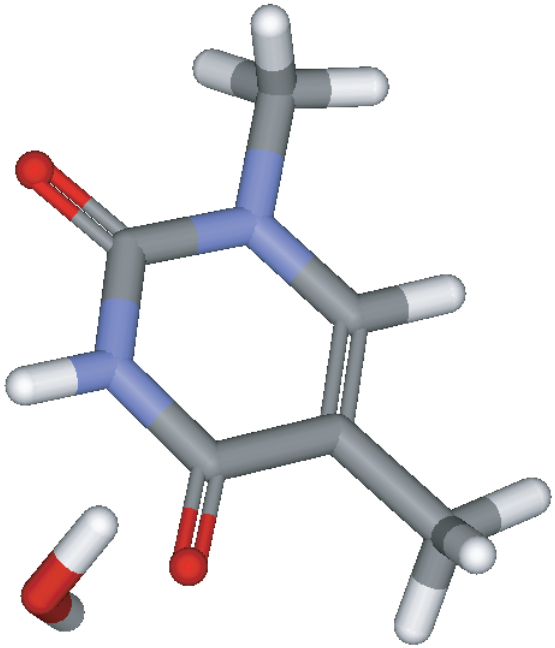
QM geometry optimization of hydrogen bonds (QM-68)

1. Calculate an optimal geometry of hydrogen-bonded dimers between thymine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

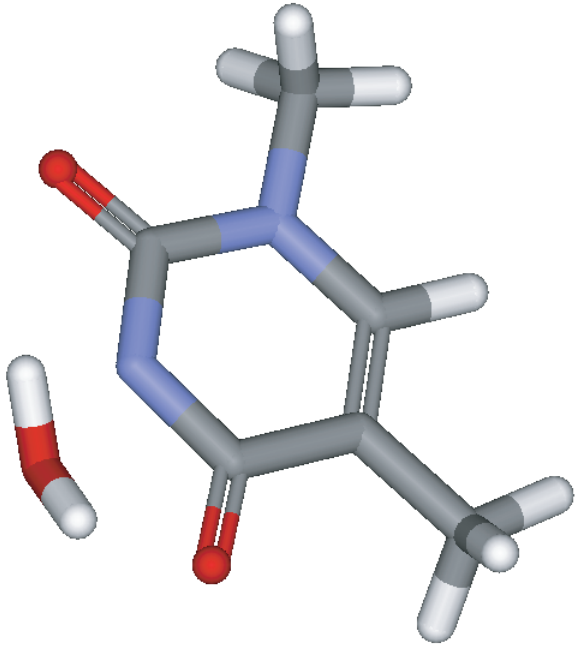
QM geometry optimization of hydrogen bonds (QM-69)

1. Calculate an optimal geometry of hydrogen-bonded dimers between thymine (deprotonated) and water, using the B3LYP/6-31+G* level of theory

2. Report in a table hydrogen bond energies of calculated dimers

3. Report in a table interatomic distances and bond angles of atoms involved in hydrogen bonds

4. Report in a table charges of atoms involved in hydrogen bonds for dimers and monomers



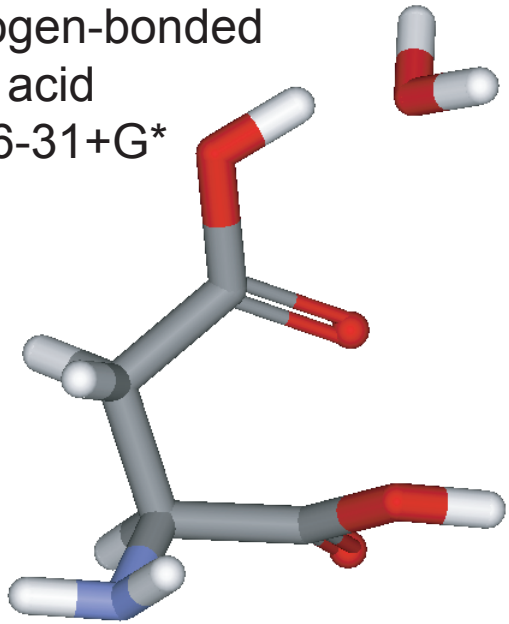
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-71)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of aspartic acid (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

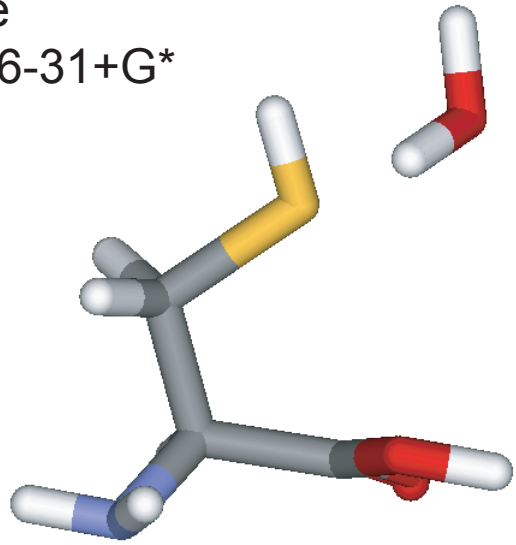
3. Report in a figure the electrostatic potential in the plane of the hydrogen bond



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-72)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of cysteine (protonated) and water, using the B3LYP/6-31+G* level of theory



2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

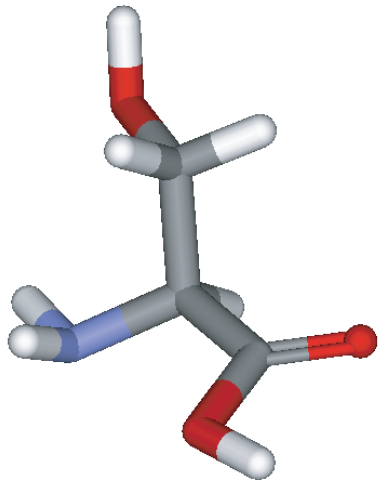
3. Report in a figure the electrostatic potential in the plane of the hydrogen bond

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-73)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of serine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule



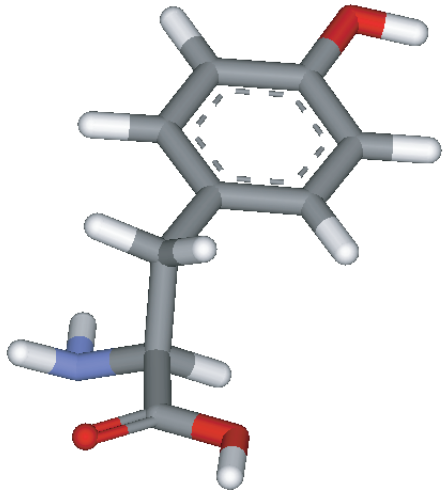
3. Report in a figure the electrostatic potential in the plane of the hydrogen bond

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-74)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of tyrosine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

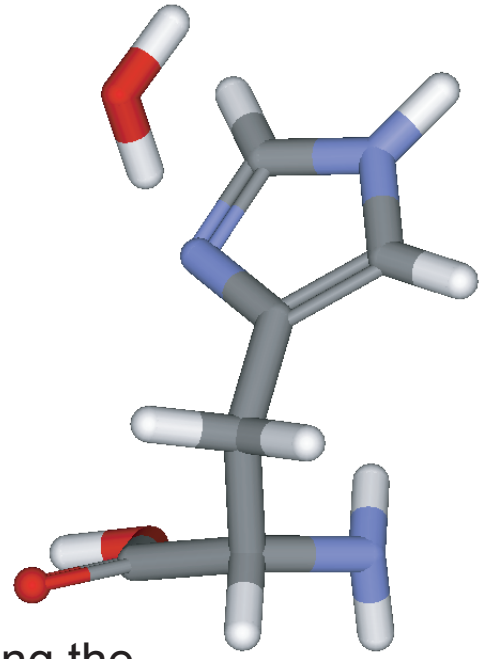


3. Report in a figure the electrostatic potential in the plane of the hydrogen bond

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-75)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of histidine (epsilon) and water, using the B3LYP/6-31+G* level of theory



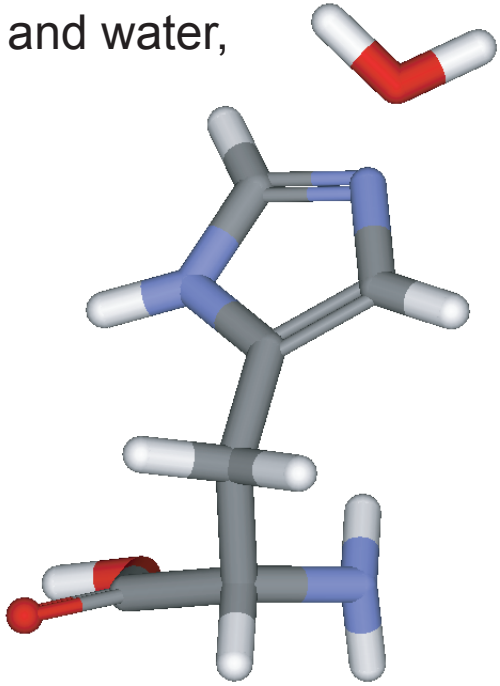
2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the hydrogen bond

4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-76)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of histidine (delta) and water, using the B3LYP/6-31+G* level of theory



2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the hydrogen bond

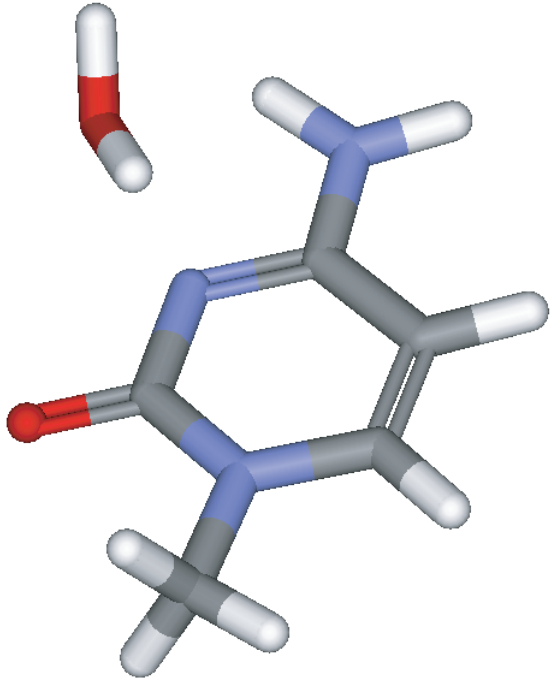
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-77)

1. Calculate an optimal geometry of hydrogen-bonded dimers between cytosine and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

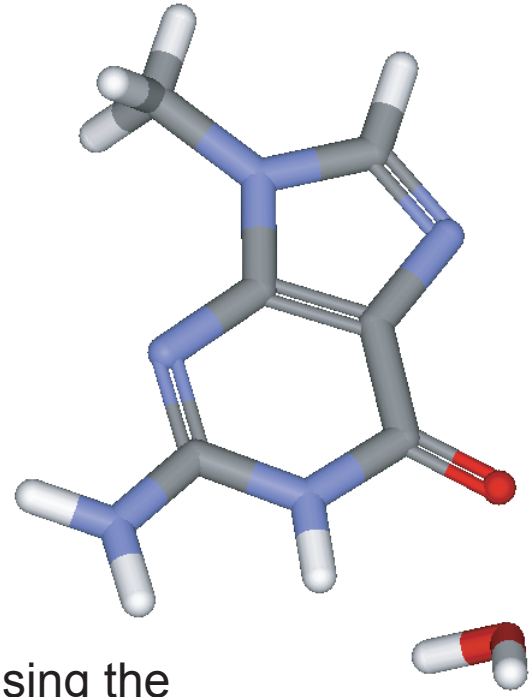
3. Report in a figure the electrostatic potential in the plane of the hydrogen bond



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-79)

