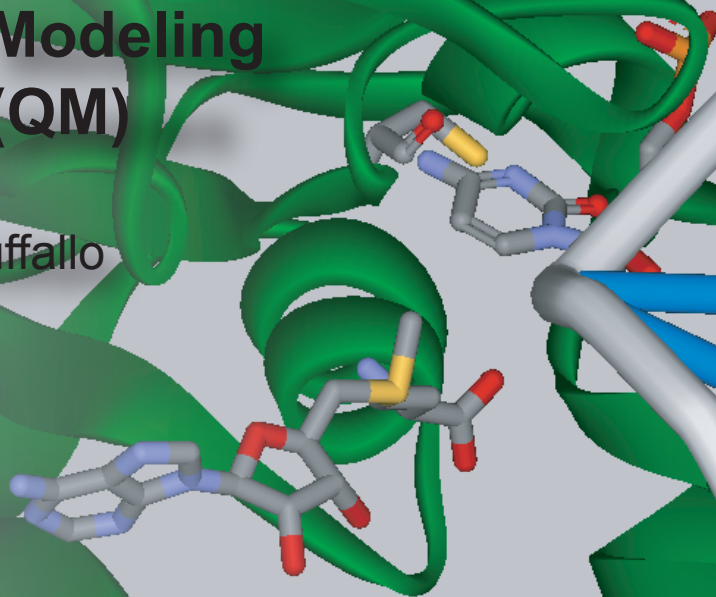


Marek
Freindorf

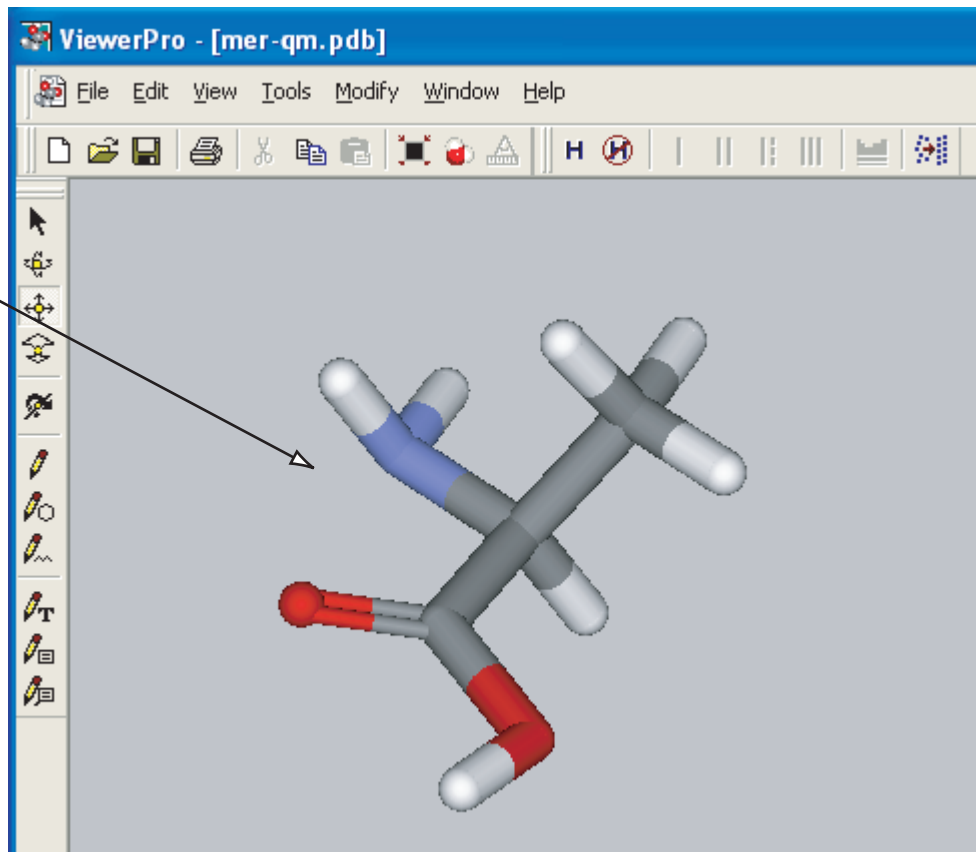
Molecular Modeling Examples (QM)

University at Buffalo
January 2007



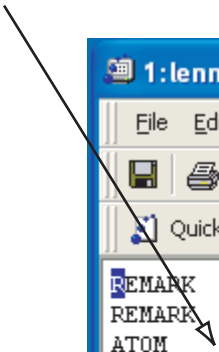
QM geometry optimization of alanine

Initial geometry
of alanine



QM geometry optimization of alanine

A PDB file of alanine



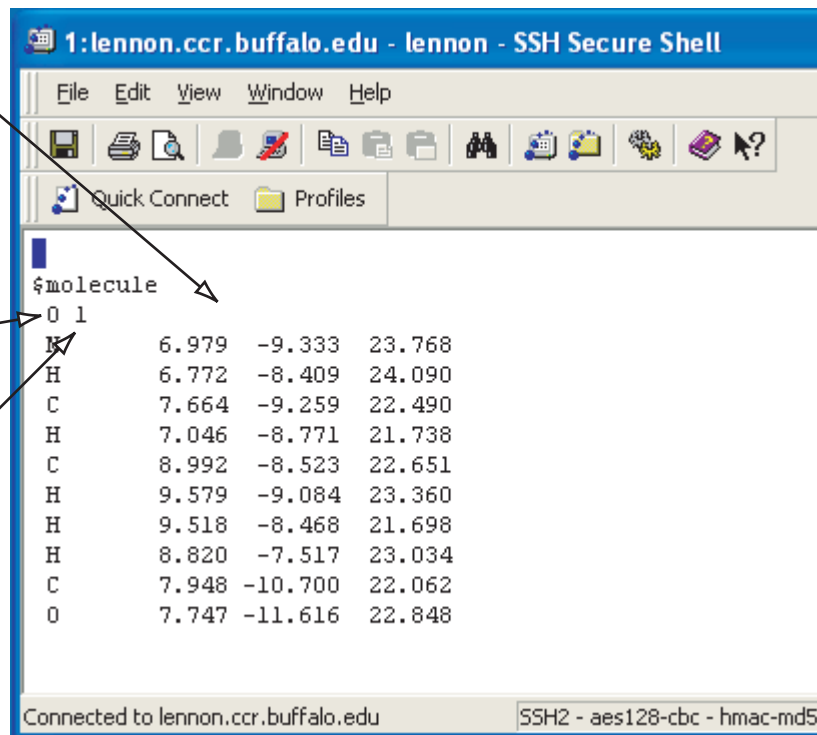
```
1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
REMARK Accelrys ViewerPro PDB file
REMARK Created: Tue Aug 29 14:13:48 Eastern Daylight
ATOM 1 N ALA 218 6.979 -9.333 23.768
ATOM 2 H ALA 218 6.772 -8.409 24.090
ATOM 3 CA ALA 218 7.664 -9.259 22.490
ATOM 4 HA ALA 218 7.046 -8.771 21.738
ATOM 5 CB ALA 218 8.992 -8.523 22.651
ATOM 6 HB1 ALA 218 9.579 -9.084 23.360
ATOM 7 HB2 ALA 218 9.518 -8.468 21.698
ATOM 8 HB3 ALA 218 8.820 -7.517 23.034
ATOM 9 C ALA 218 7.948 -10.700 22.062
ATOM 10 O ALA 218 7.747 -11.616 22.848
ATOM 11 O2O ALA 218 8.470 -10.989 20.686
"ala.pdb" [dos] 16L, 1176C
Connected to lennon.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5
```

QM geometry optimization of alanine

Copy and paste the
coordinates

Molecular charge

Multiplicity of the
electronic wave
function



```
$molecule
0 1
K      6.979  -9.333  23.768
H      6.772  -8.409  24.090
C      7.664  -9.259  22.490
H      7.046  -8.771  21.738
C      8.992  -8.523  22.651
H      9.579  -9.084  23.360
H      9.518  -8.468  21.698
H      8.820  -7.517  23.034
C      7.948 -10.700  22.062
C      7.747 -11.616  22.848
```

QM geometry optimization of alanine

Geometry
optimization

Hamiltonian

Basis set

Memory allocation

```
1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

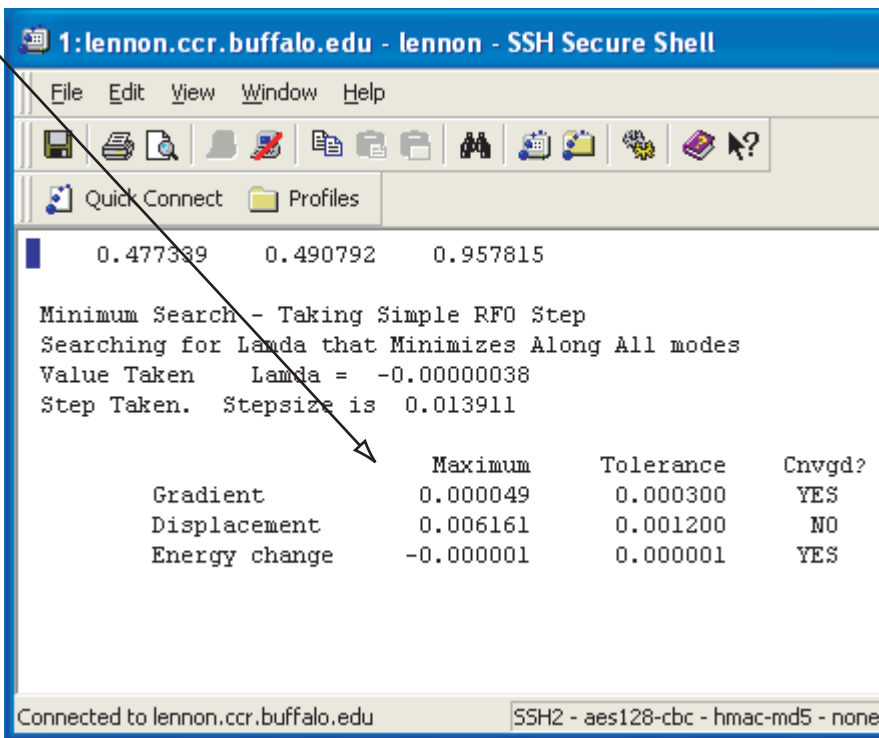
O      8.470 -10.989  20.686
H      7.565  -9.794  24.435
H      8.598 -11.974  20.577
$end

$rem
jobtype      opt      ! geometry optimizat
exchange     b3lyp    ! hybrid exchange
basis        6-31+G*  ! Pople's double zet
mem_static   512      ! Static memory
mem_total    2000     ! Total memory
$end

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```

QM geometry optimization of alanine

Geometry optimized



```
1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

0.477389 0.490792 0.957815

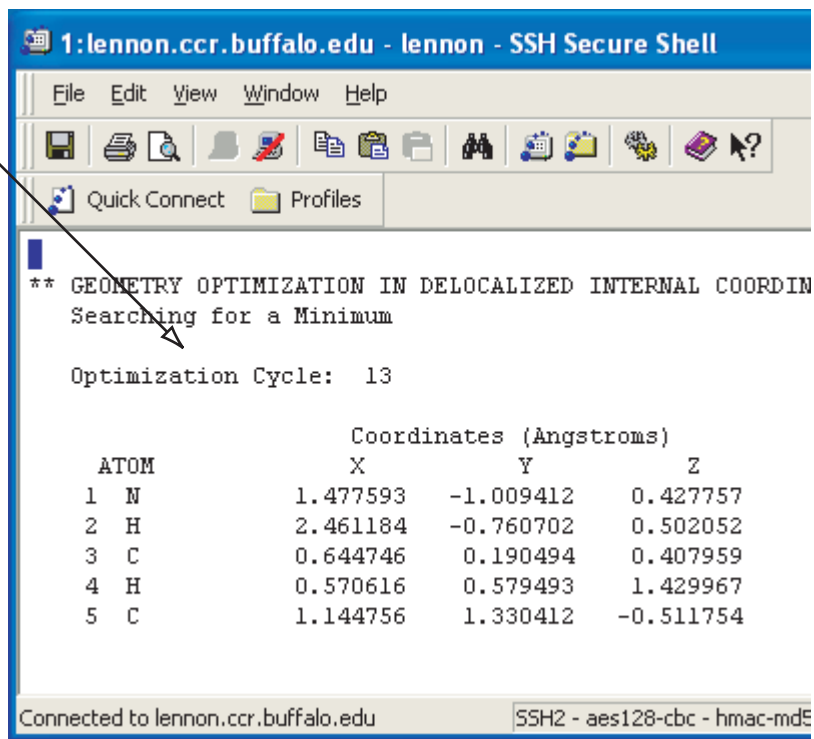
Minimum Search - Taking Simple RFO Step
Searching for Lambda that Minimizes Along All modes
Value Taken Lambda = -0.00000038
Step Taken. Stepsize is 0.013911

      Maximum      Tolerance      Cnvgd?
Gradient      0.000049      0.000300      YES
Displacement  0.006161      0.001200      NO
Energy change -0.000001      0.000001      YES

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none
```

QM geometry optimization of alanine

Final geometry



```
1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDIN
Searching for a Minimum

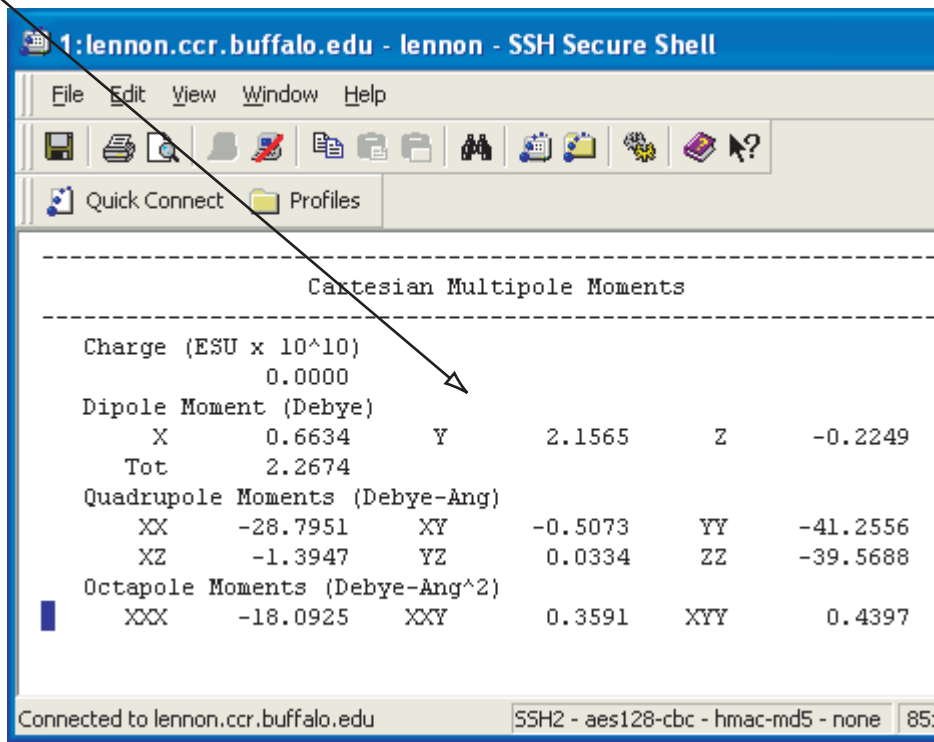
Optimization Cycle: 13

Coordinates (Angstroms)
ATOM      X      Y      Z
1  N      1.477593 -1.009412  0.427757
2  H      2.461184 -0.760702  0.502052
3  C      0.644746  0.190494  0.407959
4  H      0.570616  0.579493  1.429967
5  C      1.144756  1.330412 -0.511754

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```

QM geometry optimization of alanine

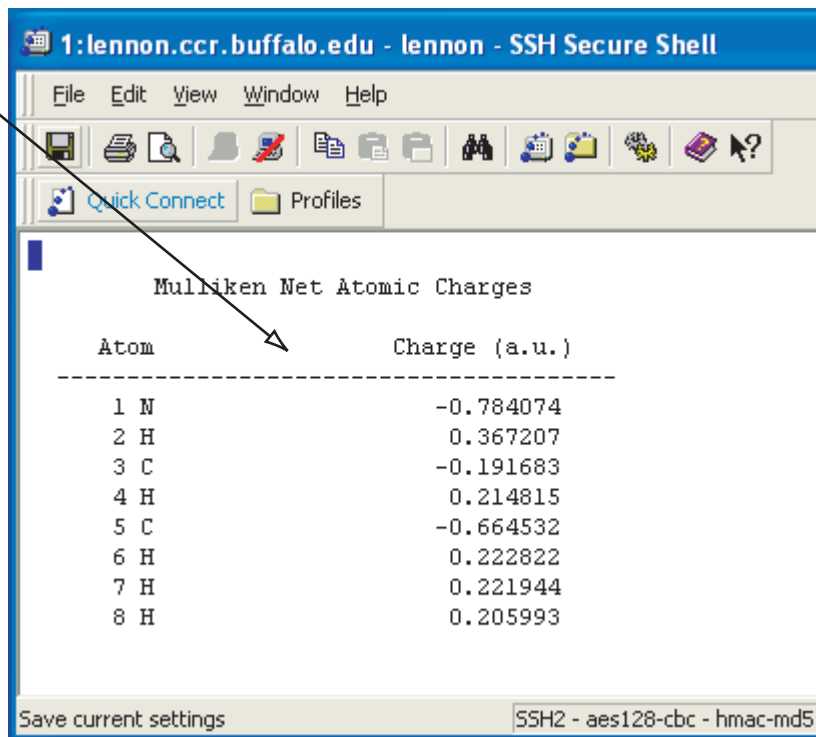
Final dipol moment



```
1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
-----
                        Cartesian Multipole Moments
-----
Charge (ESU x 10^10)
0.0000
Dipole Moment (Debye)
  X    0.6634    Y    2.1565    Z    -0.2249
Tot    2.2674
Quadrupole Moments (Debye-Ang)
  XX   -28.7951  XY   -0.5073  YY   -41.2556
  XZ   -1.3947  YZ    0.0334  ZZ   -39.5688
Octapole Moments (Debye-Ang^2)
  XXX  -18.0925  XXY    0.3591  XYY    0.4397
Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none  85
```


QM geometry optimization of alanine

Atomic charges



1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell

File Edit View Window Help

Quick Connect Profiles

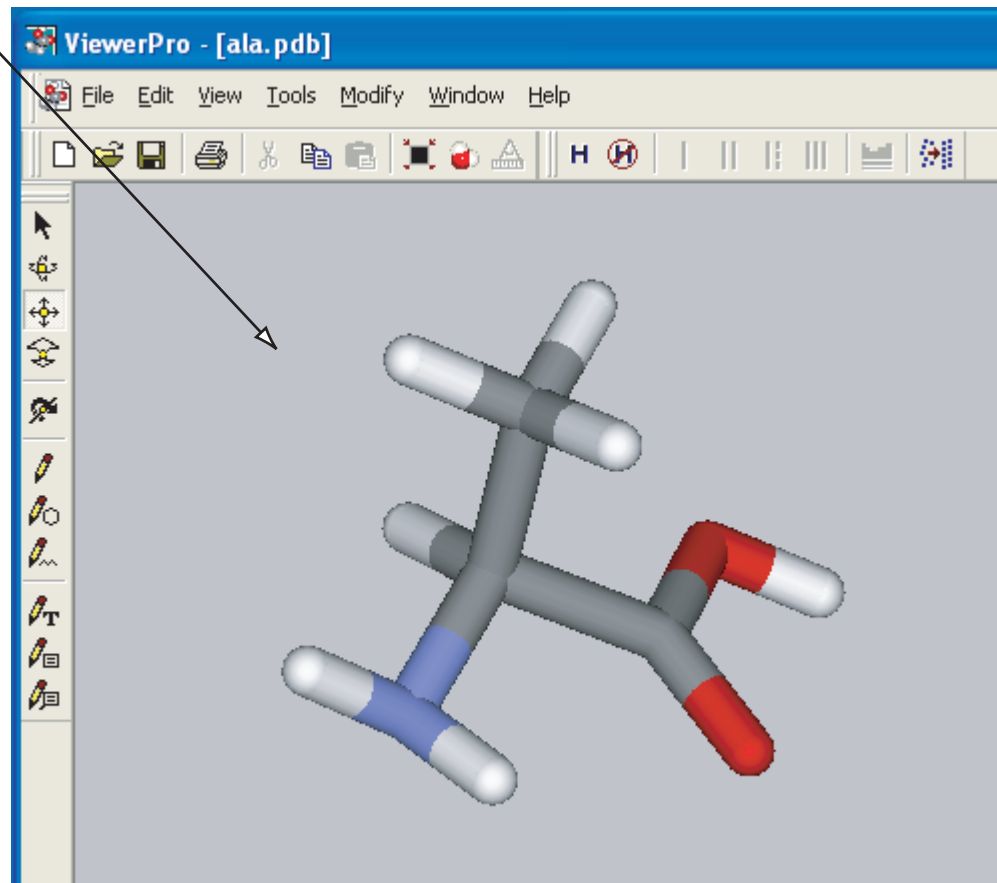
Mulliken Net Atomic Charges

Atom	Charge (a.u.)
1 N	-0.784074
2 H	0.367207
3 C	-0.191683
4 H	0.214815
5 C	-0.664532
6 H	0.222822
7 H	0.221944
8 H	0.205993

Save current settings SSH2 - aes128-cbc - hmac-md5

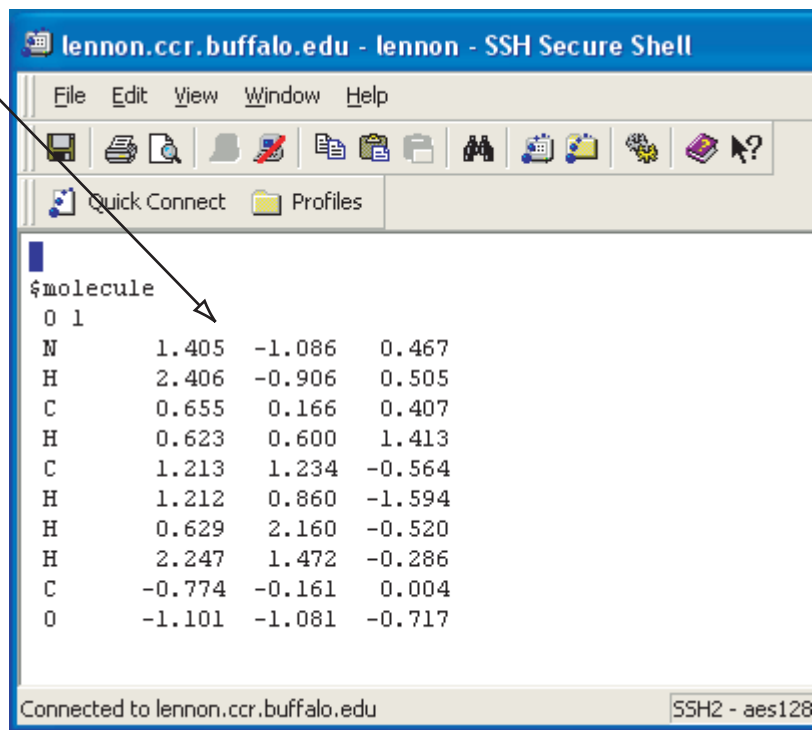
QM geometry optimization of alanine

Geometry optimized



QM oscillations of alanine

Coordinates after
geometry optimization



lennon.ccr.buffalo.edu - lennon - SSH Secure Shell

File Edit View Window Help

Quick Connect Profiles

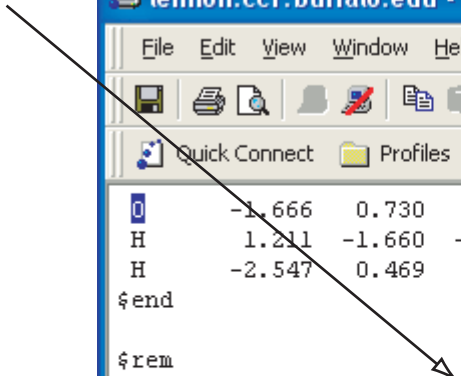
```
$molecule
O 1
N      1.405  -1.086   0.467
H      2.406  -0.906   0.505
C      0.655   0.166   0.407
H      0.623   0.600   1.413
C      1.213   1.234  -0.564
H      1.212   0.860  -1.594
H      0.629   2.160  -0.520
H      2.247   1.472  -0.286
C     -0.774  -0.161   0.004
O     -1.101  -1.081  -0.717
```

Connected to lennon.ccr.buffalo.edu

SSH2 - aes128

QM oscillations of alanine

Molecular oscillations calculations



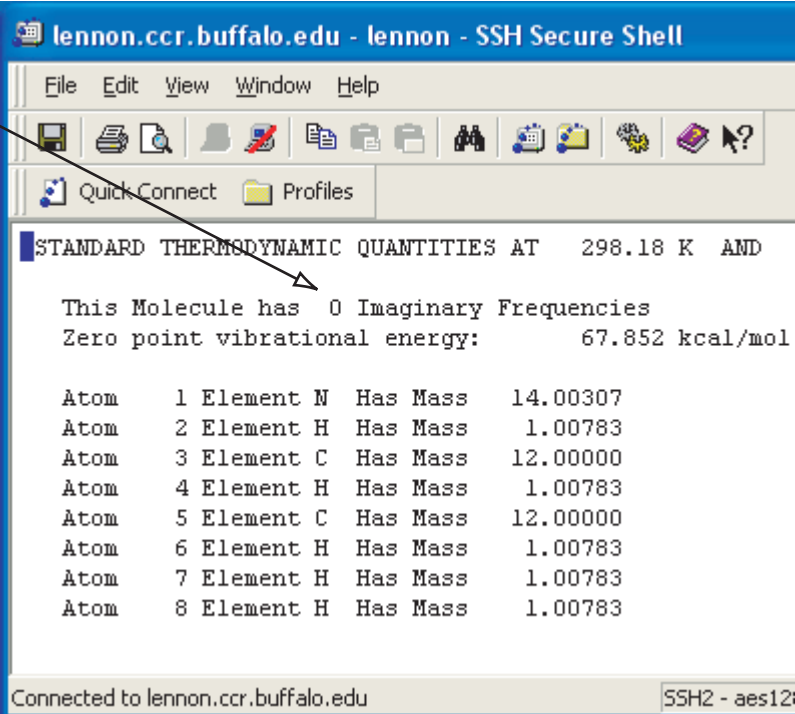
```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
O      -1.666   0.730   0.501
H       1.211  -1.660  -0.352
H      -2.547   0.469   0.172
$end

$rem
jobtype          freq      ! geometry optimization
exchange         b3lyp     ! hybrid exchange
basis            6-31+G*    ! Pople's double zeta
mem_static       512       ! Static memory
mem_total       2000       ! Total memory
$end

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128
```

QM oscillations of alanine

Results of oscillations calculations



```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 67.852 kcal/mol

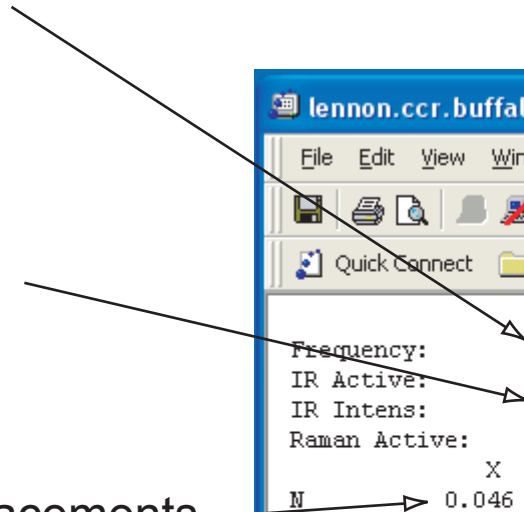
Atom 1 Element N Has Mass 14.00307
Atom 2 Element H Has Mass 1.00783
Atom 3 Element C Has Mass 12.00000
Atom 4 Element H Has Mass 1.00783
Atom 5 Element C Has Mass 12.00000
Atom 6 Element H Has Mass 1.00783
Atom 7 Element H Has Mass 1.00783
Atom 8 Element H Has Mass 1.00783
Connected to lennon.ccr.buffalo.edu SSH2 - aes128
```

QM oscillations of alanine

Frequency

IR intensity

Atomic displacements

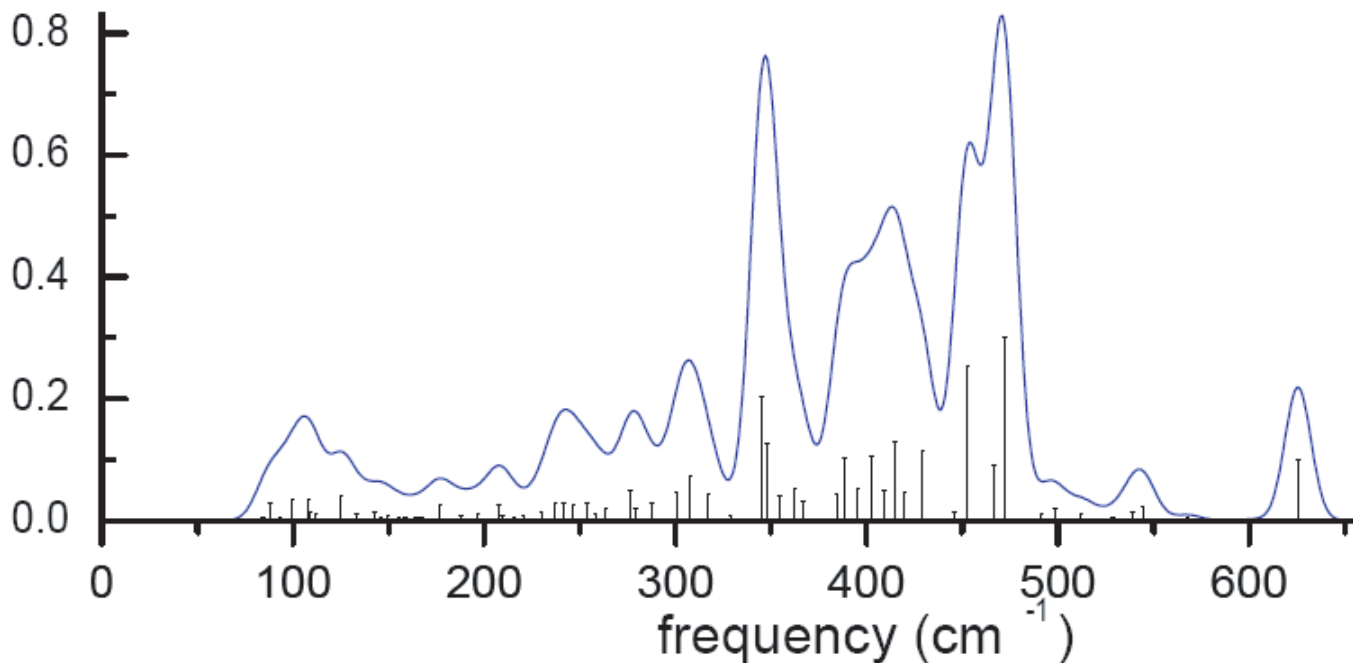


lennon.ccr.buffalo.edu - lennon - SSH Secure Shell							
File Edit View Window Help							
Quick Connect Profiles							
Frequency:	924.71			1034.90			
IR Active:	YES			YES			
IR Intens:	8.729			7.448			
Raman Active:	YES			YES			
	X	Y	Z	X	Y	Z	
N	0.046	-0.072	-0.023	-0.069	0.071	-0.017	
H	0.022	-0.019	0.138	-0.136	0.407	-0.021	
C	-0.145	-0.053	0.053	-0.036	-0.128	0.003	
H	-0.236	-0.258	0.135	-0.135	-0.292	0.077	
C	-0.022	0.154	-0.054	0.137	0.029	-0.004	
H	0.049	-0.240	0.086	-0.242	-0.041	0.018	
	0.319	0.384	-0.491	-0.254	-0.213	0.054	

Connected to lennon.ccr.buffalo.edu SSH2 - aes128

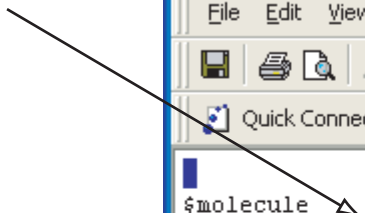
QM oscillations of alanine

IR intensity as a function
of oscillation frequency



QM electrostatic potential of alanine

Copy and paste
optimal geometry



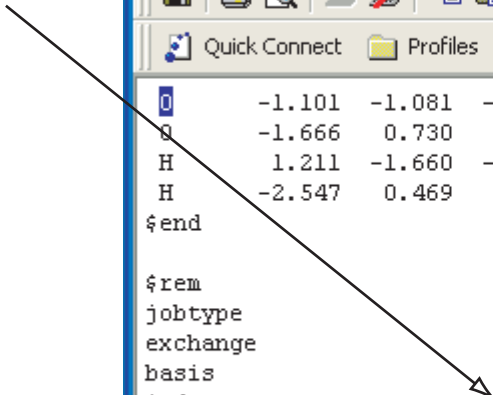
```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

$molecule
0 1
N      1.405  -1.086   0.467
H      2.406  -0.906   0.505
C      0.655   0.166   0.407
H      0.623   0.600   1.413
C      1.213   1.234  -0.564
H      1.212   0.860  -1.594
H      0.629   2.160  -0.520
H      2.247   1.472  -0.286
C     -0.774  -0.161   0.004
O     -1.101  -1.081  -0.717
O     -1.666   0.730   0.501
"ala-ele.in" 27L, 786C

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac
```

QM electrostatic potential of alanine

Electrostatic
potential at the
atomic positions



```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

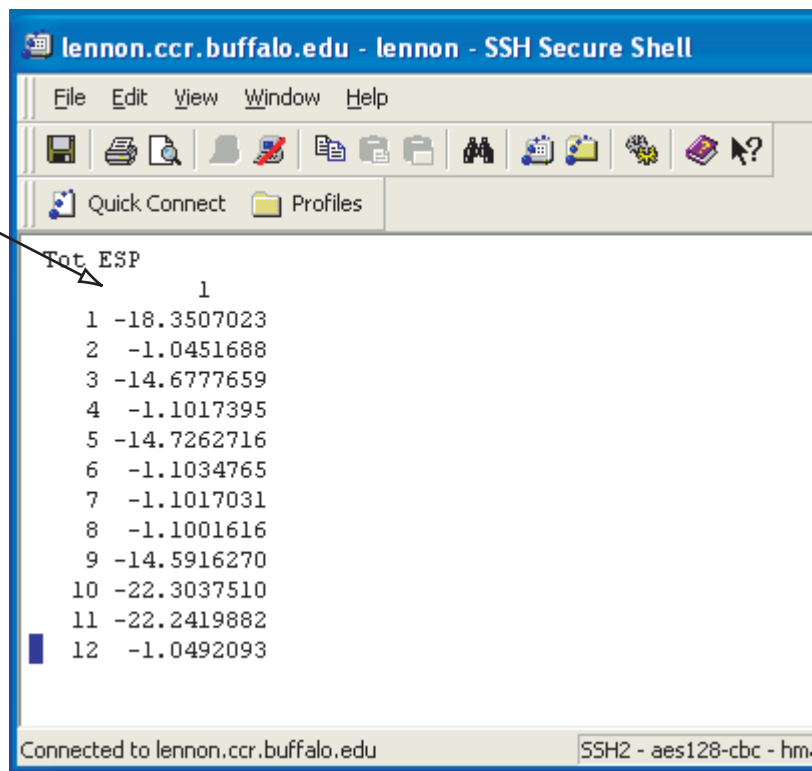
0      -1.101  -1.081  -0.717
O      -1.666   0.730   0.501
H       1.211  -1.660  -0.352
H      -2.547   0.469   0.172
$end

$rem
jobtype          sp          ! geometry optimizati
exchange         b3lyp       ! hybrid exchange
basis            6-31+G*     ! Pople's double zeta
igdsp            0           ! electrostatic poten
mem_static       512         ! Static memory
mem_total       2000        ! Total memory
$end

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac
```

QM electrostatic potential of alanine

Final values of the
electrostatic
potential at the
atomic positions



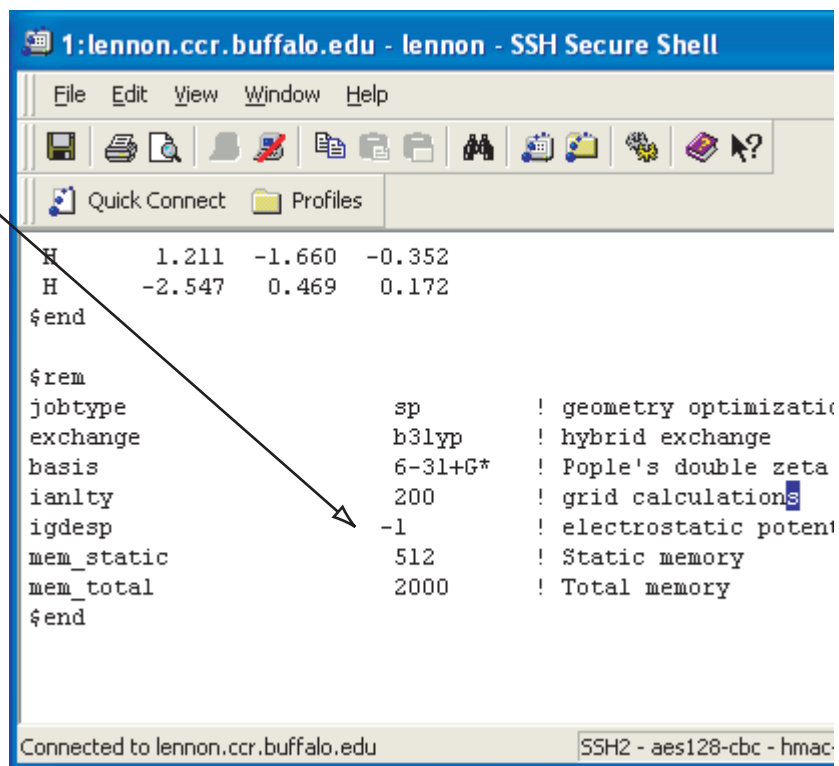
```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

Tot ESP
1
1 -18.3507023
2 -1.0451688
3 -14.6777659
4 -1.1017395
5 -14.7262716
6 -1.1034765
7 -1.1017031
8 -1.1001616
9 -14.5916270
10 -22.3037510
11 -22.2419882
12 -1.0492093

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hm.
```

QM electrostatic potential of alanine

Electrostatic potential
at the grid points



```
1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

H      1.211  -1.660  -0.352
H      -2.547   0.469   0.172
$end

$rem
jobtype                sp      ! geometry optimization
exchange               b3lyp   ! hybrid exchange
basis                  6-31+G* ! Pople's double zeta
ianlty                 200     ! grid calculations
igdesp                 -1      ! electrostatic potential
mem_static             512     ! Static memory
mem_total              2000    ! Total memory
$end

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac
```

QM electrostatic potential of alanine

Definition of the grid points

Number of grid points in the x direction

Minimum and maximum values

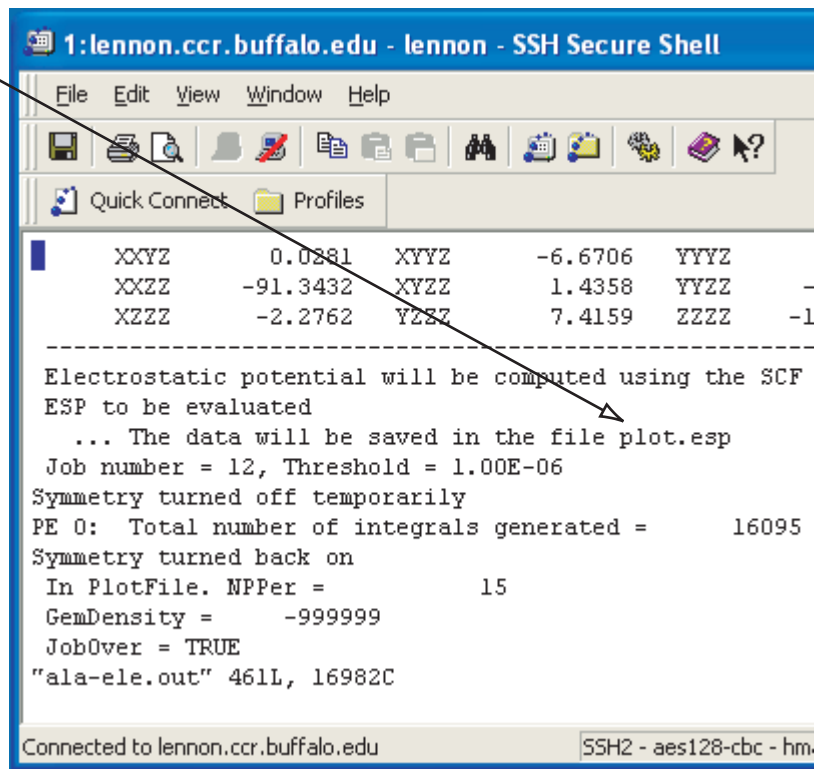
```
1: lennon.ccr.buffalo.edu - lennon* - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

ianlty                200      !
igdesp                -1      ! electrostatic pot
mem_static            512      ! Static memory
mem_total             2000     ! Total memory
$end

$plots
Electrostatic potential on a grid
1 5.0 5.0
1 5.0 5.0
1 5.0 5.0
0 0 0 0
0
$end
ala-ele.in" 37L, 942C
Connected to lennon.ccr.buffalo.edu
```


QM electrostatic potential of alanine

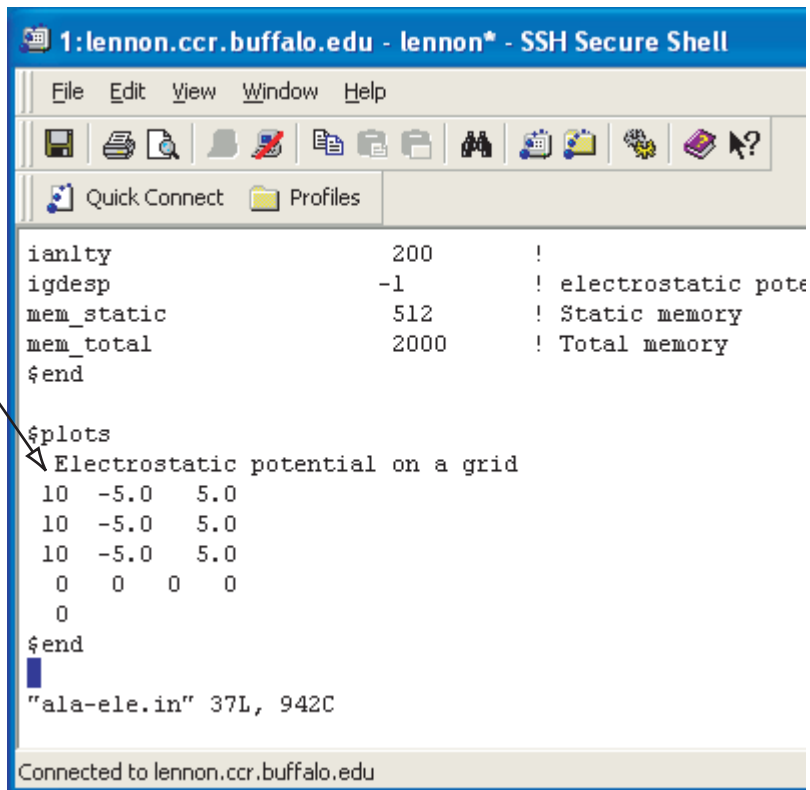
Results are written in
the plot.esp file



```
1:lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
XYZ 0.0281 XYZ -6.6706 YYZ
XXZZ -91.3432 XYZ 1.4358 YYZZ -
XZZZ -2.2762 YZZ 7.4159 ZZZZ -1
-----
Electrostatic potential will be computed using the SCF
ESP to be evaluated
... The data will be saved in the file plot.esp
Job number = 12, Threshold = 1.00E-06
Symmetry turned off temporarily
PE 0: Total number of integrals generated = 16095
Symmetry turned back on
In PlotFile. NPPer = 15
GemDensity = -999999
JobOver = TRUE
"ala-ele.out" 461L, 16982C
Connected to lennon.ccr.buffalo.edu SSH2 - aes128-cbc - hm.
```