1. Calculate an optimal geometry of hydrogen-bonded dimers between guanine (protonated) and water, using the B3LYP/6-31+G* level of theory



2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the hydrogen bond

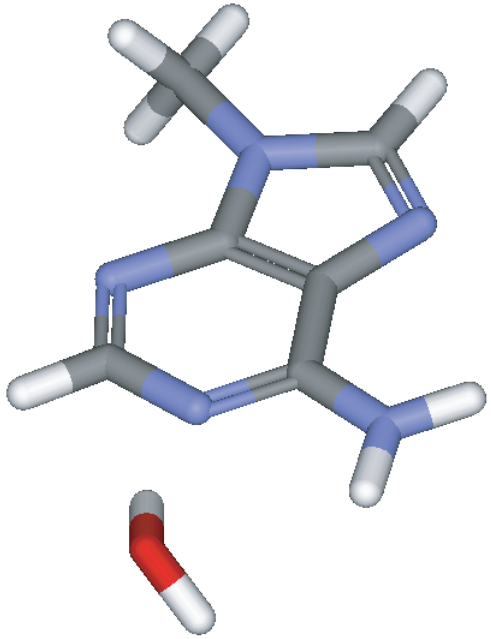
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-80)

1. Calculate an optimal geometry of hydrogen-bonded dimers between adenine and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

3. Report in a figure the electrostatic potential in the plane of the hydrogen bond



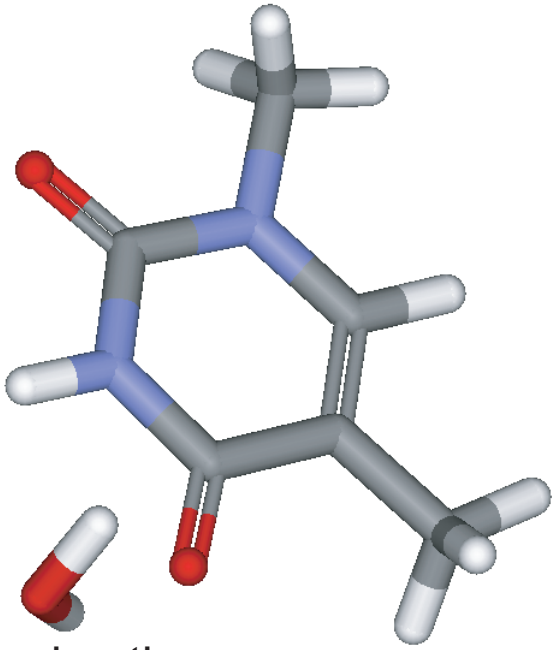
4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM electrostatic potential of hydrogen bonds (QM-81)

1. Calculate an optimal geometry of hydrogen-bonded dimers between thymine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the most stable dimer, calculate the electrostatic potential around the molecule

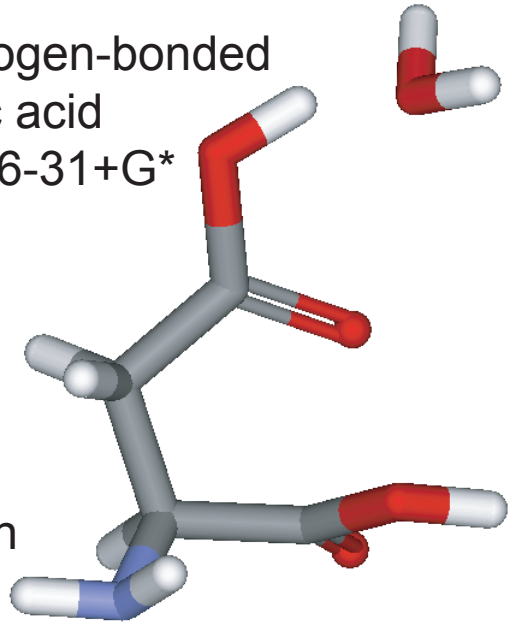
3. Report in a figure the electrostatic potential in the plane of the hydrogen bond



4. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of hydrogen bonds (QM-82)

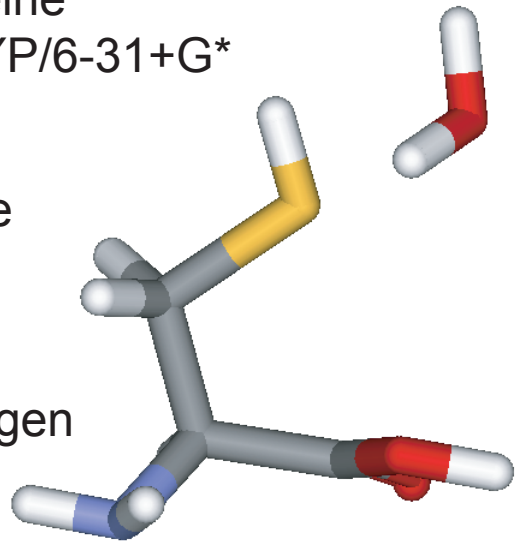
1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of aspartic acid (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the most stable dimer, calculate the molecular vibrations
3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms



4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of hydrogen bonds (QM-83)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of cysteine (protonated) and water, using the B3LYP/6-31+G* level of theory



2. For the most stable dimer, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

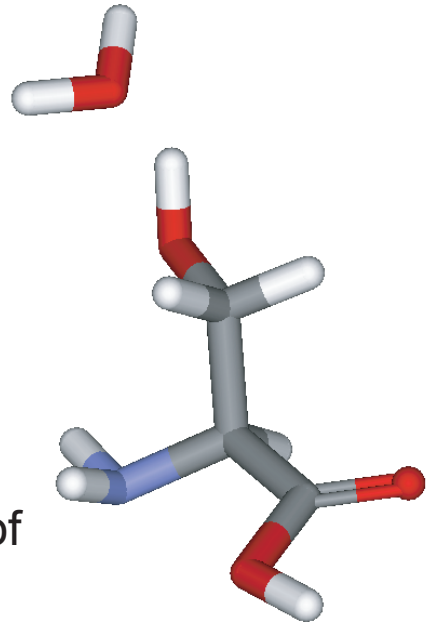
QM molecular vibrations of hydrogen bonds (QM-84)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of serine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the most stable dimer, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms

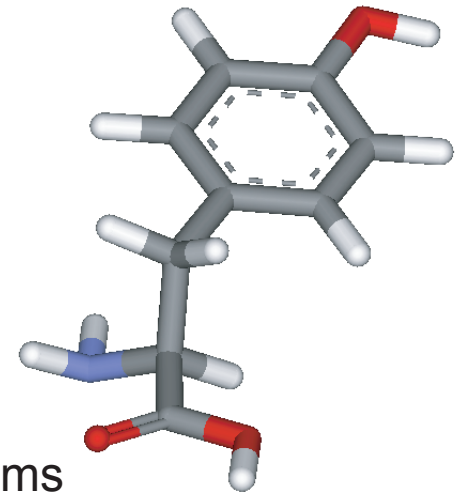


5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of hydrogen bonds (QM-85)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of tyrosine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the most stable dimer, calculate the molecular vibrations



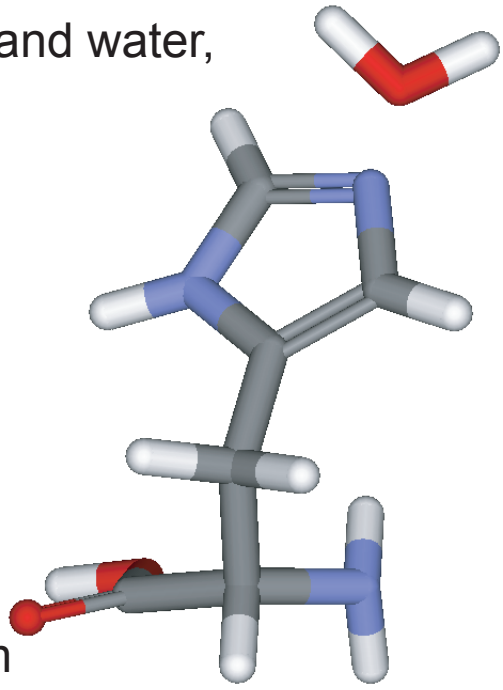
3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of hydrogen bonds (QM-86)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of histidine (delta) and water, using the B3LYP/6-31+G* level of theory



2. For the most stable dimer, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

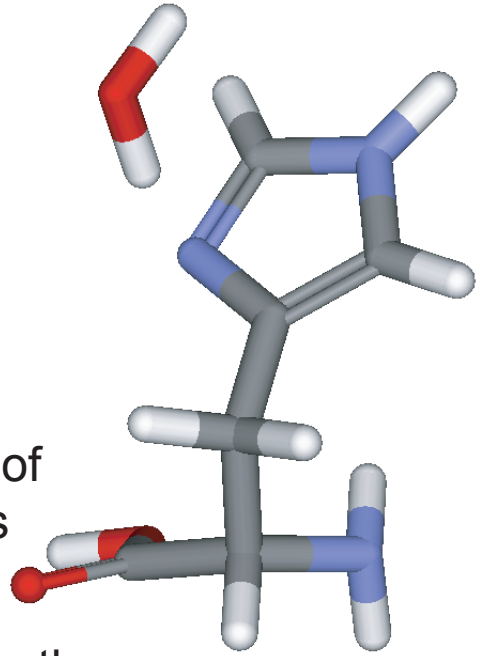
QM molecular vibrations of hydrogen bonds (QM-87)

1. Calculate an optimal geometry of hydrogen-bonded dimers between the side chain of histidine (epsilon) and water, using the B3LYP/6-31+G* level of theory

2. For the most stable dimer, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

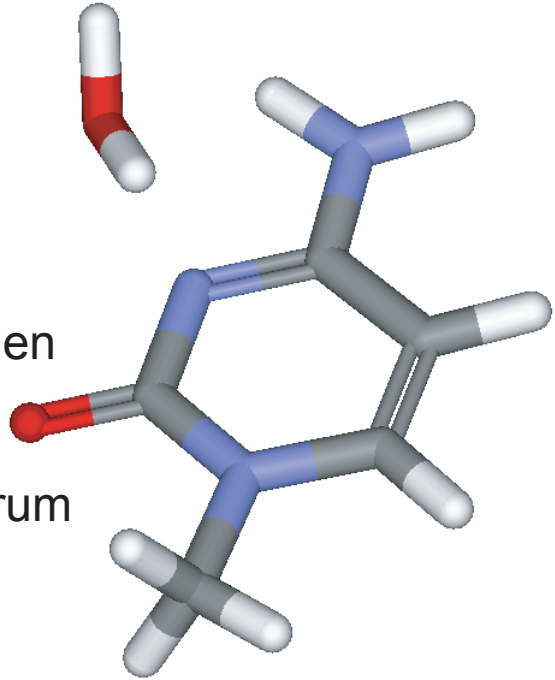
QM molecular vibrations of hydrogen bonds (QM-88)

1. Calculate an optimal geometry of hydrogen-bonded dimers between cytosine and water, using the B3LYP/6-31+G* level of theory

2. For the most stable dimer, calculate the molecular vibrations

3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

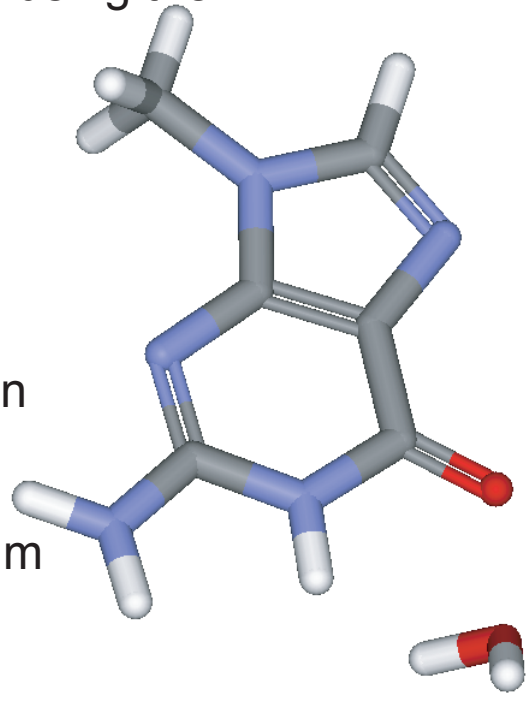
4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of hydrogen bonds (QM-89)

1. Calculate an optimal geometry of hydrogen-bonded dimers between guanine (protonated) and water, using the B3LYP/6-31+G* level of theory



2. For the most stable dimer, calculate the molecular vibrations

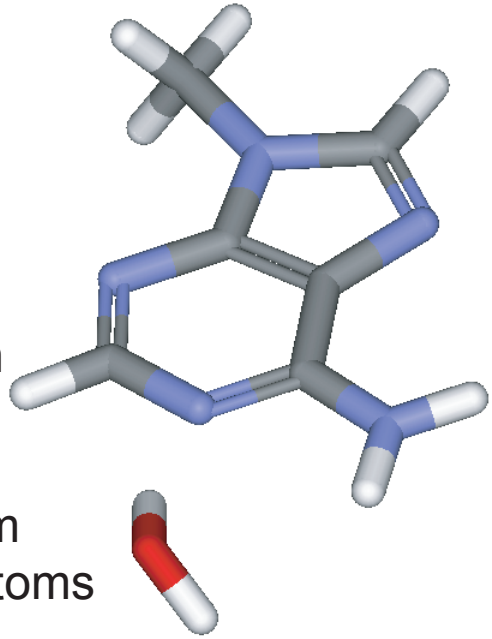
3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM molecular vibrations of hydrogen bonds (QM-90)

1. Calculate an optimal geometry of hydrogen-bonded dimers between adenine and water, using the B3LYP/6-31+G* level of theory



2. For the most stable dimer, calculate the molecular vibrations

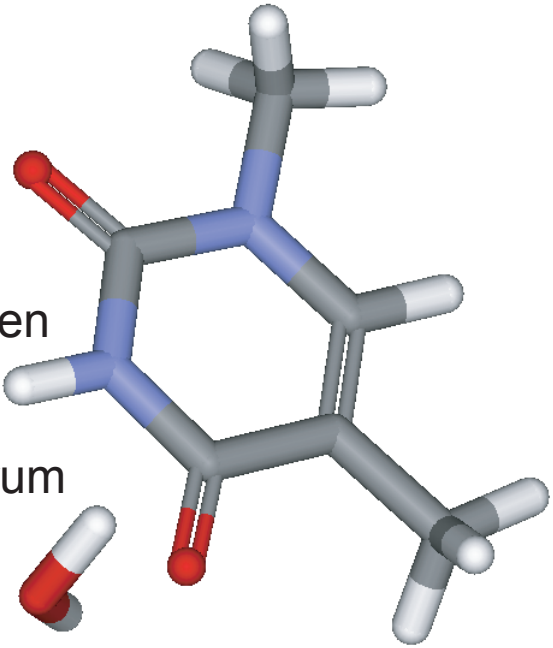
3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms

4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

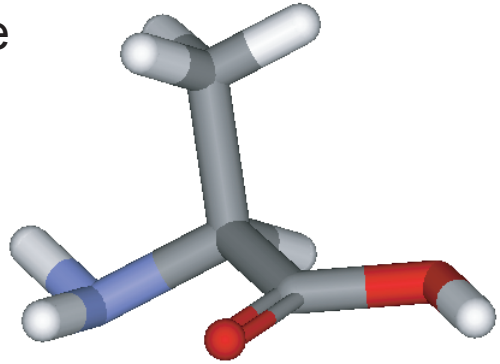
QM molecular vibrations of hydrogen bonds (QM-91)

1. Calculate an optimal geometry of hydrogen-bonded dimers between thymine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the most stable dimer, calculate the molecular vibrations
3. Report in a table frequencies and IR intensities of vibrations involving hydrogen bonded atoms
4. Report in a figure a theoretical IR spectrum of vibrations involving hydrogen bonded atoms



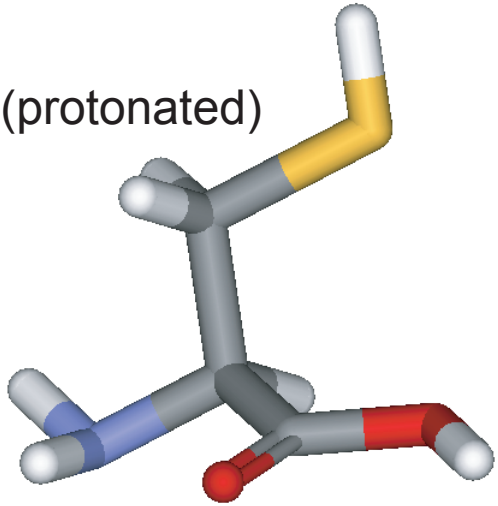
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM calculations of internal rotations (QM-92)



1. Calculate an optimal geometry of alanine using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the CH3- internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion angle
4. Report in a figure the potential energy surface of the CH3- internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM calculations of internal rotation (QM-93)



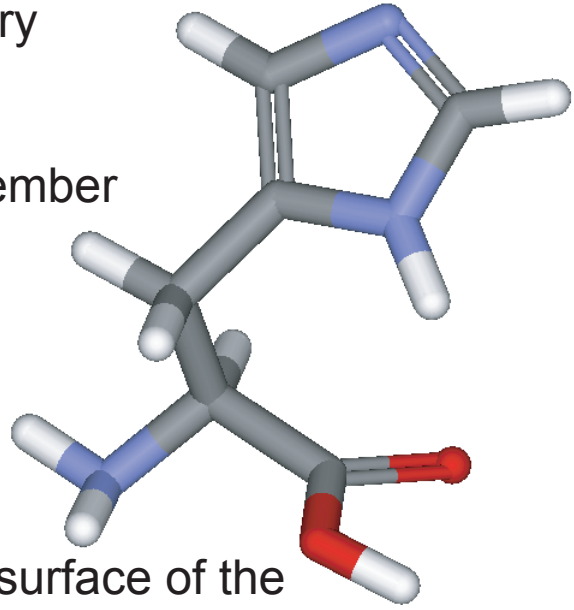
1. Calculate an optimal geometry of cysteine (protonated) using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the CH2SH- internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion
4. Report in a figure the potential energy surface of the CH2SH- internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM calculations of internal rotation (QM-94)

1. Calculate an optimal geometry of histidine (delat) using the B3LYP/6-31+G* level of theory

2. Calculated an optimal geometry for a constrained torsion angle of the 5th member ring internal rotation

3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion

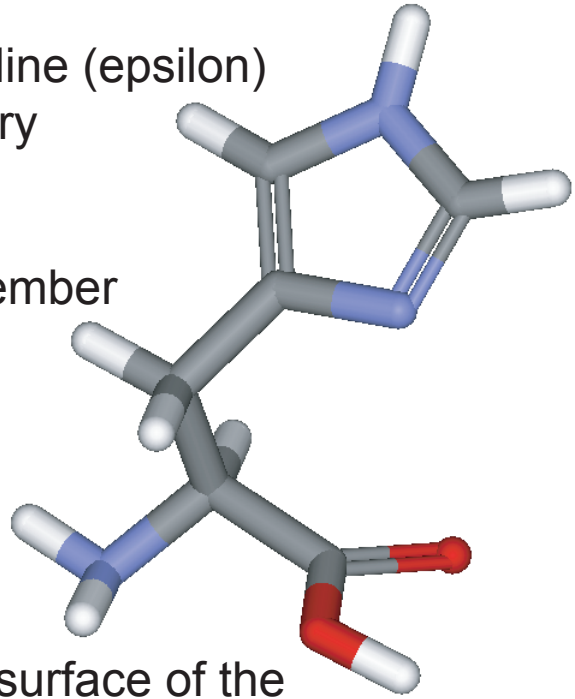


4. Report in a figure the potential energy surface of the ring internal rotation

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM calculations of internal rotation (QM-95)

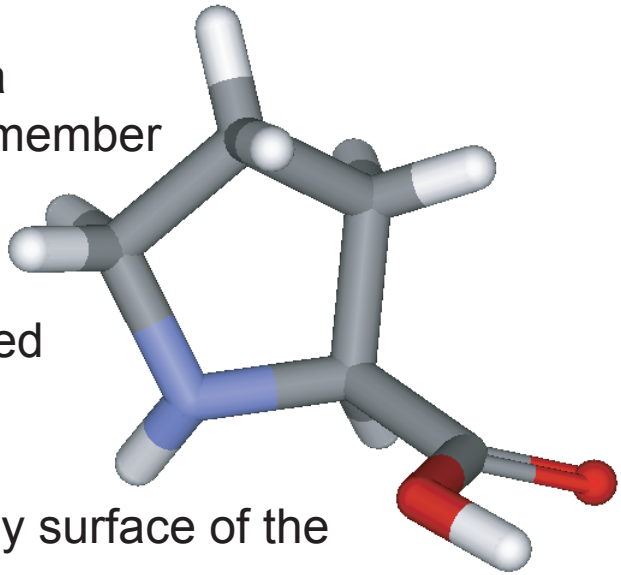
1. Calculate an optimal geometry of histidine (epsilon) using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the 5th member ring internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion



4. Report in a figure the potential energy surface of the ring internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM calculations of internal rotation (QM-96)

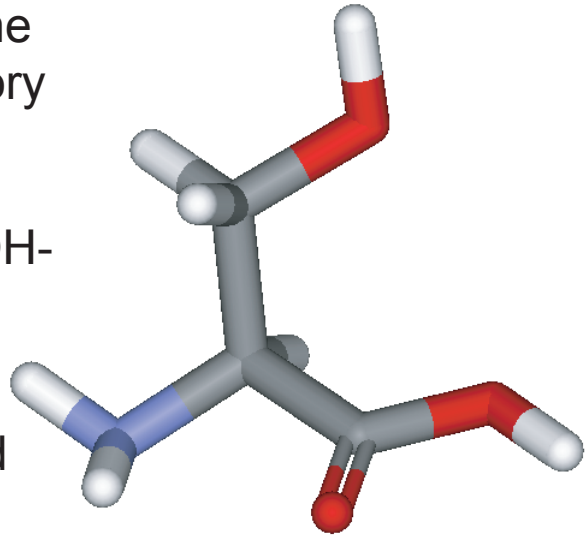
1. Calculate an optimal geometry of proline using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the 5th member ring internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion



4. Report in a figure the potential energy surface of the ring internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM calculations of internal rotation (QM-97)

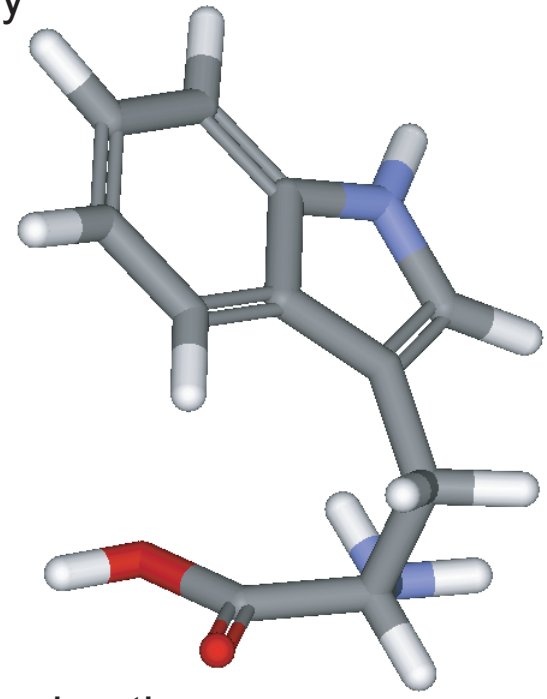
1. Calculate an optimal geometry of serine using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the CH2OH- internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion



4. Report in a figure the potential energy surface of the CH2OH- internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

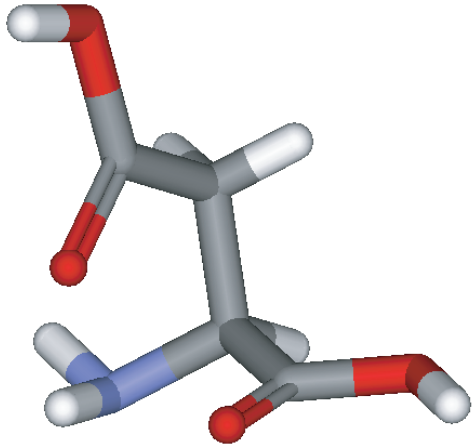
QM calculations of internal rotation (QM-98)

1. Calculate an optimal geometry of triptophan using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the ring internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion
4. Report in a figure the potential energy surface of the ring internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM calculations of internal rotation (QM-99)

1. Calculate an optimal geometry of aspartic acid using the B3LYP/6-31+G* level of theory



2. Calculated an optimal geometry for a constrained torsion angle of the COOH- internal rotation

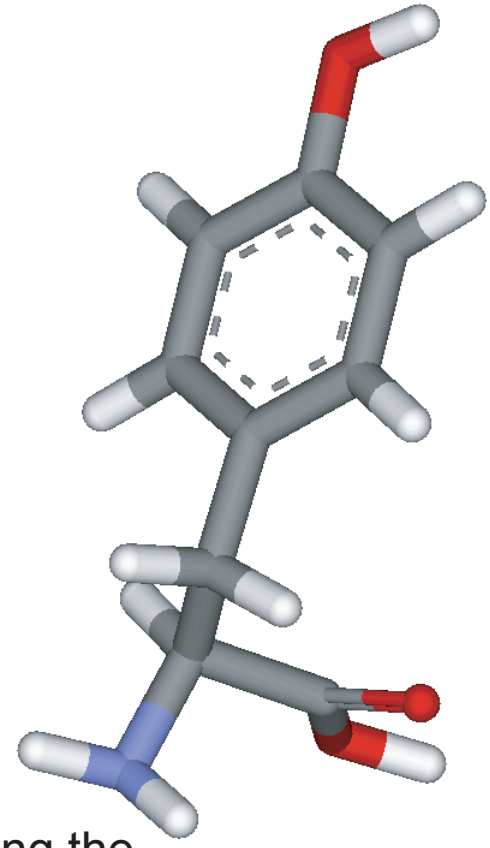
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion

4. Report in a figure the potential energy surface of the COOH- internal rotation

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

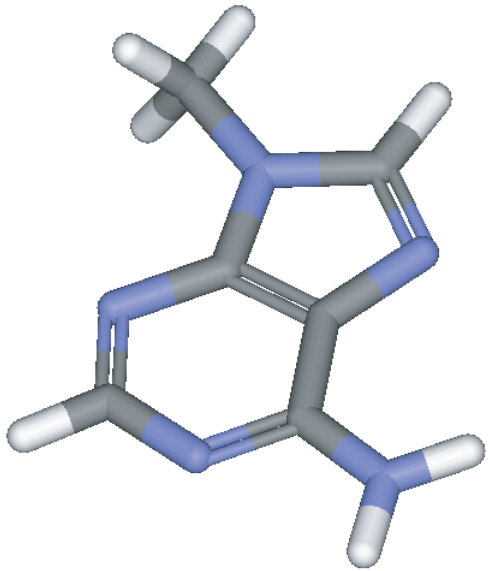
QM calculations of internal rotation (QM-100)

1. Calculate an optimal geometry of tyrosine using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the ring internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion
4. Report in a figure the potential energy surface of the ring internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM calculations of internal rotation (QM-101)

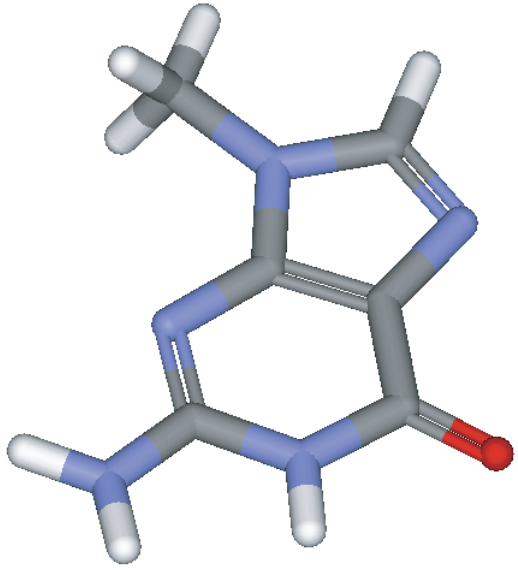
1. Calculate an optimal geometry of adenine using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the CH3- internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion



4. Report in a figure the potential energy surface of the CH3- internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

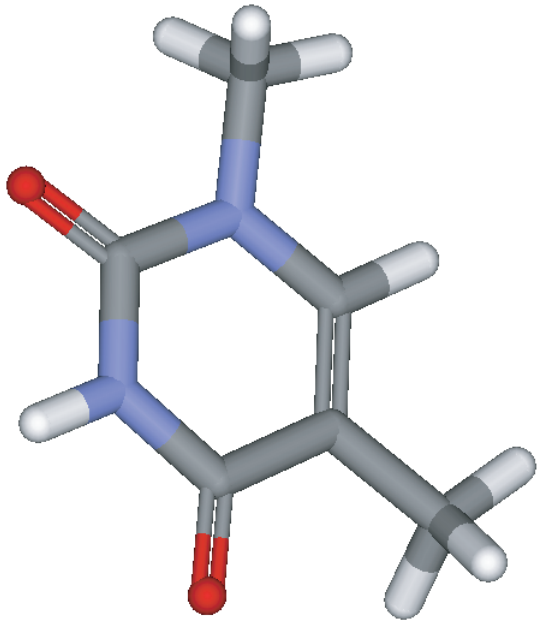
QM calculations of internal rotation (QM-102)

1. Calculate an optimal geometry of guanine using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of the NH2- internal rotation
3. Repeat calculations of geometry optimization for a series of constrained different values of the torsion
4. Report in a figure the potential energy surface of the NH2- internal rotation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



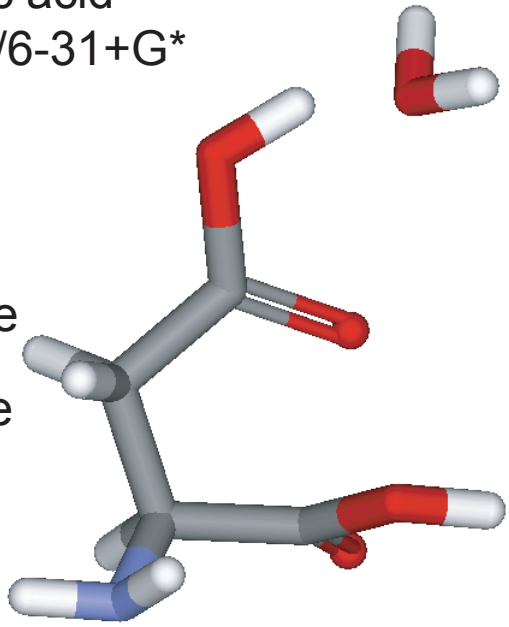
QM calculations of internal rotation (QM-103)

1. Calculate an optimal geometry of thymine using the B3LYP/6-31+G* level of theory
2. Calculated an optimal geometry for a constrained torsion angle of both CH3- internal rotations
3. Repeat calculations of geometry optimization for a series of constrained different values of both torsions
4. Report in a figure the potential energy surface of both internal rotations
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



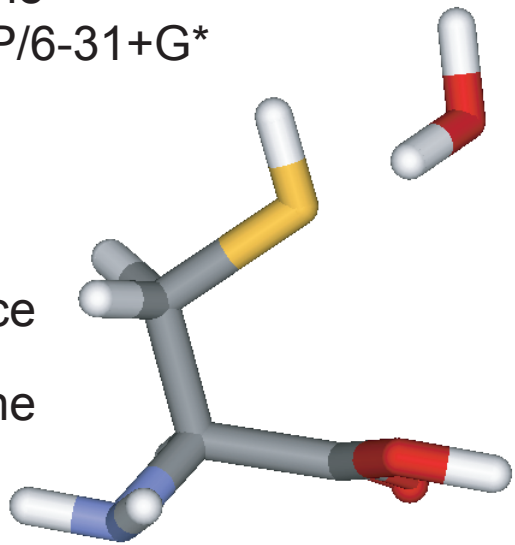
QM potential energy surface of hydrogen bonds (QM-104)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of aspartic acid (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O...H distance
3. Repeat the calculations for a series of the constrained O...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



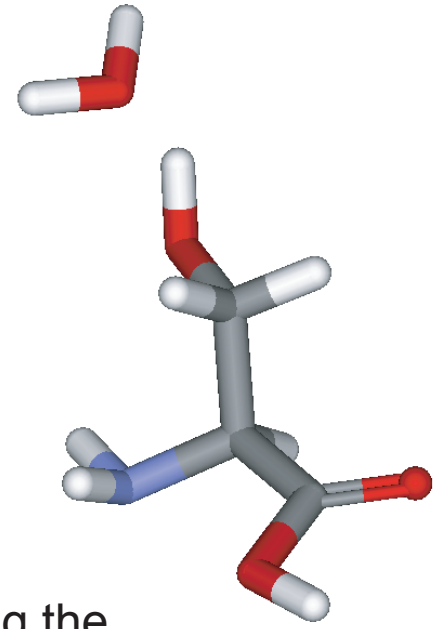
QM potential energy surface of hydrogen bonds (QM-106)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of cysteine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained S...H distance
3. Repeat the calculations for a series of the constrained S...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM potential energy surface of hydrogen bonds (QM-107)

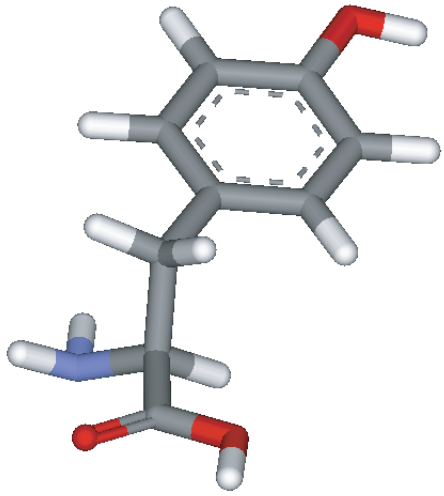
1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of serine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O...H distance
3. Repeat the calculations for a series of the constrained O...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM potential energy surface of hydrogen bonds (QM-108)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of tyrosine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O...H distance



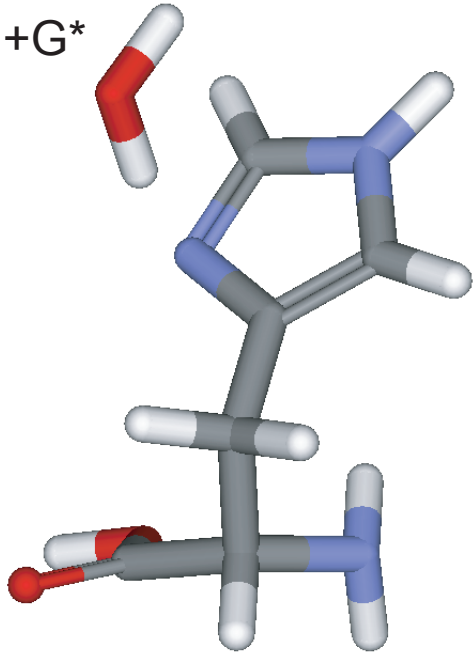
3. Repeat the calculations for a series of the constrained O...H distance