QM electrostatic potential of alanine

Three dimensional grid
definition



```
1:lennon.ccr.buffalo.edu - lennon* - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Open, Save, Print, Run, Stop, Help]
Quick Connect Profiles

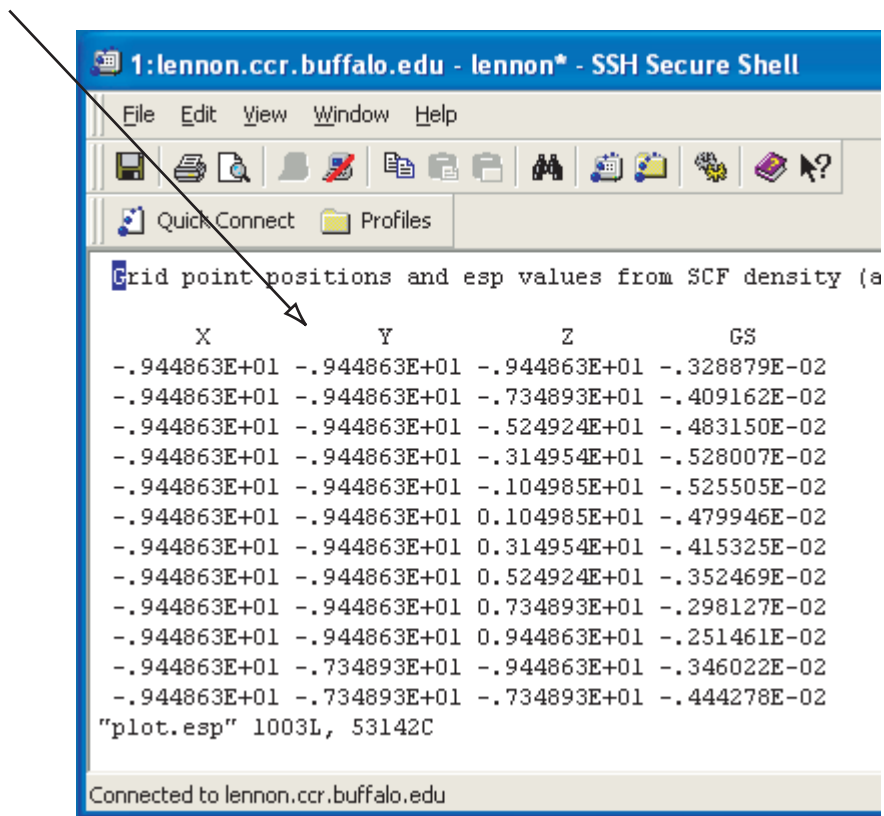
ianlty                200      !
igdesp                -1       ! electrostatic pote
mem_static            512      ! Static memory
mem_total             2000     ! Total memory
$end

$plots
Electrostatic potential on a grid
10 -5.0  5.0
10 -5.0  5.0
10 -5.0  5.0
0  0  0  0
0
$end
"ala-ele.in" 37L, 942C

Connected to lennon.ccr.buffalo.edu
```

QM electrostatic potential of alanine

Results of electrostatic potential grid calculations



```
1:lennon.ccr.buffalo.edu - lennon* - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

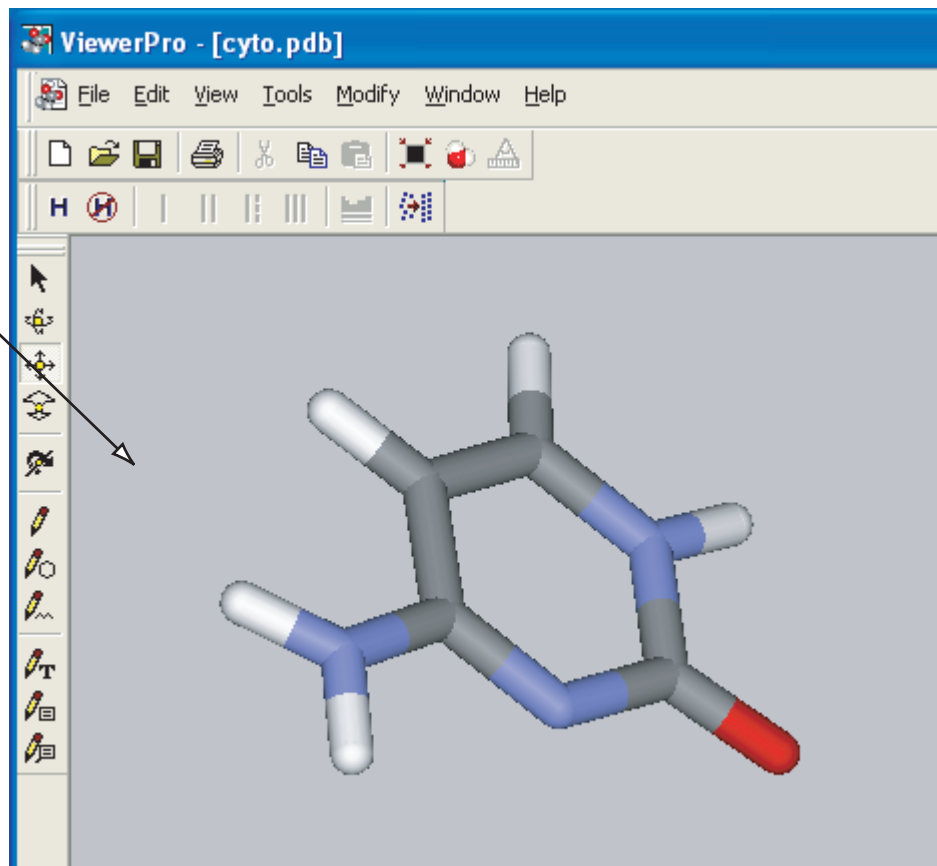
Grid point positions and esp values from SCF density (a

      X              Y              Z              GS
-.944863E+01 -.944863E+01 -.944863E+01 -.328879E-02
-.944863E+01 -.944863E+01 -.734893E+01 -.409162E-02
-.944863E+01 -.944863E+01 -.524924E+01 -.483150E-02
-.944863E+01 -.944863E+01 -.314954E+01 -.528007E-02
-.944863E+01 -.944863E+01 -.104985E+01 -.525505E-02
-.944863E+01 -.944863E+01  0.104985E+01 -.479946E-02
-.944863E+01 -.944863E+01  0.314954E+01 -.415325E-02
-.944863E+01 -.944863E+01  0.524924E+01 -.352469E-02
-.944863E+01 -.944863E+01  0.734893E+01 -.298127E-02
-.944863E+01 -.944863E+01  0.944863E+01 -.251461E-02
-.944863E+01 -.734893E+01 -.944863E+01 -.346022E-02
-.944863E+01 -.734893E+01 -.734893E+01 -.444278E-02
"plot.esp" 1003L, 53142C

Connected to lennon.ccr.buffalo.edu
```

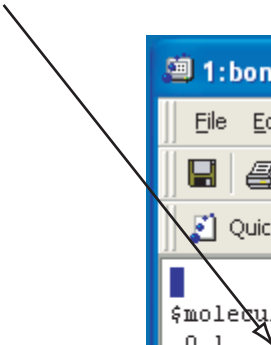
QM geometry optimization of cytosine

Initial geometry of
cytosine



QM geometry optimization of cytosine

Initial geometry of
cytosine



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
$ molecule
O 1
H -24.740 28.764 104.076
N -24.228 29.262 104.873
C -22.885 29.324 104.812
H -22.265 28.993 103.942
C -22.246 29.750 105.940
H -21.163 29.800 105.934
C -22.952 30.269 107.035
N -22.447 30.614 108.183
H -22.864 31.344 108.756
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5
```

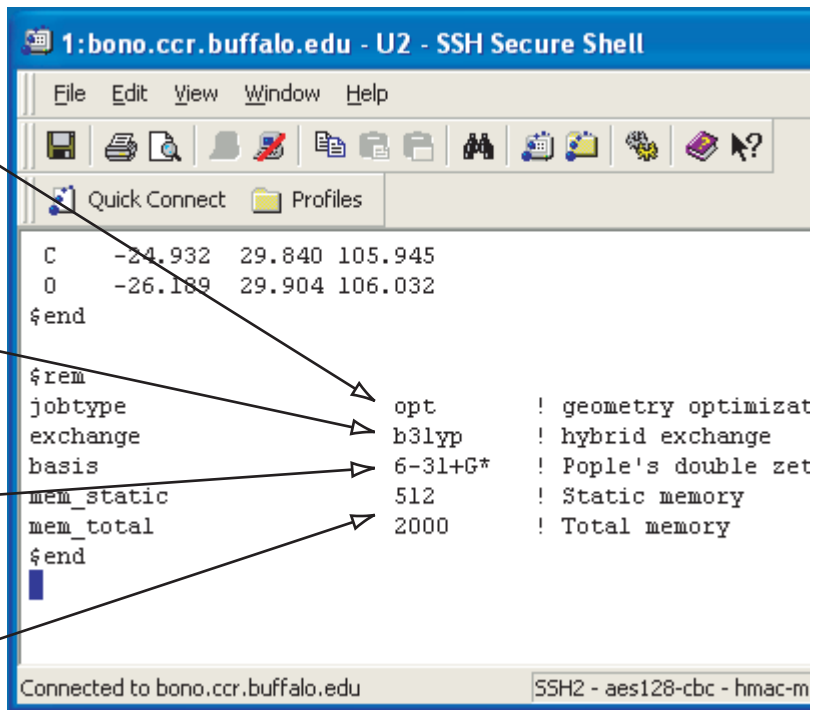

QM geometry optimization of cytosine

Geometry optimization

Hamiltonian

Basis set

Memory allocation



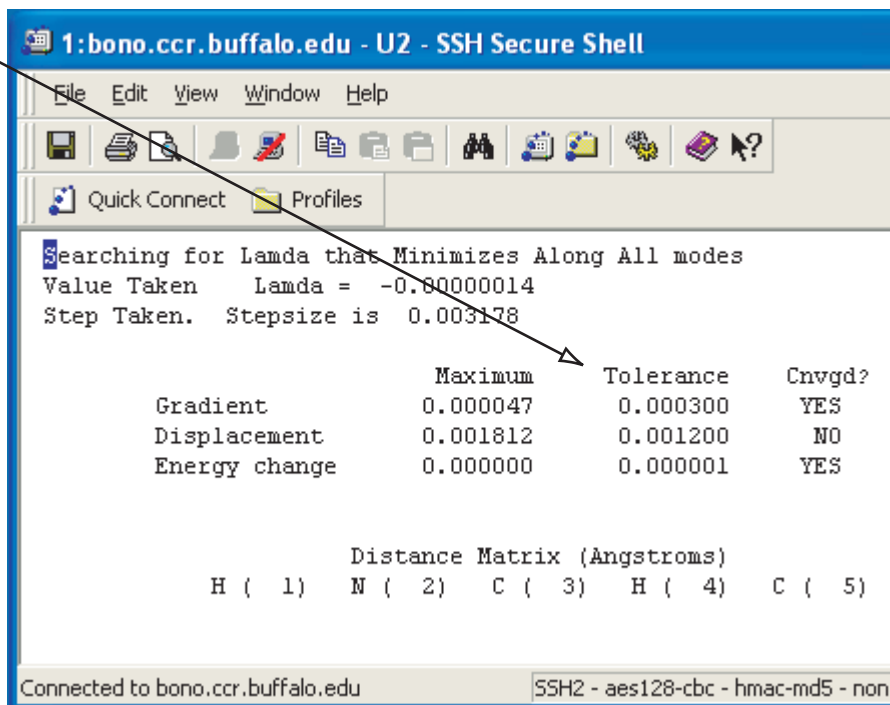
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
C -24.932 29.840 105.945
O -26.189 29.904 106.032
$end

$rem
jobtype opt ! geometry optimizat
exchange b3lyp ! hybrid exchange
basis 6-31+G* ! Pople's double zet
mem_static 512 ! Static memory
mem_total 2000 ! Total memory
$end
█

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-m
```

QM geometry optimization of cytosine

Geometry optimization
is converged



```
1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

Searching for Lamda that Minimizes Along All modes
Value Taken Lamda = -0.80000014
Step Taken. Stepsize is 0.003178

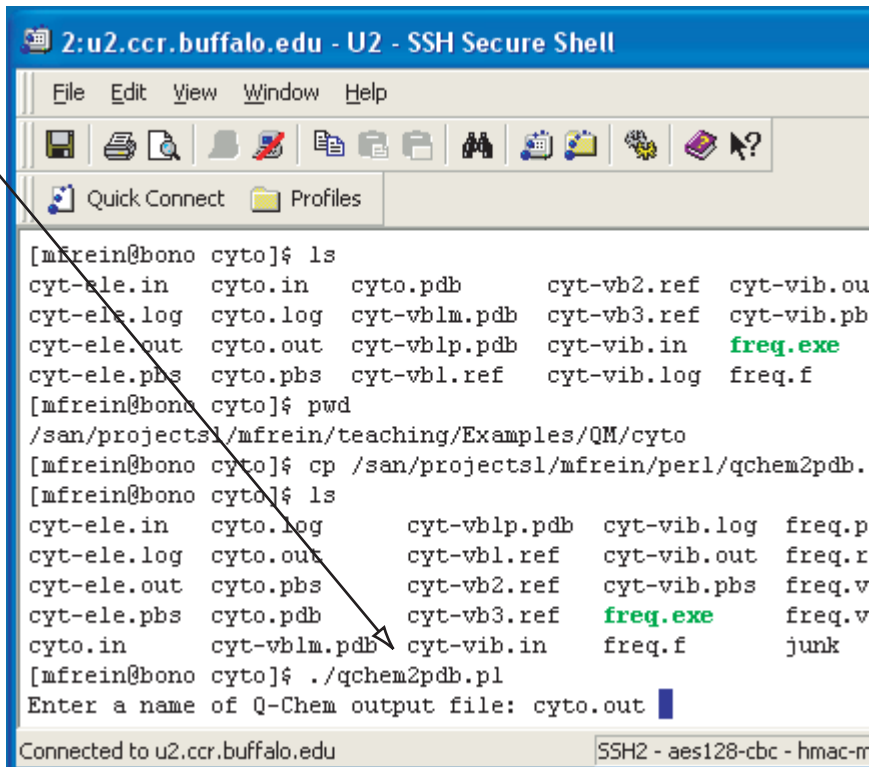
      Maximum      Tolerance      Convgd?
Gradient      0.000047      0.000300      YES
Displacement  0.001812      0.001200      NO
Energy change 0.000000      0.000001      YES

      Distance Matrix (Angstroms)
H ( 1)  N ( 2)  C ( 3)  H ( 4)  C ( 5)

Connected to bono.ccr.buffalo.edu      SSH2 - aes128-cbc - hmac-md5 - non
```

QM geometry optimization of cytosine

Converting qchem
output into a PDB file



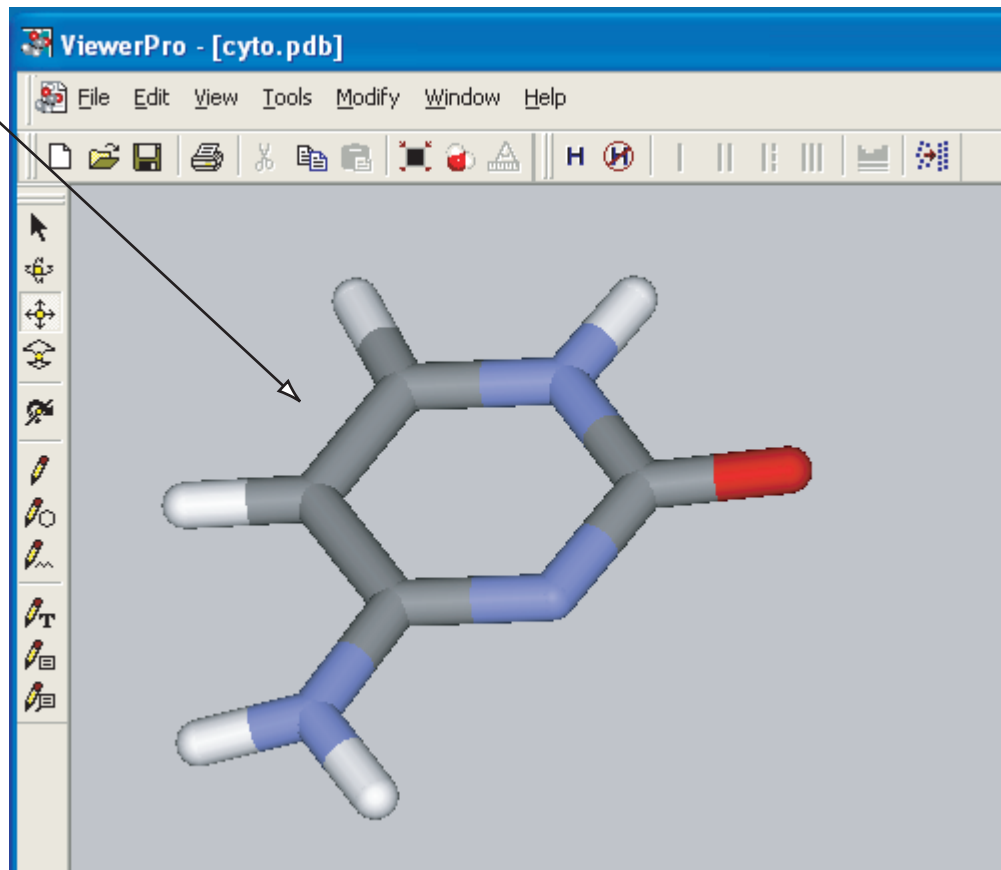
The screenshot shows an SSH terminal window titled "2:u2.ccr.buffalo.edu - U2 - SSH Secure Shell". The terminal displays the following commands and output:

```
[mfrein@bono cyto]$ ls
cyt-ele.in  cyto.in  cyto.pdb  cyt-vb2.ref  cyt-vib.ou
cyt-ele.log cyto.log  cyt-vblm.pdb  cyt-vb3.ref  cyt-vib.pb
cyt-ele.out cyto.out  cyt-vb1p.pdb  cyt-vib.in  freq.exe
cyt-ele.pbs cyto.pbs  cyt-vbl.ref  cyt-vib.log  freq.f
[mfrein@bono cyto]$ pwd
/san/projects1/mfrein/teaching/Examples/QM/cyto
[mfrein@bono cyto]$ cp /san/projects1/mfrein/perl/qchem2pdb.
[mfrein@bono cyto]$ ls
cyt-ele.in  cyto.log  cyt-vb1p.pdb  cyt-vib.log  freq.p
cyt-ele.log cyto.out  cyt-vbl.ref  cyt-vib.out  freq.r
cyt-ele.out cyto.pbs  cyt-vb2.ref  cyt-vib.pbs  freq.v
cyt-ele.pbs cyto.pdb  cyt-vb3.ref  freq.exe    freq.v
cyto.in     cyt-vblm.pdb  cyt-vib.in  freq.f      junk
[mfrein@bono cyto]$ ./qchem2pdb.pl
Enter a name of Q-Chem output file: cyto.out
```

The terminal window includes a menu bar (File, Edit, View, Window, Help) and a toolbar with icons for file operations. The status bar at the bottom indicates "Connected to u2.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-sha1".

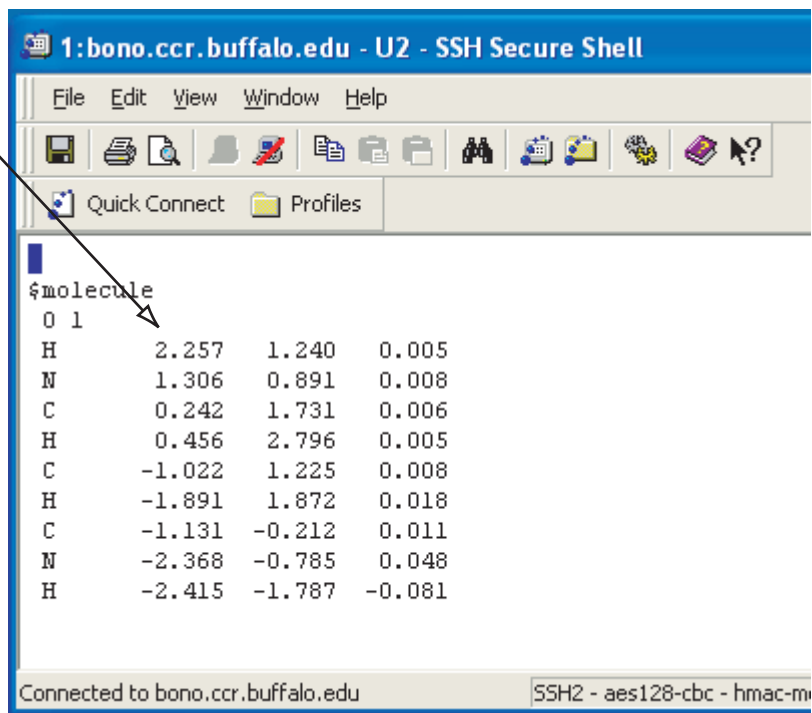
QM geometry optimization of cytosine

Final geometry of
cytosine



QM molecular oscillations of cytosine

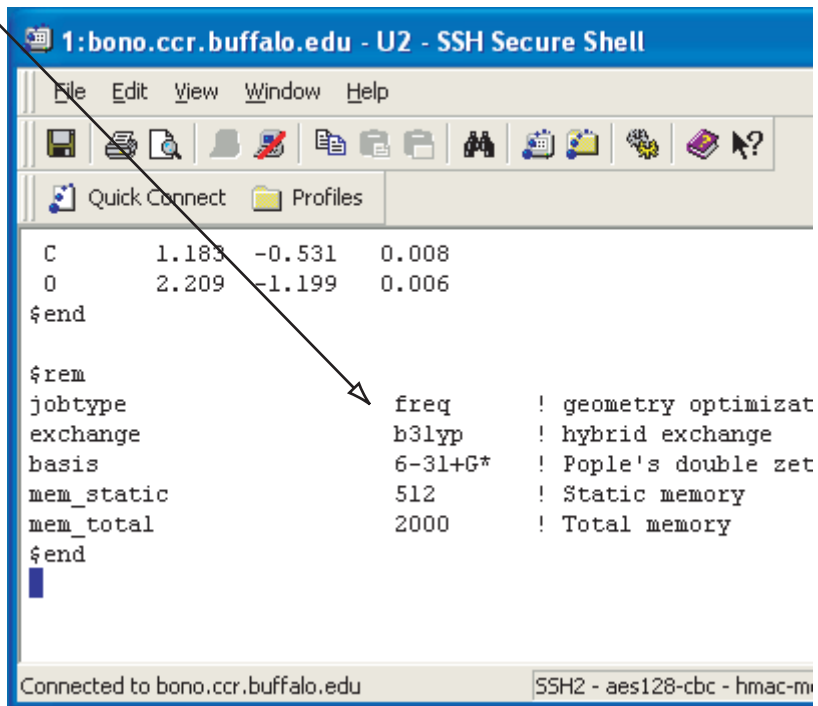
Coordinates after
geometry optimization



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
$ molecule
O 1
H      2.257   1.240   0.005
N      1.306   0.891   0.008
C      0.242   1.731   0.006
H      0.456   2.796   0.005
C     -1.022   1.225   0.008
H     -1.891   1.872   0.018
C     -1.131  -0.212   0.011
N     -2.368  -0.785   0.048
H     -2.415  -1.787  -0.081
Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-m
```

QM molecular oscillations of cytosine

Frequency calculations



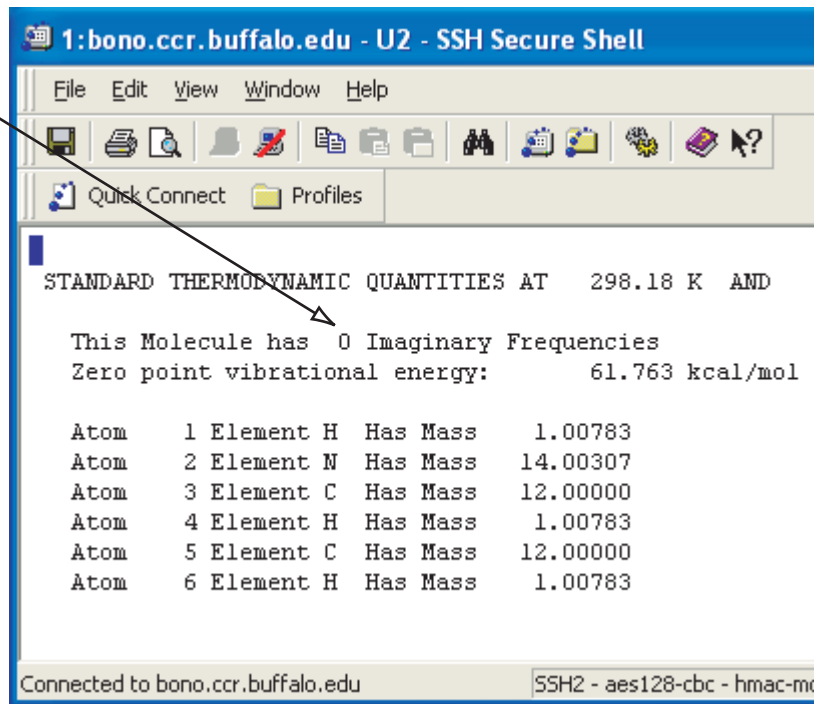
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
C      1.183  -0.531  0.008
O      2.209  -1.199  0.006
$end

$rem
jobtype          freq      ! geometry optimizat
exchange         b3lyp     ! hybrid exchange
basis            6-31+G*   ! Pople's double zet
mem_static       512       ! Static memory
mem_total        2000      ! Total memory
$end
█

Connected to bono.ccr.buffalo.edu      SSH2 - aes128-cbc - hmac-m
```

QM molecular oscillations of cytosine

Calculations are finished
correctly



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

STANDARD THERMODYNAMIC QUANTITIES AT 298.18 K AND

This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 61.763 kcal/mol

Atom 1 Element H Has Mass 1.00783
Atom 2 Element N Has Mass 14.00307
Atom 3 Element C Has Mass 12.00000
Atom 4 Element H Has Mass 1.00783
Atom 5 Element C Has Mass 12.00000
Atom 6 Element H Has Mass 1.00783

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-mk
```

QM molecular oscillations of cytosine


Frequency (cm⁻¹)

IR Intensity

Atomic
displacements

1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell

File Edit View Window Help



Quick Connect Profiles

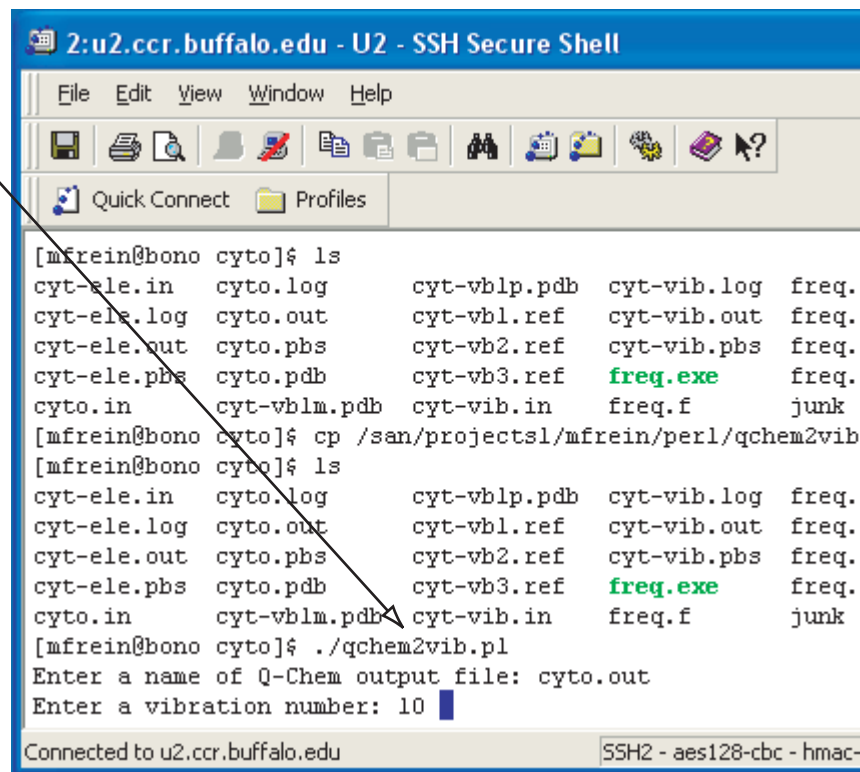
Mode:	19	20				
Frequency:	1143.81	1228.29				
Force Cnst:	1.1814	1.2325				
Red. Mass:	1.5326	1.3866				
IR Active:	YES	YES				
IR Intens:	2.870	50.156				
Raman Active:	YES	YES				
	X	Y	Z	X	Y	Z
H	-0.263	0.396	-0.001	-0.203	0.497	-0.001
N	-0.123	0.064	0.000	-0.037	0.082	0.000
C	0.003	-0.102	0.001	0.086	-0.058	-0.001

Connected to bono.ccr.buffalo.edu

SSH2 - aes128-cbc - hmac-md5

QM molecular oscillations of cytosine

Generating two pdb files
of a molecular oscillation
from q-chem output

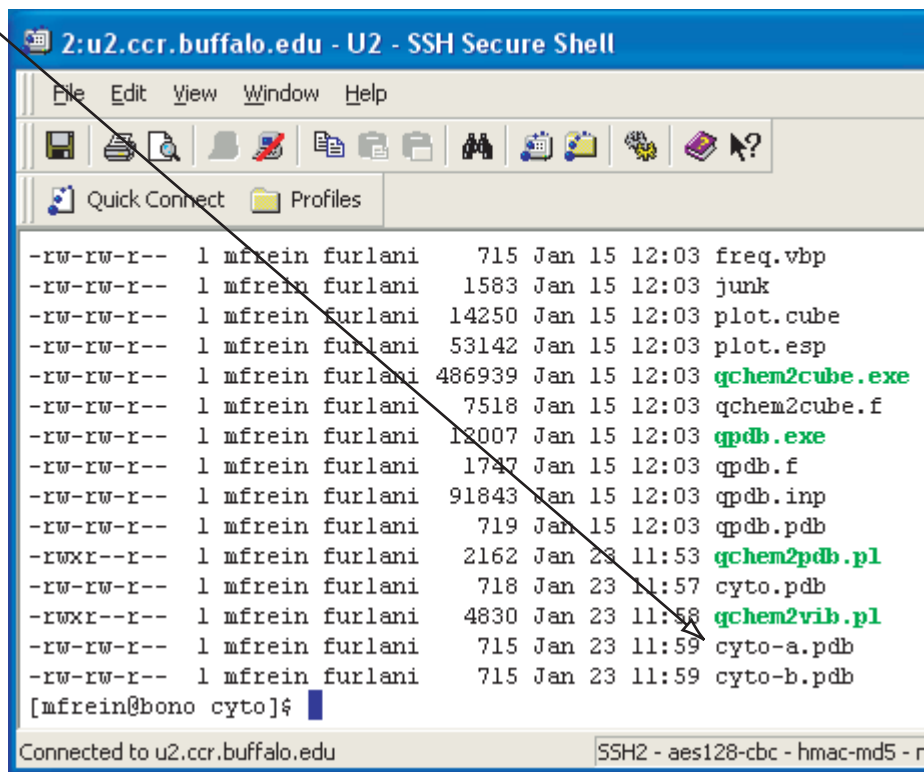


```
2:u2.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

[mfrein@bono cyto]$ ls
cyt-ele.in  cyto.log      cyt-vb1p.pdb  cyt-vib.log  freq.
cyt-ele.log cyto.out      cyt-vb1.ref   cyt-vib.out  freq.
cyt-ele.out cyto.pbs      cyt-vb2.ref   cyt-vib.pbs  freq.
cyt-ele.pbs cyto.pdb      cyt-vb3.ref   freq.exe     freq.
cyto.in     cyt-vb1m.pdb  cyt-vib.in    freq.f       junk
[mfrein@bono cyto]$ cp /san/projects1/mfrein/perl/qchem2vib
[mfrein@bono cyto]$ ls
cyt-ele.in  cyto.log      cyt-vb1p.pdb  cyt-vib.log  freq.
cyt-ele.log cyto.out      cyt-vb1.ref   cyt-vib.out  freq.
cyt-ele.out cyto.pbs      cyt-vb2.ref   cyt-vib.pbs  freq.
cyt-ele.pbs cyto.pdb      cyt-vb3.ref   freq.exe     freq.
cyto.in     cyt-vb1m.pdb  cyt-vib.in    freq.f       junk
[mfrein@bono cyto]$ ./qchem2vib.pl
Enter a name of Q-Chem output file: cyto.out
Enter a vibration number: 10
Connected to u2.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-
```

QM molecular oscillations of cytosine

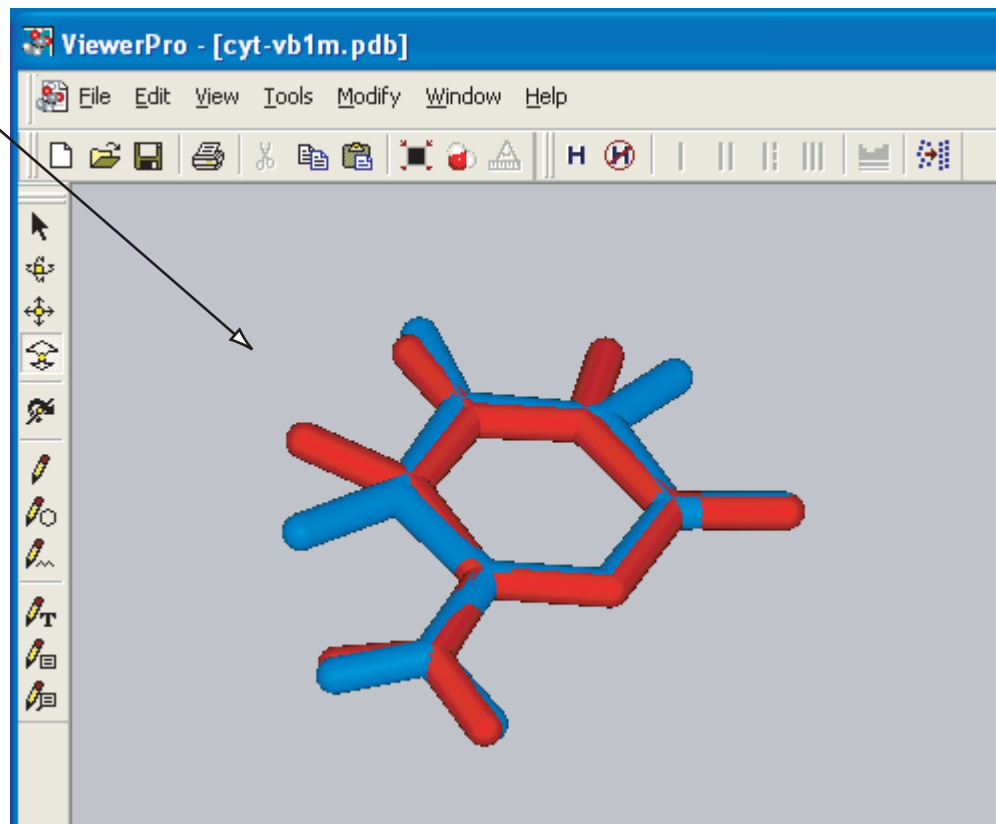
The program generates
two PDB files of two
phases of the oscillation



```
2:u2.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
-rw-rw-r-- 1 mfrein furlani 715 Jan 15 12:03 freq.vbp
-rw-rw-r-- 1 mfrein furlani 1583 Jan 15 12:03 junk
-rw-rw-r-- 1 mfrein furlani 14250 Jan 15 12:03 plot.cube
-rw-rw-r-- 1 mfrein furlani 53142 Jan 15 12:03 plot.esp
-rw-rw-r-- 1 mfrein furlani 486939 Jan 15 12:03 qchem2cube.exe
-rw-rw-r-- 1 mfrein furlani 7518 Jan 15 12:03 qchem2cube.f
-rw-rw-r-- 1 mfrein furlani 12007 Jan 15 12:03 qpdb.exe
-rw-rw-r-- 1 mfrein furlani 1747 Jan 15 12:03 qpdb.f
-rw-rw-r-- 1 mfrein furlani 91843 Jan 15 12:03 qpdb.inp
-rw-rw-r-- 1 mfrein furlani 719 Jan 15 12:03 qpdb.pdb
-rwxr--r-- 1 mfrein furlani 2162 Jan 23 11:53 qchem2pdb.pl
-rw-rw-r-- 1 mfrein furlani 718 Jan 23 11:57 cyto.pdb
-rwxr--r-- 1 mfrein furlani 4830 Jan 23 11:58 qchem2vib.pl
-rw-rw-r-- 1 mfrein furlani 715 Jan 23 11:59 cyto-a.pdb
-rw-rw-r-- 1 mfrein furlani 715 Jan 23 11:59 cyto-b.pdb
[mfrein@bono cyto]$
Connected to u2.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - r
```

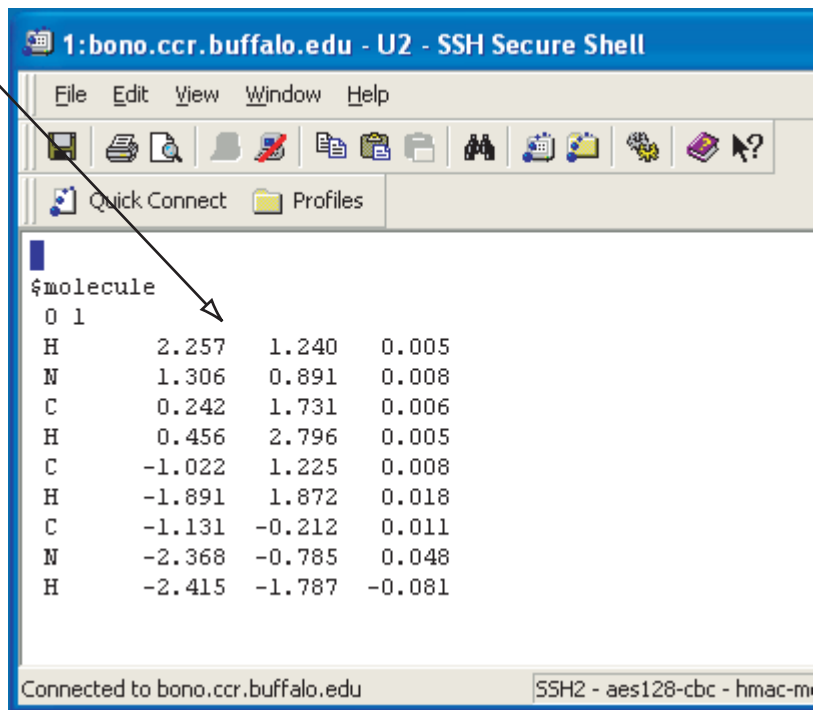
QM molecular oscillations of cytosine

Visualization of the
molecular
oscillation



QM electrostatic potential of cytosine

Optimal coordinates after
geometry optimization



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

$ molecule
0 1
H      2.257   1.240   0.005
N      1.306   0.891   0.008
C      0.242   1.731   0.006
H      0.456   2.796   0.005
C     -1.022   1.225   0.008
H     -1.891   1.872   0.018
C     -1.131  -0.212   0.011
N     -2.368  -0.785   0.048
H     -2.415  -1.787  -0.081

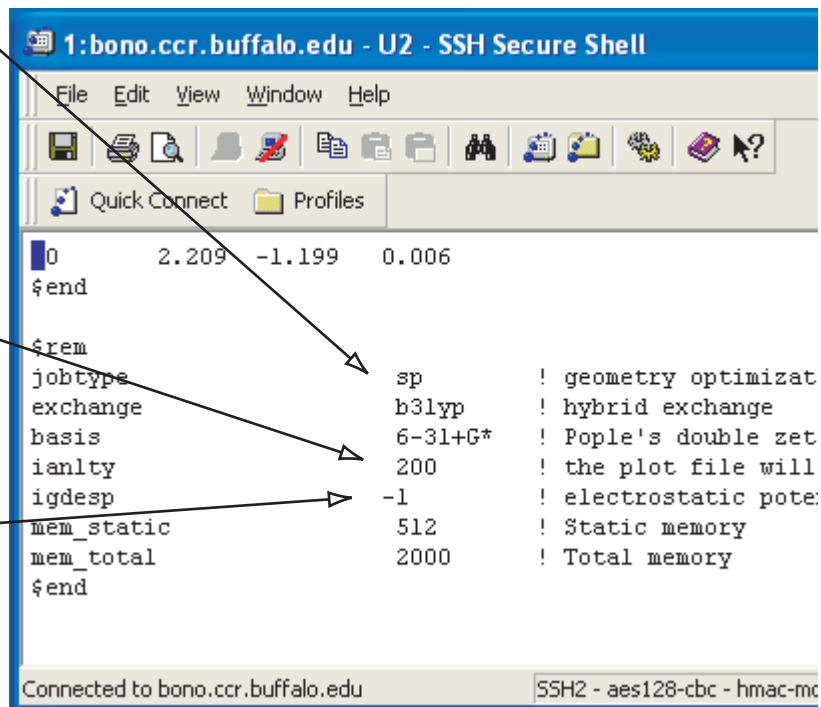
Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-m
```

QM electrostatic potential of cytosine

Single point calculations
(no geometry optimization)

Generating the
plot file

Generating the
electrostatic
potential



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

0      2.209  -1.199   0.006
$end

$rem
jobtype      sp          ! geometry optimizat
exchange     b3lyp       ! hybrid exchange
basis        6-31+G*     ! Pople's double zet
ianlty       200         ! the plot file will
igdesp       -1          ! electrostatic pote
mem_static   512         ! Static memory
mem_total    2000        ! Total memory
$end