4. Report in a figure the potential energy surface of the hydrogen bond

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

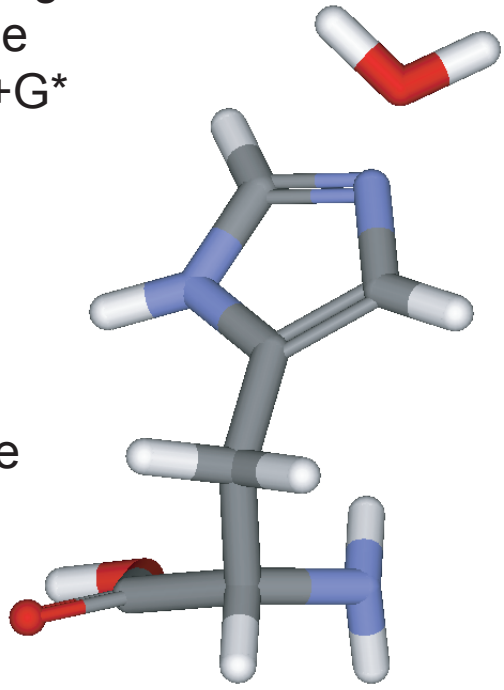
QM potential energy surface of hydrogen bonds (QM-109)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of histidine (epsilon) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O(N)...H
3. Repeat the calculations for a series of the constrained O(N)...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



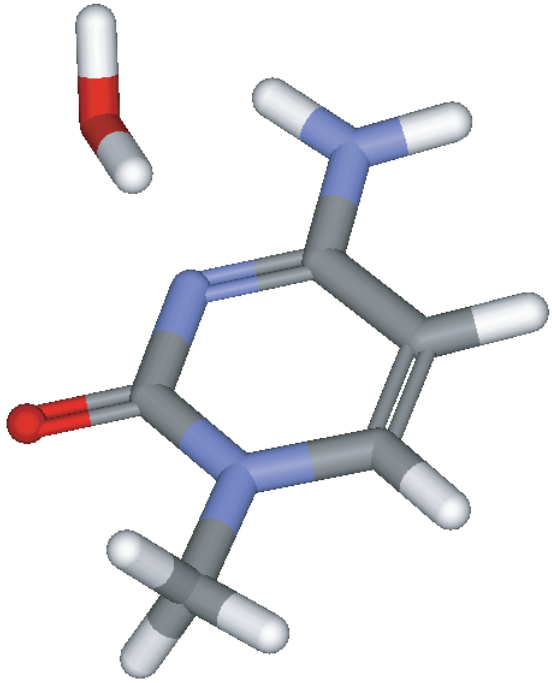
QM potential energy surface of hydrogen bonds (QM-110)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of histidine (delta) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O(N)...H
3. Repeat the calculations for a series of the constrained O(N)...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



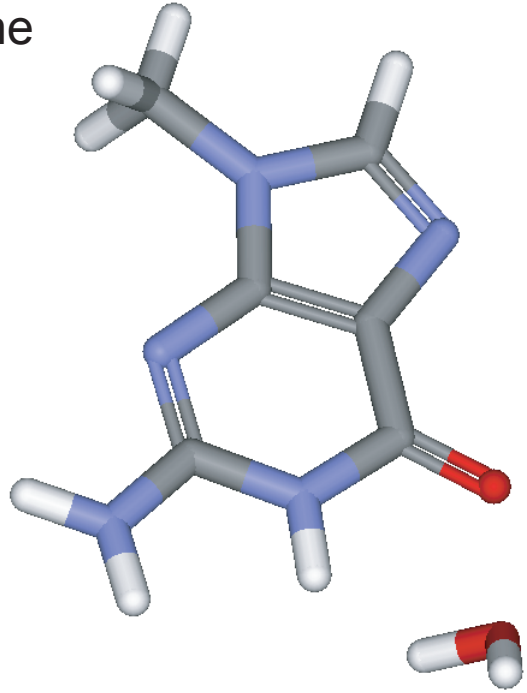
QM potential energy surface of hydrogen bonds (QM-111)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of cytosine and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O(N)...H
3. Repeat the calculations for a series of the constrained O(N)...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM potential energy surface of hydrogen bonds (QM-112)

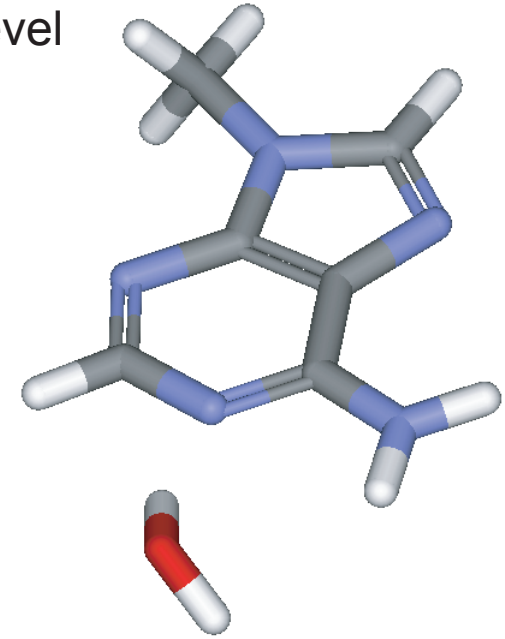
1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of guanine (protonated) and water, using the B3LYP/6-31+G* level of theory



2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O(N)...H
3. Repeat the calculations for a series of the constrained O(N)...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

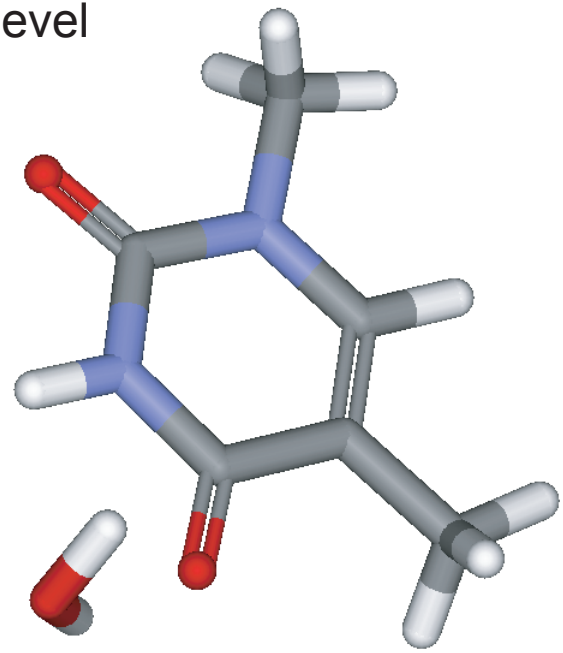
QM potential energy surface of hydrogen bonds (QM-113)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of adenine and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O(N)...H
3. Repeat the calculations for a series of the constrained O(N)...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



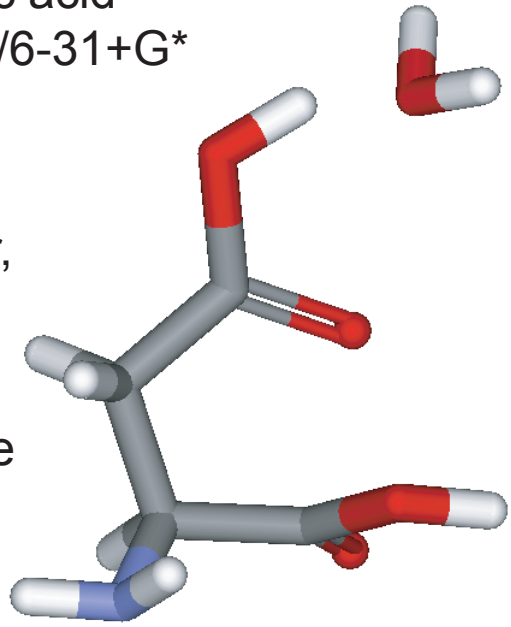
QM potential energy surface of hydrogen bonds (QM-114)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of thymine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the most stable dimer, calculate the optimal geometry for a constrained O(N)...H
3. Repeat the calculations for a series of the constrained O(N)...H distance
4. Report in a figure the potential energy surface of the hydrogen bond
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



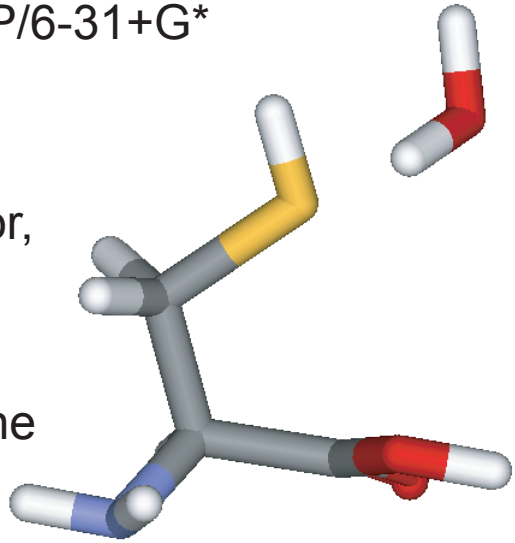
QM deprotonation in hydrogen bonds (QM-115)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of aspartic acid (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained O-H distance
3. Repeat the calculations for a series of the constrained O-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



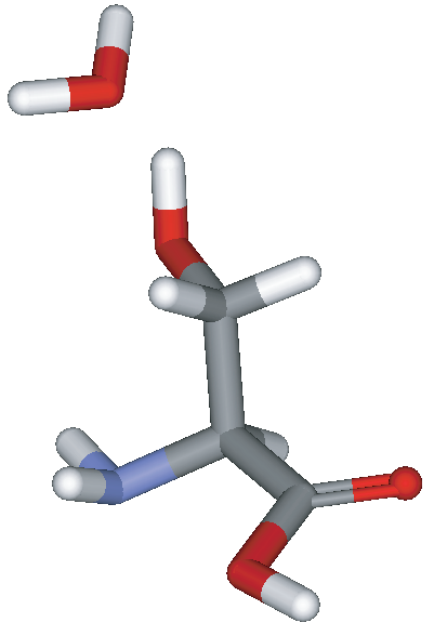
QM deprotonation in hydrogen bonds (QM-116)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of cysteine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained S-H distance
3. Repeat the calculations for a series of the constrained S-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM deprotonation in hydrogen bonds (QM-117)

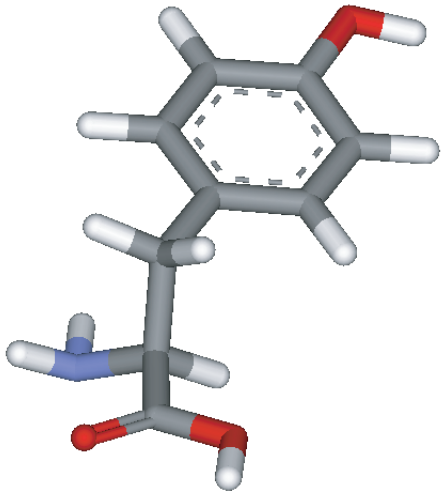
1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of serine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained O-H distance
3. Repeat the calculations for a series of the constrained O-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM deprotonation in hydrogen bonds (QM-118)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of tyrosine (protonated) and water, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained O-H distance



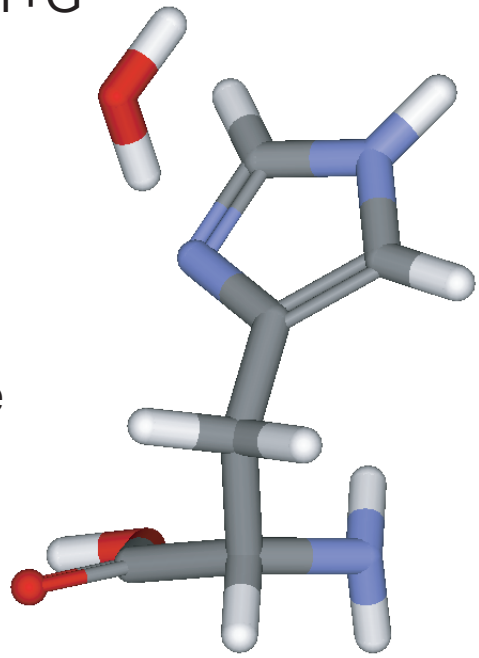
3. Repeat the calculations for a series of the constrained O-H distance

4. Report in a figure the potential energy surface of acid deprotonation

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

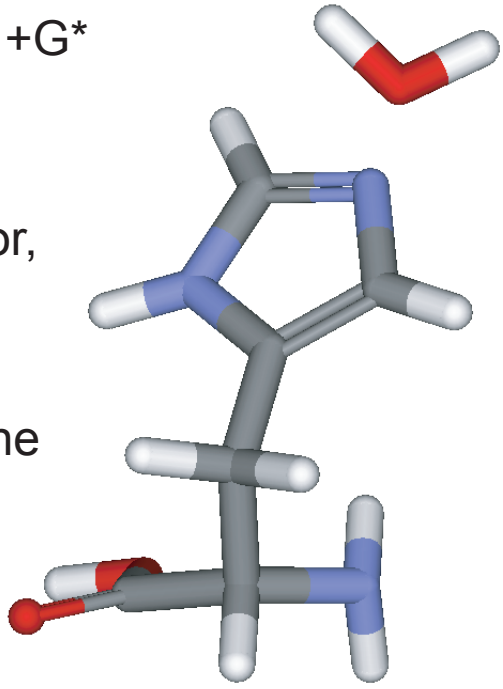
QM deprotonation in hydrogen bonds (QM-119)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of histidine (epsilon) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained N-H distance
3. Repeat the calculations for a series of the constrained N-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



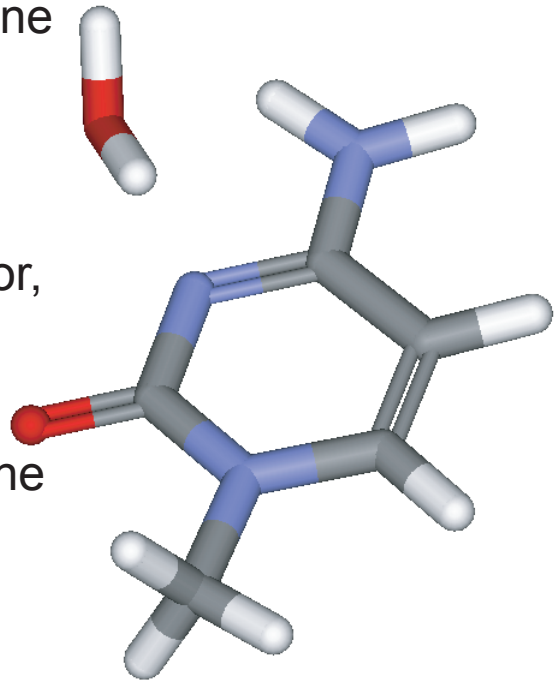
QM deprotonation in hydrogen bonds (QM-120)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of histidine (delta) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained N-H distance
3. Repeat the calculations for a series of the constrained N-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



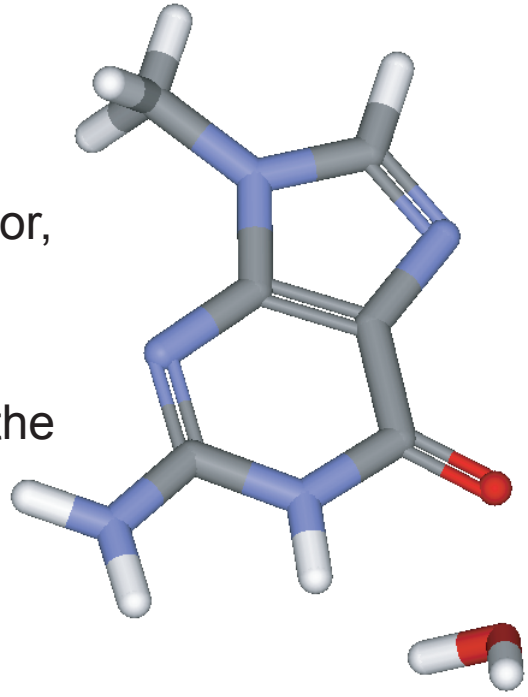
QM deprotonation in hydrogen bonds (QM-121)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of cytosine and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained N-H distance
3. Repeat the calculations for a series of the constrained N-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



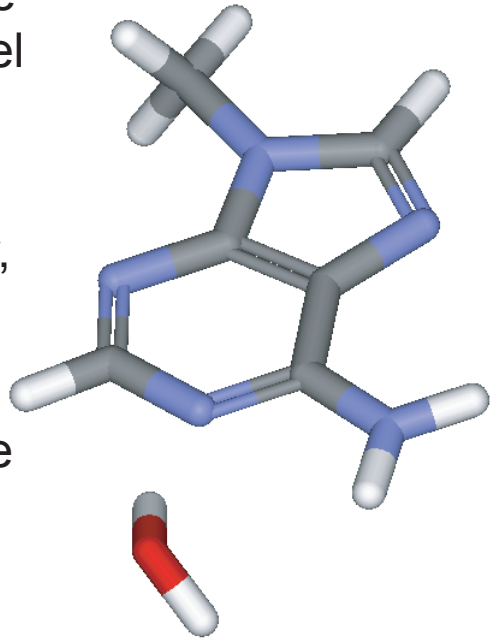
QM deprotonation in hydrogen bonds (QM-122)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of guanine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained N-H distance
3. Repeat the calculations for a series of the constrained N-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



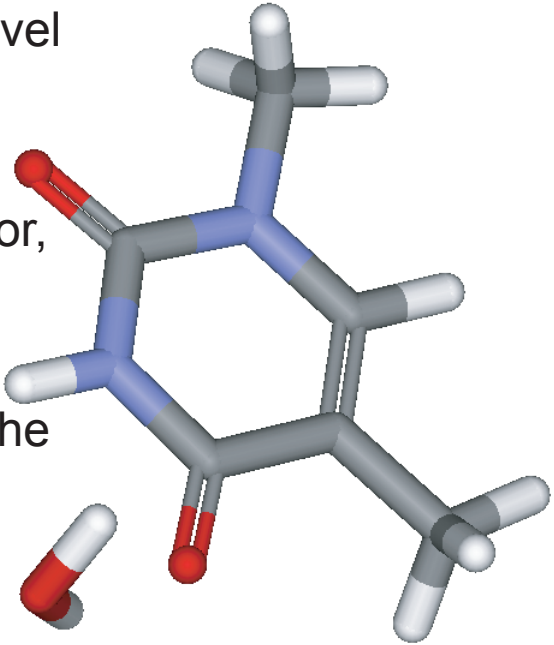
QM deprotonation in hydrogen bonds (QM-123)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of adenine and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained N-H distance
3. Repeat the calculations for a series of the constrained N-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



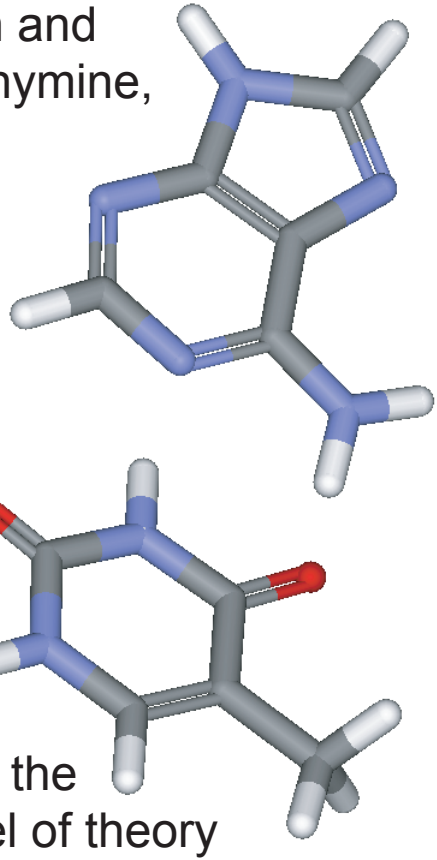
QM deprotonation in hydrogen bonds (QM-124)

1. Calculate an optimal geometry of all hydrogen-bonded dimers between the side chain of thymine (protonated) and water, using the B3LYP/6-31+G* level of theory
2. For the optimal geometry of the dimer where the acid is a hydrogen atom donor, calculate the optimal geometry for a constrained N-H distance
3. Repeat the calculations for a series of the constrained N-H distance
4. Report in a figure the potential energy surface of acid deprotonation
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



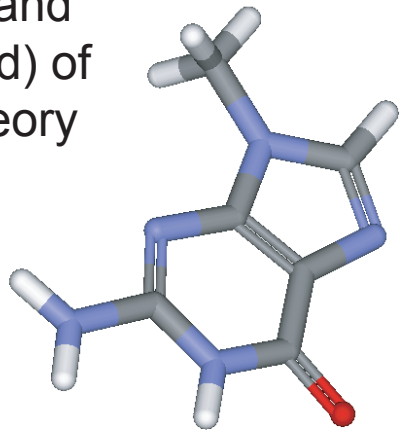
QM calculations of proton transfer in base pairs (QM-125)

1. Calculate an optimal geometry of a thymine-adenine dimer for a constrained distance between hydrogen and nitrogen (involved in the hydrogen bond) of thymine, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of that distance
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer, where thymine is a hydrogen atom acceptor
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

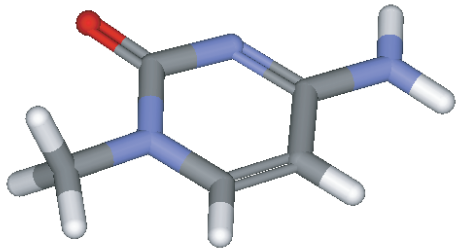


QM calculations of proton transfer in base pairs (QM-126)

1. Calculate an optimal geometry of a cytosine-guanine dimer for a constrained distance between hydrogen and nitrogen (involved in the central hydrogen bond) of guanine, using the B3LYP/6-31+G* level of theory



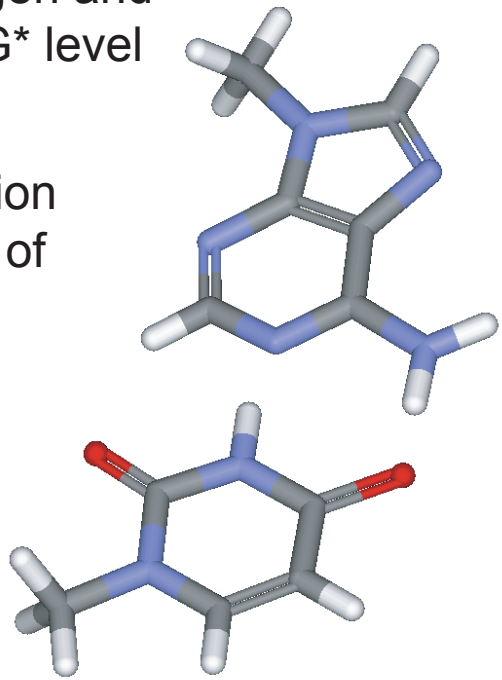
2. Repeat calculations of geometry optimization for a series of constrained different values of that distance
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer, where guanine is a hydrogen atom acceptor



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM calculations of proton transfer in base pairs (QM-127)