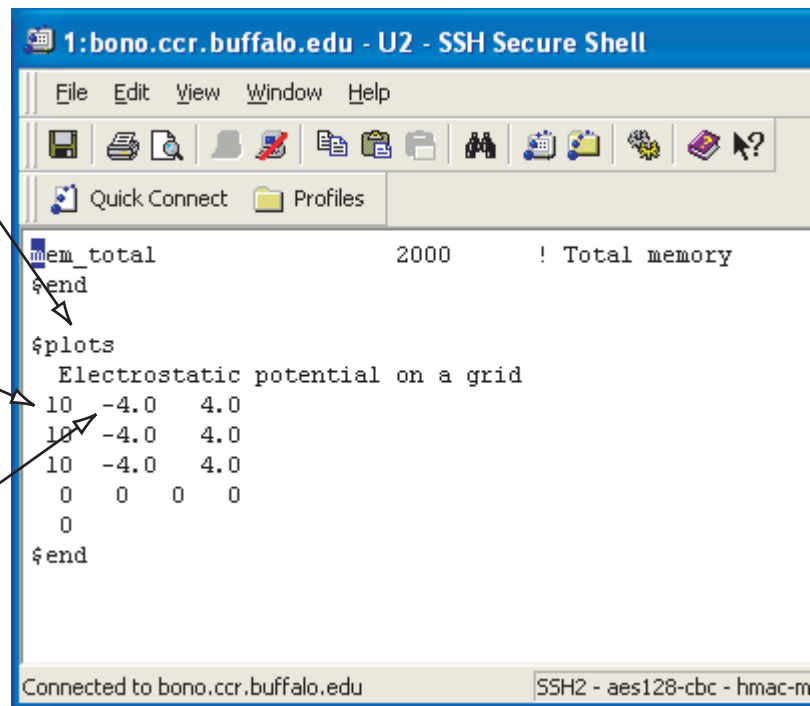
Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-mc
```

QM electrostatic potential of cytosine

Details of the plot
calculations

Number of points
in the x direction

Minimum and maximum
values of the grid in the
x direction



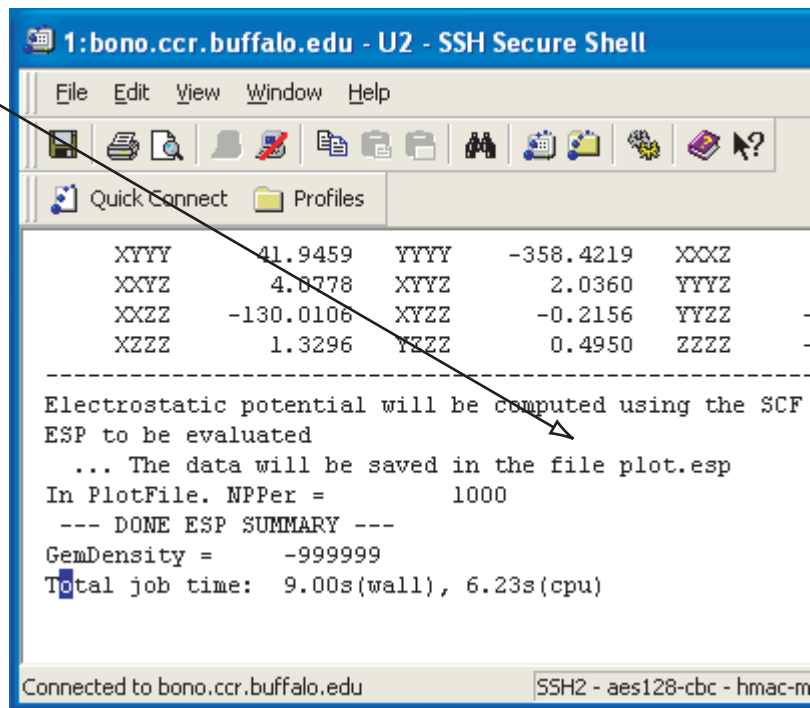
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
mem_total                2000      ! Total memory
$end

$plots
Electrostatic potential on a grid
10 -4.0  4.0
10 -4.0  4.0
10 -4.0  4.0
0  0  0  0
0
$end

Connected to bono.ccr.buffalo.edu      SSH2 - aes128-cbc - hmac-m
```

QM electrostatic potential of cytosine

Results of the grid calculations are written in the plot.esp file



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
-----
      XYYY      41.9459      YYYY      -358.4219      XXXZ
      XXYZ       4.8778      XXYZ       2.0360      YYYZ
      XXZZ     -130.0106      XZZZ      -0.2156      YYZZ      -
      XZZZ       1.3296      YZZZ       0.4950      ZZZZ      -
-----
Electrostatic potential will be computed using the SCF
ESP to be evaluated
... The data will be saved in the file plot.esp
In PlotFile. NPPer =          1000
--- DONE ESP SUMMARY ---
GemDensity =      -999999
Total job time:  9.00s(wall), 6.23s(cpu)
-----
Connected to bono.ccr.buffalo.edu      SSH2 - aes128-cbc - hmac-m
```

QM electrostatic potential of cytosine

Executing the
converting
program

```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

cyt-ele.in  cyt-ele.pbs  cyto.out  cyt-vib.in  cyt-vib.pbs  qchem2cu
cyt-ele.log cyto.in      cyto.pbs  cyt-vib.log plot.cube    qchem2cu
cyt-ele.out cyto.log     cyto.pdb  cyt-vib.out plot.esp     qpdb.exe
[mfrein@bono cyto]$ module load intel
intel/9.0(36):ERROR:150: Module 'intel/9.0' conflicts with the current
'intel/8.1'
intel/9.0(36):ERROR:102: Tcl command execution failed: conflict intel/

[mfrein@bono cyto]$ ls
cyt-ele.in  cyt-ele.pbs  cyto.out  cyt-vib.in  cyt-vib.pbs  qchem2cu
cyt-ele.log cyto.in      cyto.pbs  cyt-vib.log plot.cube    qchem2cu
cyt-ele.out cyto.log     cyto.pdb  cyt-vib.out plot.esp     qpdb.exe
[mfrein@bono cyto]$ ./qchem2cube.exe l cyt-ele.out plot.esp plot.cube

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none  89x13
```

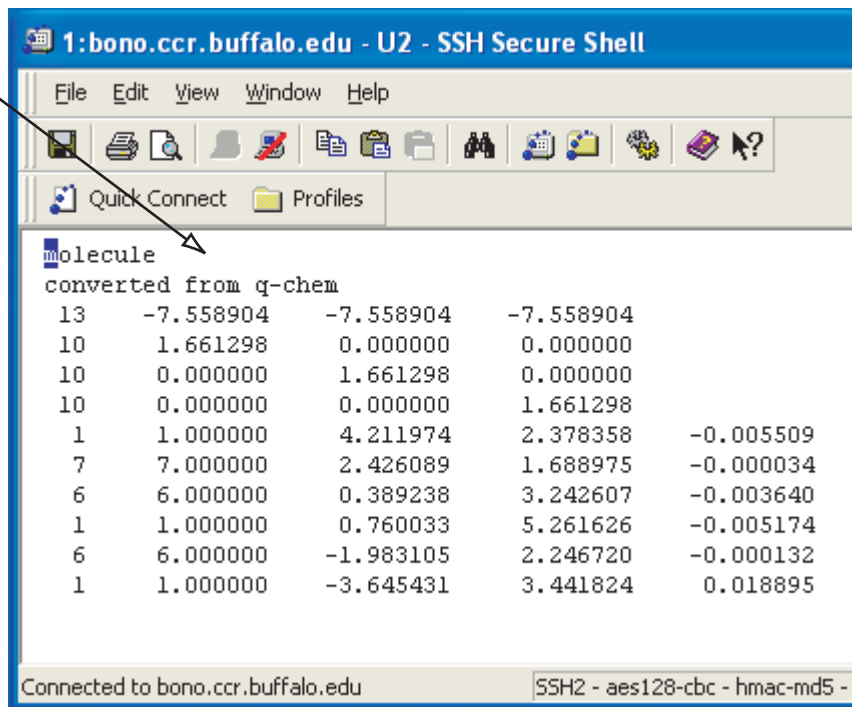
Output from
qchem

Plot file from
qchem

Cube file

QM electrostatic potential of cytosine

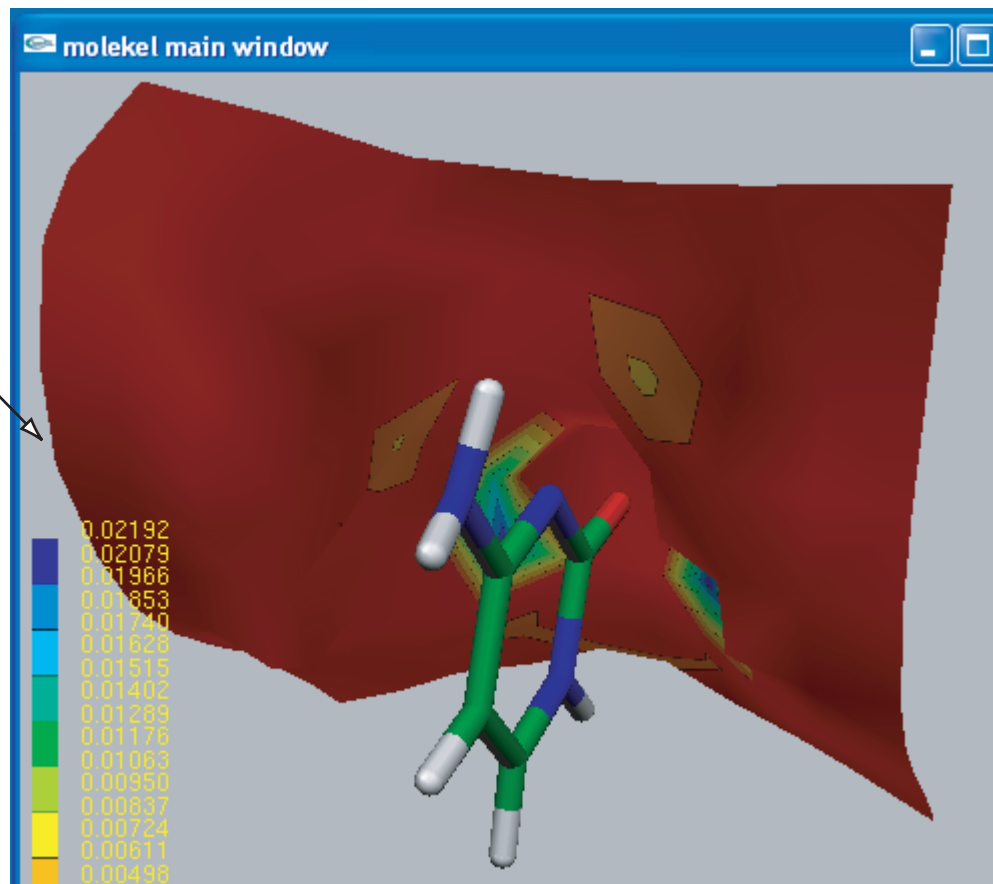
Cube file



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
molecule
converted from q-chem
13 -7.558904 -7.558904 -7.558904
10 1.661298 0.000000 0.000000
10 0.000000 1.661298 0.000000
10 0.000000 0.000000 1.661298
1 1.000000 4.211974 2.378358 -0.005509
7 7.000000 2.426089 1.688975 -0.000034
6 6.000000 0.389238 3.242607 -0.003640
1 1.000000 0.760033 5.261626 -0.005174
6 6.000000 -1.983105 2.246720 -0.000132
1 1.000000 -3.645431 3.441824 0.018895
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 -
```

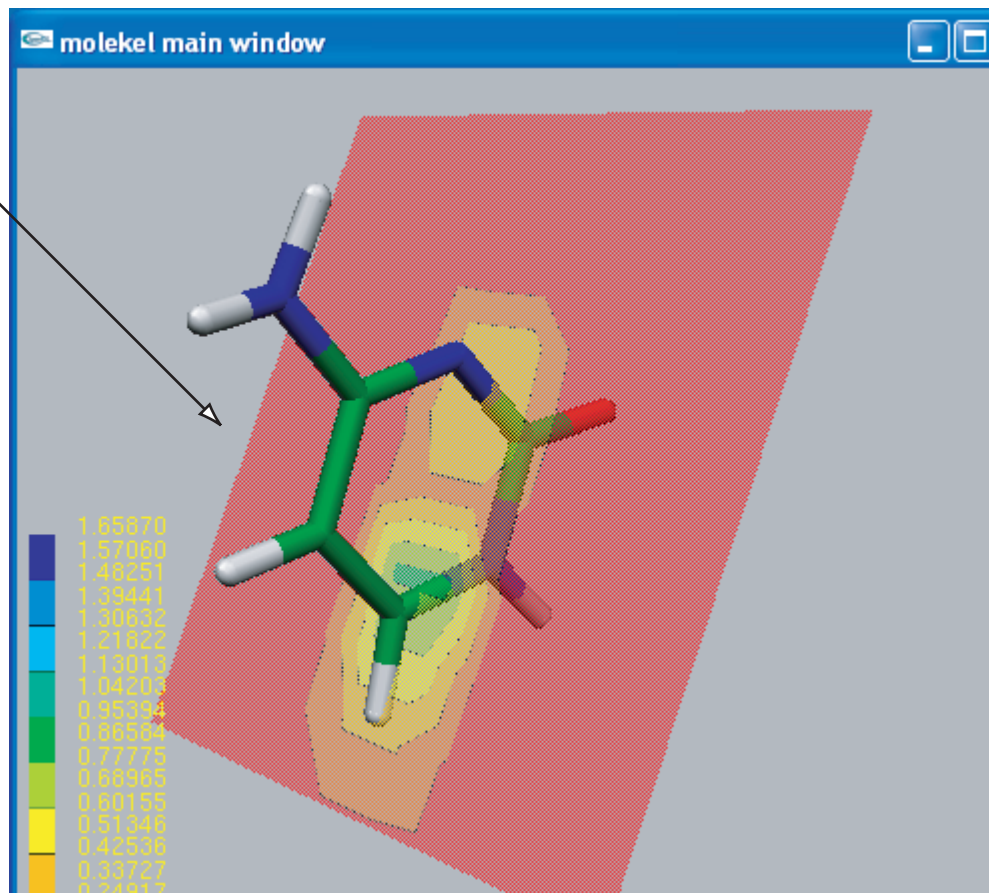
QM electrostatic potential of cytosine

Visualization of
the electrostatic
potential using
the Molekel
program



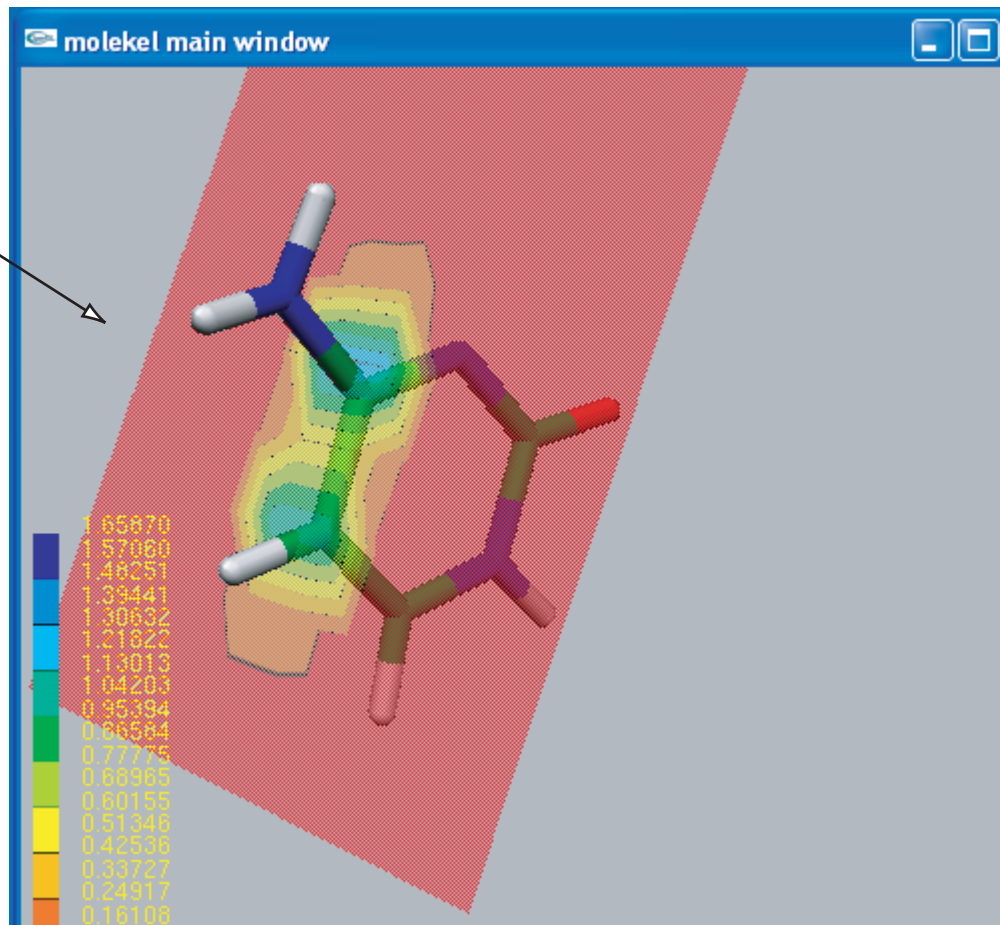
QM electrostatic potential of cytosine

Plane cut through
the electrostatic
potential



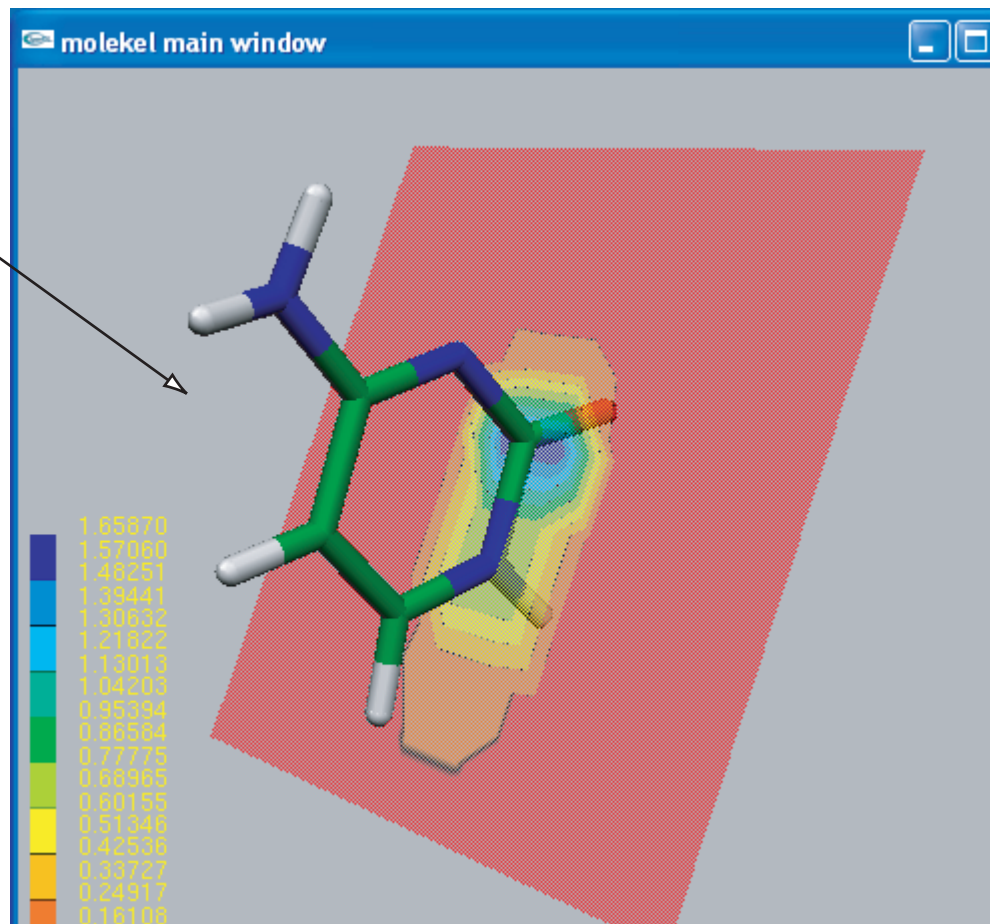
QM electrostatic potential of cytosine

Plane cut through
the electrostatic
potential



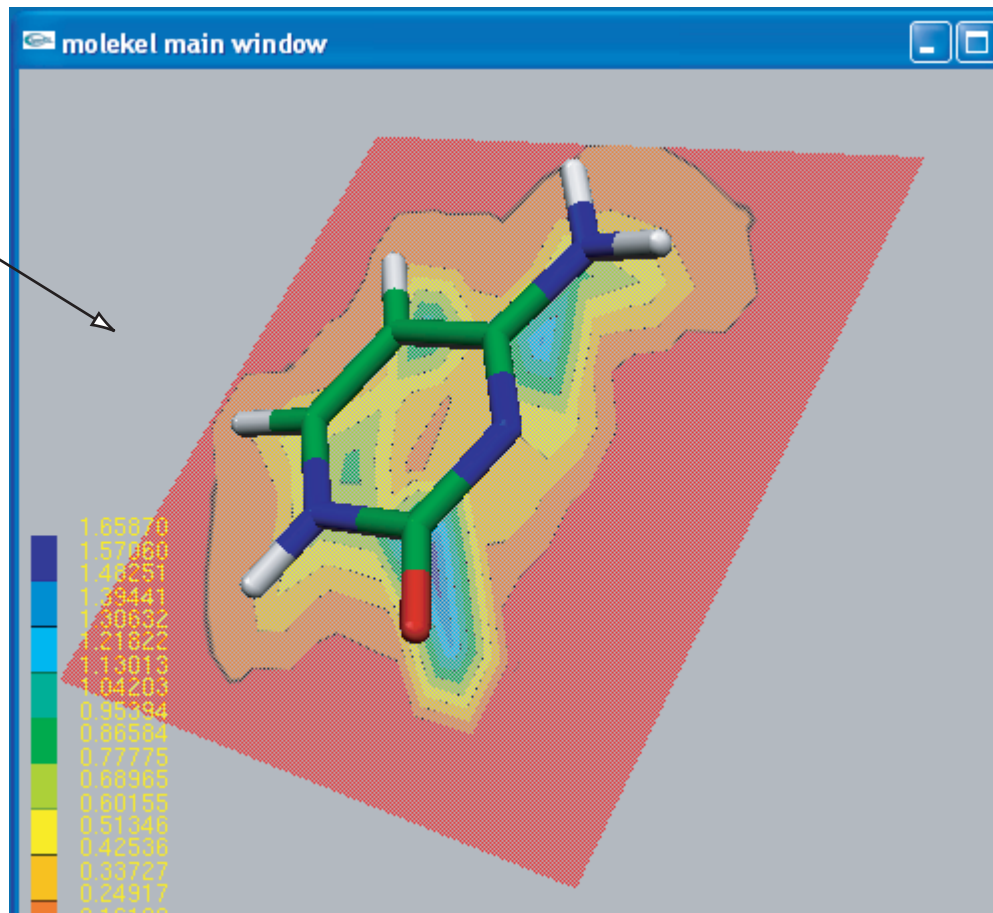
QM electrostatic potential of cytosine

Plane cut through
the electrostatic
potential



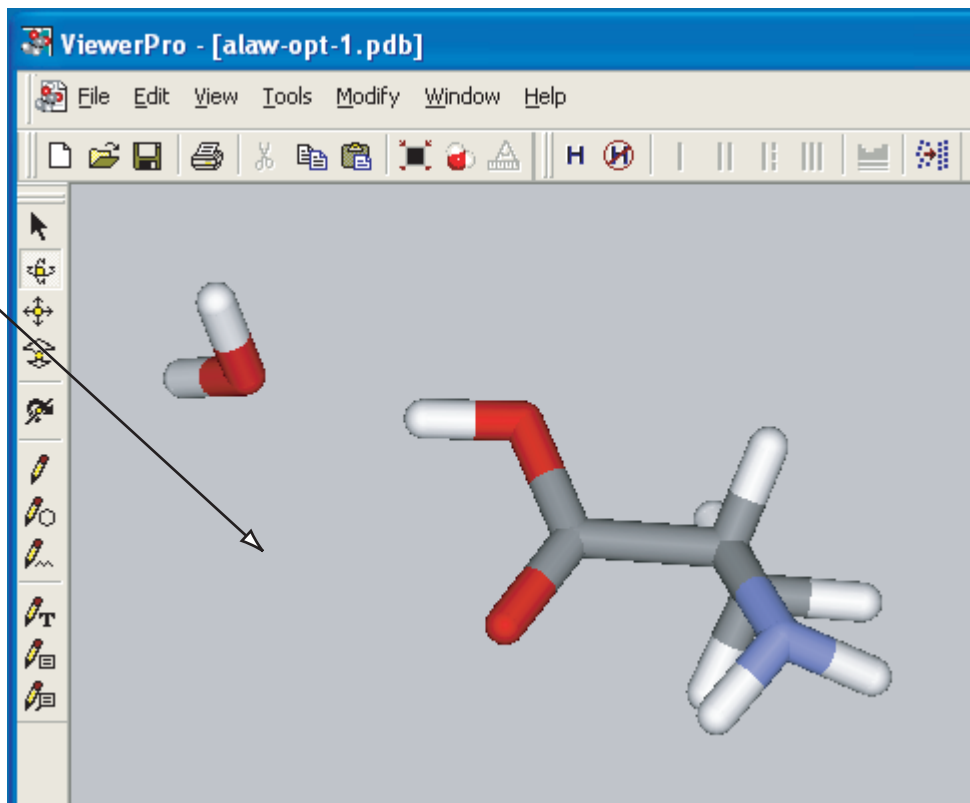
QM electrostatic potential of cytosine

Plane cut through
the electrostatic
potential



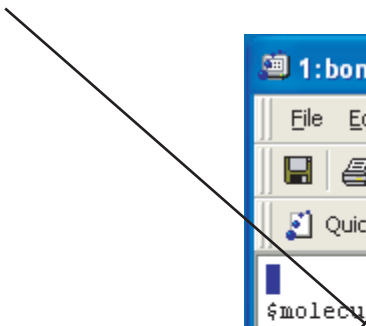
QM geometry optimization of alanine and water

Initial geometry
of an alanine
and water dimer



QM geometry optimization of alanine and water

Initial coordinates of the dimer



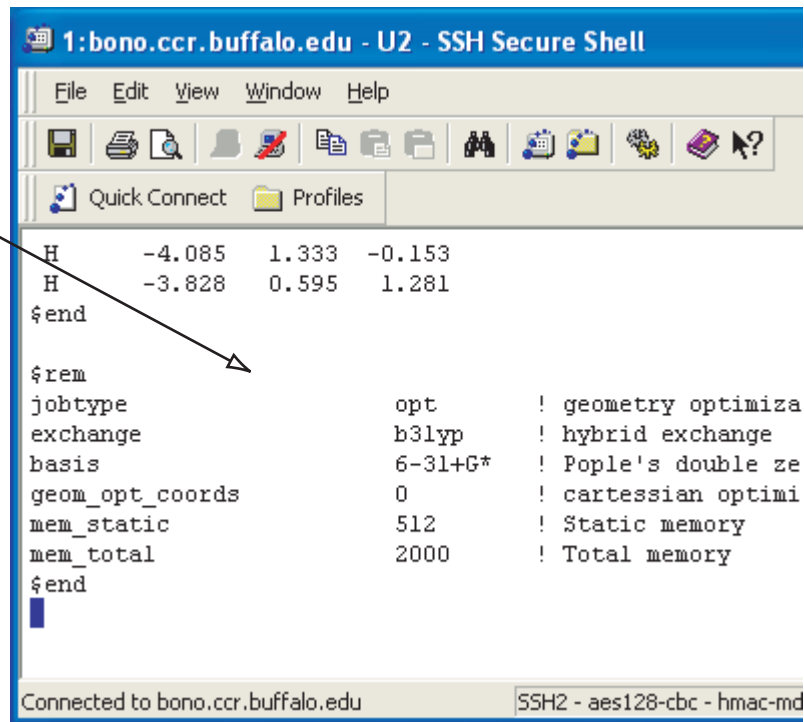
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

$ molecule
0 1
N      2.007  -1.174   0.295
H      3.010  -1.089   0.151
C      1.375   0.140   0.382
H      1.526   0.537   1.393
C      1.892   1.190  -0.631
H      1.730   0.848  -1.660
H      1.394   2.158  -0.495
H      2.968   1.340  -0.485
C     -0.123  -0.035   0.187
O     -0.616  -0.953  -0.459

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-mc
```


QM geometry optimization of alanine and water

Geometry optimization
using cartessian
coordinates



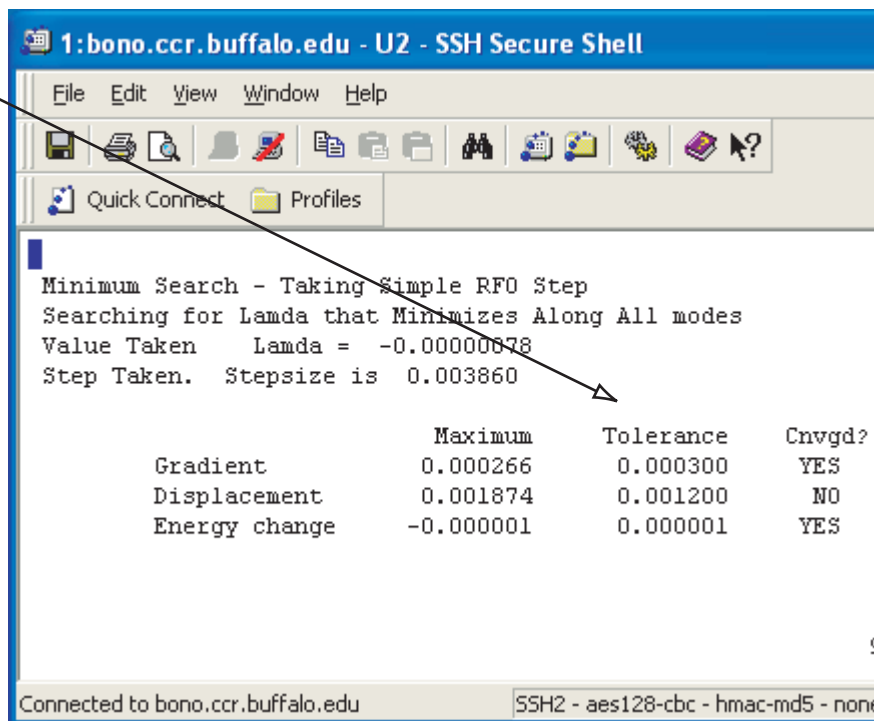
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
H      -4.085   1.333  -0.153
H      -3.828   0.595   1.281
$end

$rem
jobtype           opt      ! geometry optimiza
exchange          b3lyp    ! hybrid exchange
basis             6-31+G*   ! Pople's double ze
geom_opt_coords   0        ! cartessian optimi
mem_static        512      ! Static memory
mem_total         2000     ! Total memory
$end
█

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md
```

QM geometry optimization of alanine and water

Optimization
converged



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

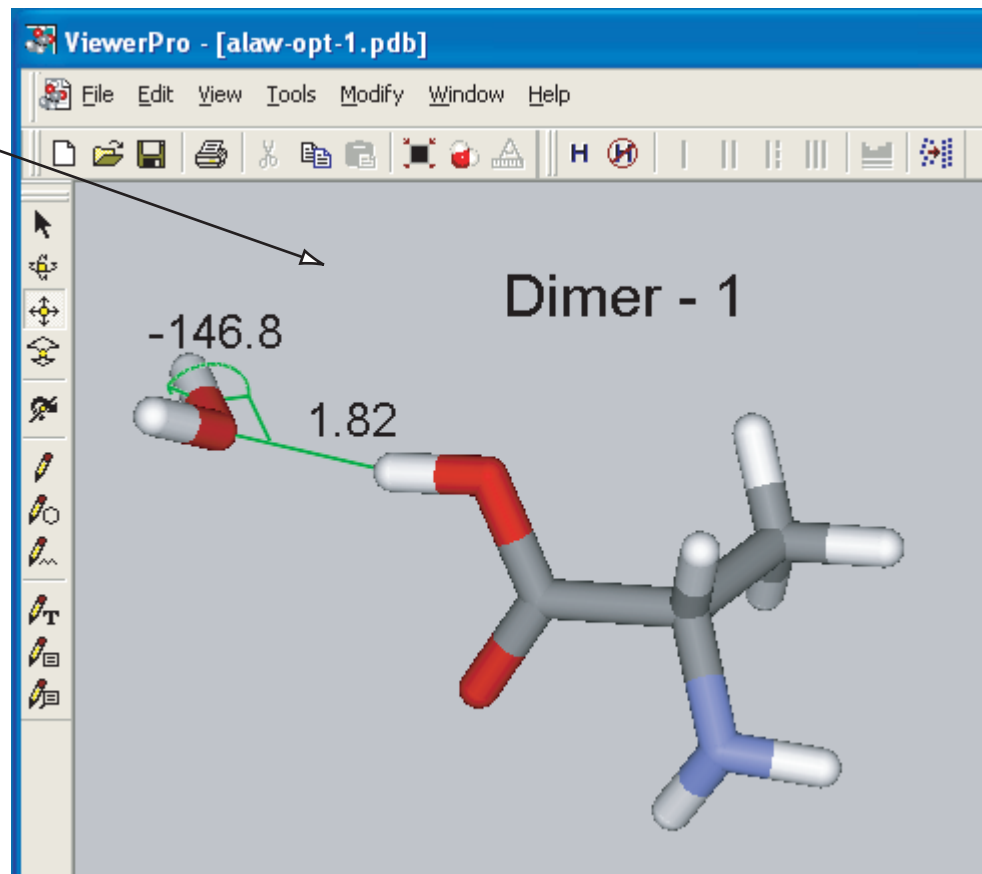
Minimum Search - Taking Simple RFO Step
Searching for Lamda that Minimizes Along All modes
Value Taken    Lamda = -0.00000678
Step Taken.    Stepsize is 0.003860

      Maximum    Tolerance    Cnvgd?
Gradient      0.000266      0.000300      YES
Displacement  0.001874      0.001200      NO
Energy change -0.000001      0.000001      YES

Connected to bono.ccr.buffalo.edu    SSH2 - aes128-cbc - hmac-md5 - none
```

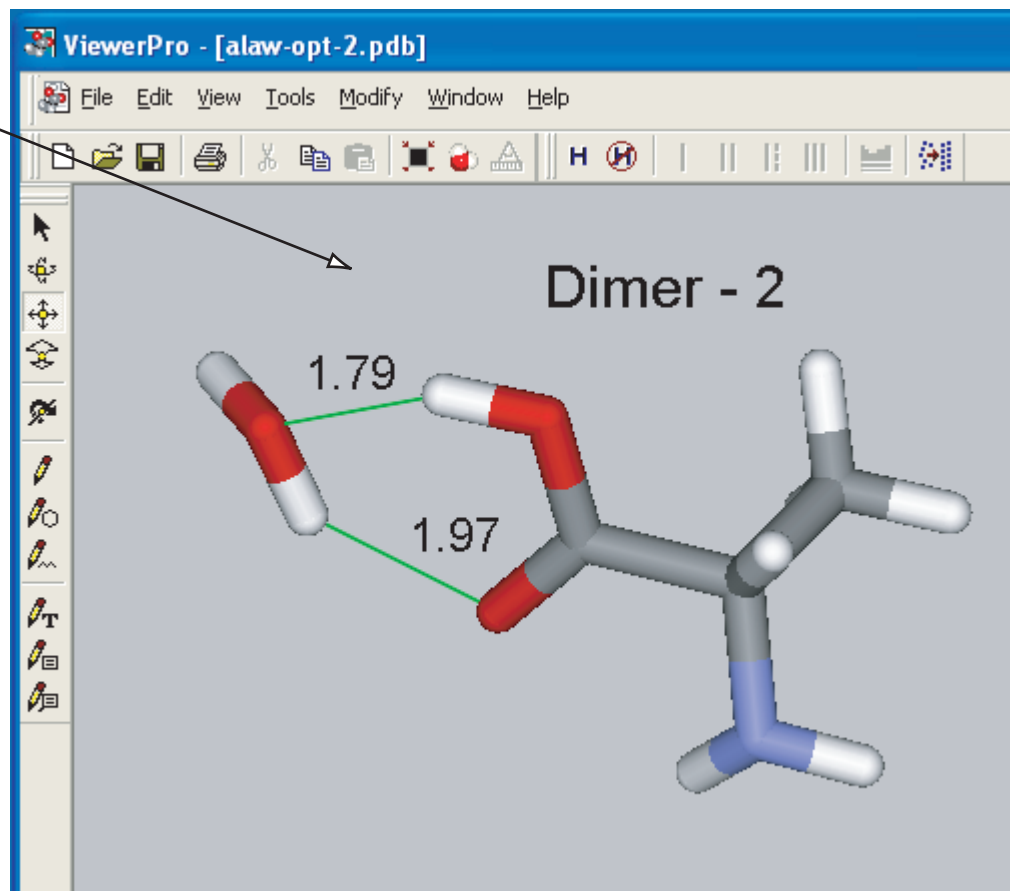
QM geometry optimization of alanine and water

Geometrical
parameters of
the dimer -1



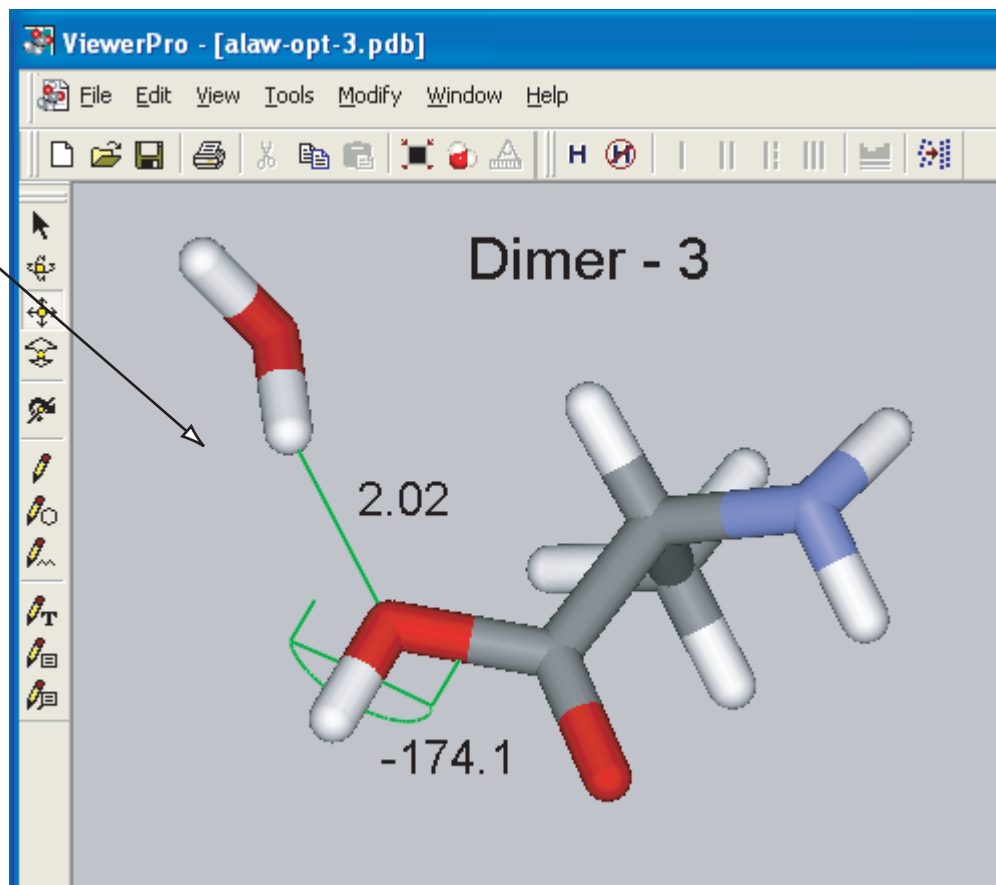
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 2



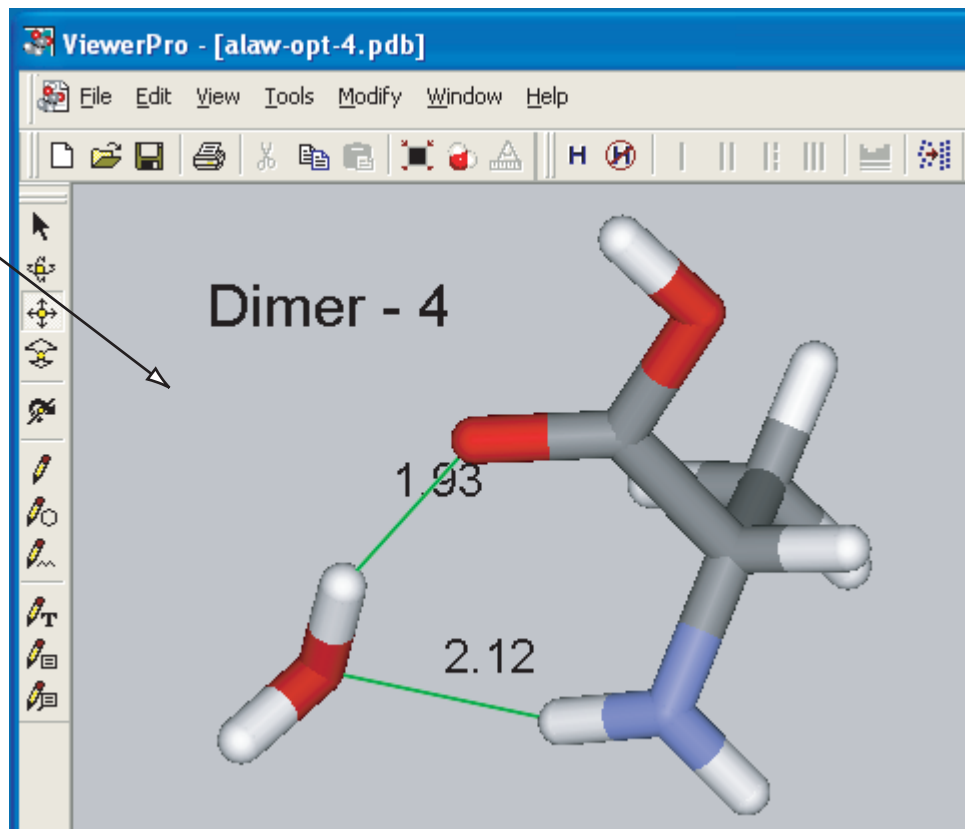
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 3



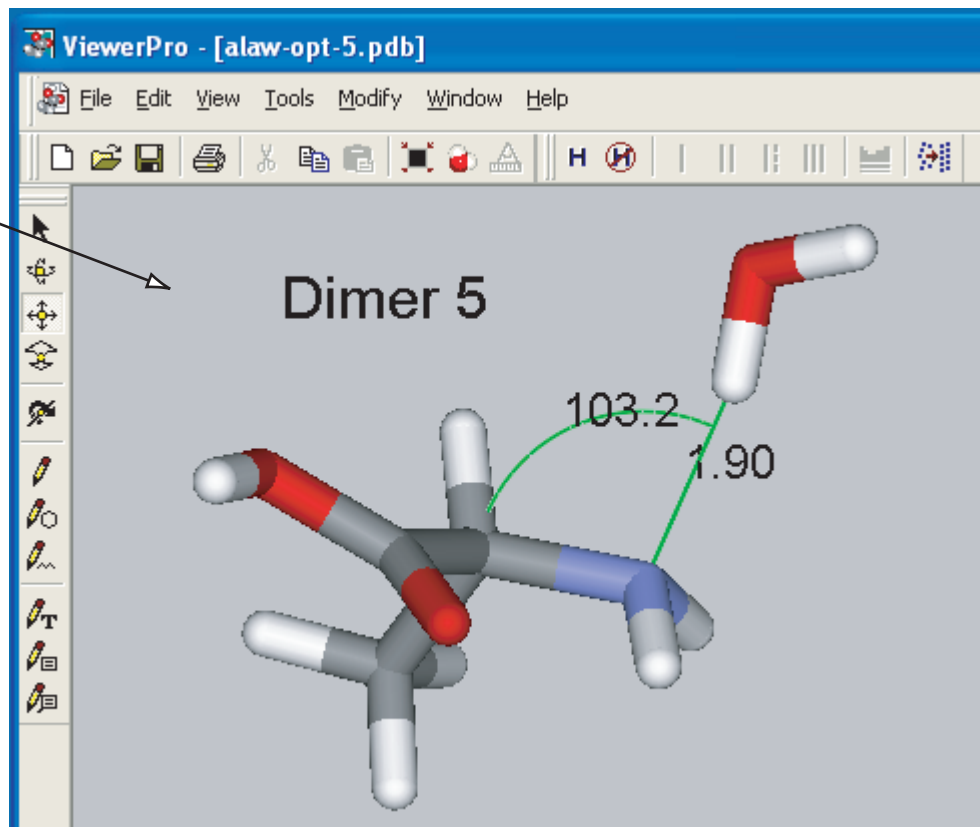
QM geometry optimization of alanine and water

Geometrical
parameters of
the dimer - 4



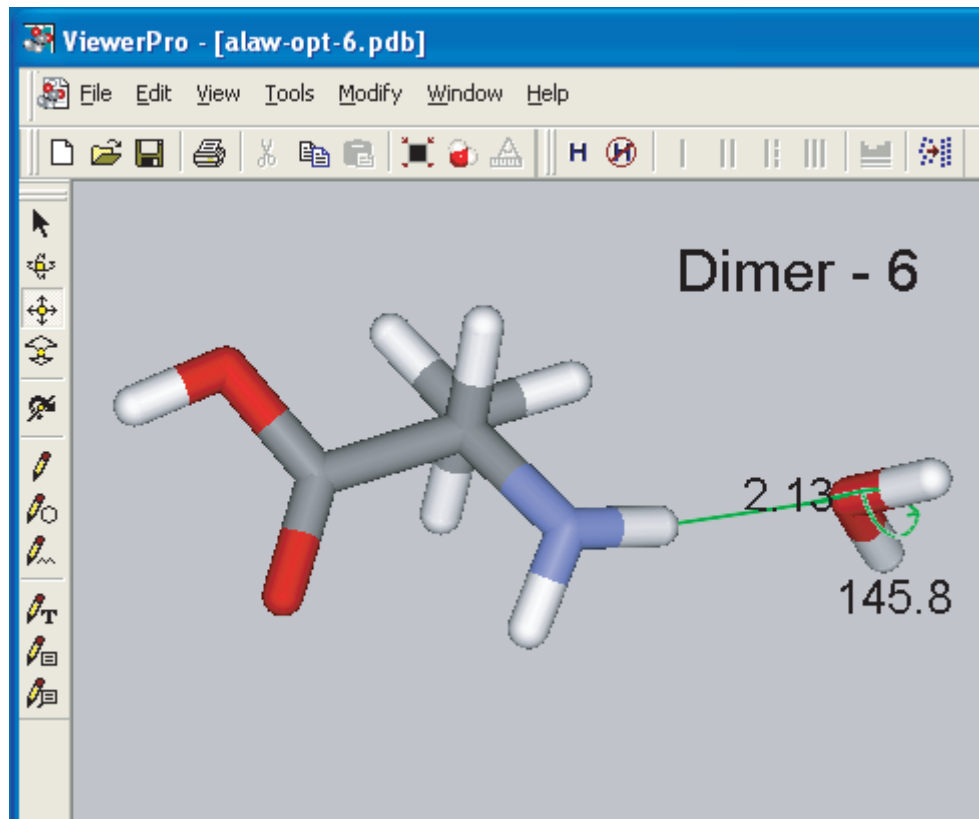
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 5



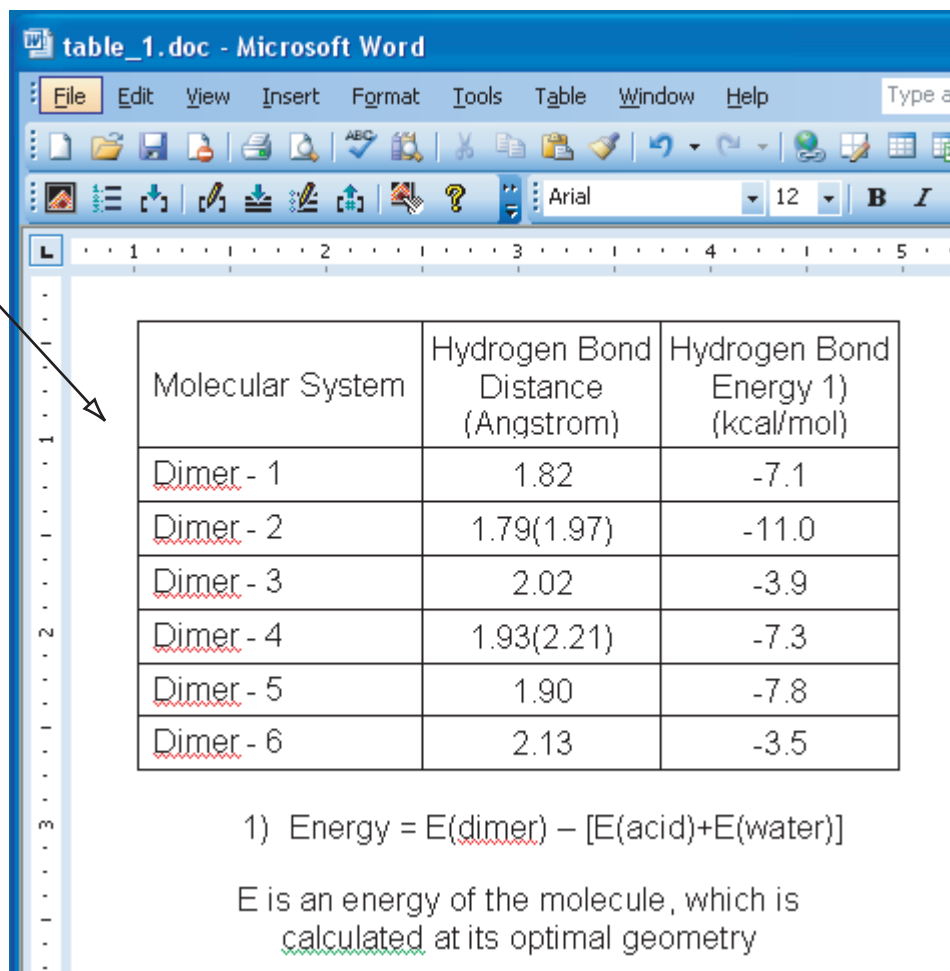
QM geometry optimization of alanine and water

Geometrical
parameters of
the dimer - 6



QM geometry optimization of alanine and water

Results of the calculations



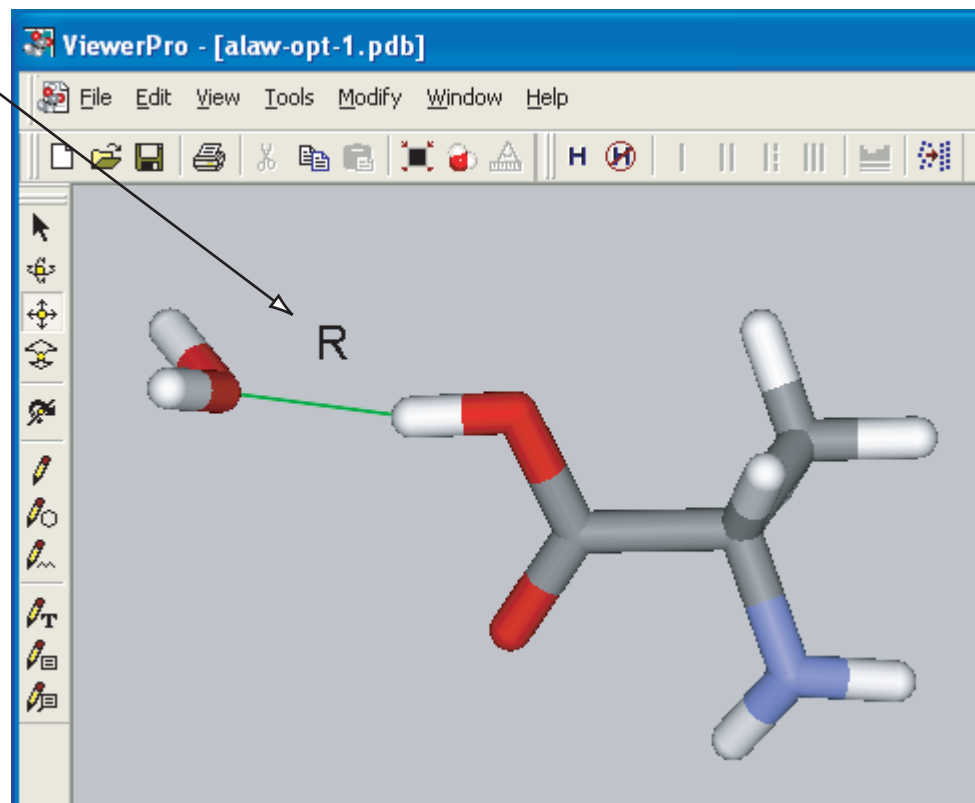
Molecular System	Hydrogen Bond Distance (Angstrom)	Hydrogen Bond Energy 1) (kcal/mol)
Dimer - 1	1.82	-7.1
Dimer - 2	1.79(1.97)	-11.0
Dimer - 3	2.02	-3.9
Dimer - 4	1.93(2.21)	-7.3
Dimer - 5	1.90	-7.8
Dimer - 6	2.13	-3.5

1) Energy = $E(\text{dimer}) - [E(\text{acid}) + E(\text{water})]$

E is an energy of the molecule, which is calculated at its optimal geometry

QM energy of alanine-water dimer

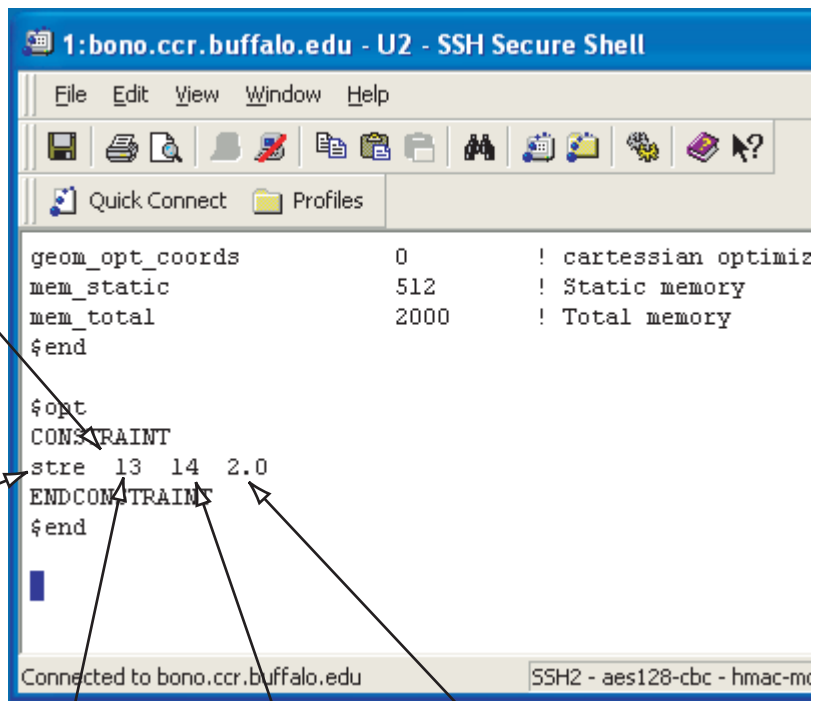
Intermolecular
distance R



QM energy of alanine-water dimer

Geometry optimization
with a constrained
distance

Distance



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
geom_opt_coords      0      ! cartesian optimiz
mem_static           512    ! Static memory
mem_total            2000   ! Total memory
$end

$opt
CONSTRAINT
stre 13 14 2.0
ENDCONSTRAINTS
$end
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-mc

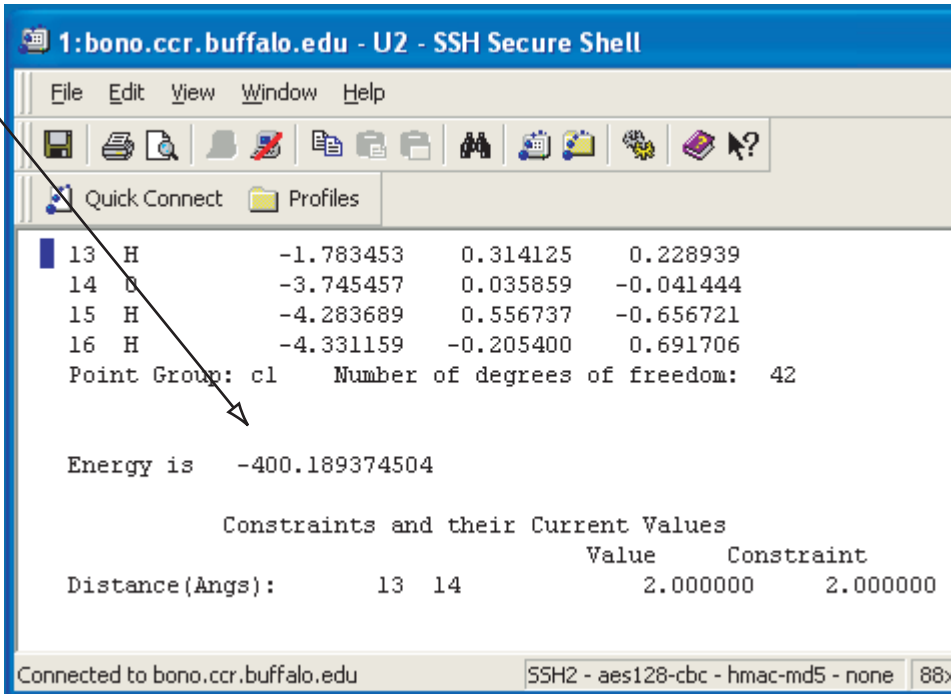
Atom #1

Atom #2

Value

QM energy of alanine-water dimer

Final energy for a
constrained distance



The screenshot shows an SSH terminal window titled "1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The terminal displays the output of a quantum mechanics calculation. An arrow points from the text "Final energy for a constrained distance" to the "Energy is" line. Below the energy, a table shows constraints and their current values. The terminal also shows a list of atoms (13 H, 14 O, 15 H, 16 H) with their coordinates. The status bar at the bottom indicates the connection is to bono.ccr.buffalo.edu using SSH2 with aes128-cbc encryption.

```
13 H      -1.783453    0.314125    0.228939
14 O      -3.745457    0.035859   -0.041444
15 H      -4.283689    0.556737   -0.656721
16 H      -4.331159   -0.205400    0.691706
Point Group: c1      Number of degrees of freedom: 42

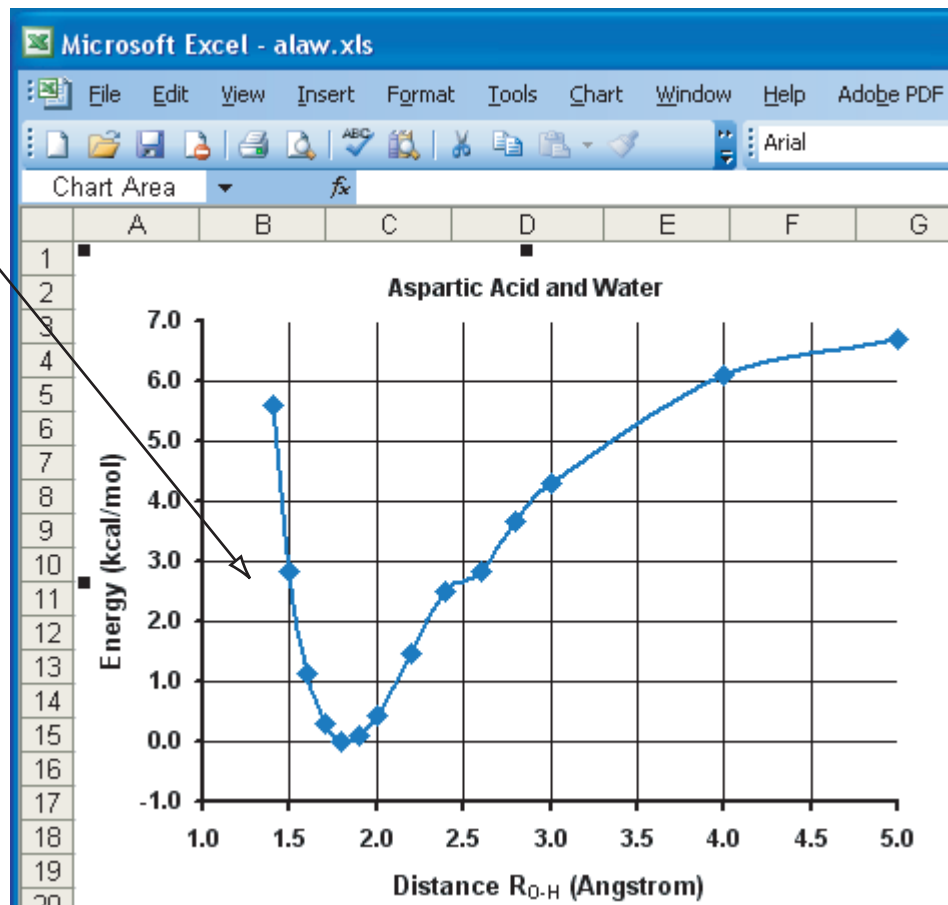
Energy is  -400.189374504

Constraints and their Current Values
                                Value      Constraint
Distance(Angs):      13  14      2.000000      2.000000
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 88x

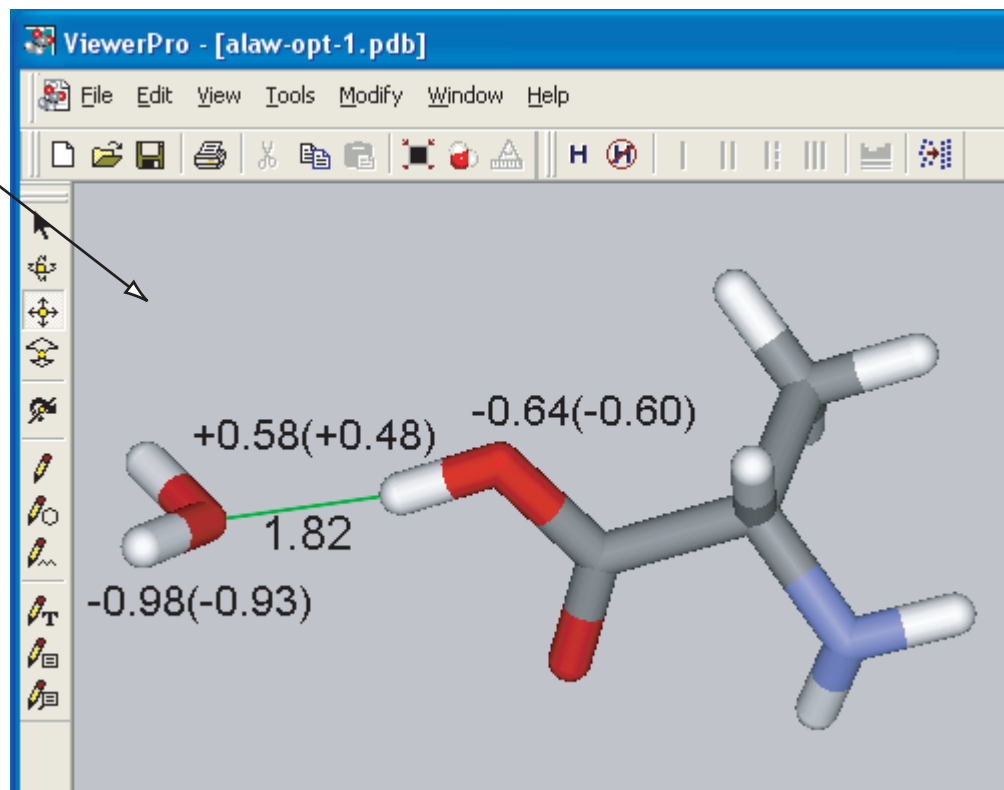
QM energy of alanine-water dimer

Final energy for a
constrained
distance



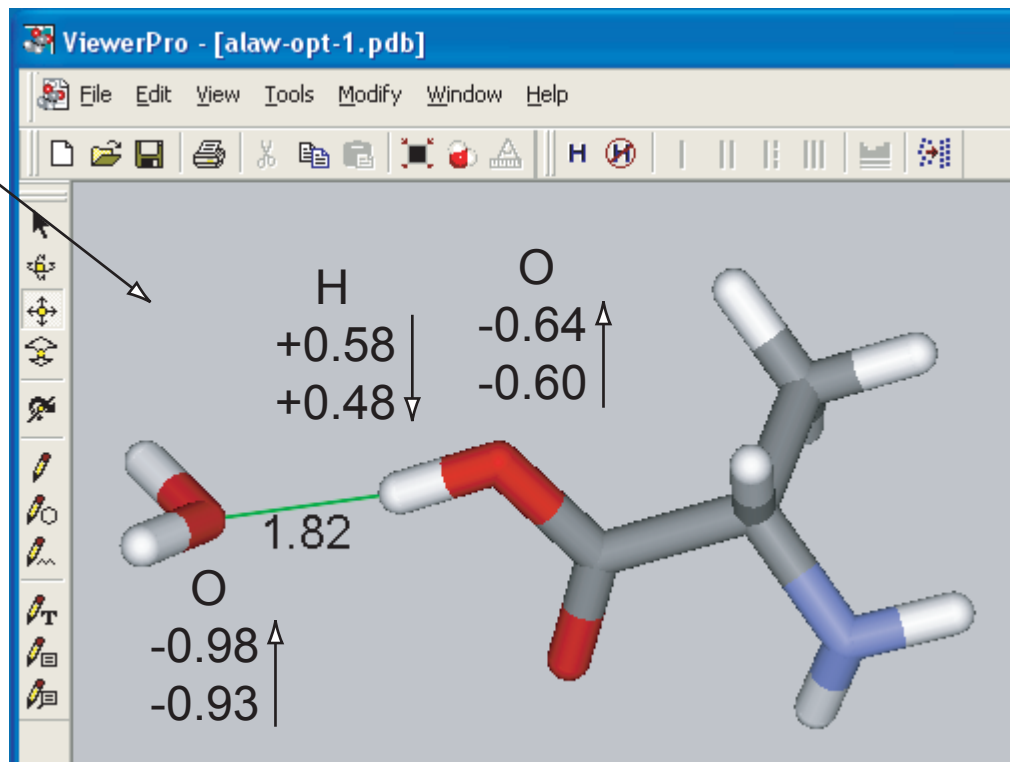
QM properties of alanine-water dimer

Atomic charges
before and after
hydrogen bonding



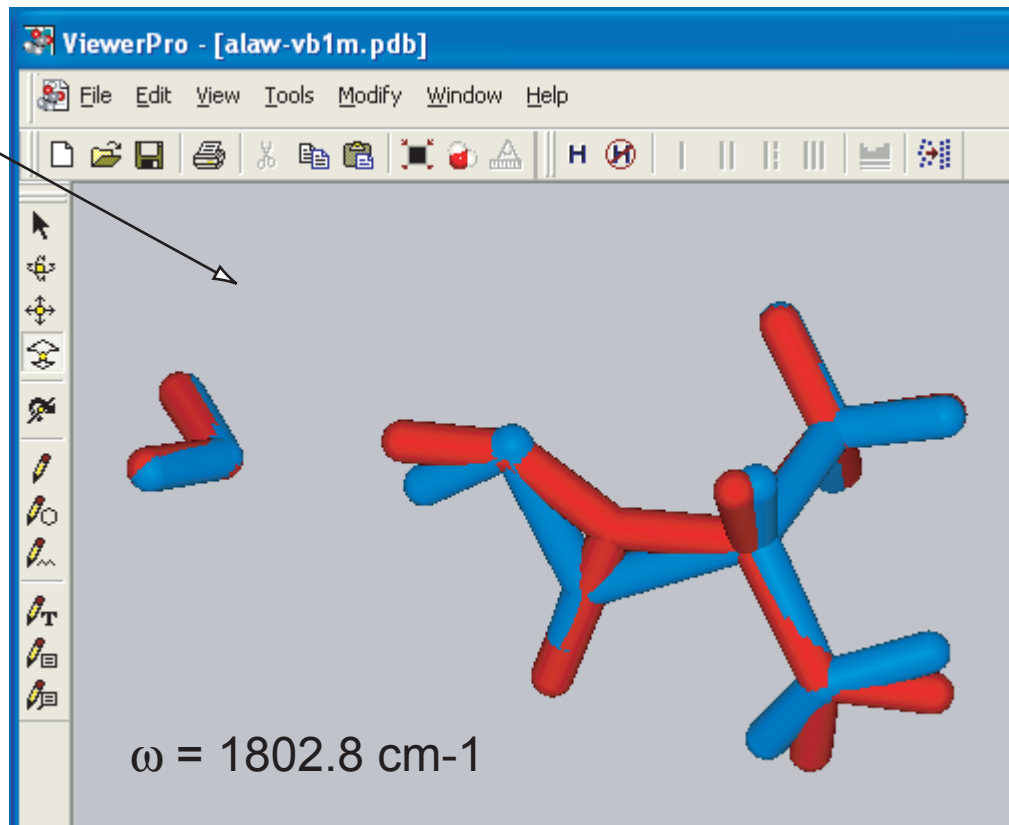
QM properties of alanine-water dimer

Atomic charges
before and after
hydrogen bonding



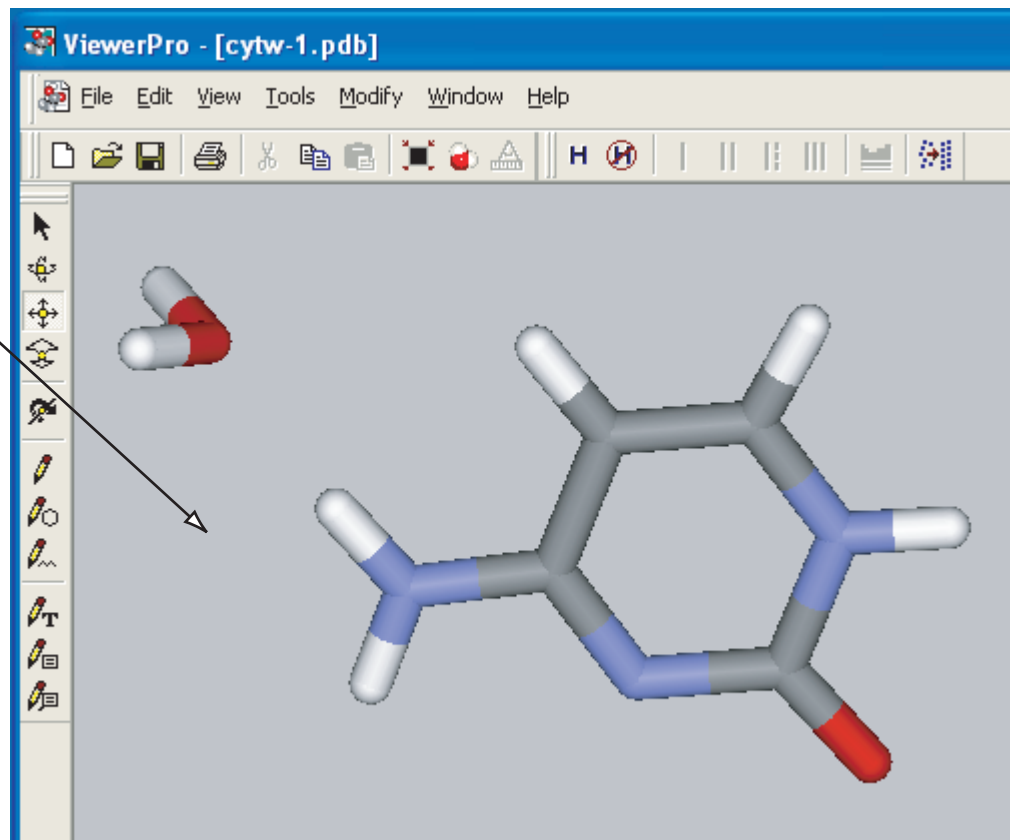
QM properties of alanine-water dimer

Vibration involving
the hydrogen
move



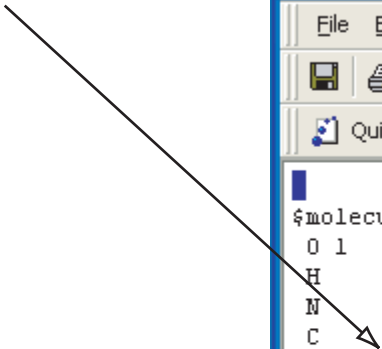
QM geometry optimization of cytosine and water

Initial geometry
of the cytosine
and water dimer



QM geometry optimization of cytosine and water

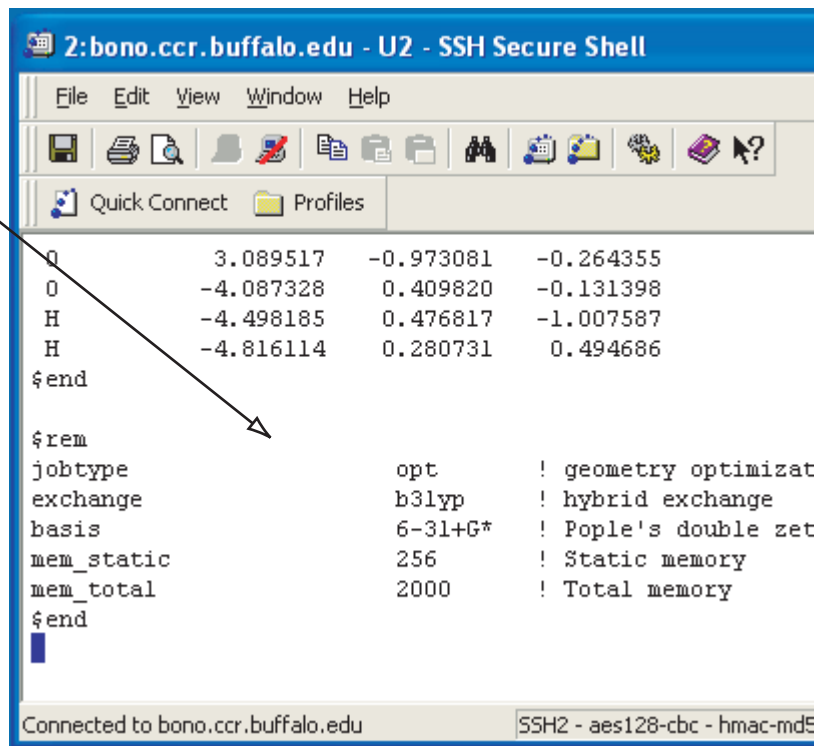
Initial geometry
of the cytosine
and water dimer



```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
$
$molecule
O 1
H      2.854630    1.437230   -0.008651
N      1.952048    0.979019    0.007872
C      0.795813    1.682251    0.128269
H      0.885746    2.761491    0.213281
C     -0.397785    1.030995    0.137191
H     -1.336697    1.562199    0.231099
C     -0.340663   -0.406544    0.014272
N     -1.499622   -1.110329    0.036949
H     -1.443742   -2.108875   -0.109189
H     -2.405717   -0.653105    0.020982
N      0.788490   -1.089530   -0.109169
"cytw-1.in" 29L, 1057C
Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-m
```

QM geometry optimization of cytosine and water

Geometry
optimization



```
2: bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
O      3.089517   -0.973081   -0.264355
O      -4.087328   0.409820   -0.131398
H      -4.498185   0.476817   -1.007587
H      -4.816114   0.280731   0.494686
$end

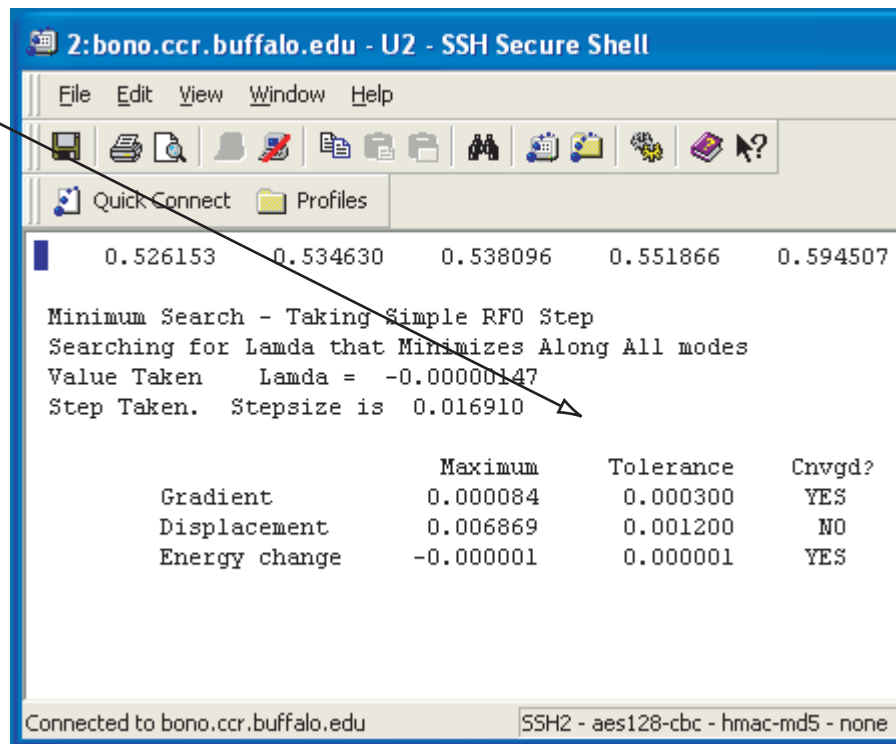
$rem
jobtype                opt          ! geometry optimization
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double zeta
mem_static             256          ! Static memory
mem_total              2000         ! Total memory
$end

[Blue cursor bar]
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5

QM geometry optimization of cytosine and water

Optimization
converged



```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
0.526153 0.534630 0.538096 0.551866 0.594507

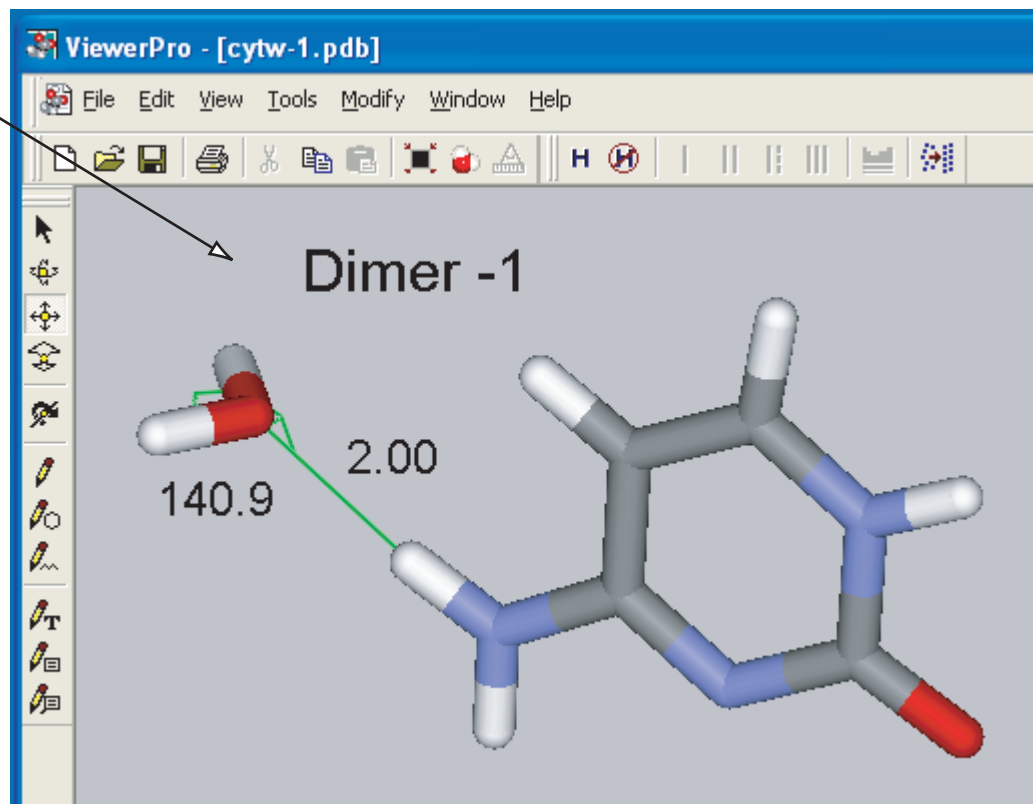
Minimum Search - Taking Simple RFO Step
Searching for Lambda that Minimizes Along All modes
Value Taken Lambda = -0.00000147
Step Taken. Stepsize is 0.016910

          Maximum      Tolerance      Cnvgd?
Gradient      0.000084      0.000300      YES
Displacement  0.006869      0.001200      NO
Energy change -0.000001      0.000001      YES