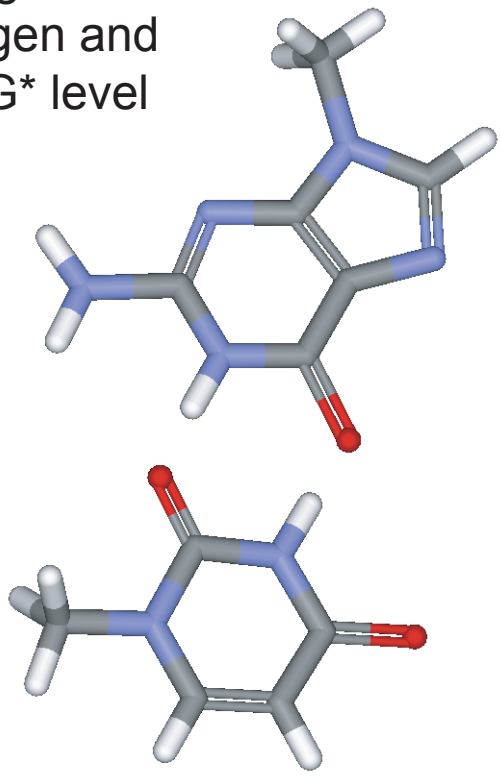
1. Calculate an optimal geometry of a uracil-adenine dimer for a constrained distance between hydrogen and nitrogen of uracil, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of that distance
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer, where uracil is a hydrogen atom acceptor



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

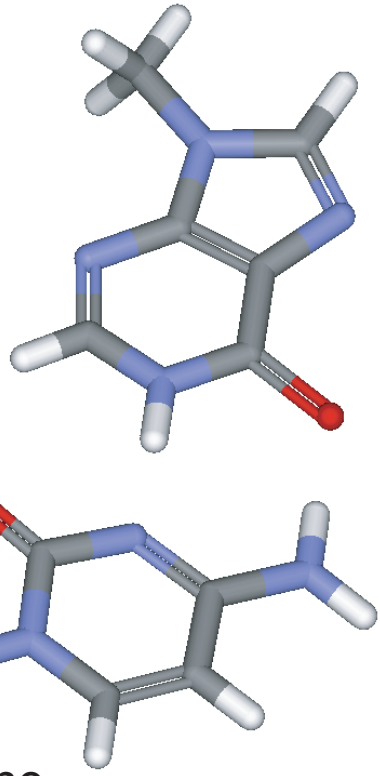
QM calculations of proton transfer in base pairs (QM-128)

1. Calculate an optimal geometry of a uracil-guanine dimer for a constrained distance between hydrogen and nitrogen of uracil, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of that distance
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer, where uracil is a hydrogen atom acceptor
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



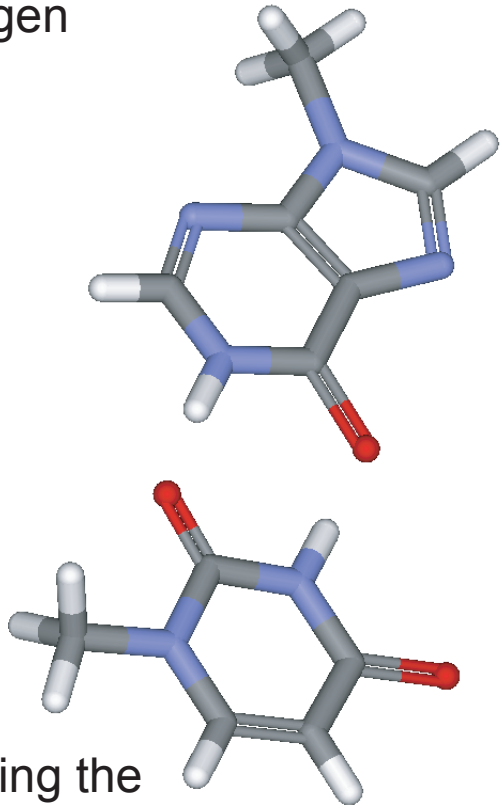
QM calculations of proton transfer in base pairs (QM-129)

1. Calculate an optimal geometry of a cytosine-inocine dimer for a constrained distance between hydrogen and nitrogen of inosine, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of that distance
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer, where inosine is a hydrogen atom acceptor
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



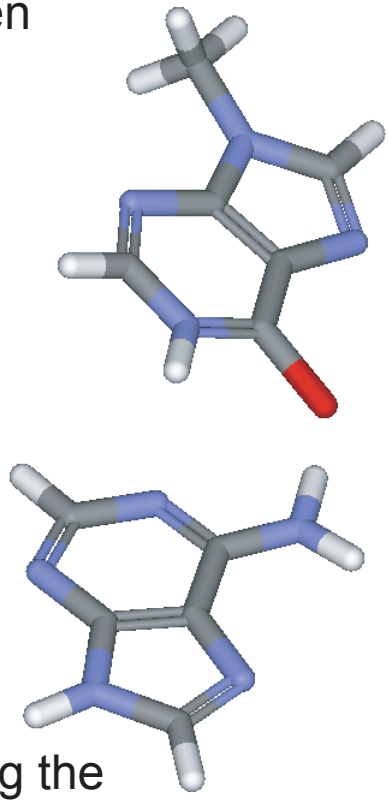
QM calculations of proton transfer in base pairs (QM-130)

1. Calculate an optimal geometry of a uracil-inocine dimer for a constrained distance between hydrogen and nitrogen of inosine, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of that distance
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer, where inosine is a hydrogen atom acceptor
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



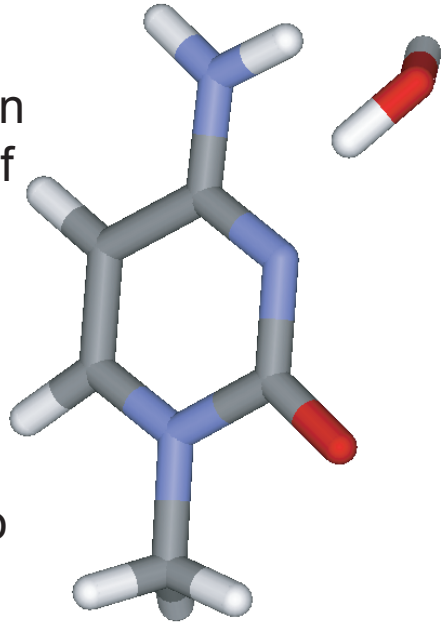
QM calculations of proton transfer in base pairs (QM-131)

1. Calculate an optimal geometry of a adenine-inocine dimer for a constrained distance between hydrogen and nitrogen of inosine, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of that distance
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer, where inosine is a hydrogen atom acceptor
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



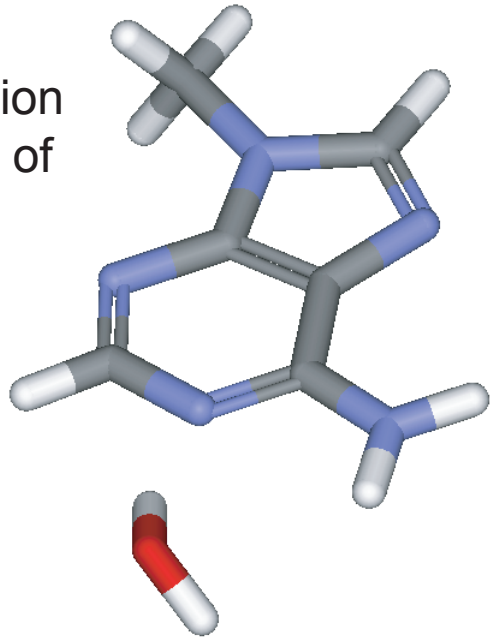
QM calculations of base tautomers (QM-132)

1. Calculate an optimal geometry of a cytosine-water dimer where cytosine is a hydrogen atom donor from one nitrogen and a hydrogen atom acceptor to another nitrogen, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of a nitrogen-hydrogen distance of cytosine
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer of cytosine with two water molecules
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



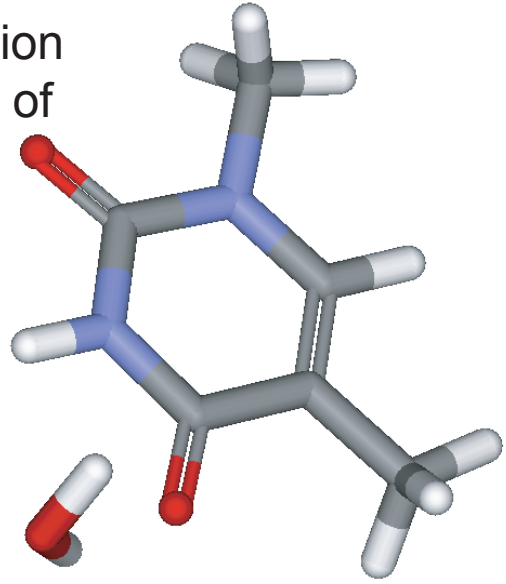
QM calculations of base tautomers (QM-133)

1. Calculate an optimal geometry of a adenine-water dimer where adenine is a hydrogen atom donor from one nitrogen and a hydrogen atom acceptor to another nitrogen, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of a nitrogen-hydrogen distance of the base
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer of the base with two water molecules
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



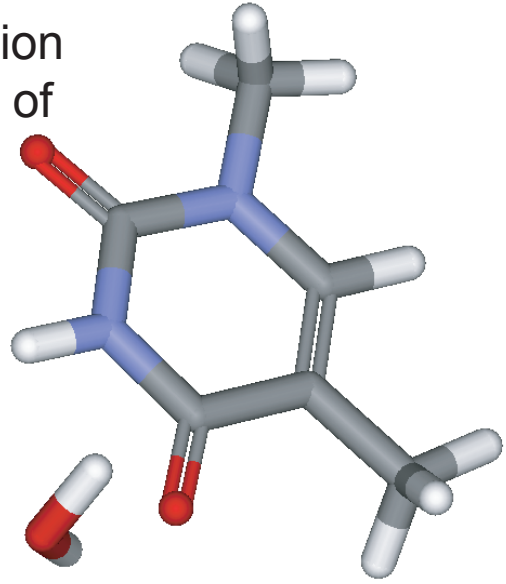
QM calculations of base tautomers (QM-134)

1. Calculate an optimal geometry of a thymine-water dimer where guanine is a hydrogen atom donor from one nitrogen and a hydrogen atom acceptor to another nitrogen, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of a nitrogen-hydrogen distance of the base
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer of the base with two water molecules
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



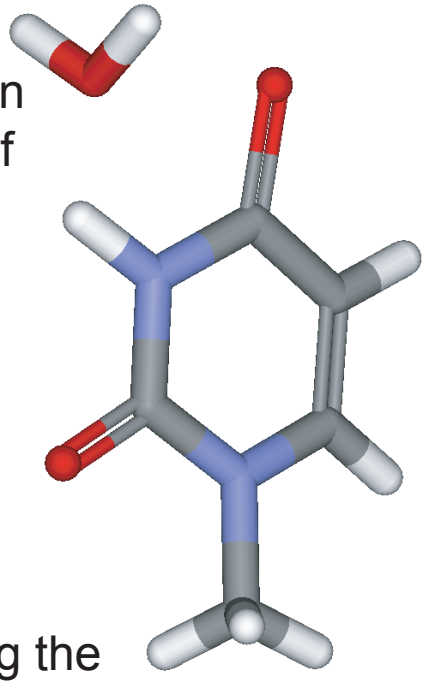
QM calculations of base tautomers (QM-135)

1. Calculate an optimal geometry of a thymine-water dimer where thymine is a hydrogen atom donor from nitrogen and a hydrogen atom acceptor to oxygen, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of a nitrogen-hydrogen distance of the base
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer of the base with two water molecules
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