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none
```

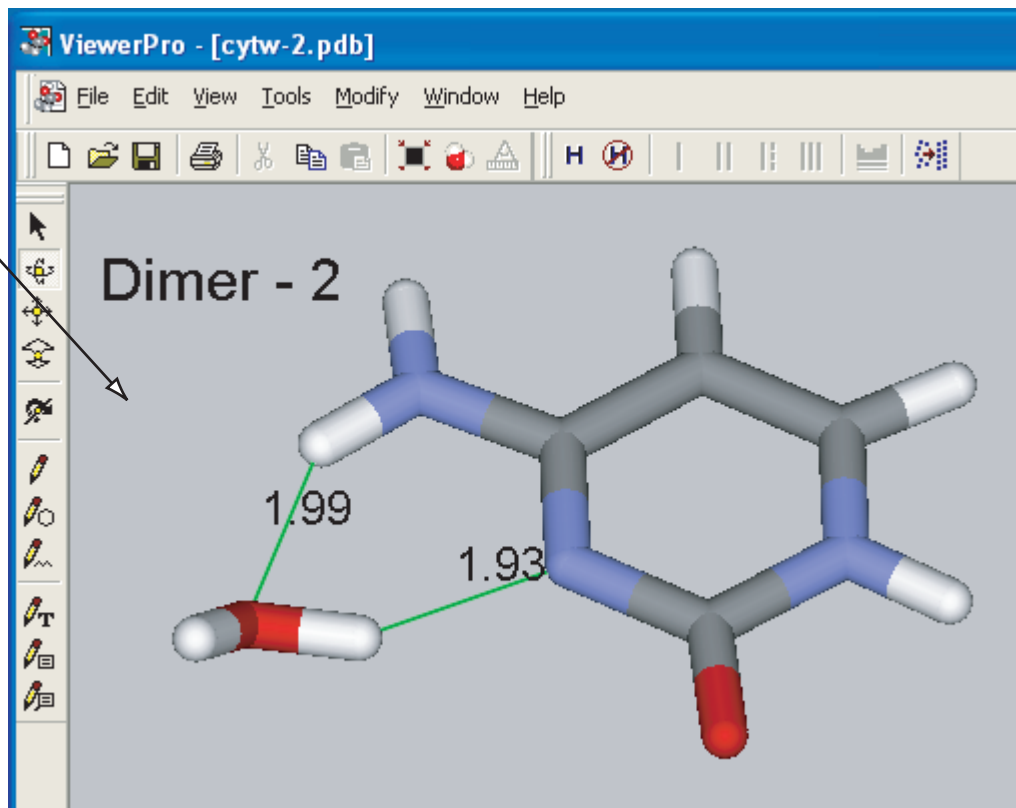
QM geometry optimization of cytosine and water

Final geometry
of Dimer -1



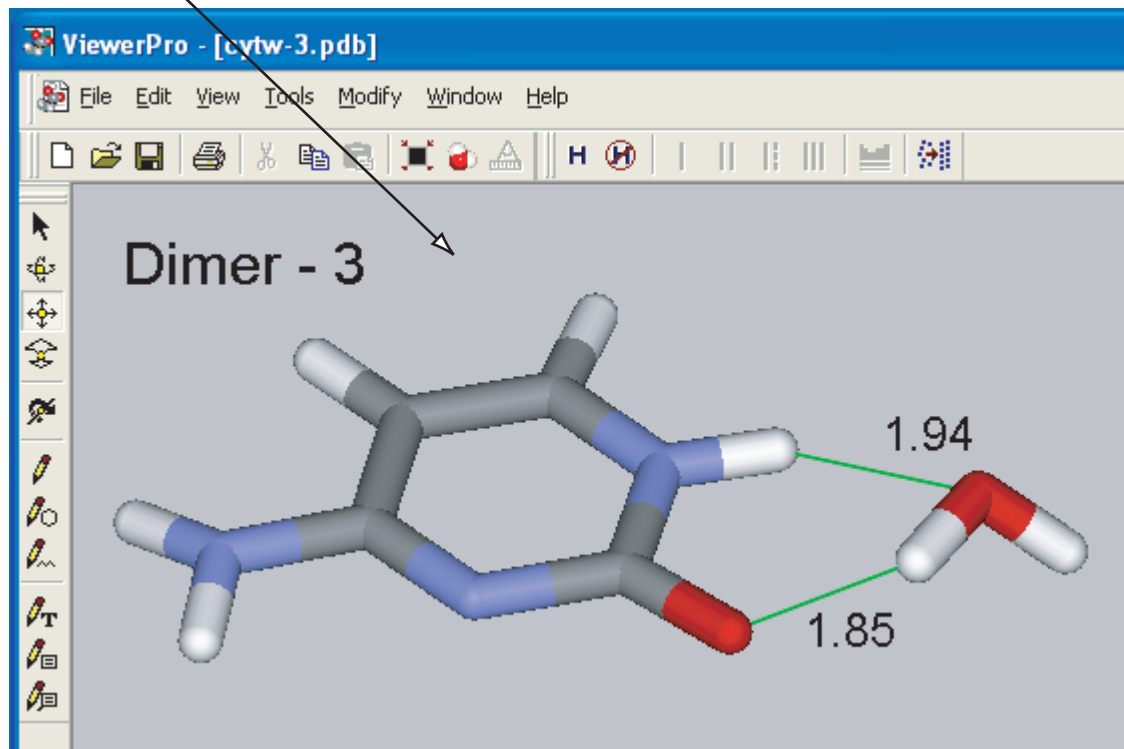
QM geometry optimization of cytosine and water

Final geometry
of Dimer -2



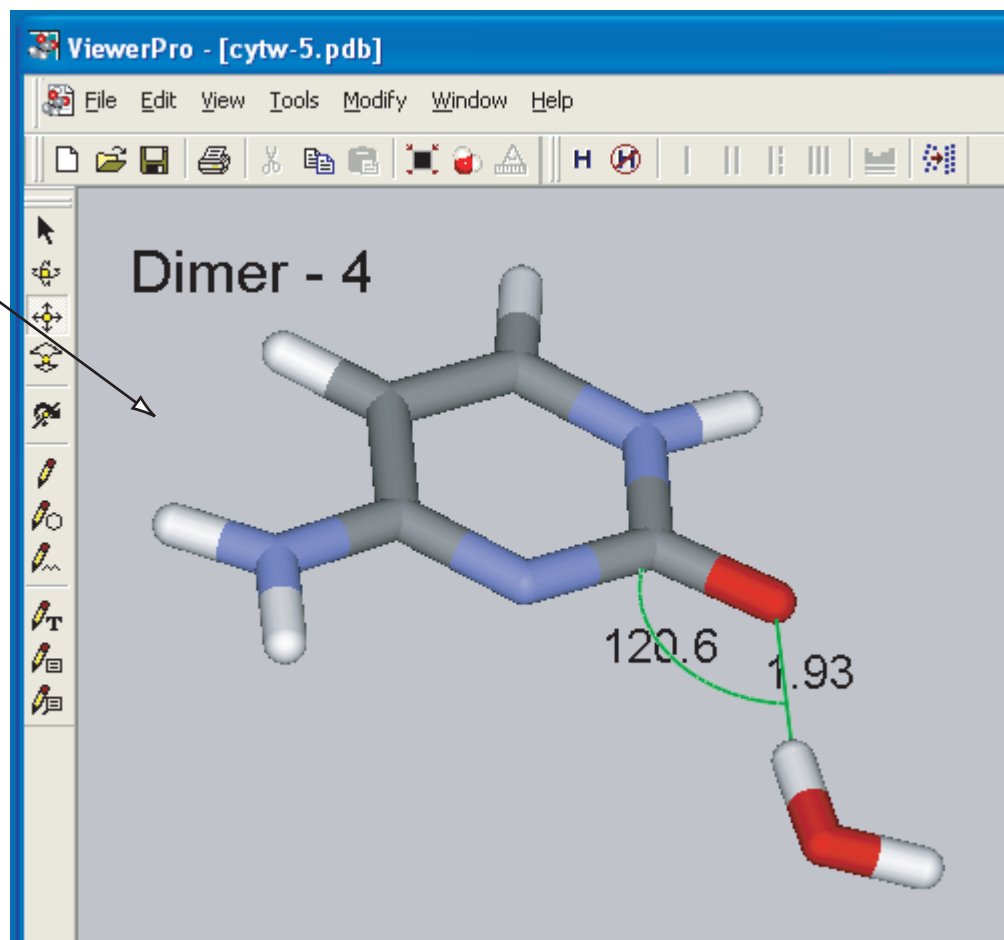
QM geometry optimization of cytosine and water

Final geometry
of Dimer - 3



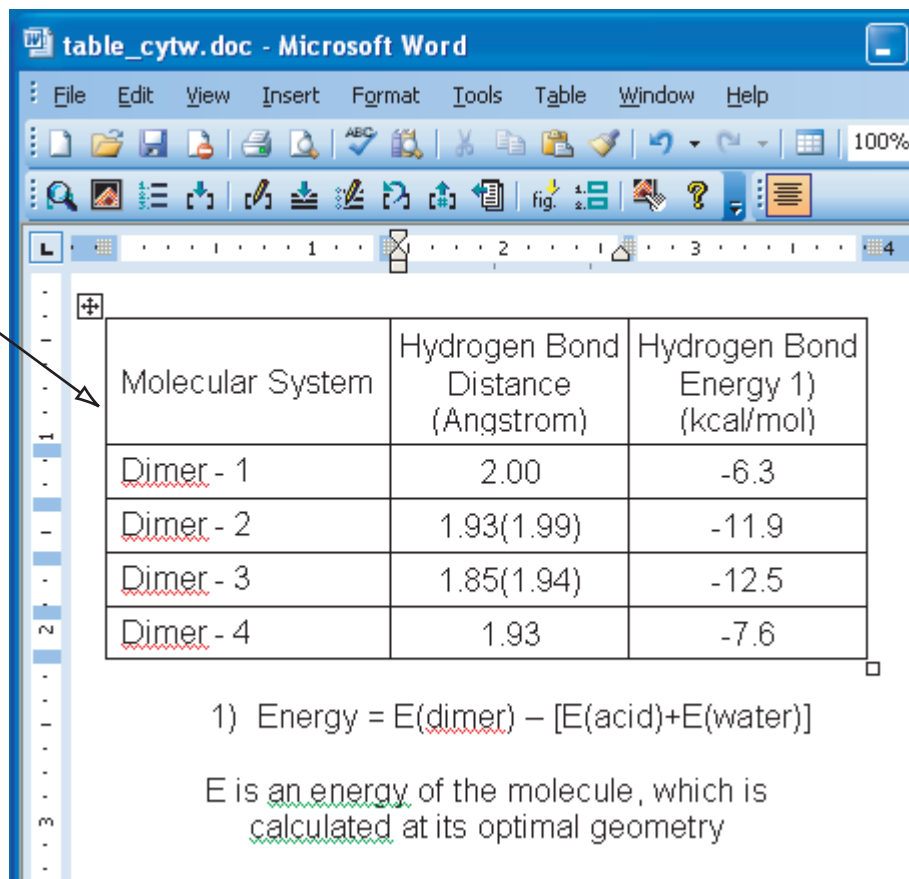
QM geometry optimization of cytosine and water

Final geometry
of Dimer - 4



QM geometry optimization of cytosine and water

Final results



The screenshot shows a Microsoft Word document titled "table_cytw.doc". The document contains a table with three columns: "Molecular System", "Hydrogen Bond Distance (Angstrom)", and "Hydrogen Bond Energy 1) (kcal/mol)". The table lists four dimers. The first row shows "Dimer - 1" with a distance of 2.00 and energy of -6.3. The second row shows "Dimer - 2" with a distance of 1.93(1.99) and energy of -11.9. The third row shows "Dimer - 3" with a distance of 1.85(1.94) and energy of -12.5. The fourth row shows "Dimer - 4" with a distance of 1.93 and energy of -7.6. Below the table, there is a footnote: "1) Energy = E(dimer) - [E(acid)+E(water)]". Below the footnote, there is a note: "E is an energy of the molecule, which is calculated at its optimal geometry".

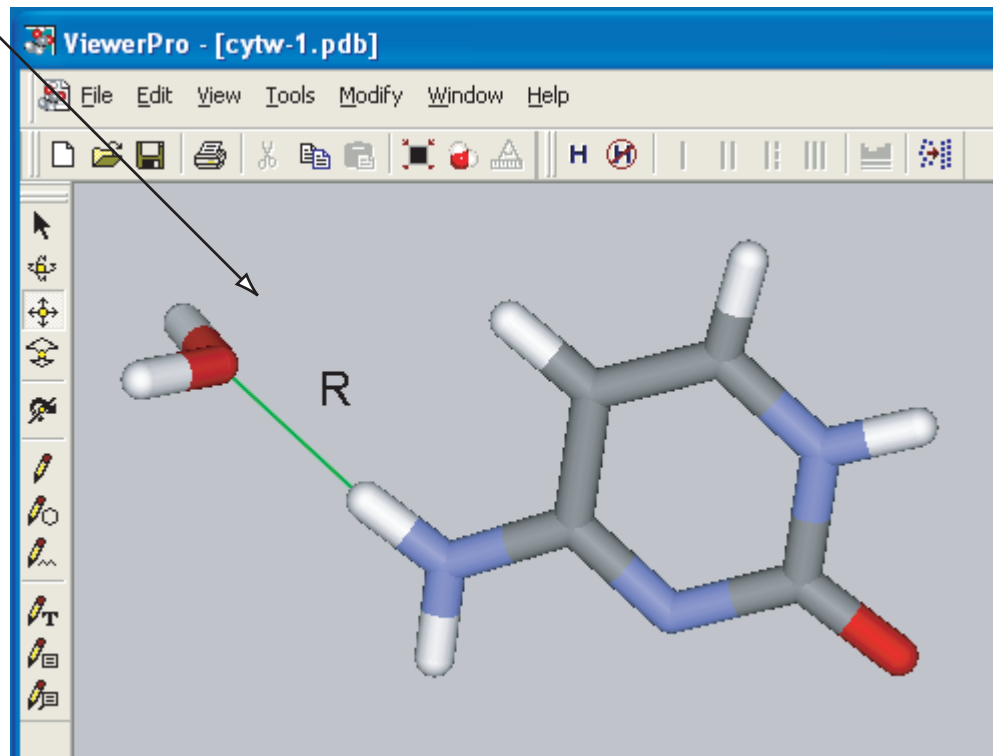
Molecular System	Hydrogen Bond Distance (Angstrom)	Hydrogen Bond Energy 1) (kcal/mol)
Dimer - 1	2.00	-6.3
Dimer - 2	1.93(1.99)	-11.9
Dimer - 3	1.85(1.94)	-12.5
Dimer - 4	1.93	-7.6

1) Energy = E(dimer) - [E(acid)+E(water)]

E is an energy of the molecule, which is calculated at its optimal geometry

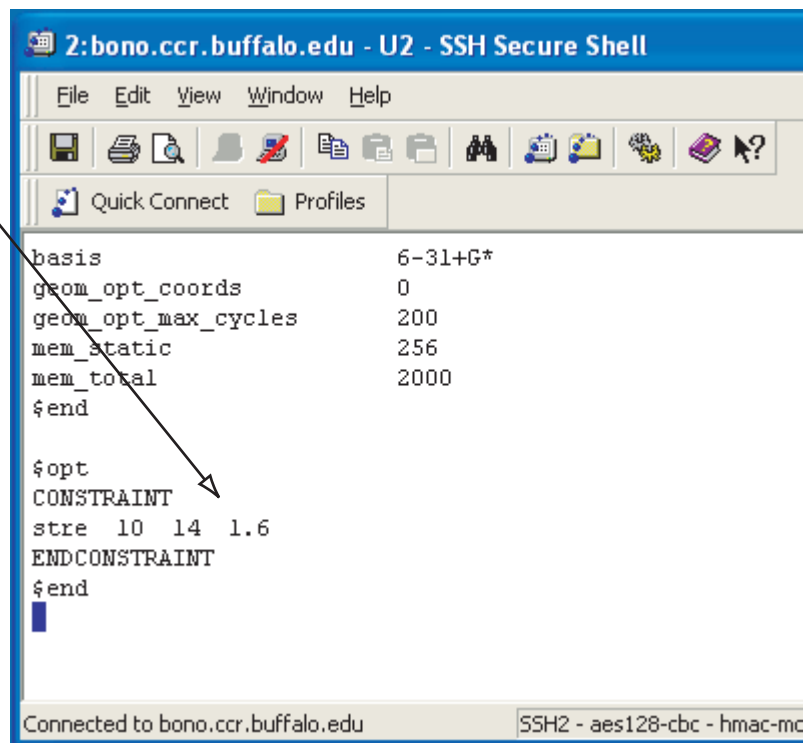
QM geometry optimization of cytosine and water

Calculations with a
constrained distance



QM geometry optimization of cytosine and water

Constrained distance
between two atoms



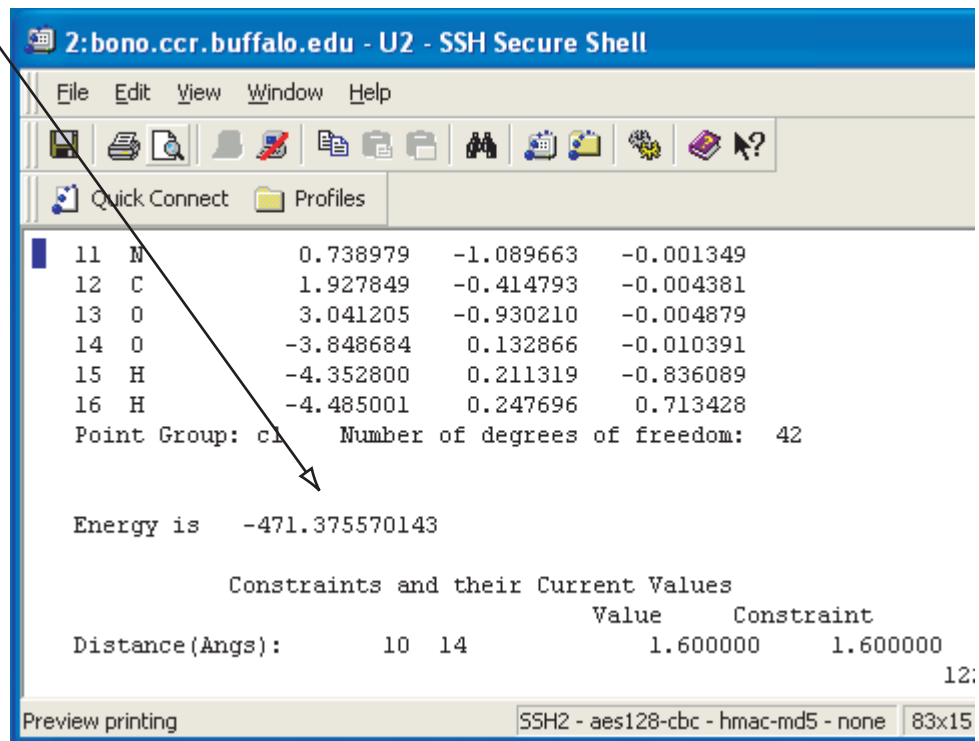
```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
basis 6-31+G*
geom_opt_coords 0
geom_opt_max_cycles 200
mem_static 256
mem_total 2000
$end

$opt
CONSTRAINT
stre 10 14 1.6
ENDCONSTRAINT
$end
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-mc

QM geometry optimization of cytosine and water

Final energy with a
constrained distance



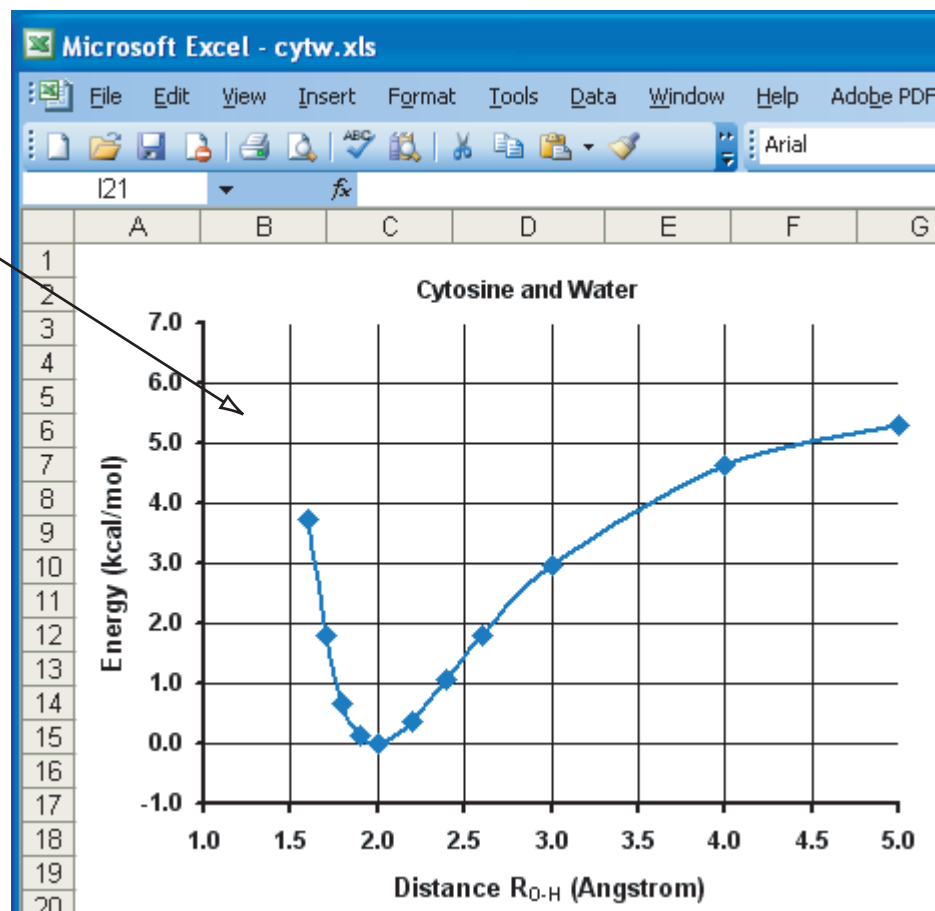
```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
11 N      0.738979  -1.089663  -0.001349
12 C      1.927849  -0.414793  -0.004381
13 O      3.041205  -0.930210  -0.004879
14 O     -3.848684   0.132866  -0.010391
15 H     -4.352800   0.211319  -0.836089
16 H     -4.485001   0.247696   0.713428
Point Group: c1      Number of degrees of freedom: 42

Energy is  -471.375570143

Constraints and their Current Values
                        Value      Constraint
Distance(Angs):      10  14      1.600000      1.600000
                                                                12:
Preview printing      SSH2 - aes128-cbc - hmac-md5 - none 83x15
```

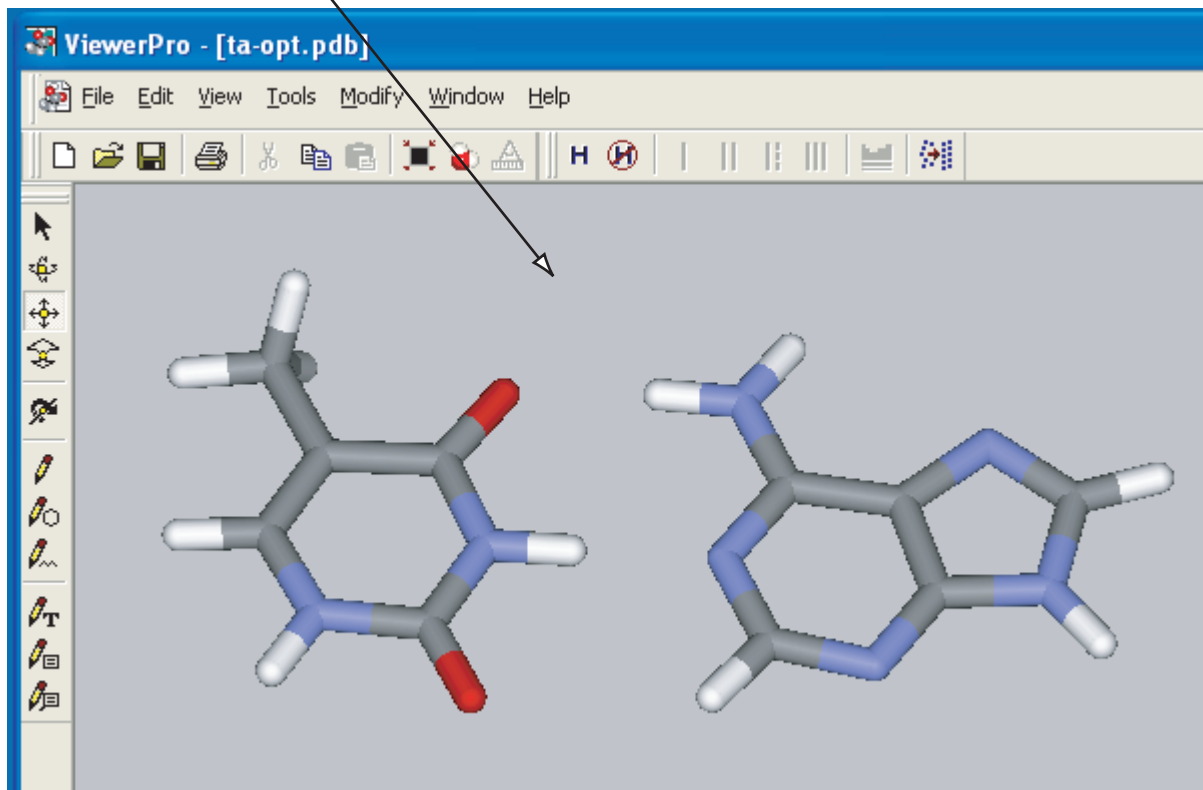
QM geometry optimization of cytosine and water

Energy as a function
of a constrained
distance



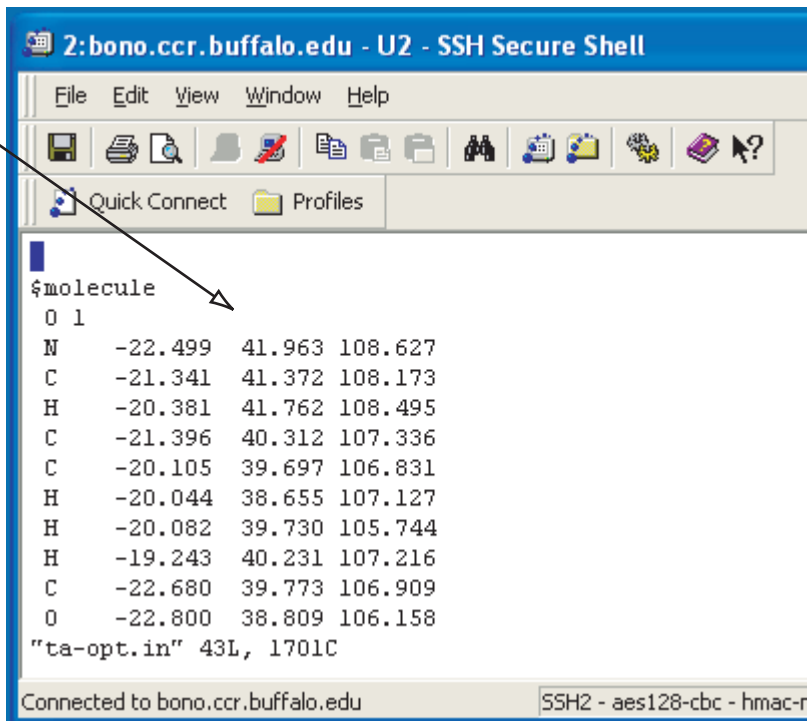
QM proton transfer in Thymine and Adenine dimer

Initial geometry of Thymine
and Adenine dimer



QM proton transfer in Thymine and Adenine dimer

Initial geometry of the dimer taken from an experimental PDB file



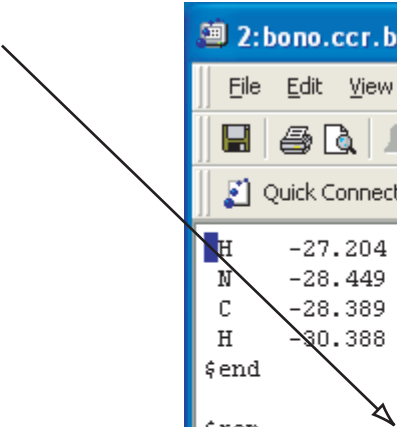
The screenshot shows a terminal window titled "2: bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window has a menu bar with "File", "Edit", "View", "Window", and "Help". Below the menu bar is a toolbar with various icons. The main area of the terminal displays the following text:

```
$molecule  
O 1  
N -22.499 41.963 108.627  
C -21.341 41.372 108.173  
H -20.381 41.762 108.495  
C -21.396 40.312 107.336  
C -20.105 39.697 106.831  
H -20.044 38.655 107.127  
H -20.082 39.730 105.744  
H -19.243 40.231 107.216  
C -22.680 39.773 106.909  
O -22.800 38.809 106.158  
"ta-opt.in" 43L, 1701C
```

At the bottom of the terminal window, it says "Connected to bono.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-r". An arrow from the text "Initial geometry of the dimer taken from an experimental PDB file" points to the first line of coordinates "O 1".

QM proton transfer in Thymine and Adenine dimer

Geometry optimization
of the dimer



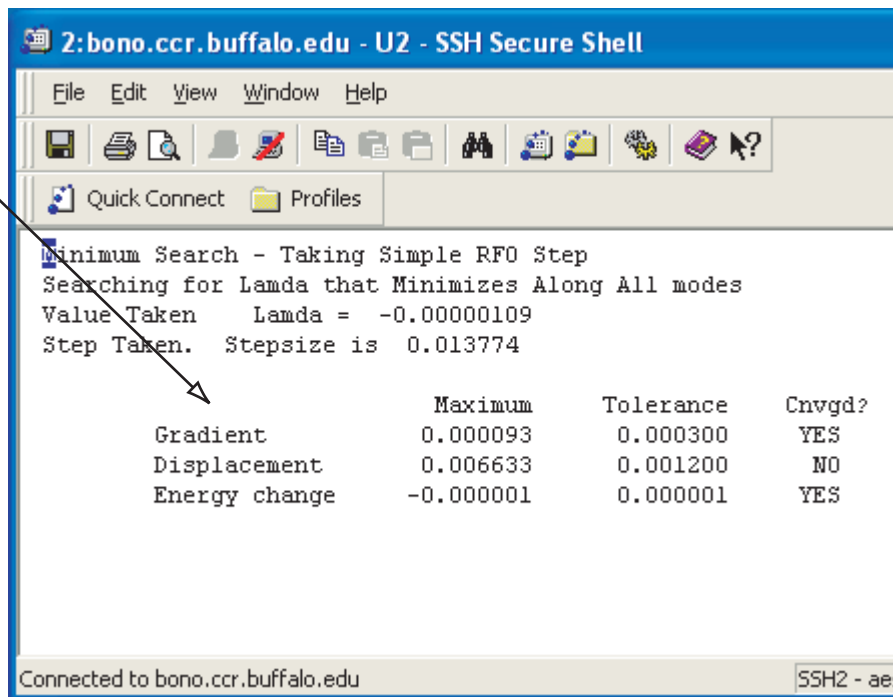
```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
H -27.204 40.710 107.330
N -28.449 39.646 106.092
C -28.389 38.735 105.082
H -30.388 38.583 104.340
$end

$rem
jobtype                opt          ! geometry optimization
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double zeta
mem_static             256          ! Static memory
mem_total              2000         ! Total memory
$end

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```


QM proton transfer in Thymine and Adenine dimer

Optimization
converged



```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

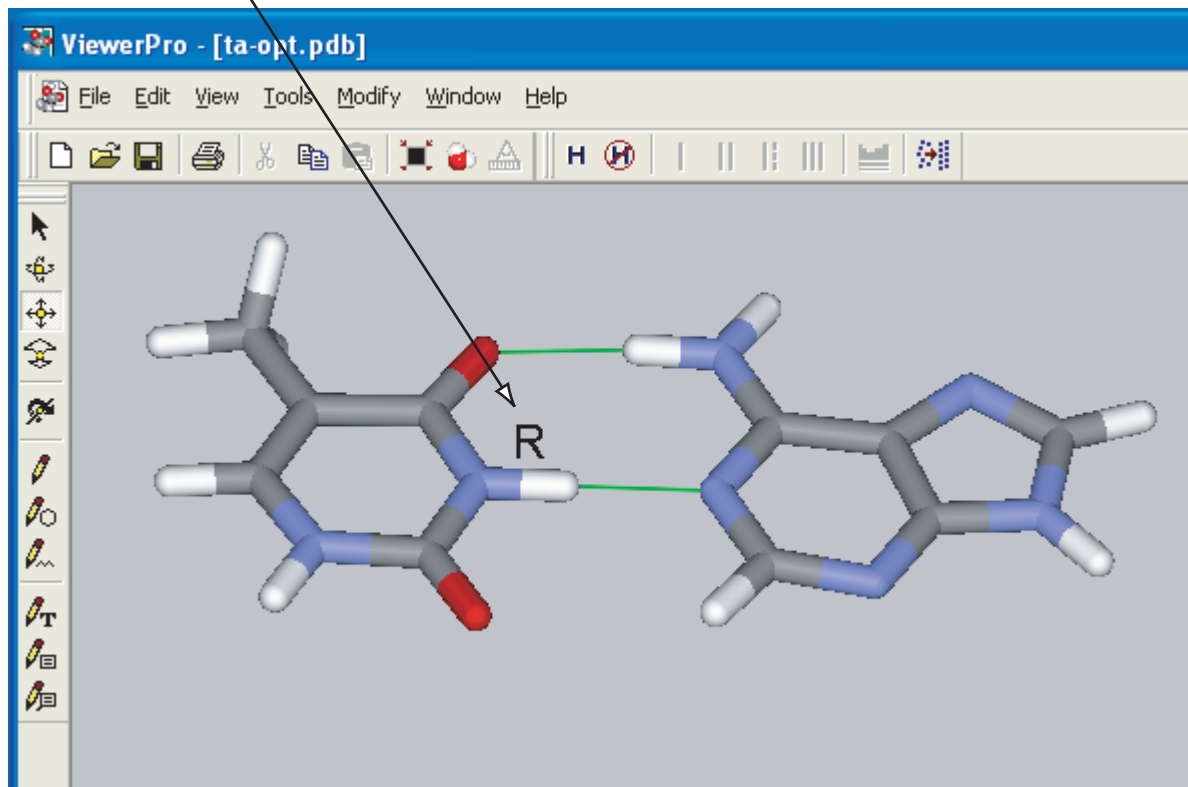
Minimum Search - Taking Simple RFO Step
Searching for Lambda that Minimizes Along All modes
Value Taken Lambda = -0.00000109
Step Taken. Stepsize is 0.013774

      Maximum      Tolerance      Cnvgd?
Gradient      0.000093      0.000300      YES
Displacement  0.006633      0.001200      NO
Energy change -0.000001      0.000001      YES

Connected to bono.ccr.buffalo.edu      SSH2 - ae:
```

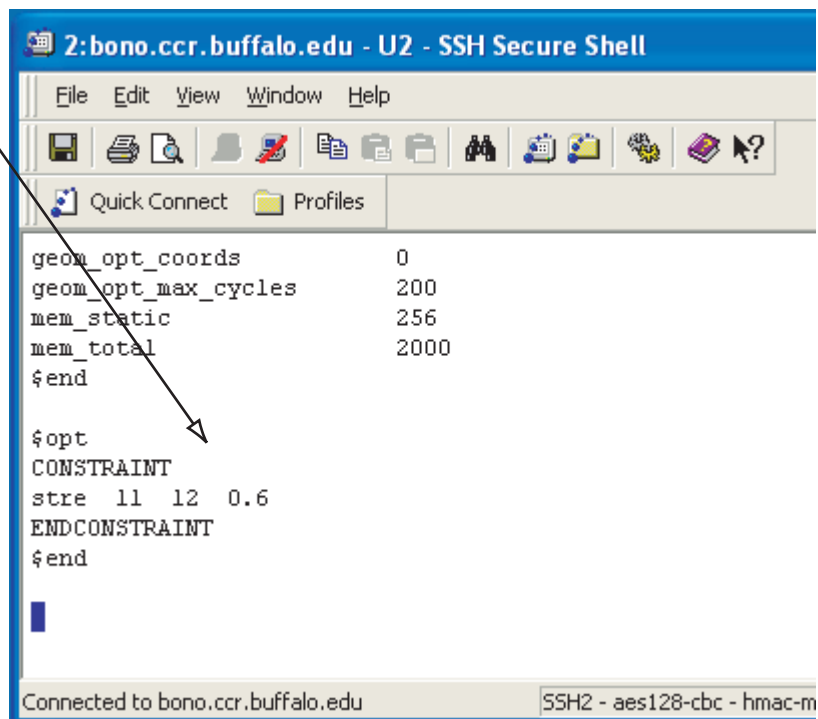
QM proton transfer in Thymine and Adenine dimer

A series of calculations for
the constrained R value



QM proton transfer in Thymine and Adenine dimer

A constrained distance
between two atoms



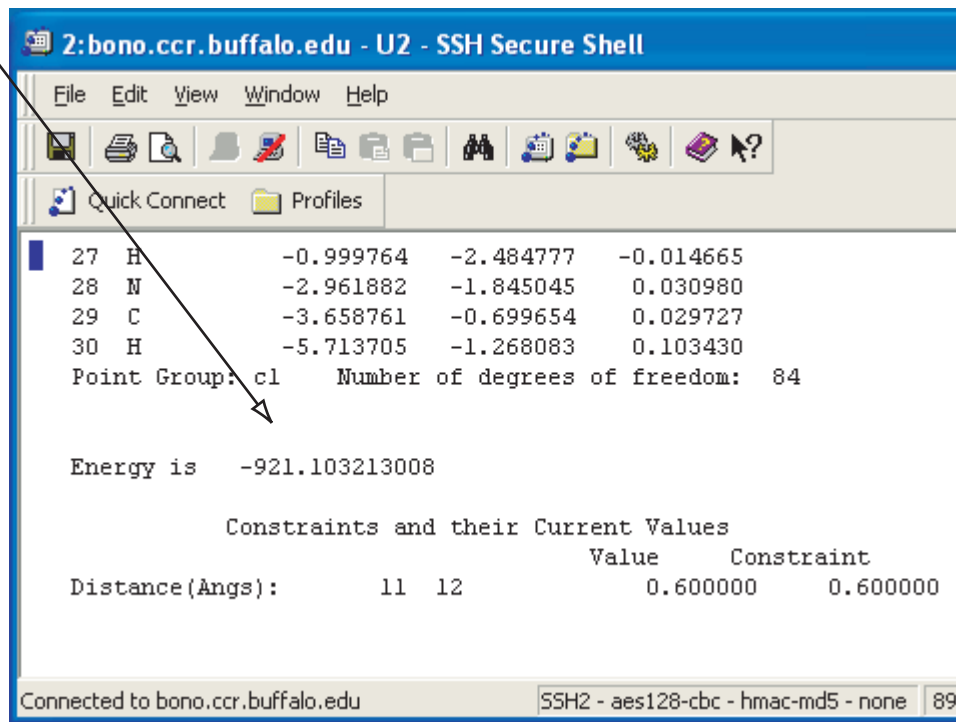
```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
geom_opt_coords      0
geom_opt_max_cycles  200
mem_static           256
mem_total            2000
$end

$opt
CONSTRAINT
stre 11 12 0.6
ENDCONSTRAINT
$end

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-m
```

QM proton transfer in Thymine and Adenine dimer

Final energy for a
constrained distance



```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
27 H -0.999764 -2.484777 -0.014665
28 N -2.961882 -1.845045 0.030980
29 C -3.658761 -0.699654 0.029727
30 H -5.713705 -1.268083 0.103430
Point Group: c1 Number of degrees of freedom: 84

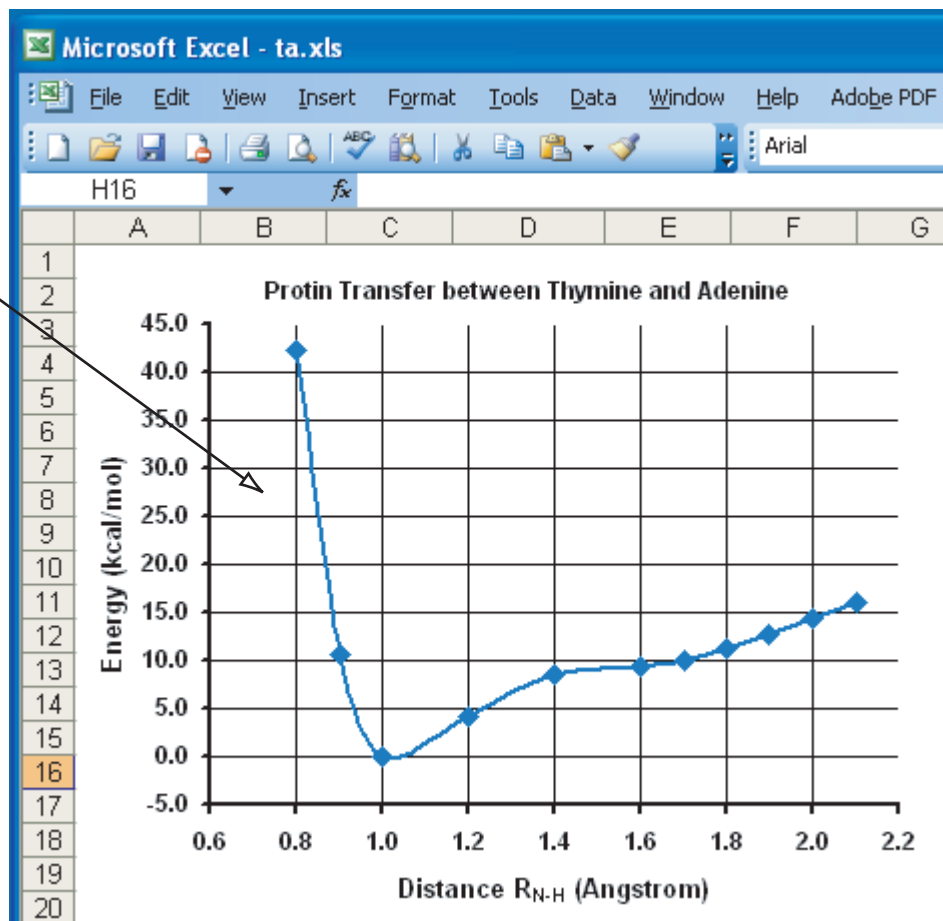
Energy is -921.103213008

Constraints and their Current Values
                        Value      Constraint
Distance(Angs):      11 12      0.600000    0.600000

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none 89
```

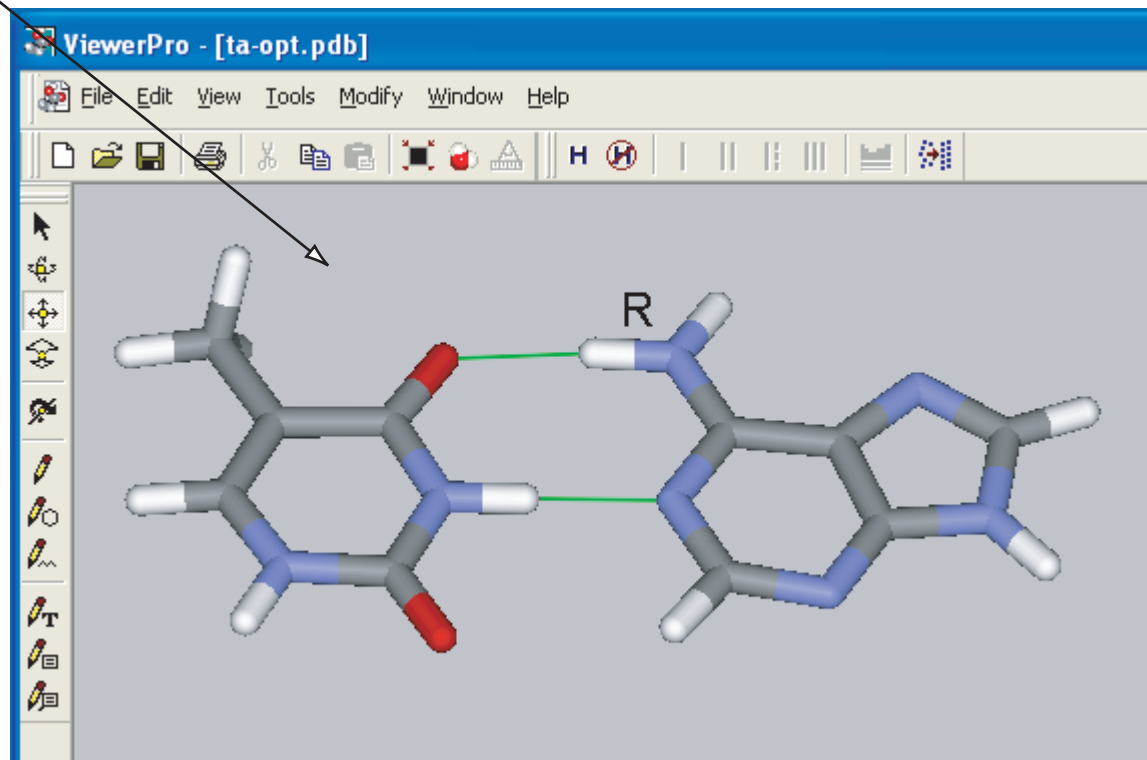
QM proton transfer in Thymine and Adenine dimer

The energy as a function of the $R(\text{N-H})$ distance



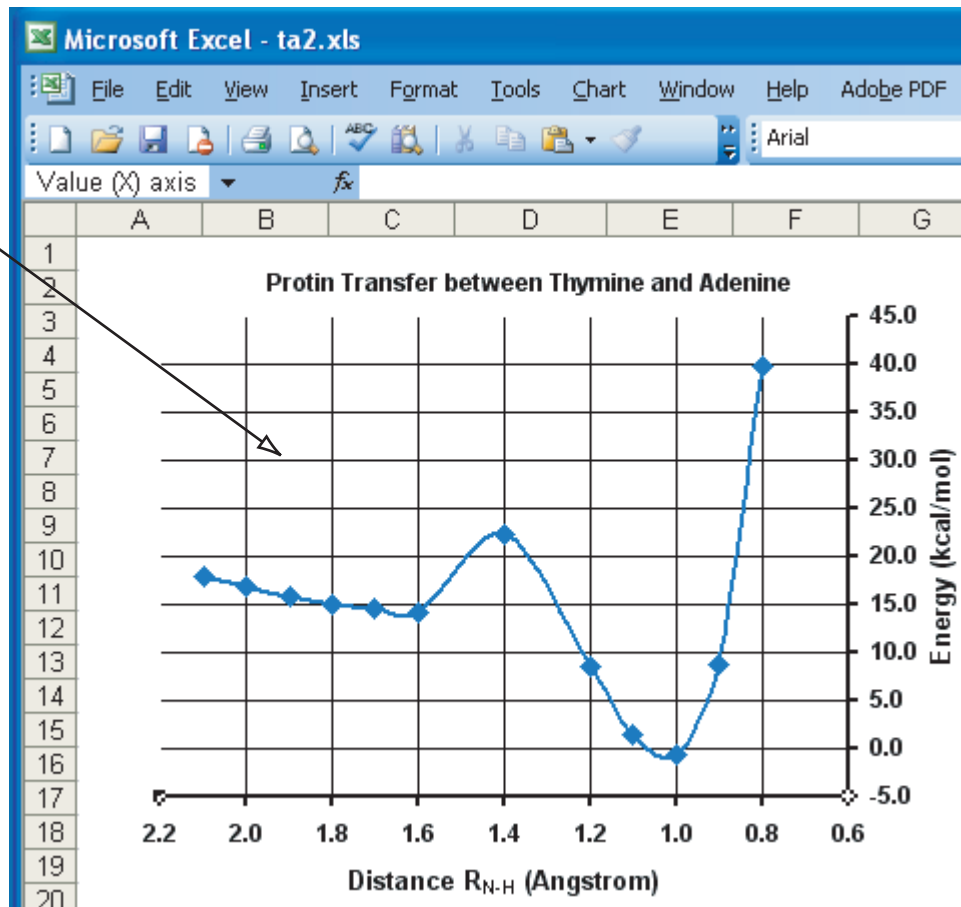
QM proton transfer in Thymine and Adenine dimer

A constrained
interatomic distance



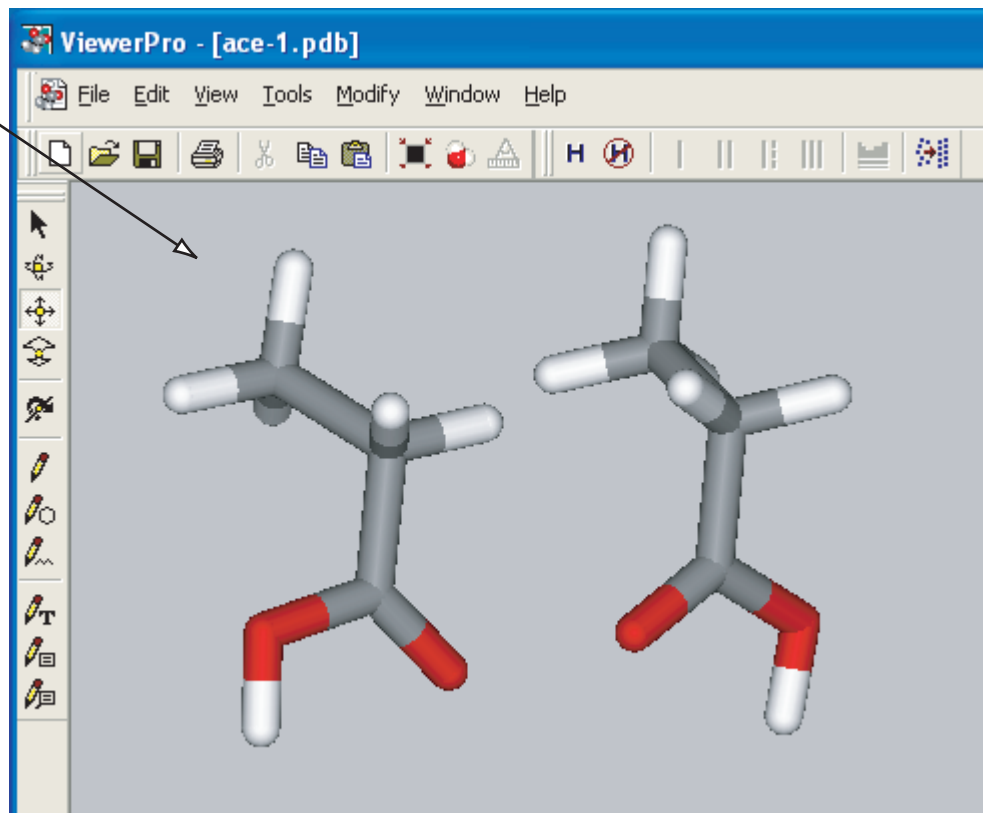
QM proton transfer in Thymine and Adenine dimer

The energy as a function of the $R(\text{N-H})$ distance



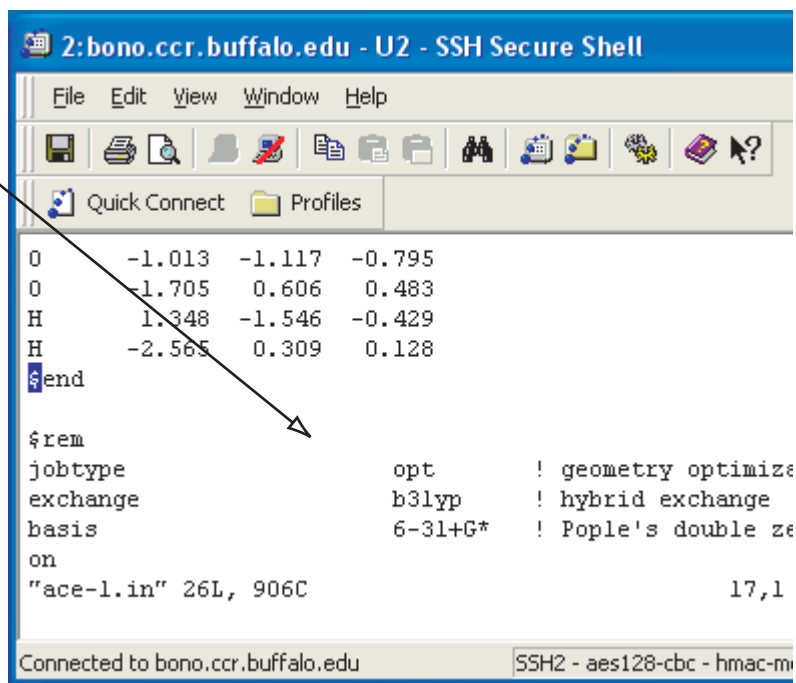
QM tautomerization - Alanine

Two tautomers
of alanine



QM tautomerization - Alanine

Geometry
optimization



```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

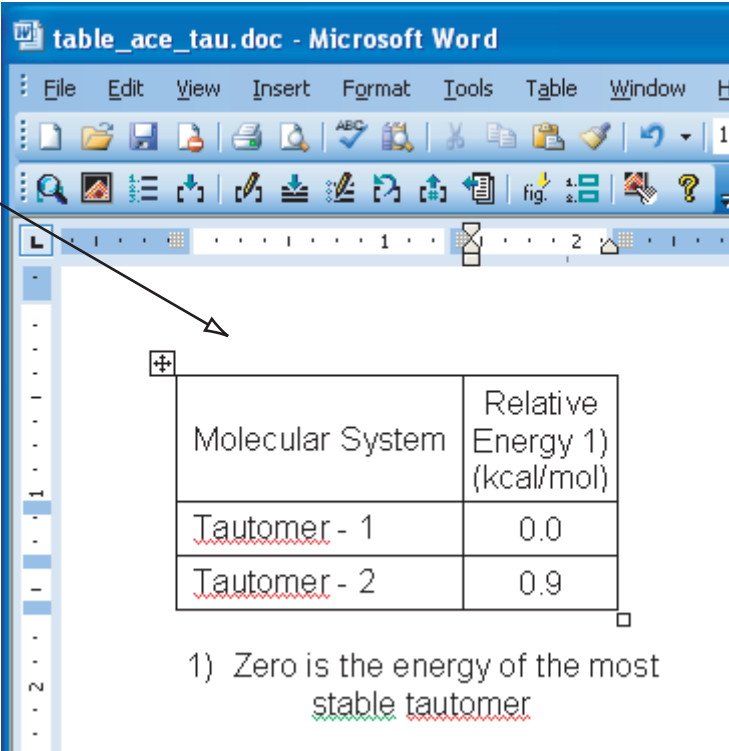
O -1.013 -1.117 -0.795
O -1.705 0.606 0.483
H 1.348 -1.546 -0.429
H -2.565 0.309 0.128
$end

$rem
jobtype opt ! geometry optimize
exchange b3lyp ! hybrid exchange
basis 6-31+G* ! Pople's double ze
on
"ace-1.in" 26L, 906C 17,1

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-m
```

QM tautomerization - Alanine

Final results



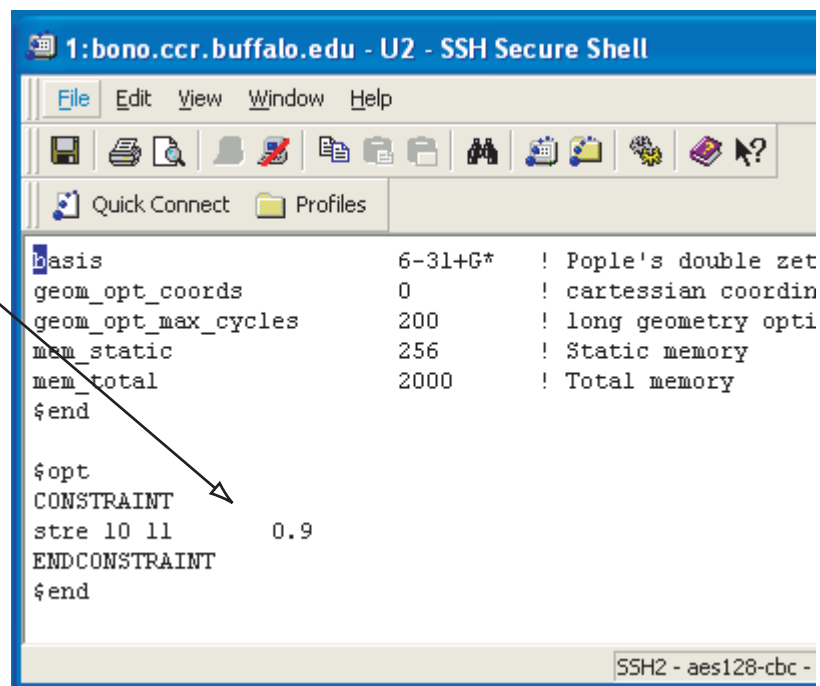
The screenshot shows a Microsoft Word window with the title 'table_ace_tau.doc'. The table below is embedded in the document. An arrow points from the text 'Final results' to the table.

Molecular System	Relative Energy 1) (kcal/mol)
<u>Tautomer - 1</u>	0.0
<u>Tautomer - 2</u>	0.9

1) Zero is the energy of the most stable tautomer

QM tautomerization - Alanine

Geometry
optimization with
a constrained
distance



The screenshot shows a terminal window titled "1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window contains Gaussian input for a geometry optimization. An arrow from the text "Geometry optimization with a constrained distance" points to the "CONSTRAINT" section of the input. The input is as follows:

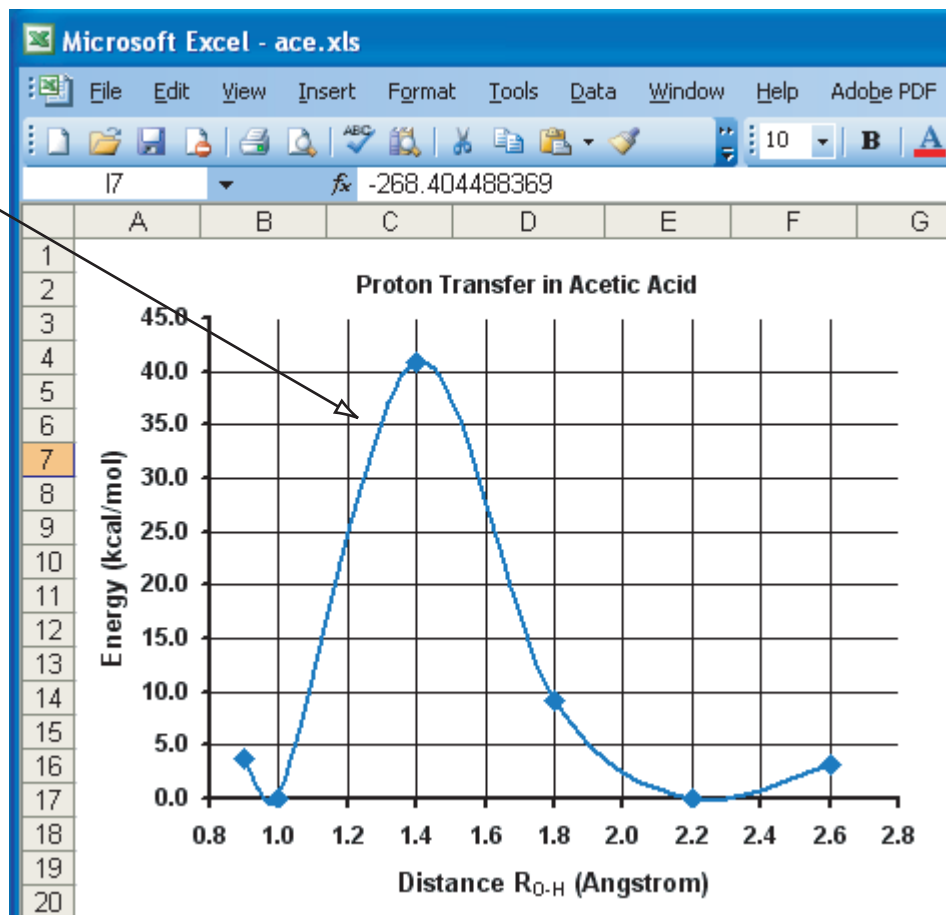
```
basis 6-31+G* ! Pople's double zet
geom_opt_coords 0 ! cartessian coordin
geom_opt_max_cycles 200 ! long geometry opti
mem_static 256 ! Static memory
mem_total 2000 ! Total memory
$end

$opt
CONSTRAINT
stre 10 11 0.9
ENDCONSTRAINT
$end
```

The terminal window also shows a menu bar (File, Edit, View, Window, Help), a toolbar with various icons, and a status bar at the bottom indicating "SSH2 - aes128-cbc -".

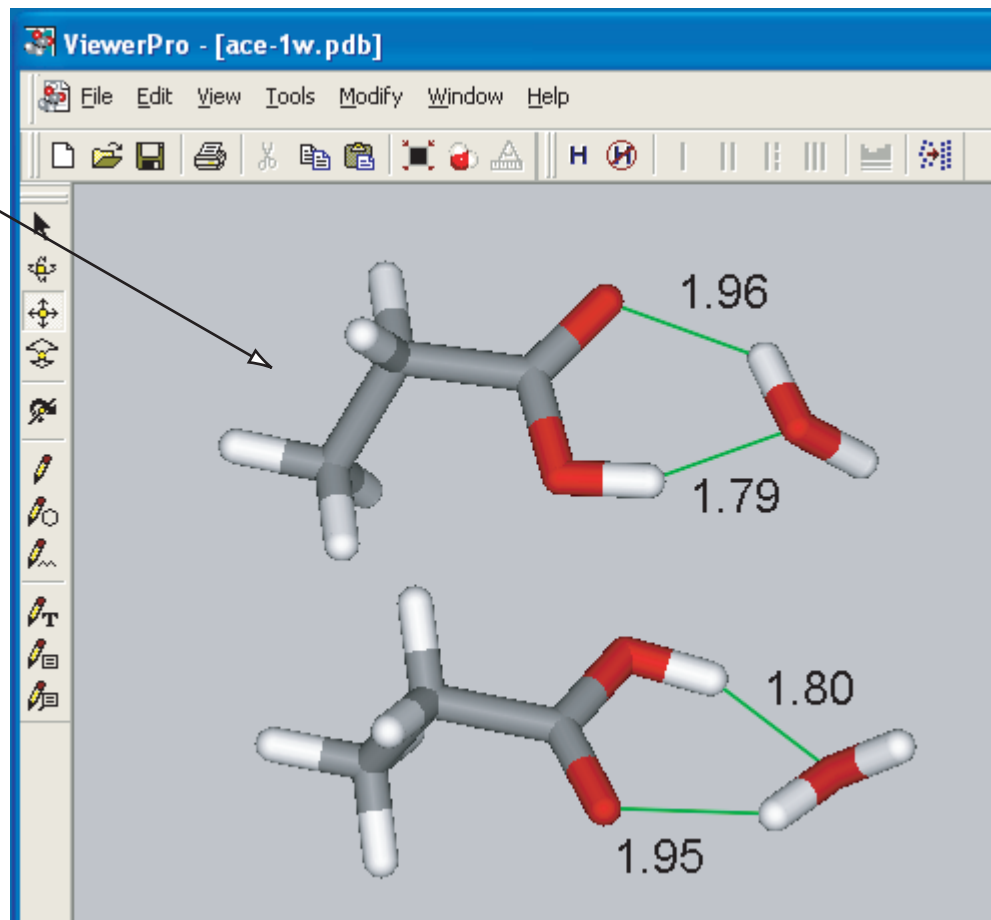
QM tautomerization - Alanine

Final results



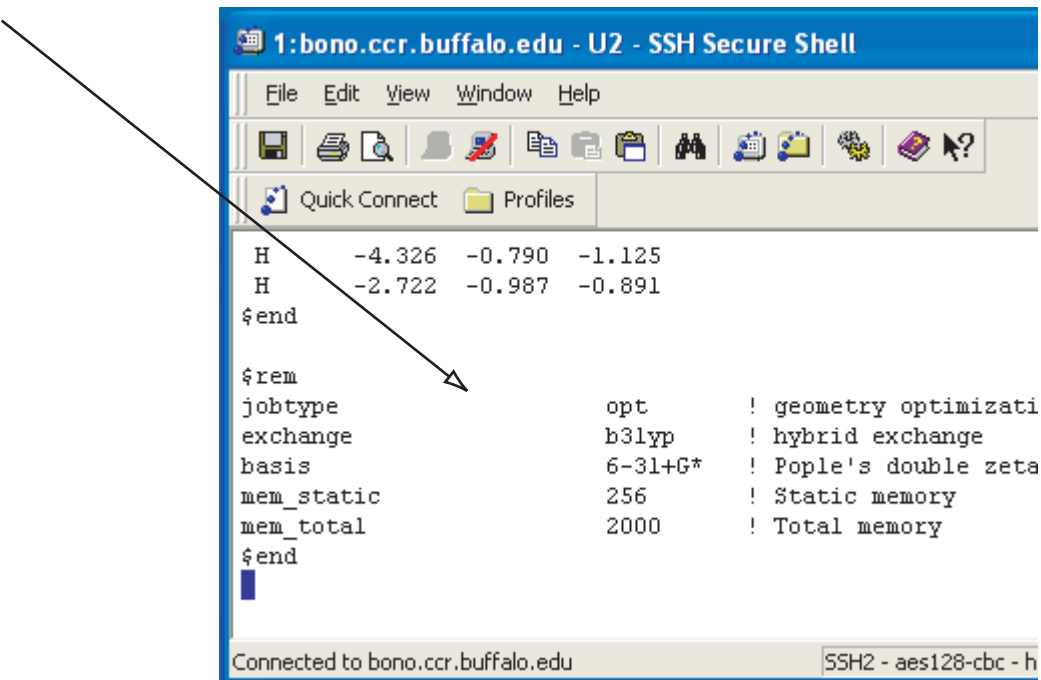
QM tautomerization - Alanine

Alanine and
water dimers



QM tautomerization - Alanine

Geometry
optimization



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
H      -4.326  -0.790  -1.125
H      -2.722  -0.987  -0.891
$end

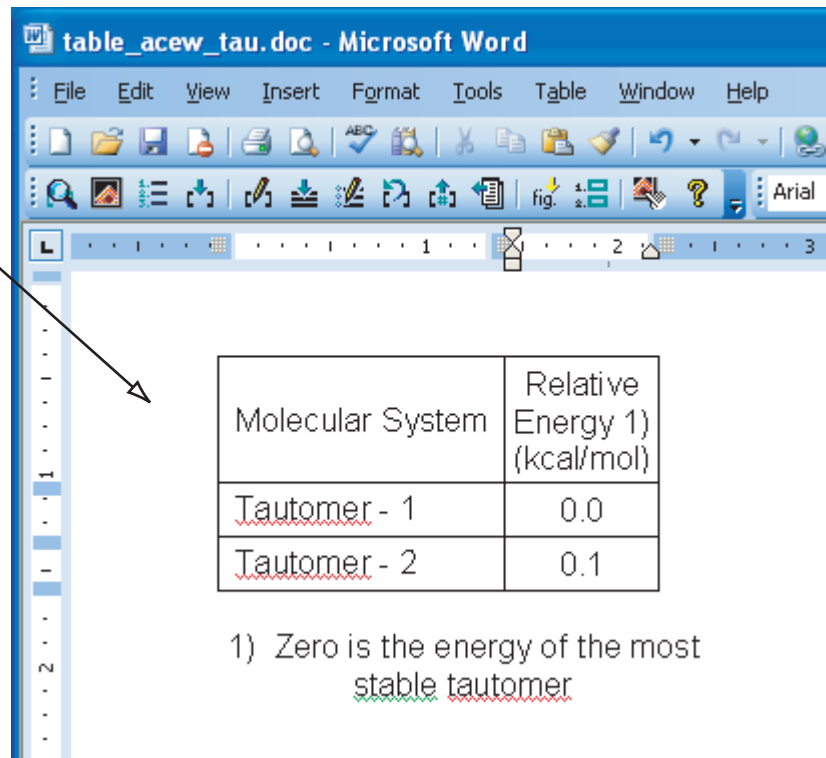
$rem
jobtype                opt      ! geometry optimizati
exchange               b3lyp    ! hybrid exchange
basis                  6-31+G*  ! Pople's double zeta
mem_static             256      ! Static memory
mem_total              2000     ! Total memory
$end

[Cursor]
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - h

QM tautomerization - Alanine

Final results



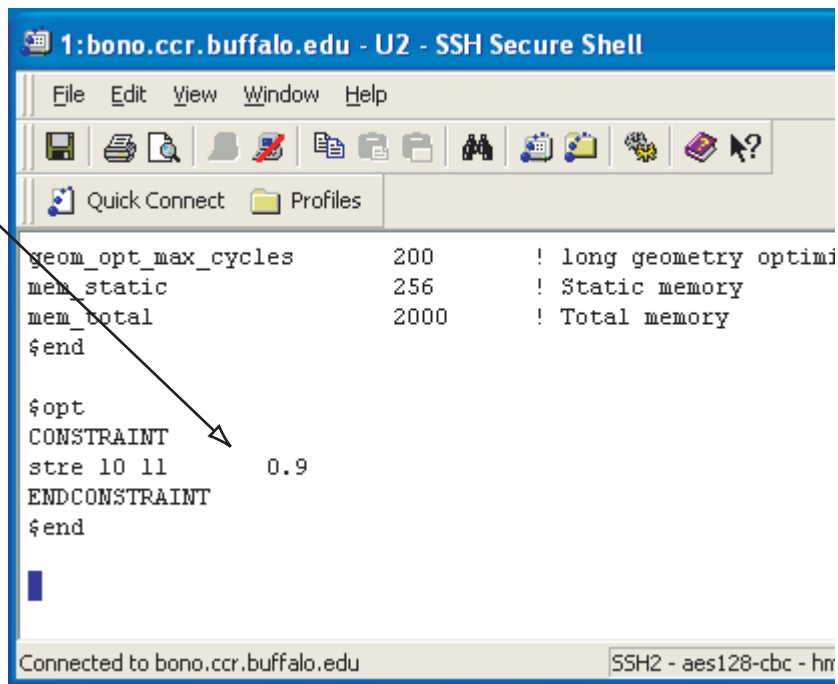
The screenshot shows a Microsoft Word document with a table containing two columns: 'Molecular System' and 'Relative Energy 1) (kcal/mol)'. The table lists two tautomers: 'Tautomer - 1' with a relative energy of 0.0, and 'Tautomer - 2' with a relative energy of 0.1. A footnote below the table states: '1) Zero is the energy of the most stable tautomer'.

Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - 1	0.0
Tautomer - 2	0.1

1) Zero is the energy of the most stable tautomer

QM tautomerization - Alanine

Calculations with a
constrained
distance



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

geom_opt_max_cycles      200      ! long geometry optimi
mem_static               256      ! Static memory
mem_total                2000     ! Total memory
$end

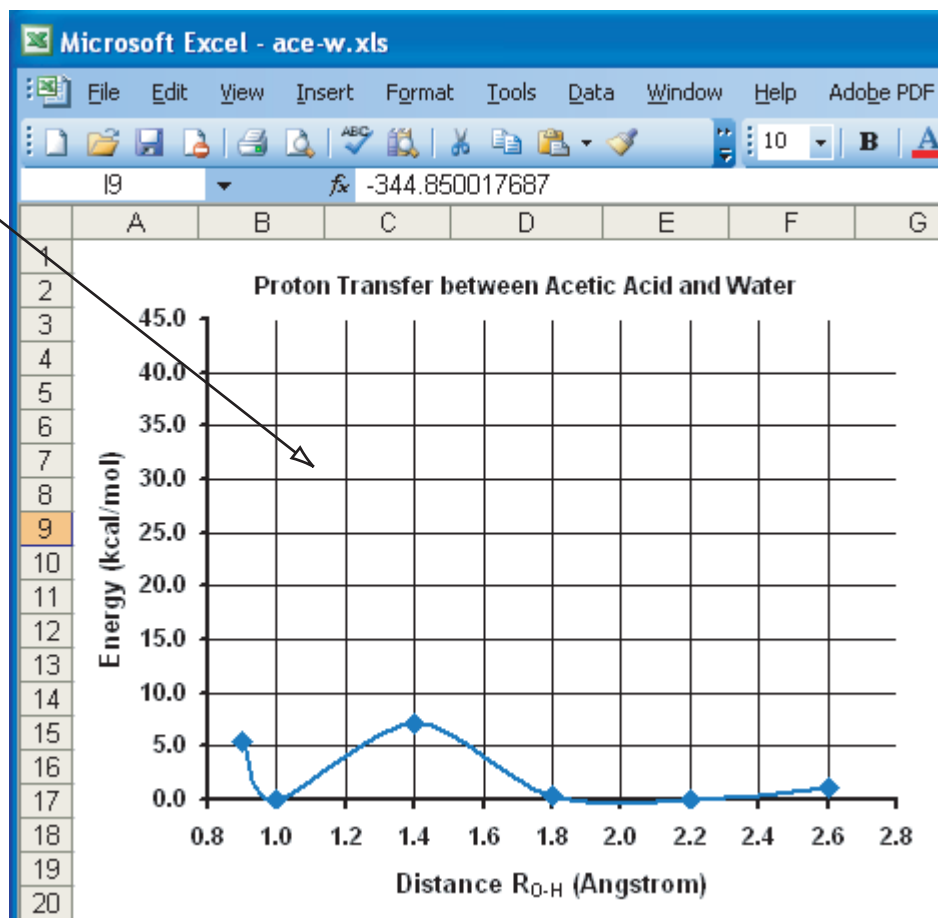
$opt
CONSTRAINT
stre 10 11      0.9
ENDCONSTRAINT
$end

[Cursor]
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hr

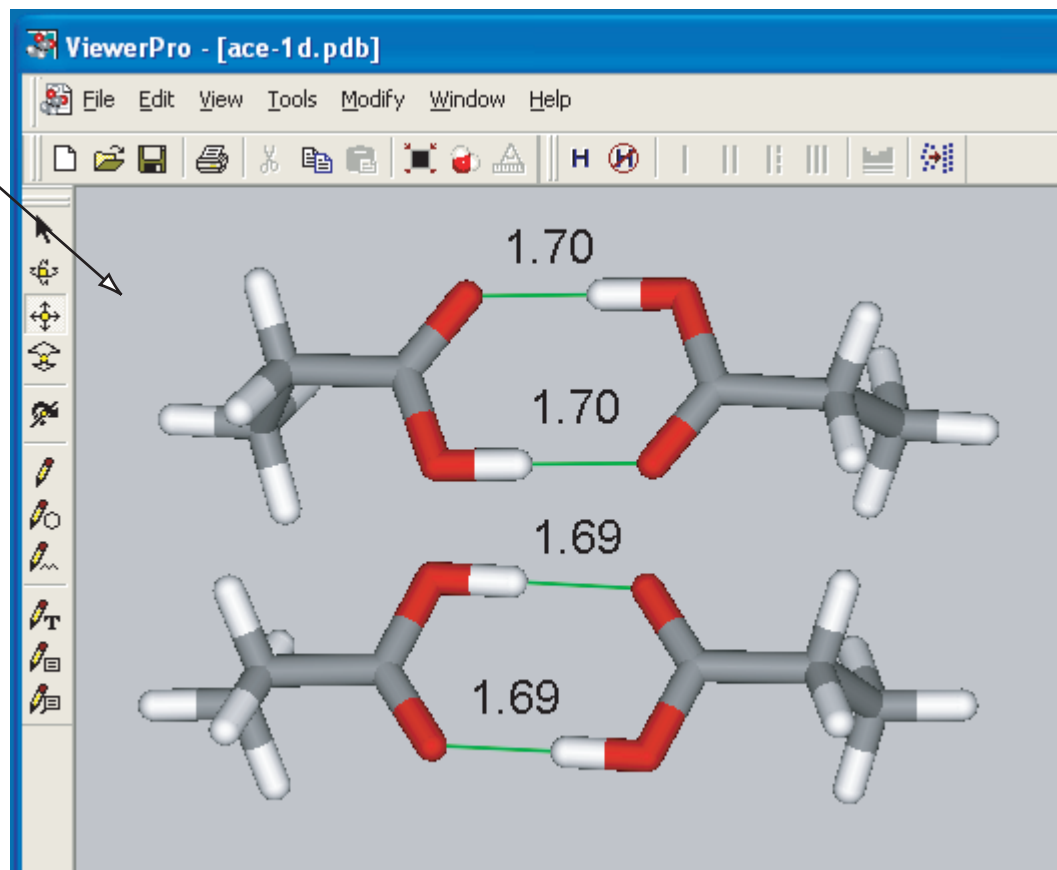
QM tautomerization - Alanine

Energy of the
proton transfer



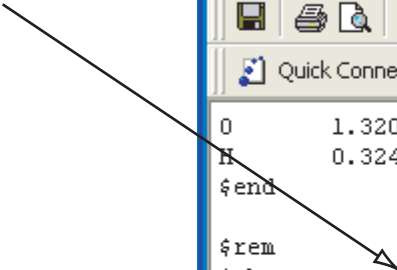
QM tautomerization - Alanine

Alanine dimers



QM tautomerization - Alanine

Geometry
optimization



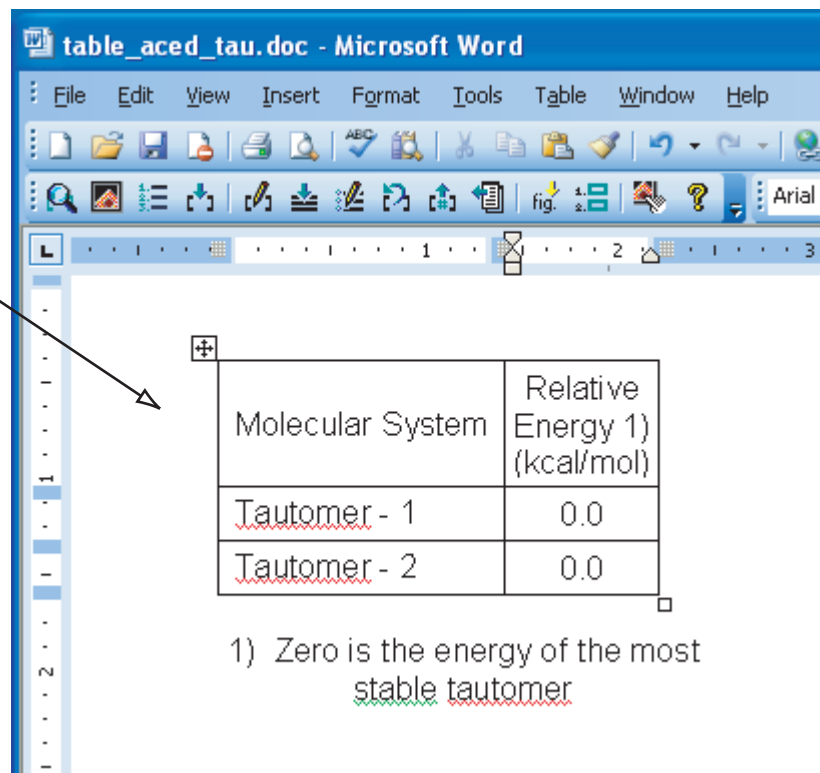
```
1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
O      1.320   1.286   0.129
H      0.324   1.161   0.142
$end

$rem
jobtype                opt          ! geometry optimizati
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double zeta
mem_static             256          ! Static memory
mem_total              2000         ! Total memory
$end

"ace-ld.in" 35L, 1311C
Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 -
```

QM tautomerization - Alanine

Final results



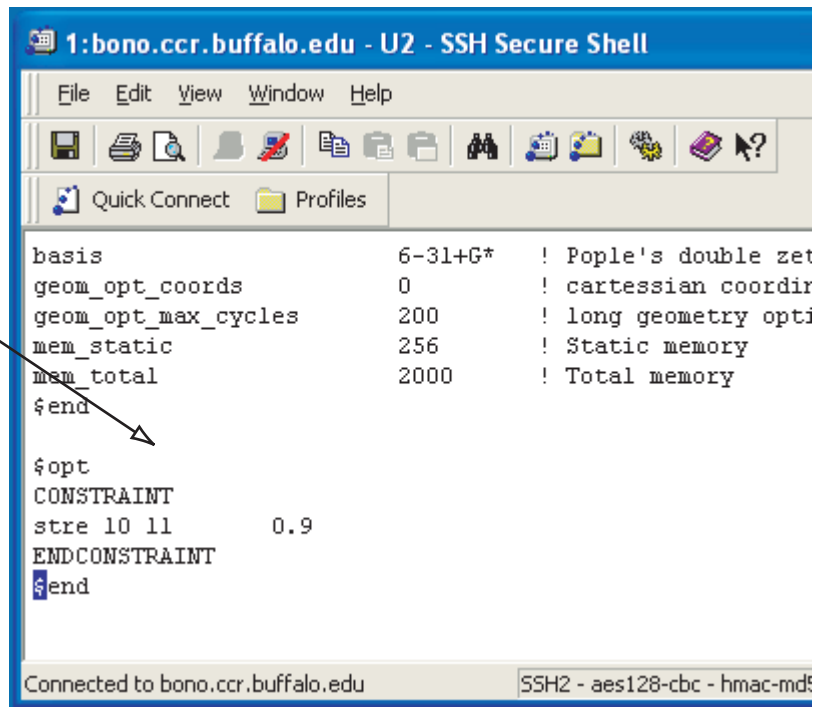
The screenshot shows a Microsoft Word window with the title 'table_aced_tau.doc'. The document contains a table with two columns: 'Molecular System' and 'Relative Energy 1) (kcal/mol)'. The table lists two tautomers, both with a relative energy of 0.0. A note below the table states: '1) Zero is the energy of the most stable tautomer'.

Molecular System	Relative Energy 1) (kcal/mol)
<u>Tautomer - 1</u>	0.0
<u>Tautomer - 2</u>	0.0

1) Zero is the energy of the most stable tautomer

QM tautomerization - Alanine

Geometry
optimization with
a constrained
distance



The screenshot shows an SSH window titled "1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window contains a text editor with a Gaussian input file. The file includes a basis set definition, geometry optimization settings, and a constraint on the distance between atoms 10 and 11. An arrow points from the text "Geometry optimization with a constrained distance" to the constraint section of the input file.

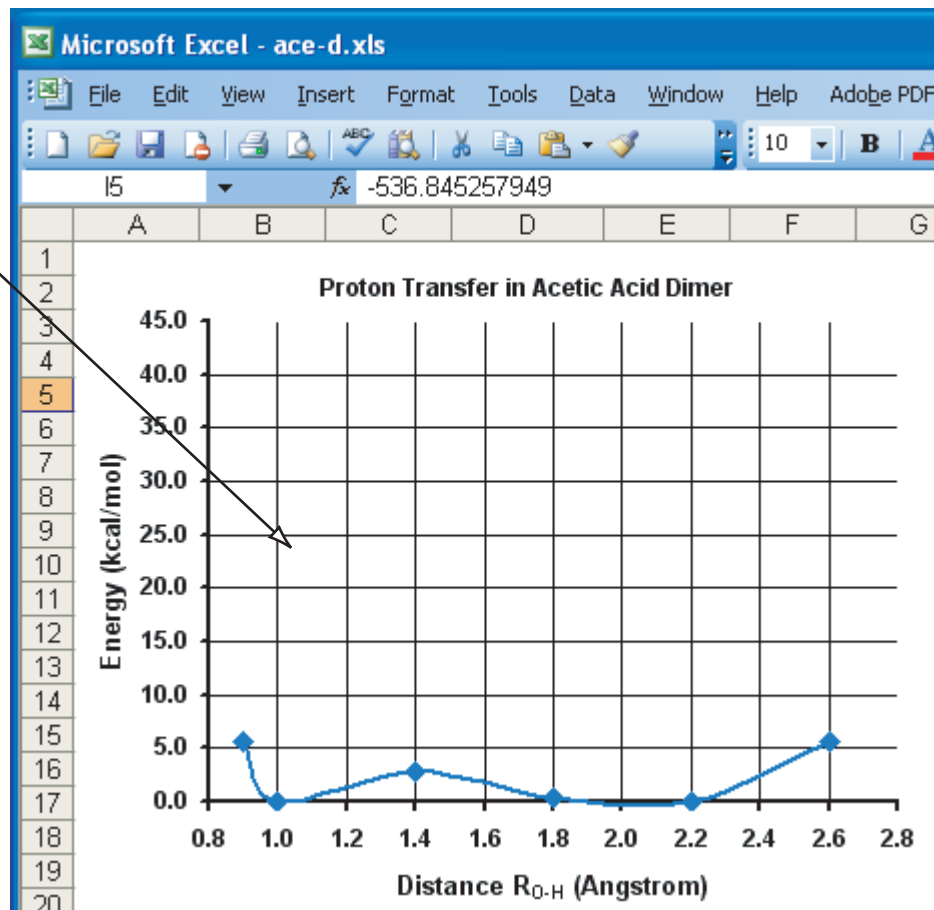
```
basis                6-31+G*    ! Pople's double zet
geom_opt_coords      0          ! cartessian coordin
geom_opt_max_cycles  200        ! long geometry opti
mem_static           256        ! Static memory
mem_total            2000       ! Total memory
$end

$opt
CONSTRAINT
stre 10 11          0.9
ENDCONSTRAINT
$end
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5