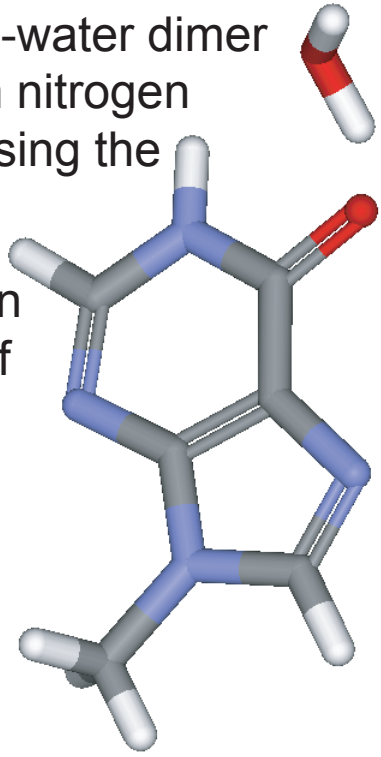
QM calculations of base tautomers (QM-136)

1. Calculate an optimal geometry of a uracil-water dimer where uracil is a hydrogen atom donor from nitrogen and a hydrogen atom acceptor to oxygen, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of a nitrogen-hydrogen distance of the base
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer of the base with two water molecules
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



QM calculations of base tautomers (QM-137)

1. Calculate an optimal geometry of an inocine-water dimer where incine is a hydrogen atom donor from nitrogen and a hydrogen atom acceptor to oxygen, using the B3LYP/6-31+G* level of theory
2. Repeat calculations of geometry optimization for a series of constrained different values of a nitrogen-hydrogen distance of the base
3. Report in a figure the potential energy surface of proton transfer
4. Repeat the same calculations for a hydrogen bonded dimer of the base with two water molecules
5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



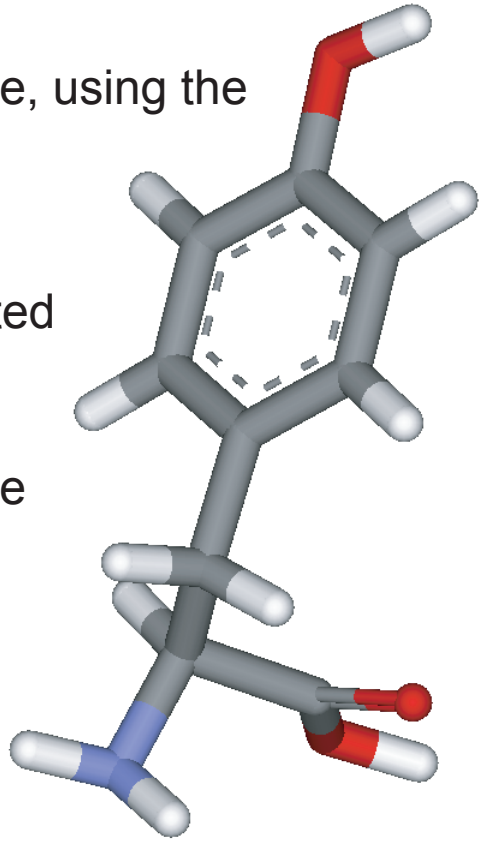
QM excited electronic states of amino acids (QM-138)

1. Calculate an optimal geometry of tyrosine, using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the ring

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

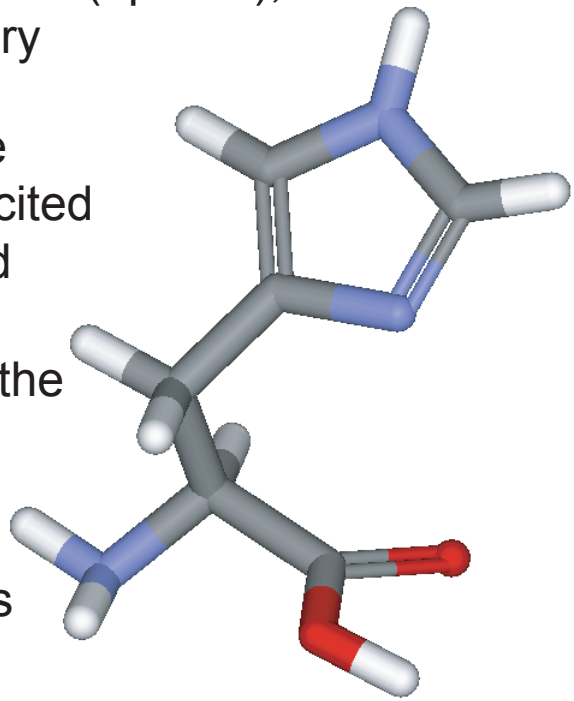
QM excited electronic states of amino acids (QM-139)

1. Calculate an optimal geometry of histidine (epsilon), using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the ring

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

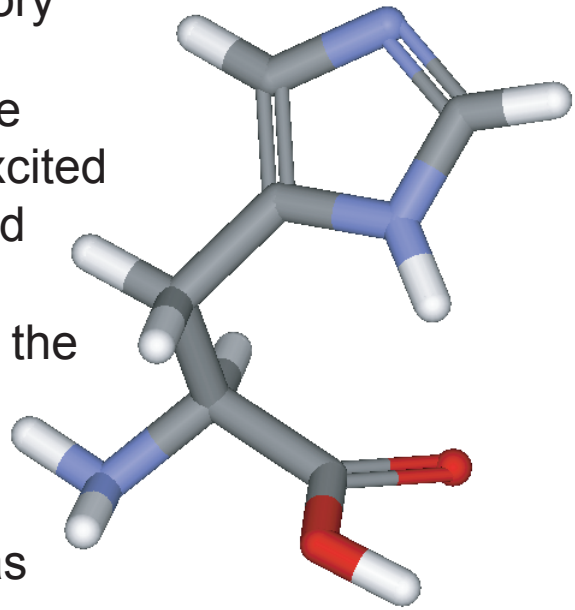
QM excited electronic states of amino acids (QM-140)

1. Calculate an optimal geometry of histidine (delta), using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the ring

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

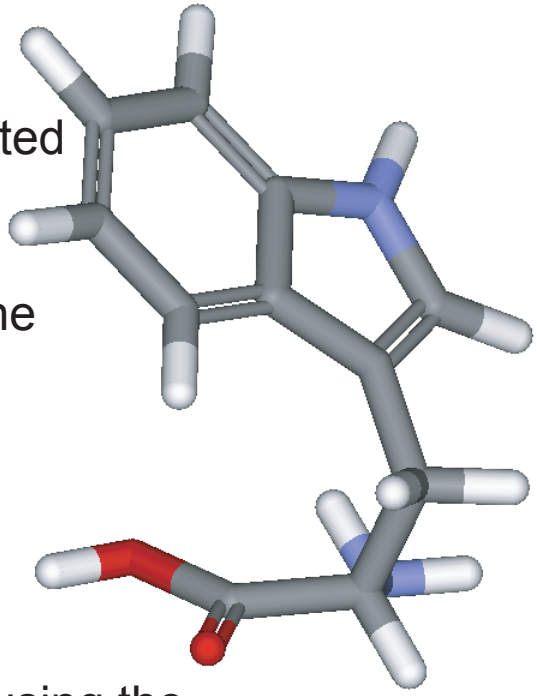
QM excited electronic states of amino acids (QM-141)

1. Calculate an optimal geometry of triptophan (protonated), using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the ring

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

QM excited electronic states of base monomers (QM-142)

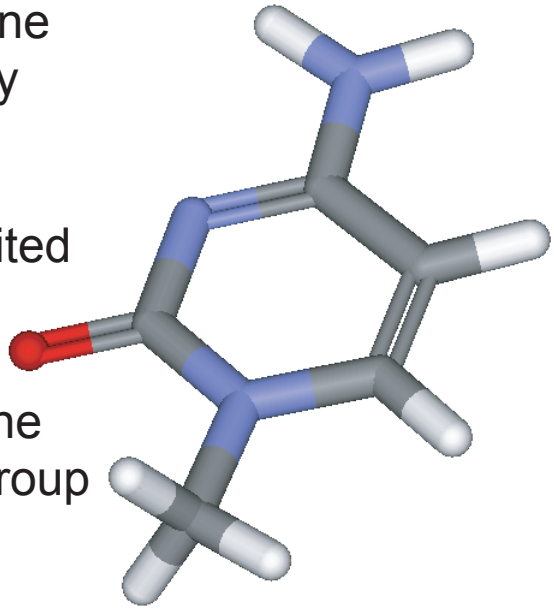
1. Calculate an optimal geometry of cytosine using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the NH2- group

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle

5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory



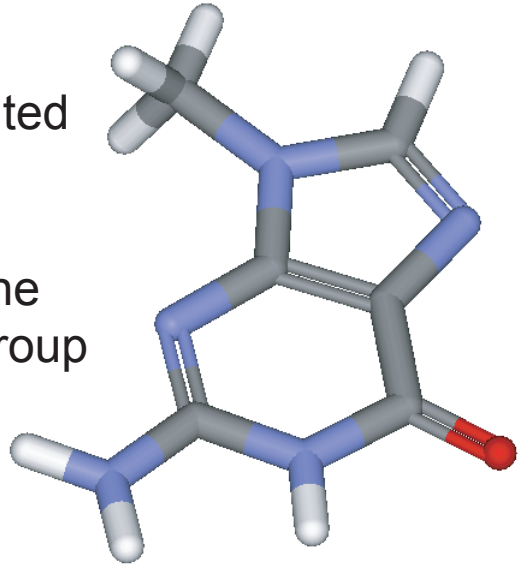
QM excited electronic states of base monomers (QM-143)

1. Calculate an optimal geometry of guanine (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the NH2- group

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

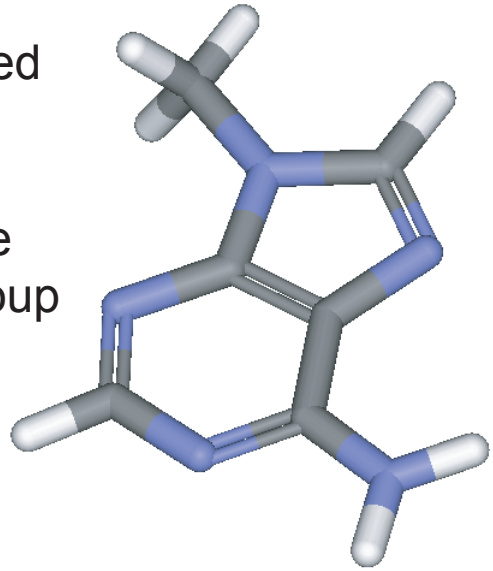
QM excited electronic states of base monomers (QM-144)

1. Calculate an optimal geometry of adenine using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the NH2- group

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory

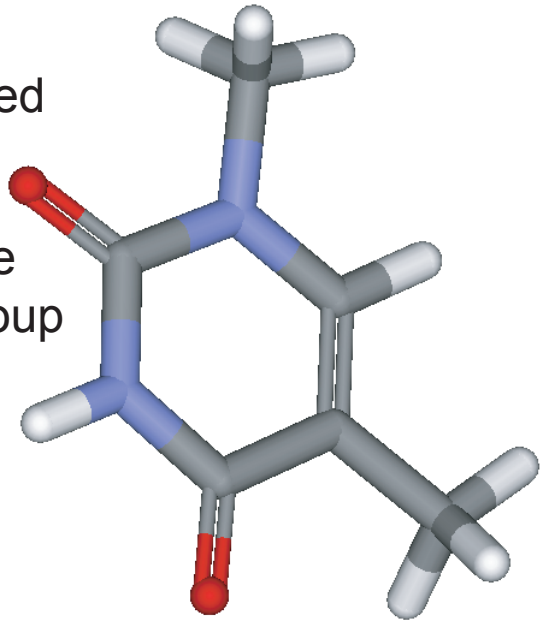
QM excited electronic states of base monomers (QM-145)

1. Calculate an optimal geometry of thymine (protonated) using the B3LYP/6-31+G* level of theory

2. For the optimal geometry, calculate the energy of the first singlet and triplet excited electronic states, using TDDFT method

3. Repeat the calculations for a series of the constrained torsion angle of the CH3- group connected to N

4. Report in a figure the energy of the ground and excited electronic states as a function of the torsion angle



5. Report results of the same calculations using the B3LYP/6-311+G*, and B3LYP/6-311+G** level of theory