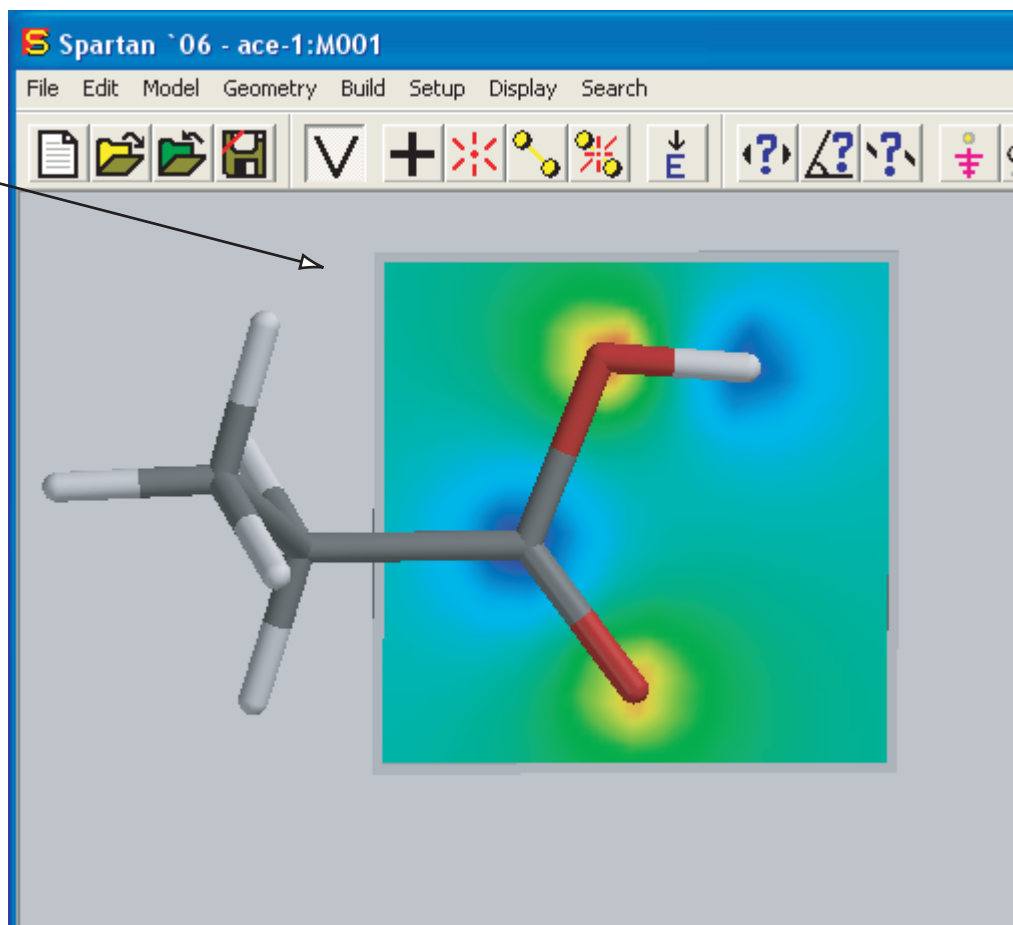
QM tautomerization - Alanine

Energy of proton transfer in the dimer



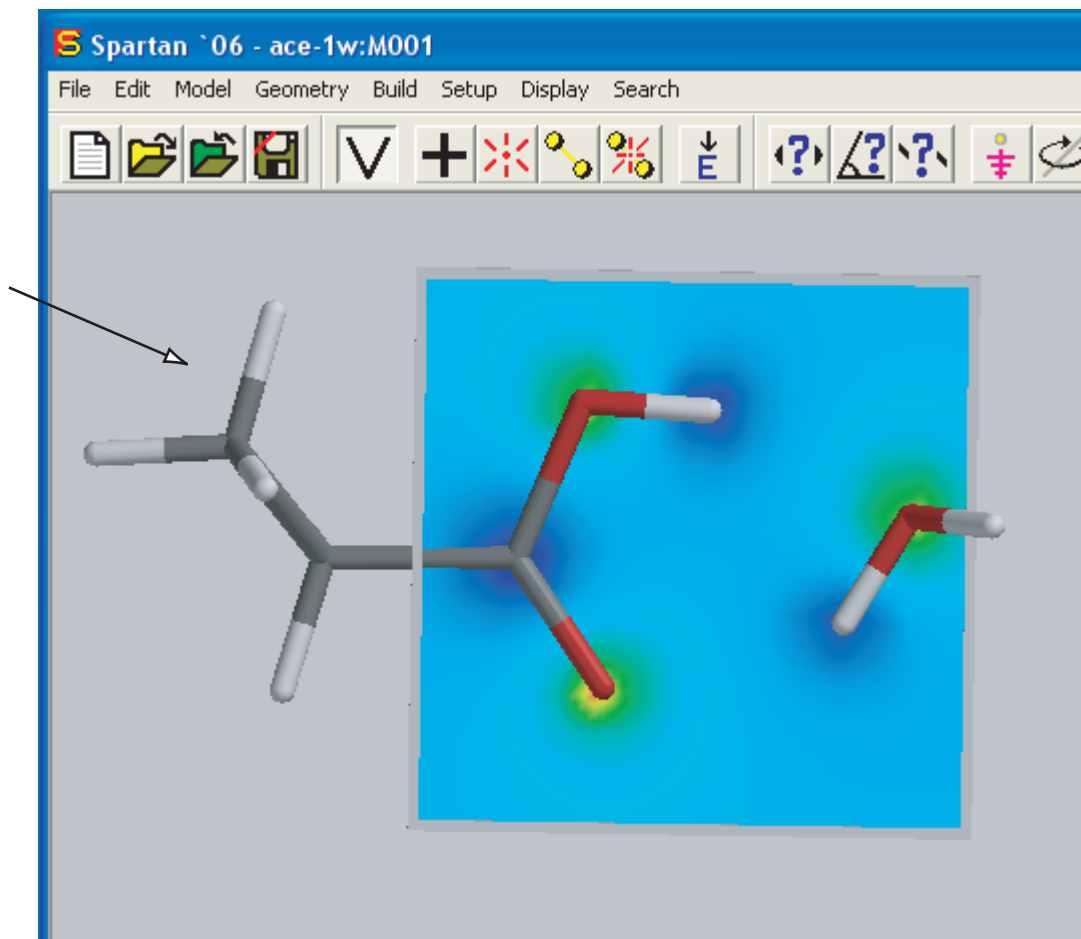
QM tautomerization - Alanine

Electrostatic
potential



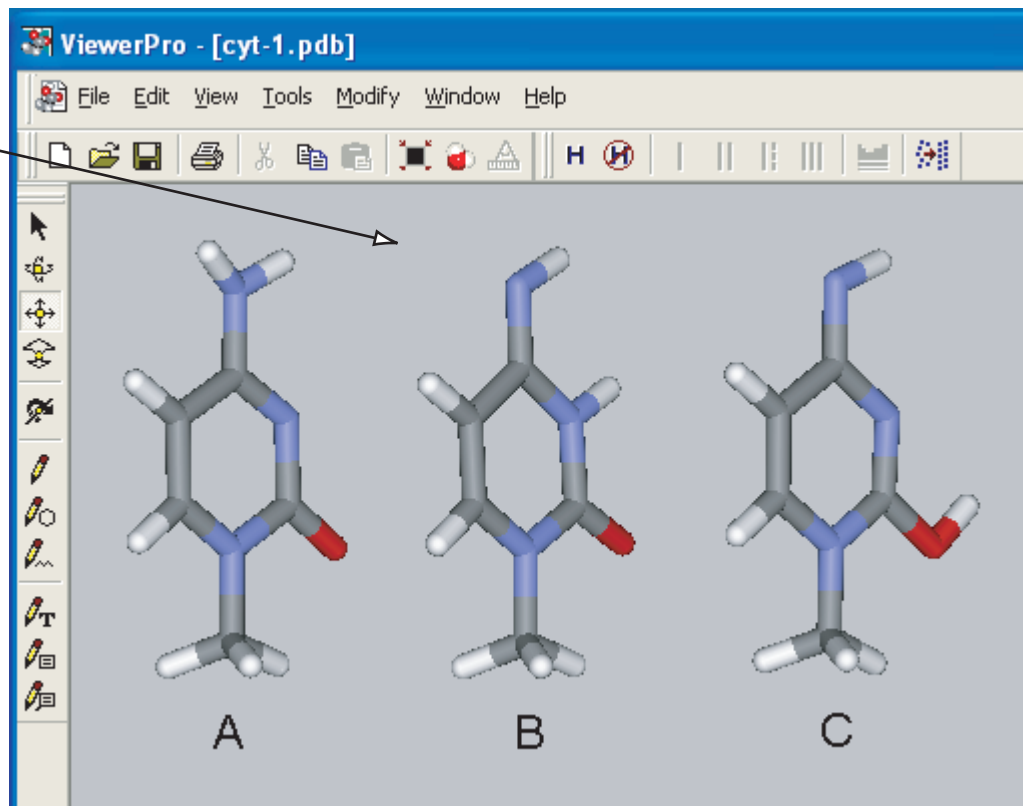
QM tautomerization - Alanine

Electrostatic
potential of
hydrogen
bonded dimer



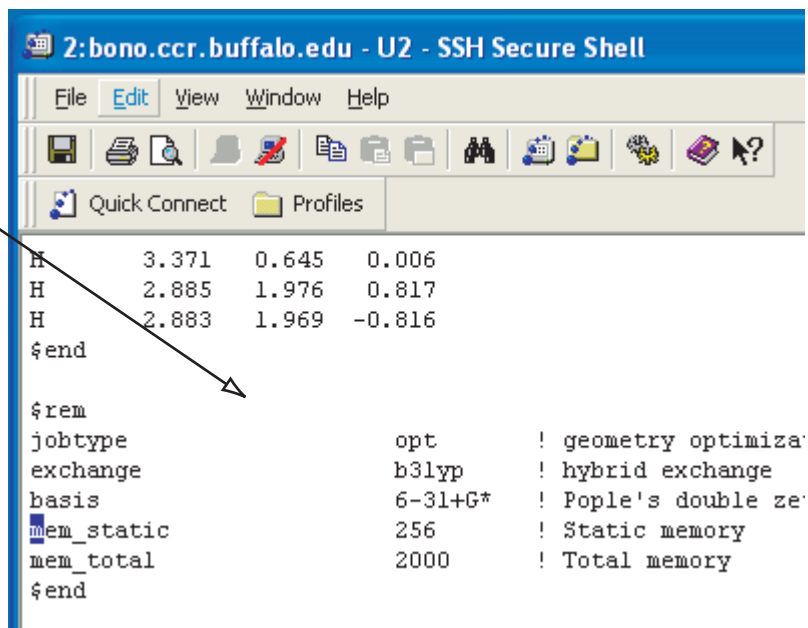
QM tautomerization - Cytosine

Geometry optimization of three cytosine tautomers



QM tautomerization - Cytosine

Geometry
optimization of
three cytosine
tautomers



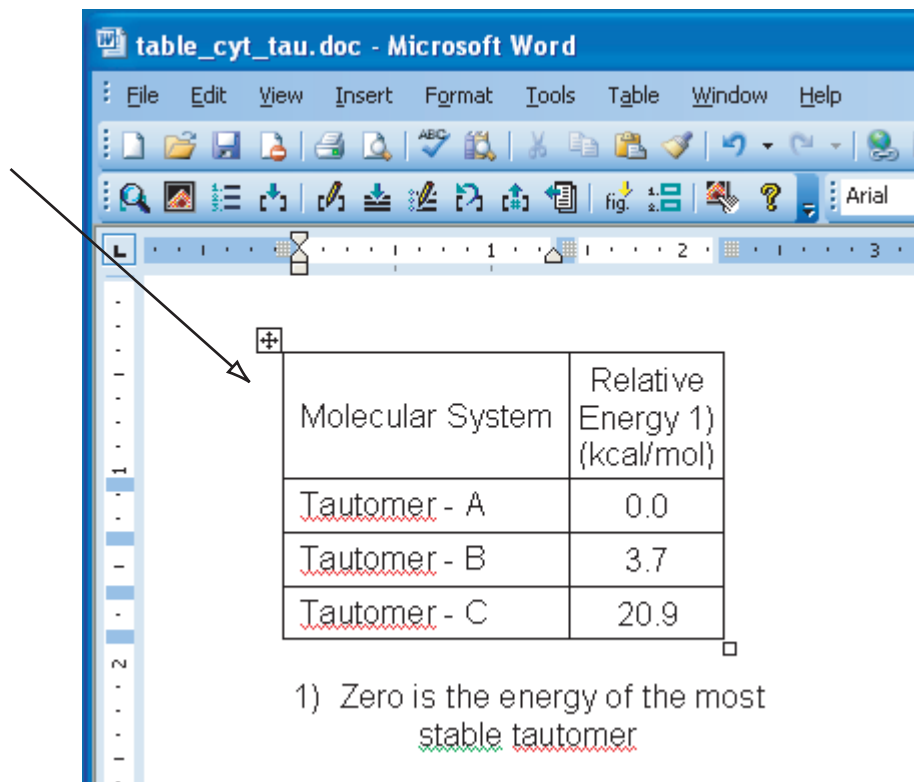
```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Open, Save As, Recent, Run, Stop, Help]
Quick Connect Profiles

H      3.371   0.645   0.006
H      2.885   1.976   0.817
H      2.883   1.969  -0.816
$end

$rem
jobtype                opt          ! geometry optimization
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double zeta
mem_static             256         ! Static memory
mem_total              2000        ! Total memory
$end
```

QM tautomerization - Cytosine

Final results of
the calculations



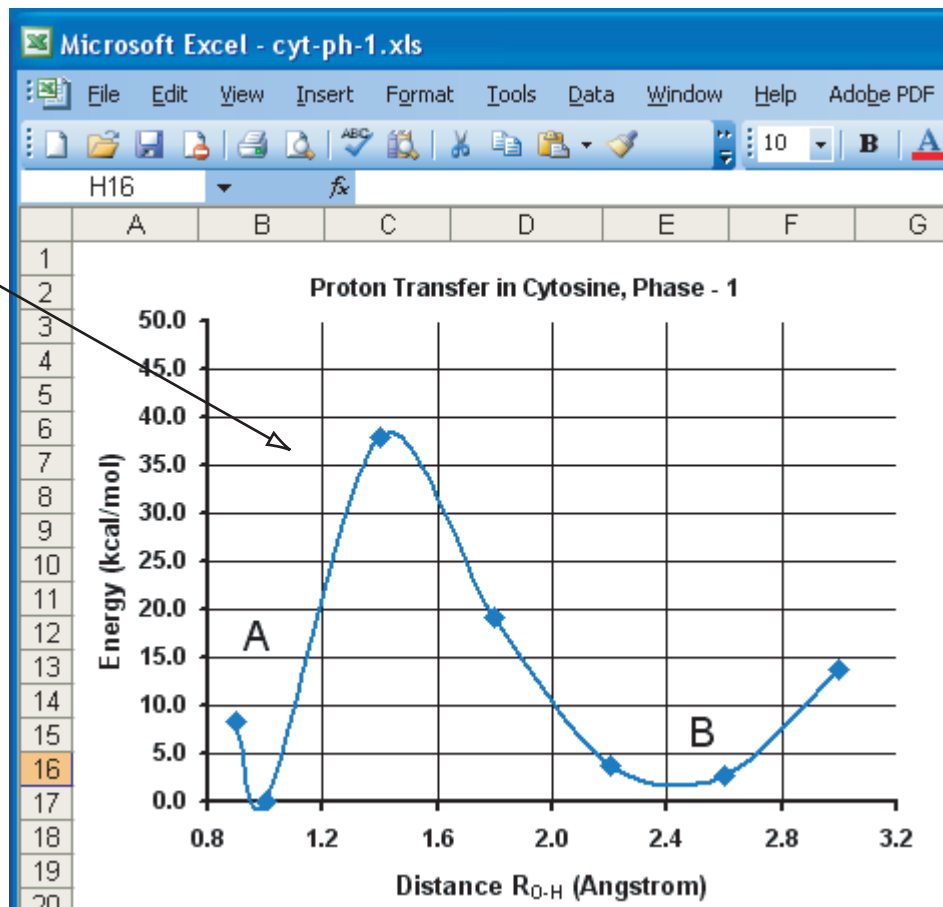
The screenshot shows a Microsoft Word document with a table containing the following data:

Molecular System	Relative Energy 1) (kcal/mol)
<u>Tautomer - A</u>	0.0
<u>Tautomer - B</u>	3.7
<u>Tautomer - C</u>	20.9

1) Zero is the energy of the most
stable tautomer

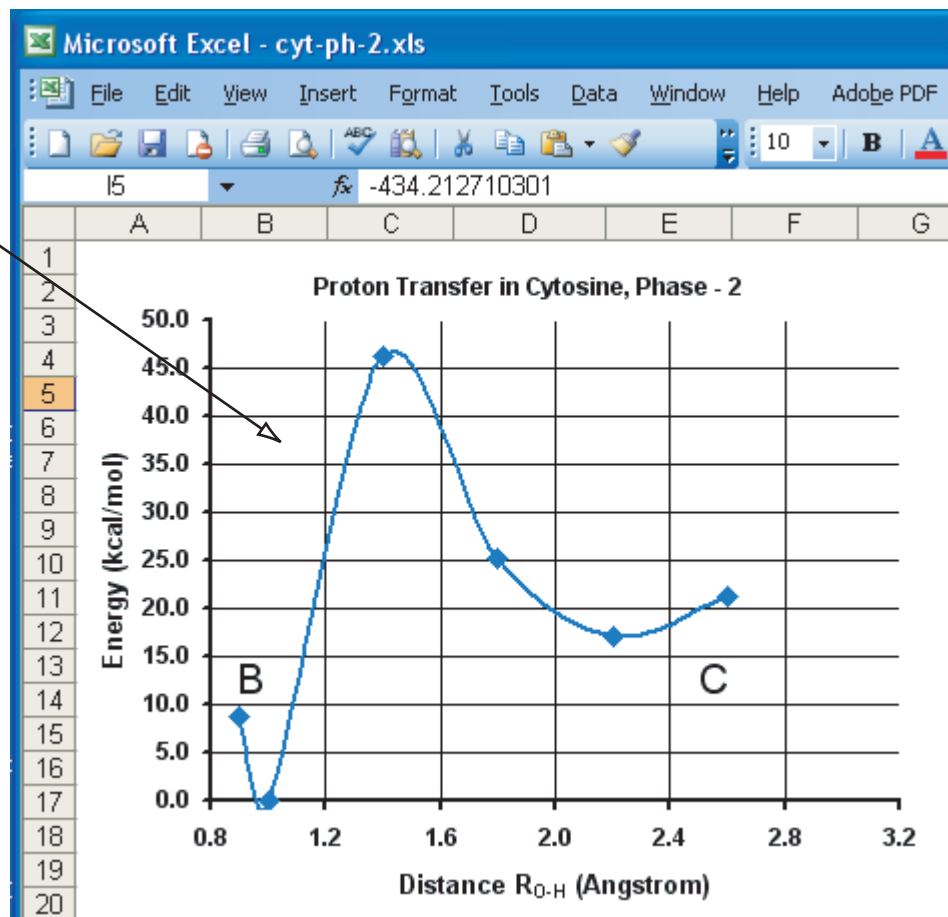
QM tautomerization - Cytosine

Energy of the
first phase of
proton transfer



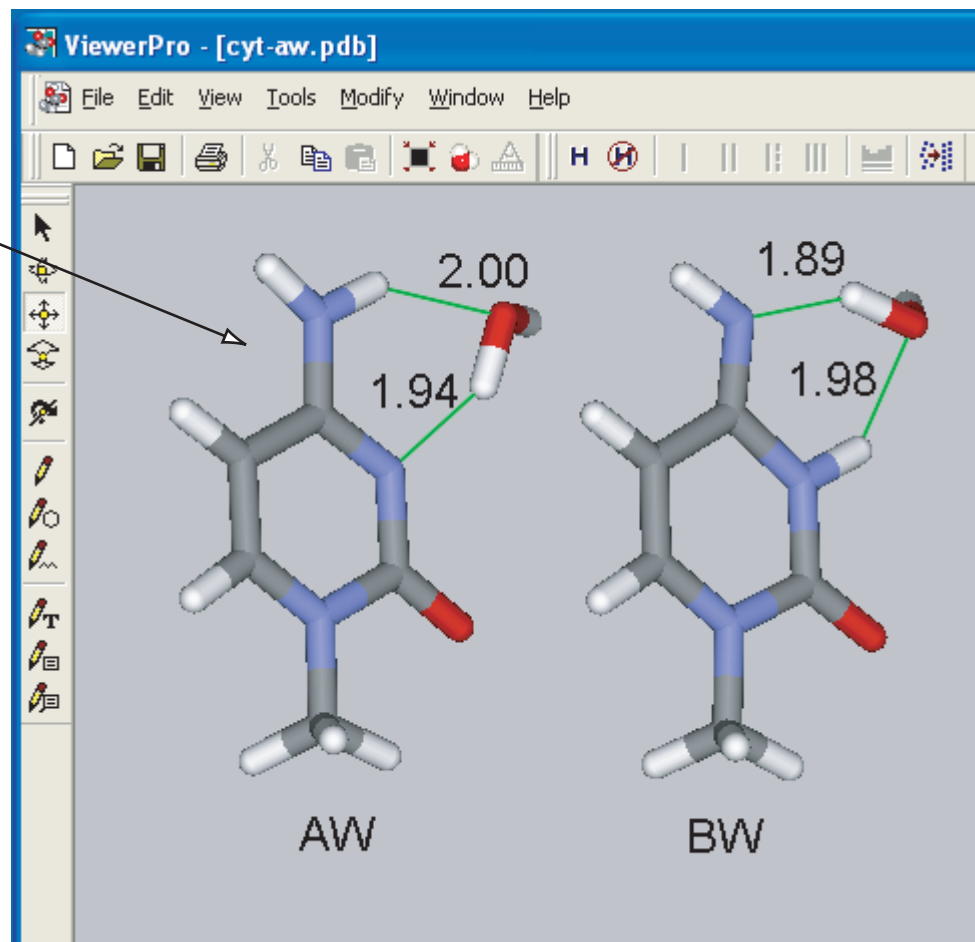
QM tautomerization - Cytosine

Energy of the
second phase of
proton transfer



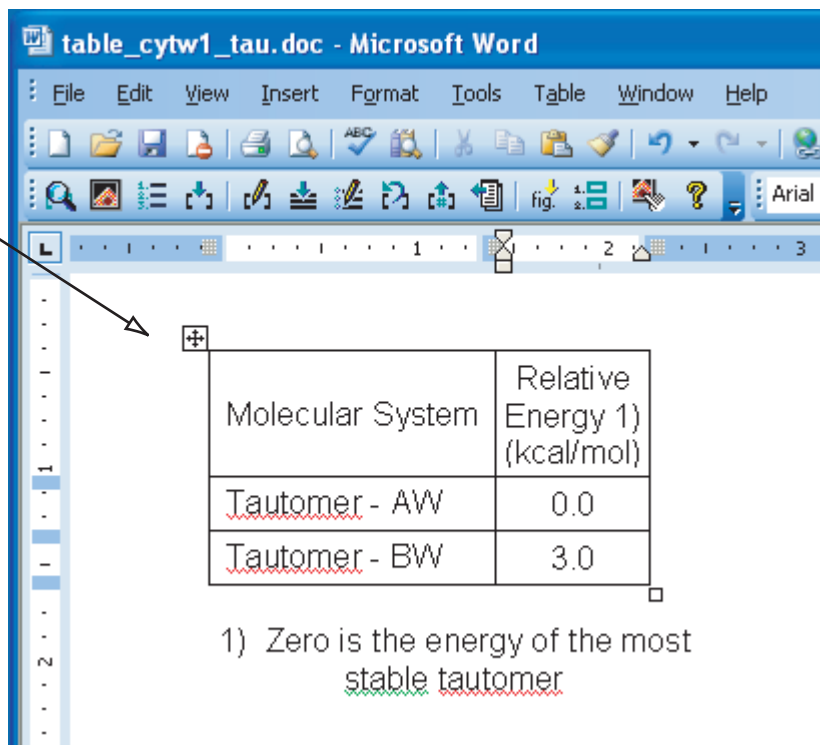
QM tautomerization - Cytosine

Two tautomers
of the cysteine
and water dimer



QM tautomerization - Cytosine

Energies of
the calculated
dimers

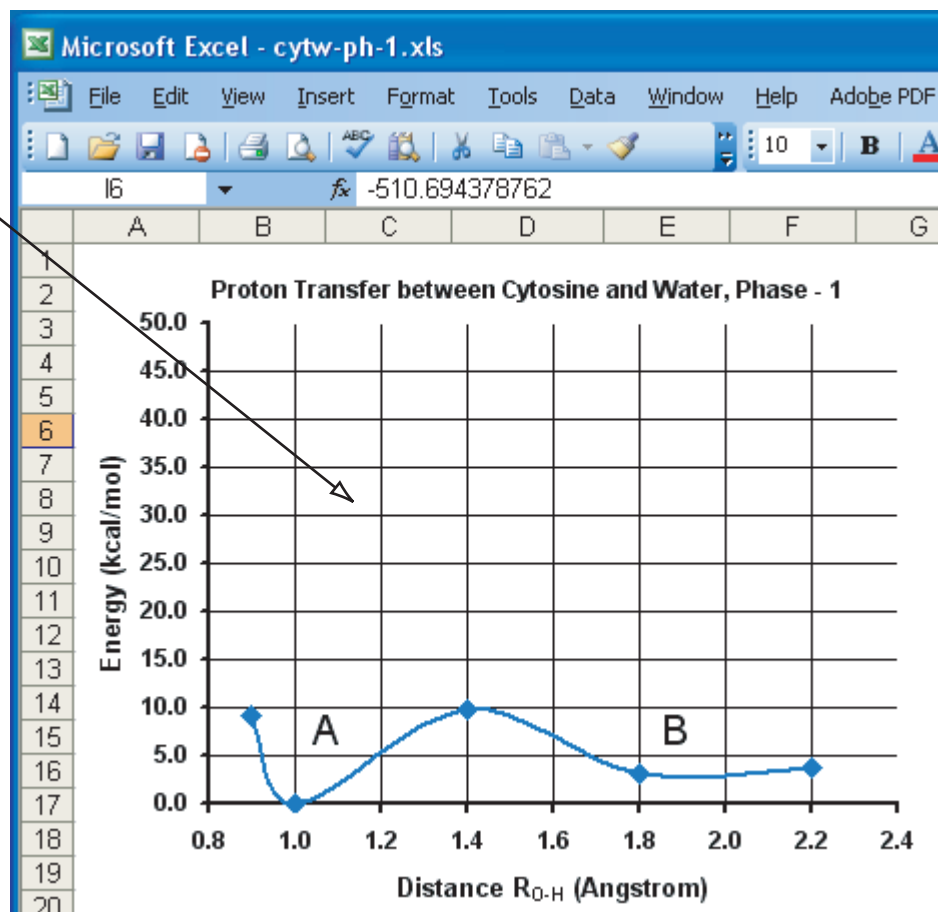


Molecular System	Relative Energy 1) (kcal/mol)
<u>Tautomer - AW</u>	0.0
<u>Tautomer - BW</u>	3.0

1) Zero is the energy of the most stable tautomer

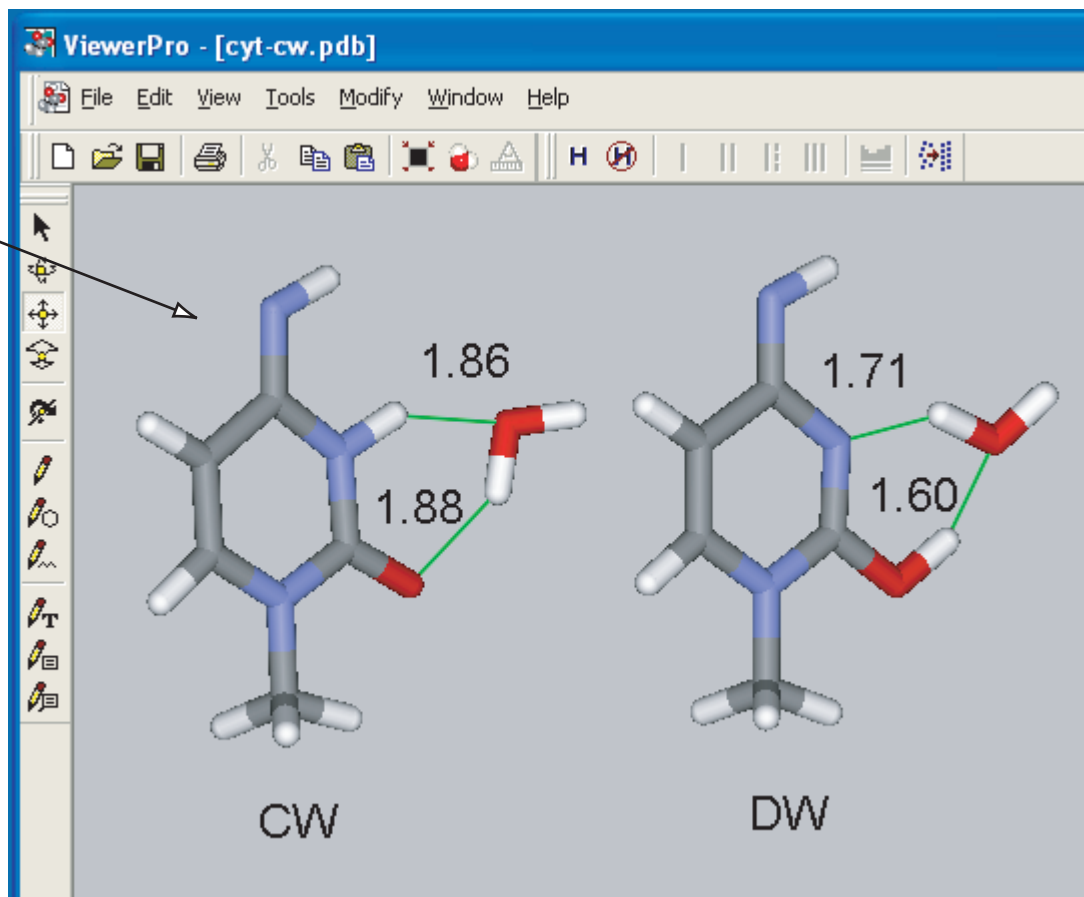
QM tautomerization - Cytosine

Energy of proton transfer



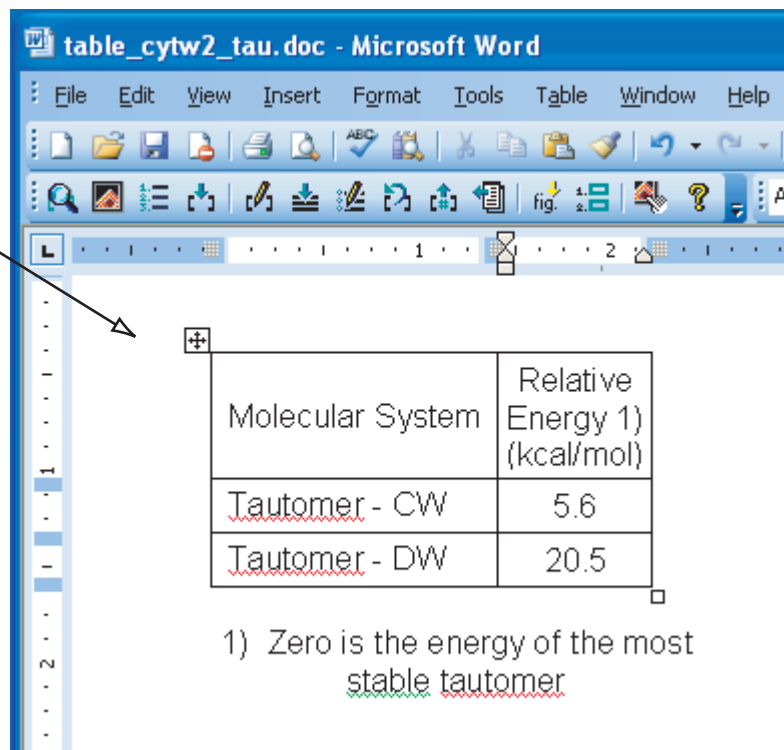
QM tautomerization - Cytosine

Two
tautomers of
the cysteine
water dimer



QM tautomerization - Cytosine

Results of the
calculations



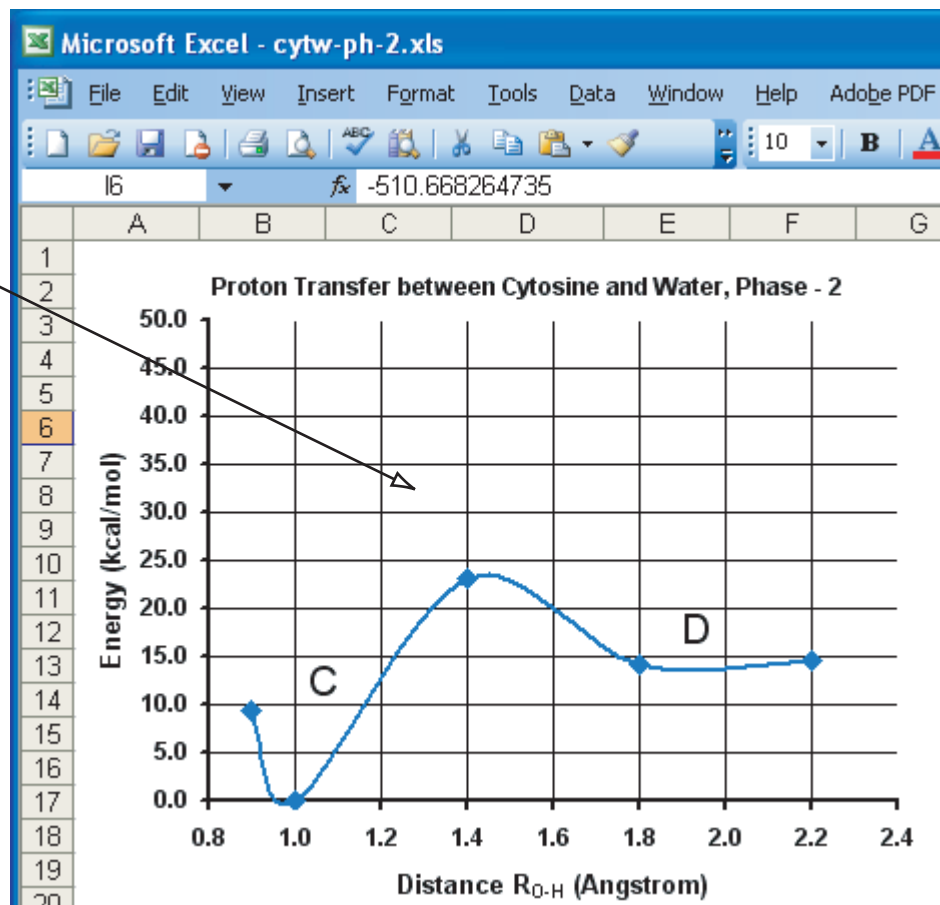
table_cytw2_tau.doc - Microsoft Word

Molecular System	Relative Energy 1) (kcal/mol)
<u>Tautomer - CW</u>	5.6
<u>Tautomer - DW</u>	20.5

1) Zero is the energy of the most
stable tautomer

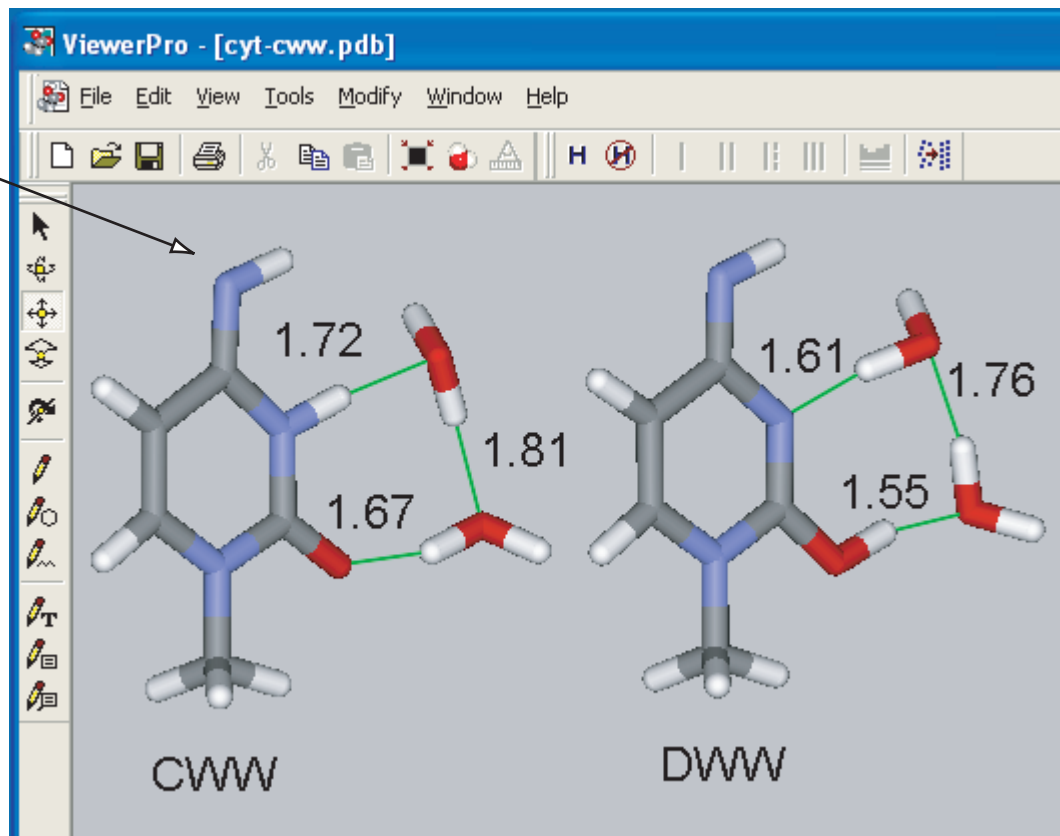
QM tautomerization - Cytosine

Energy of proton transfer between tautomers of the dimer



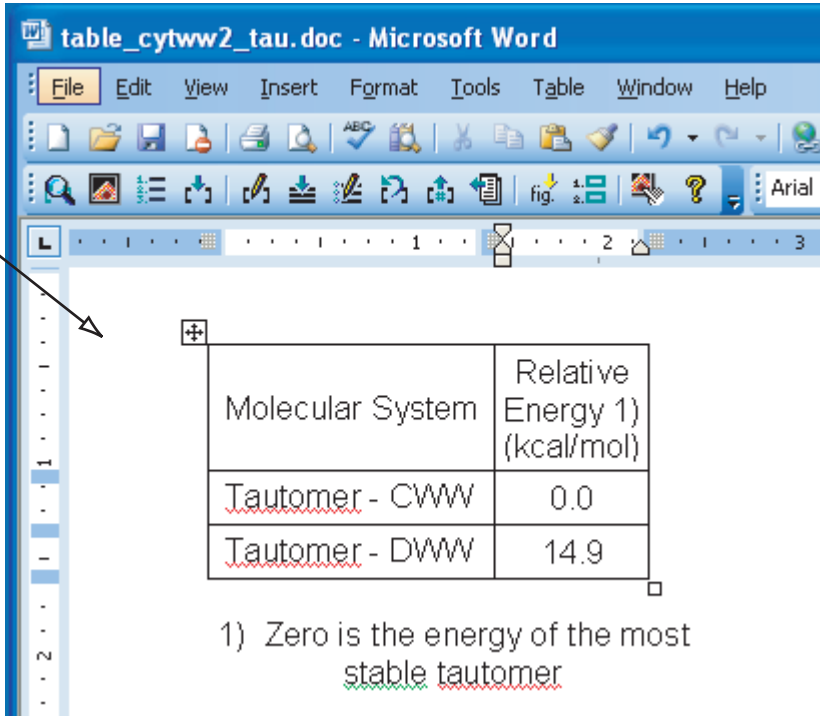
QM tautomerization - Cytosine

Two tautomers
of a cytosine
water trimer



QM tautomerization - Cytosine

Results of the
calculations



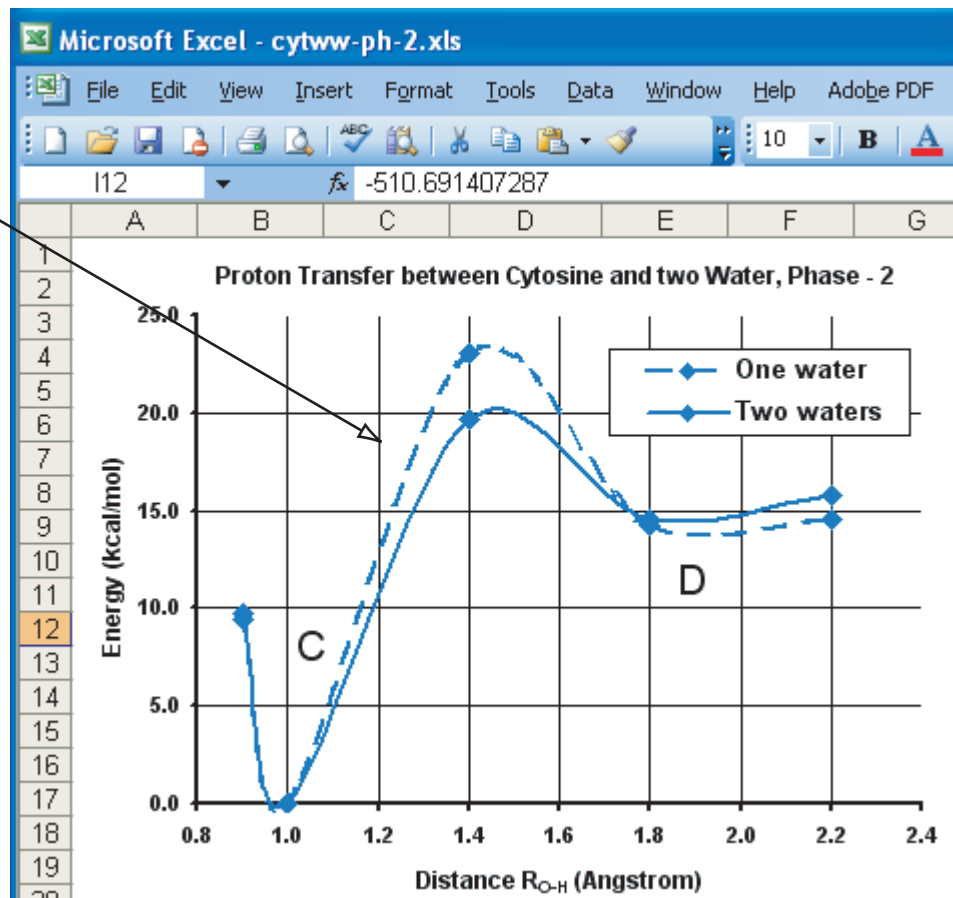
The screenshot shows a Microsoft Word window with the title 'table_cytww2_tau.doc'. The document contains a table with two columns: 'Molecular System' and 'Relative Energy 1) (kcal/mol)'. The table lists two tautomers: 'Tautomer - CWW' with a relative energy of 0.0, and 'Tautomer - DWW' with a relative energy of 14.9. A footnote below the table states: '1) Zero is the energy of the most stable tautomer'.

Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - CWW	0.0
Tautomer - DWW	14.9

1) Zero is the energy of the most stable tautomer

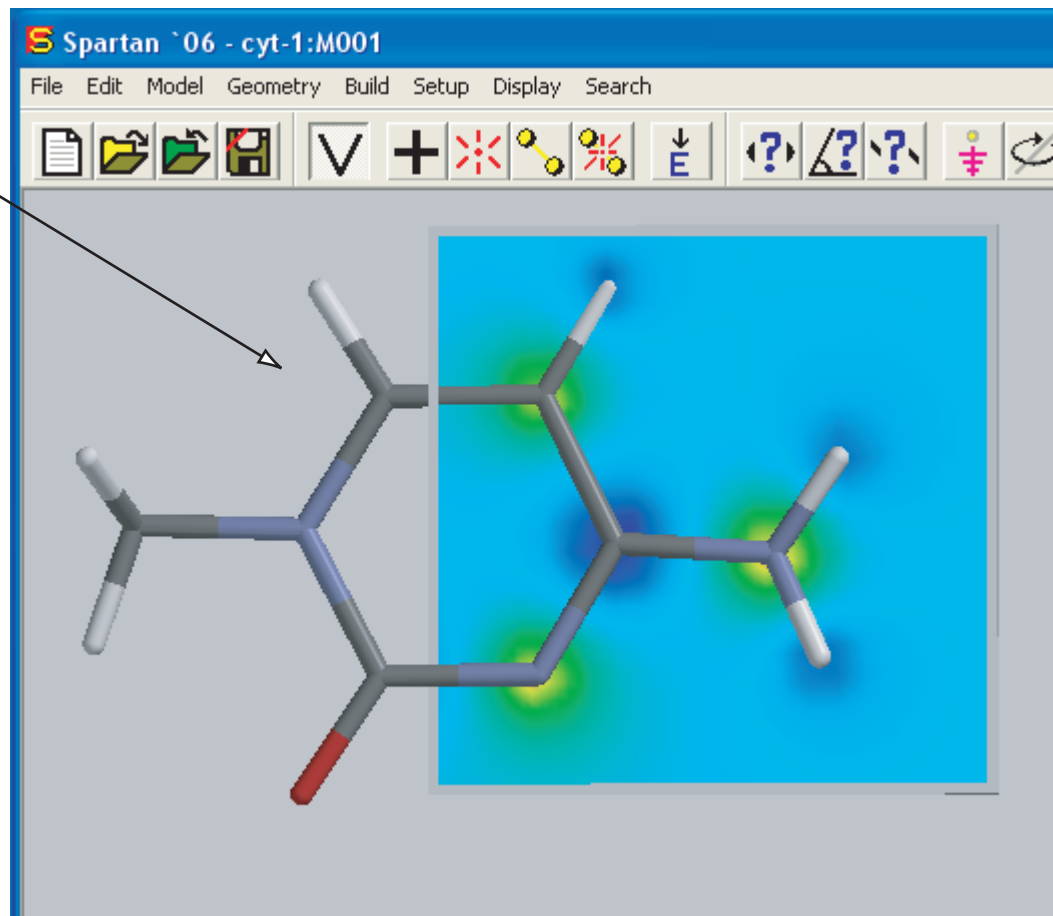
QM tautomerization - Cytosine

Energy of proton transfer in cytosine dimer and trimer



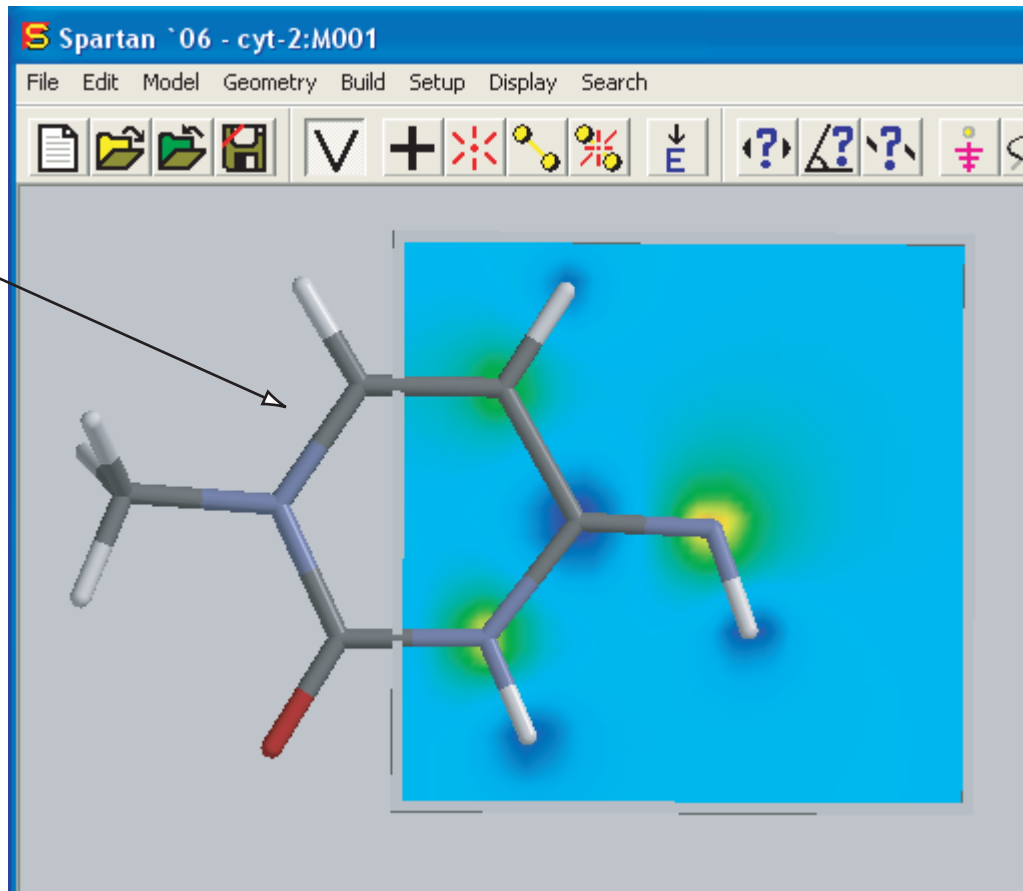
QM tautomerization - Cytosine

Electrostatic
potential of
cytosine
tautomer - 1



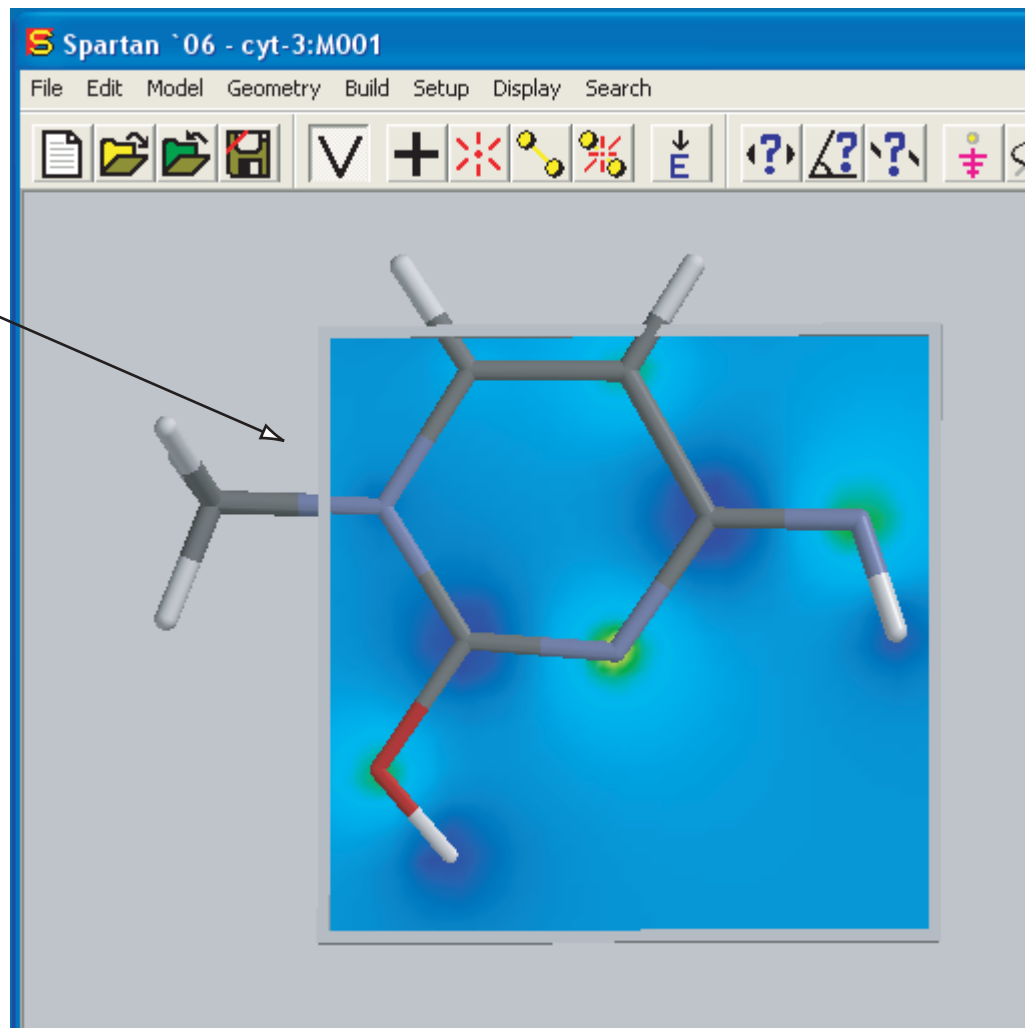
QM tautomerization - Cytosine

Electrostatic
potential of
cytosine
tautomer - 2



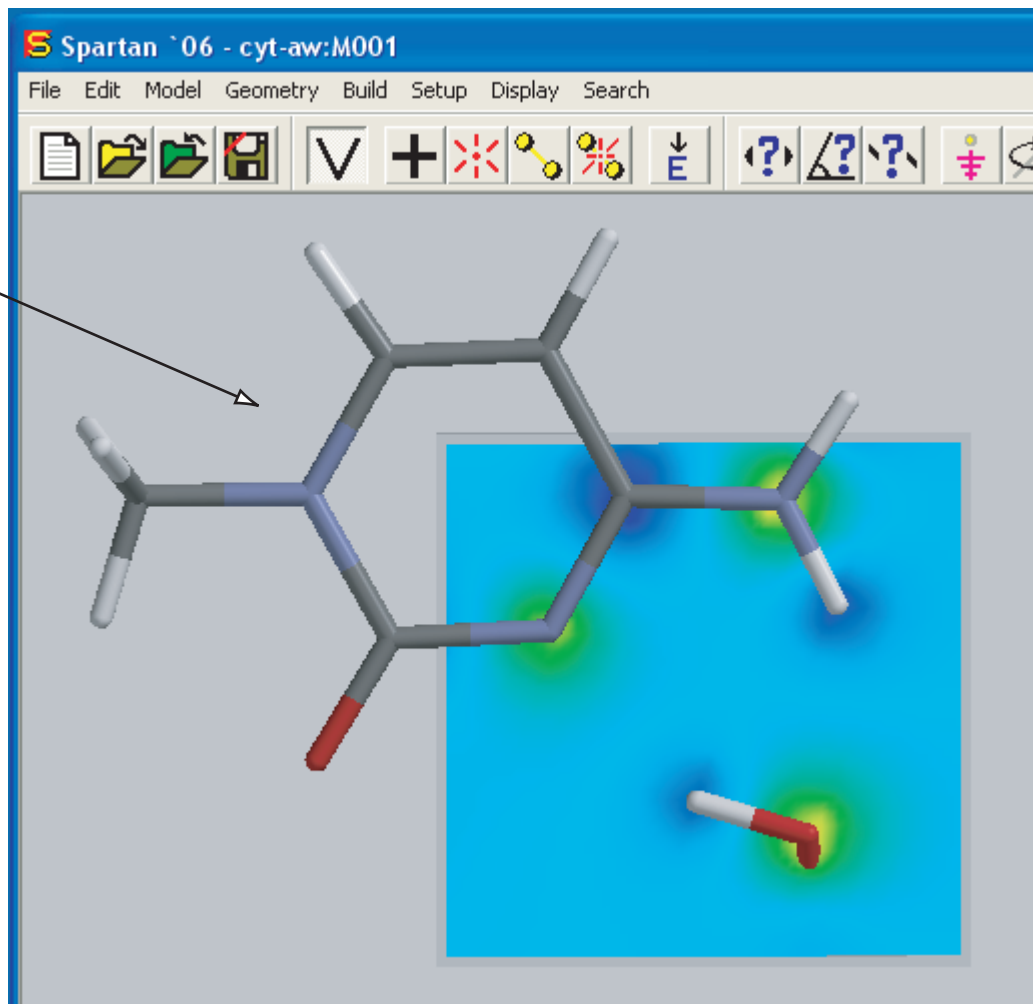
QM tautomerization - Cytosine

Electrostatic
potential of
cytosine
tautomer - 3



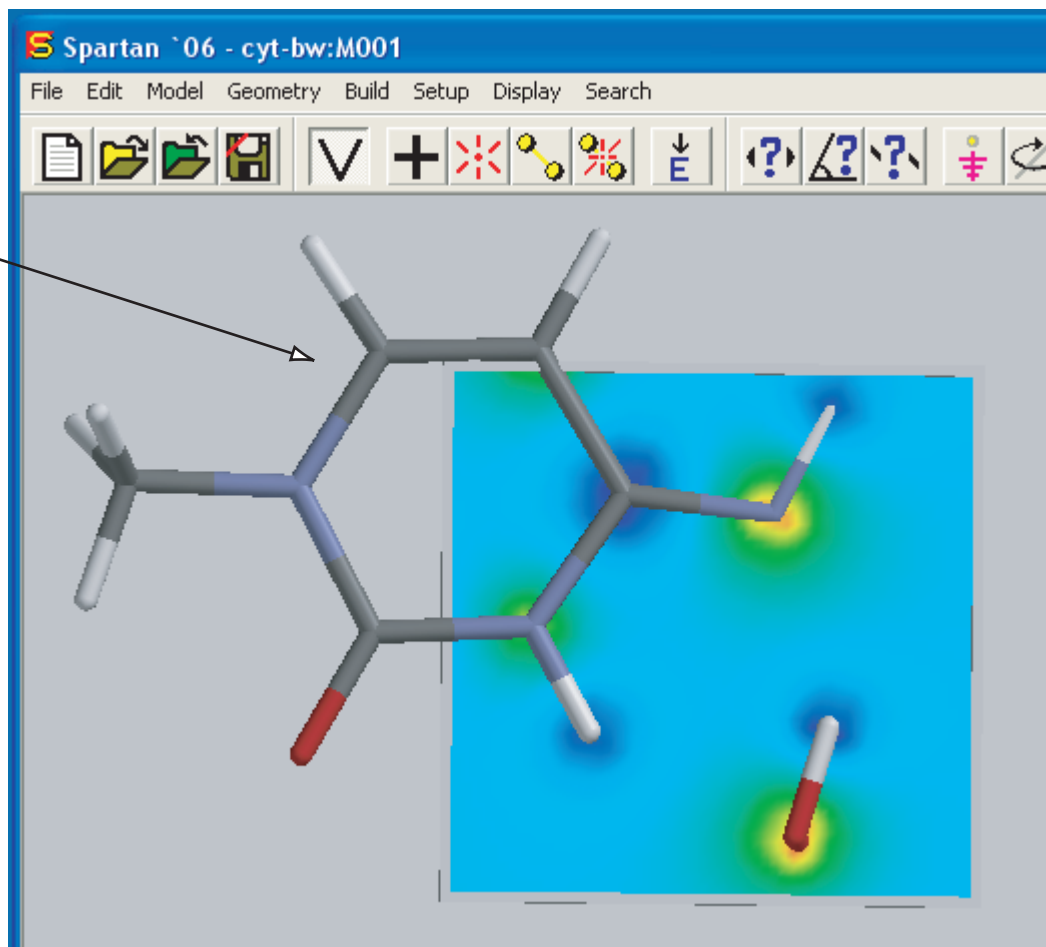
QM tautomerization - Cytosine

Electrostatic
potential of
cytosine water
dimer (AW)



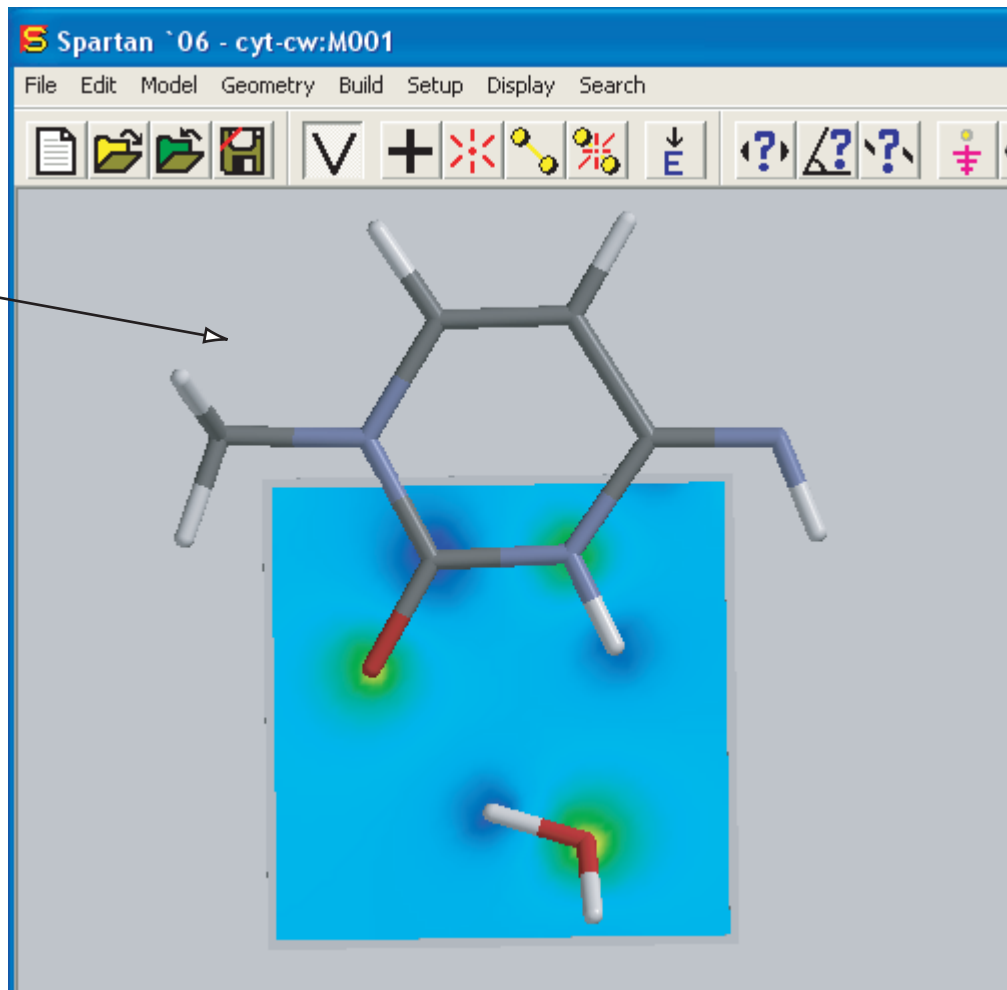
QM tautomerization - Cytosine

Electrostatic
potential of
cytosine water
dimer (BW)



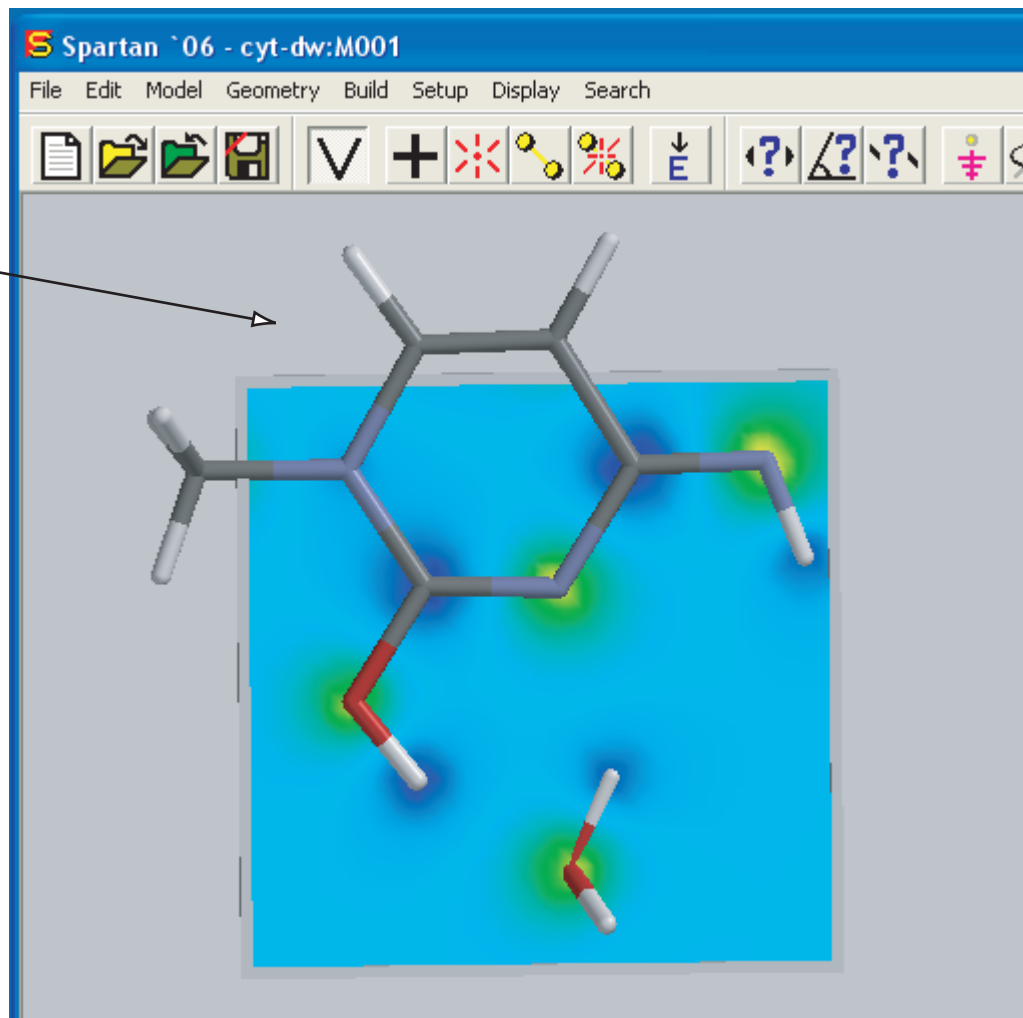
QM tautomerization - Cytosine

Electrostatic
potential of
cytosine water
dimer (CW)



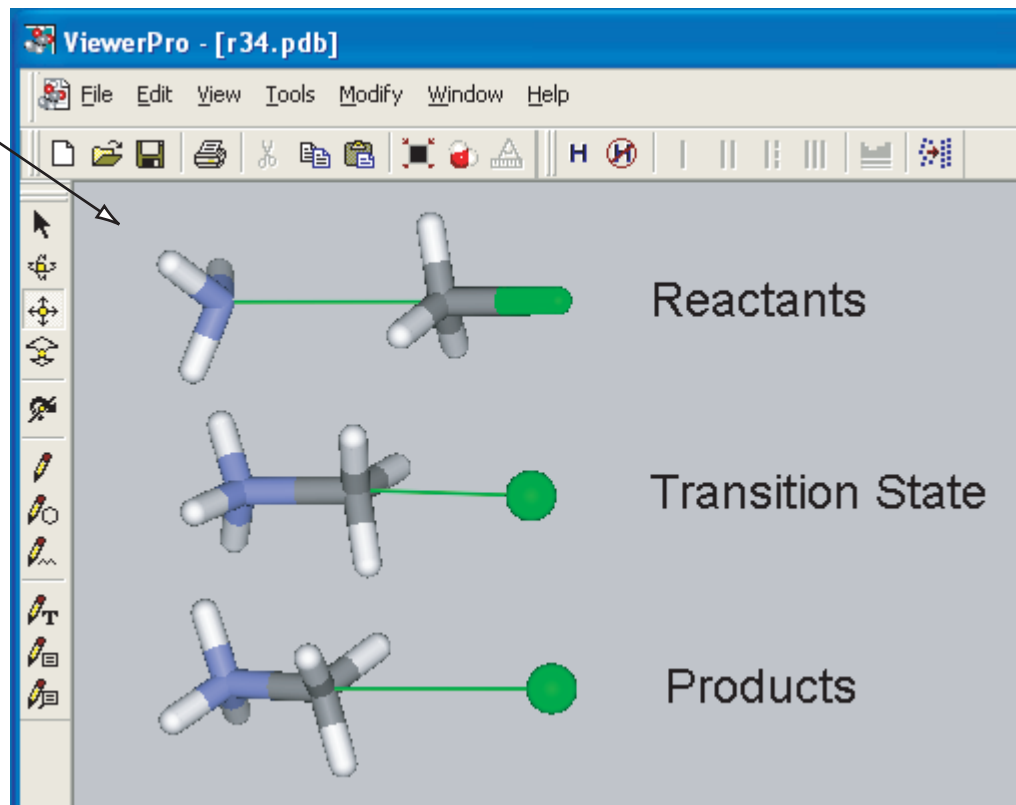
QM tautomerization - Cytosine

Electrostatic
potential of
cytosine water
dimer (DW)



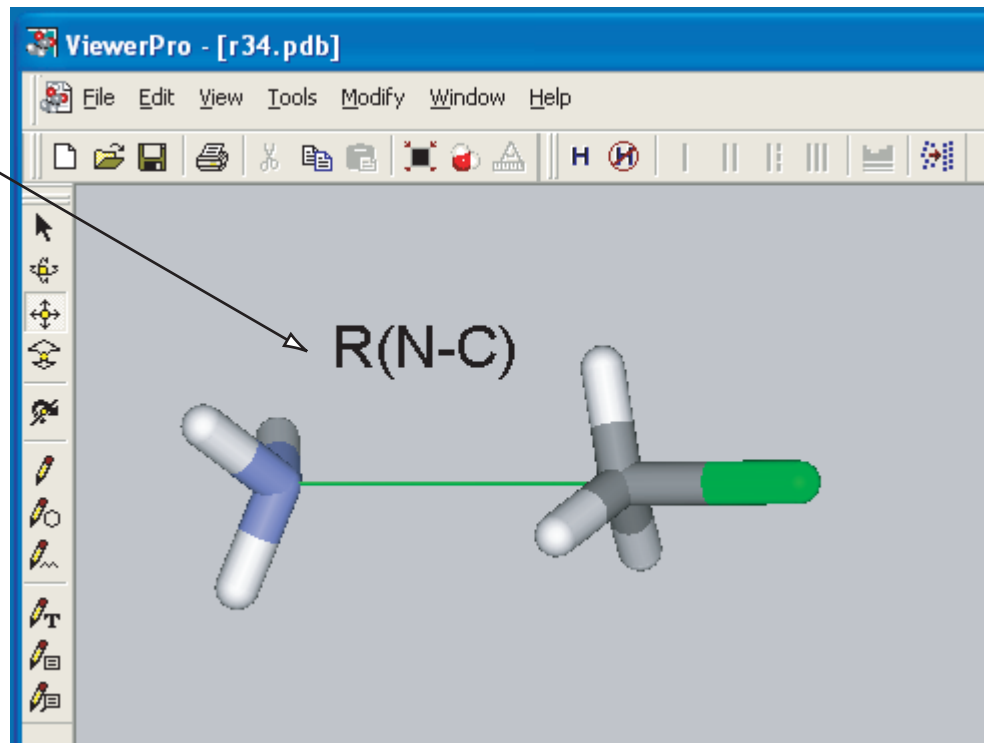
QM Reaction Profiles - Menshutkin reaction

Menshutkin
reaction



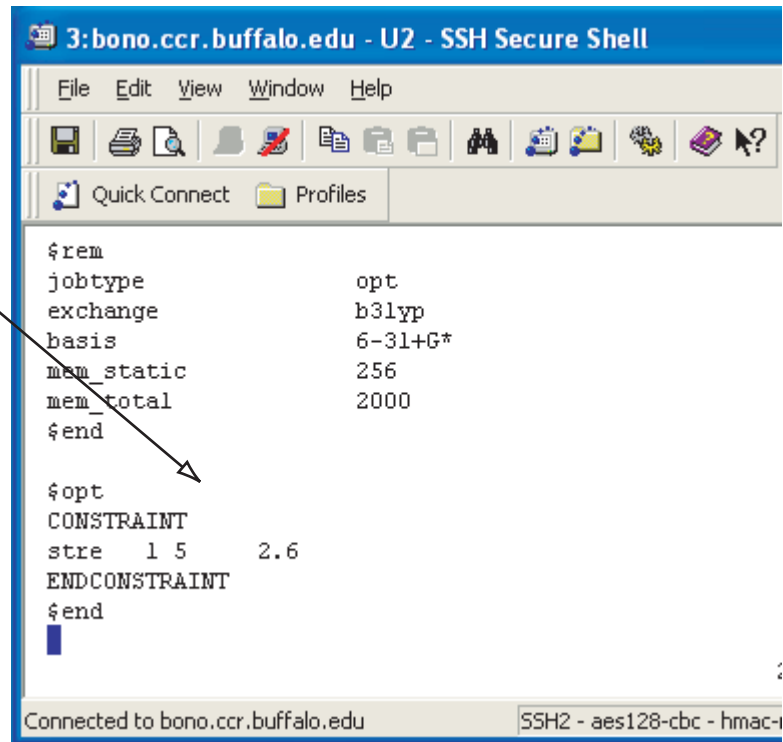
QM Reaction Profiles - Menshutkin reaction

Reaction
coordinate for
reactants



QM Reaction Profiles - Menshutkin reaction

Constrained
geometry
optimization



```
3: bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

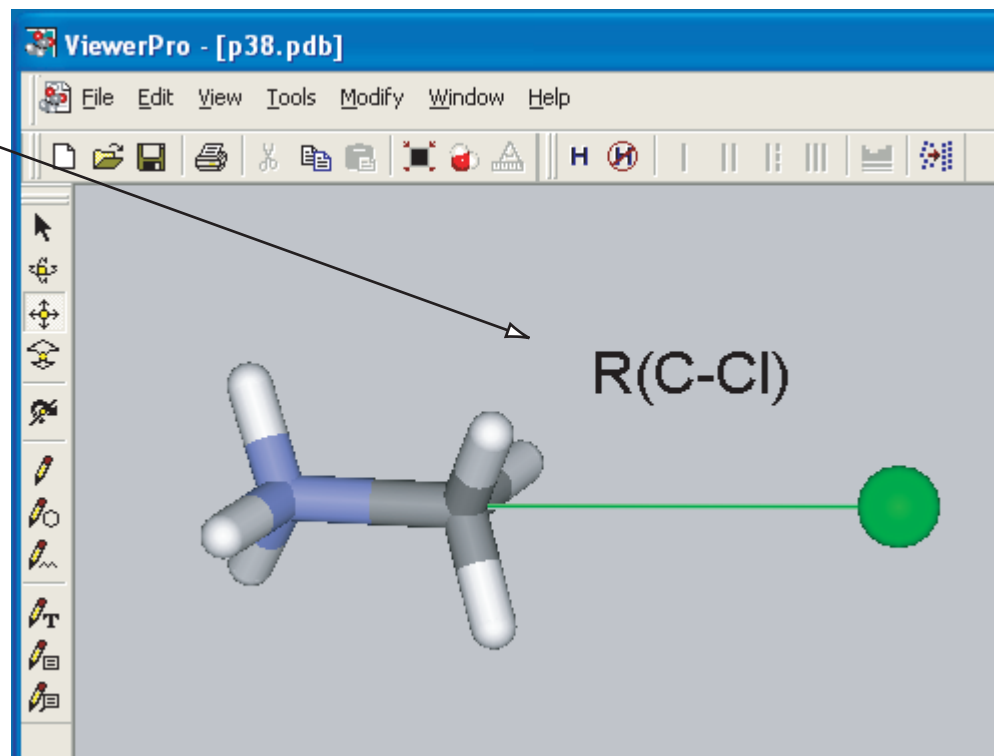
$rem
jobtype                opt
exchange               b3lyp
basis                  6-31+G*
mem_static              256
mem_total               2000
$end

$opt
CONSTRAINT
stre 1 5      2.6
ENDCONSTRAINT
$end
█

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-sha1
```

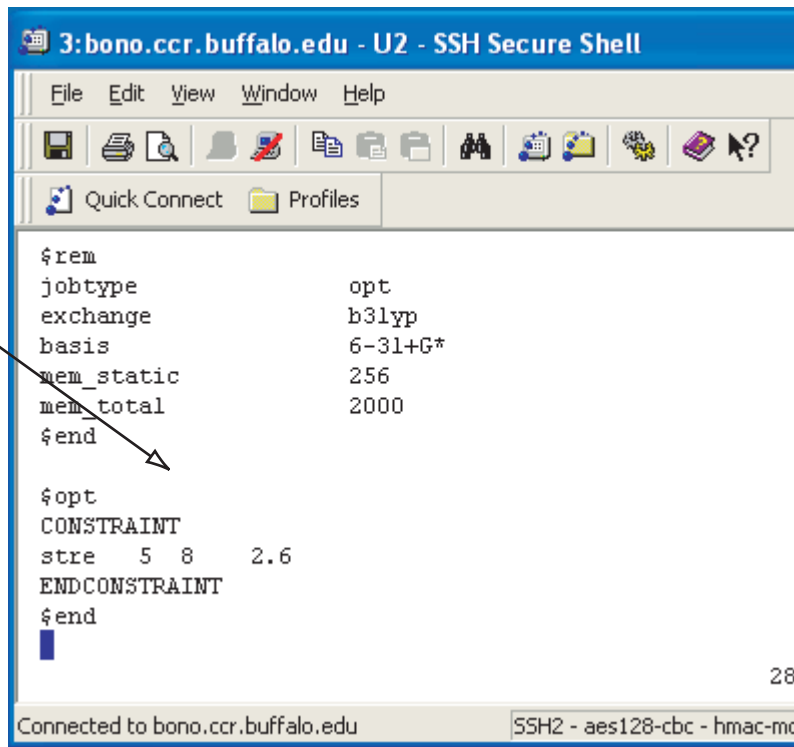

QM Reaction Profiles - Menshutkin reaction

Reaction
coordinate for
products



QM Reaction Profiles - Menshutkin reaction

Constrained
geometry
optimization



```
$rem
jobtype                opt
exchange               b3lyp
basis                  6-31+G*
mem_static              256
mem_total               2000
$end

$opt
CONSTRAINT
stre  5  8    2.6
ENDCONSTRAINT
$end
```

28

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md

QM Reaction Profiles - Menshutkin reaction

Results of the
calculations

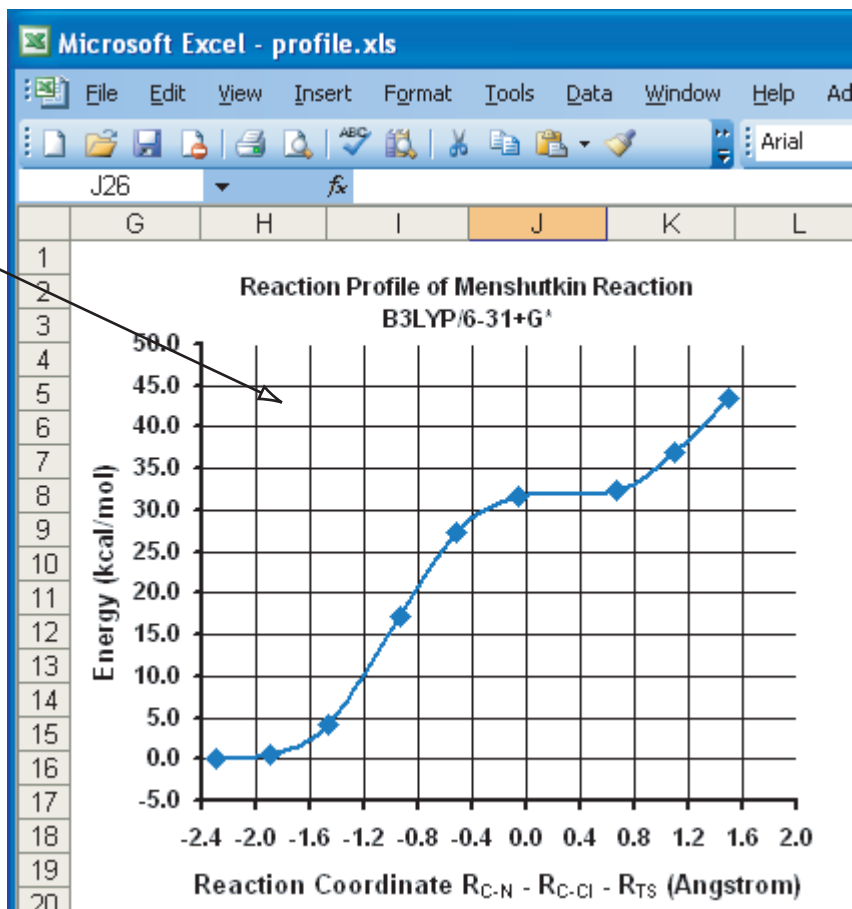
Reactants

Products

	A	B	C	D	E	F
1	R(CCL)	R(CN)	R-Del	Energy	kcal/m	
2	1.84	3.40	-2.30	-556.6657	0.00	
3	1.85	3.00	-1.89	-556.6649	0.47	
4	1.88	2.60	-1.46	-556.6593	4.05	
5	2.00	2.20	-0.94	-556.6384	17.11	
6	2.22	2.00	-0.52	-556.6223	27.22	
7	2.60	1.92	-0.06	-556.6151	31.73	
8	3.00	1.60	0.66	-556.6143	32.28	
9	3.40	1.56	1.10	-556.6069	36.91	
10	3.80	1.56	1.50	-556.5965	43.45	
11						
12				-556.6657		
13						

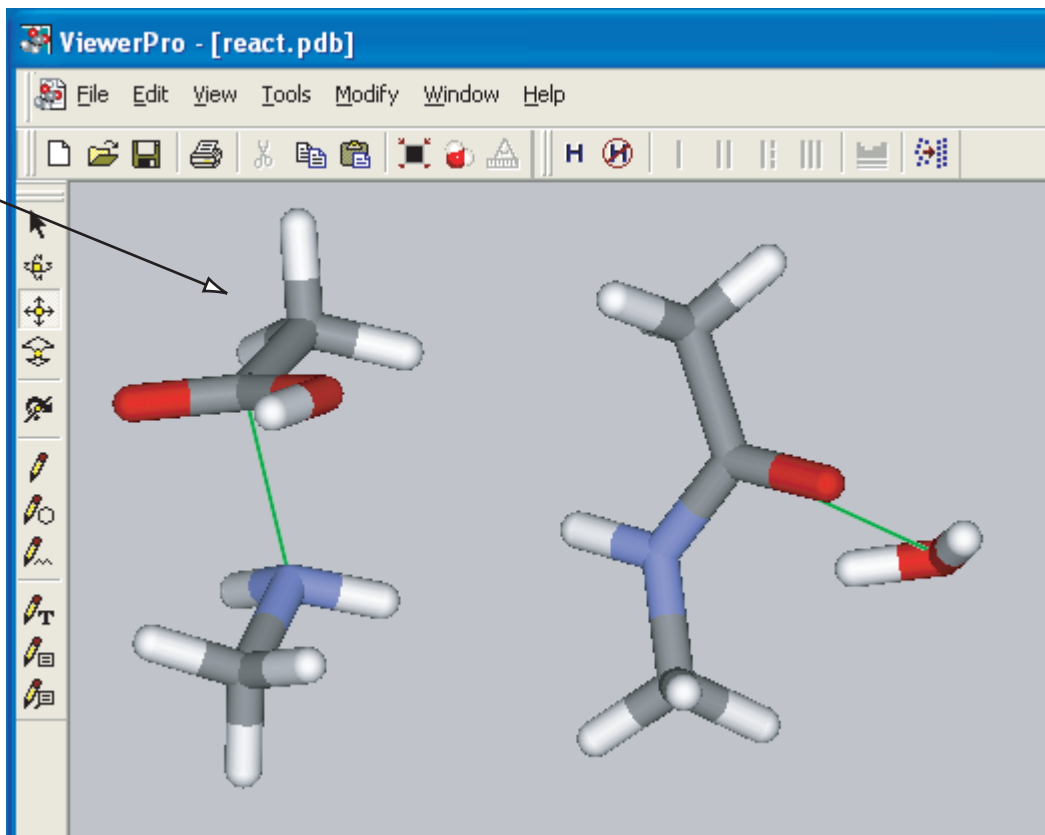
QM Reaction Profiles - Menshutkin reaction

Reaction profile



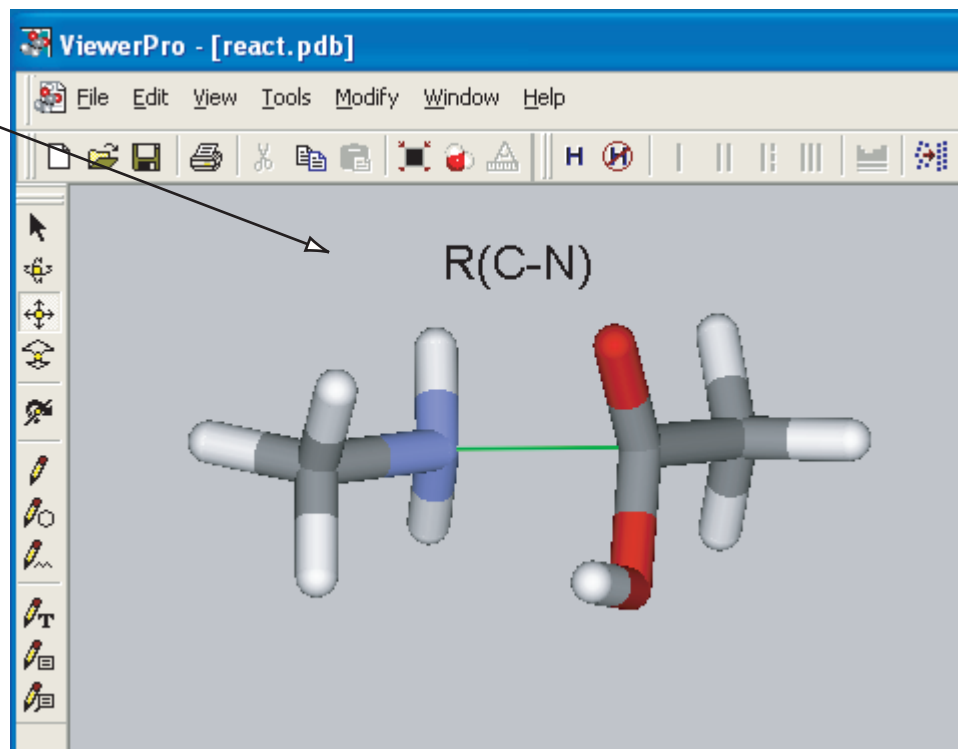
QM Reaction Profiles - Peptide Reaction

Creating a
peptide bond



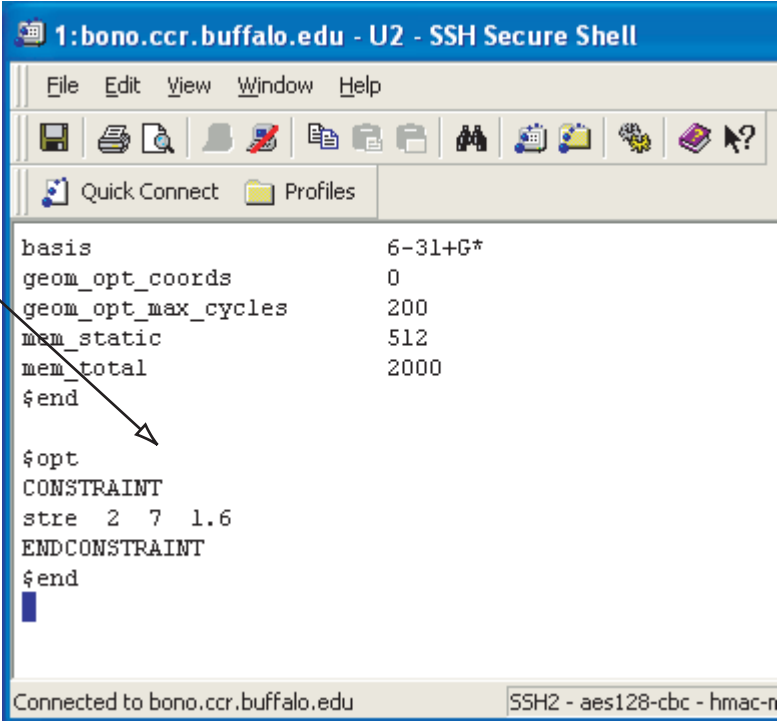
QM Reaction Profiles - Peptide Reaction

Reaction
coordinate in
reactants



QM Reaction Profiles - Peptide Reaction

Geometry
optimization with
a constrained
distance



The screenshot shows an SSH window titled "1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window contains a text editor with the following Gaussian input file content:

```
basis 6-31+G*
geom_opt_coords 0
geom_opt_max_cycles 200
mem_static 512
mem_total 2000
$end

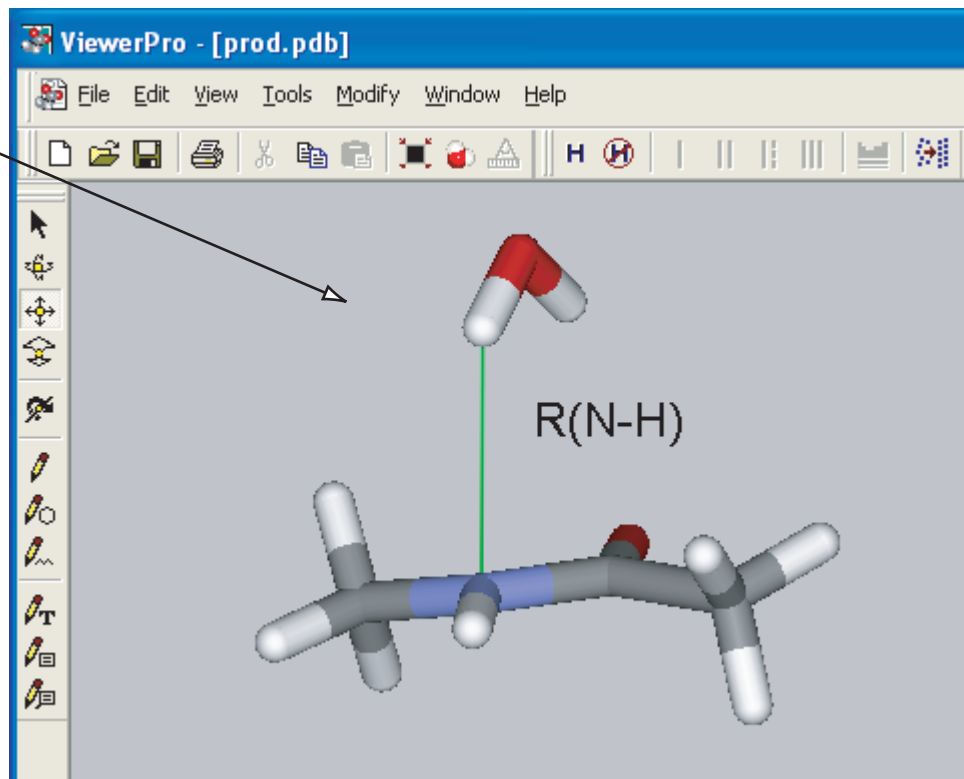
$opt
CONSTRAINT
stre 2 7 1.6
ENDCONSTRAINT
$end
```

An arrow points from the text "Geometry optimization with a constrained distance" to the "CONSTRAINT" section of the input file.

At the bottom of the window, it says "Connected to bono.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-n".

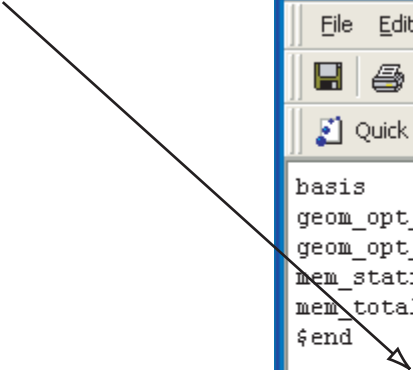
QM Reaction Profiles - Peptide Reaction

Reaction
coordinate in
products



QM Reaction Profiles - Peptide Reaction

Geometry optimization
with a constrained
distance



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
basis 6-31+G*
geom_opt_coords 0
geom_opt_max_cycles 200
mem_static 512
mem_total 2000
$end

$opt
CONSTRAINT
stre 2 5 2.6
ENDCONSTRAINT
$end
"prod-26.in" 36L, 1034C
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-m
```

QM Reaction Profiles - Peptide Reaction

Results of the
calculations

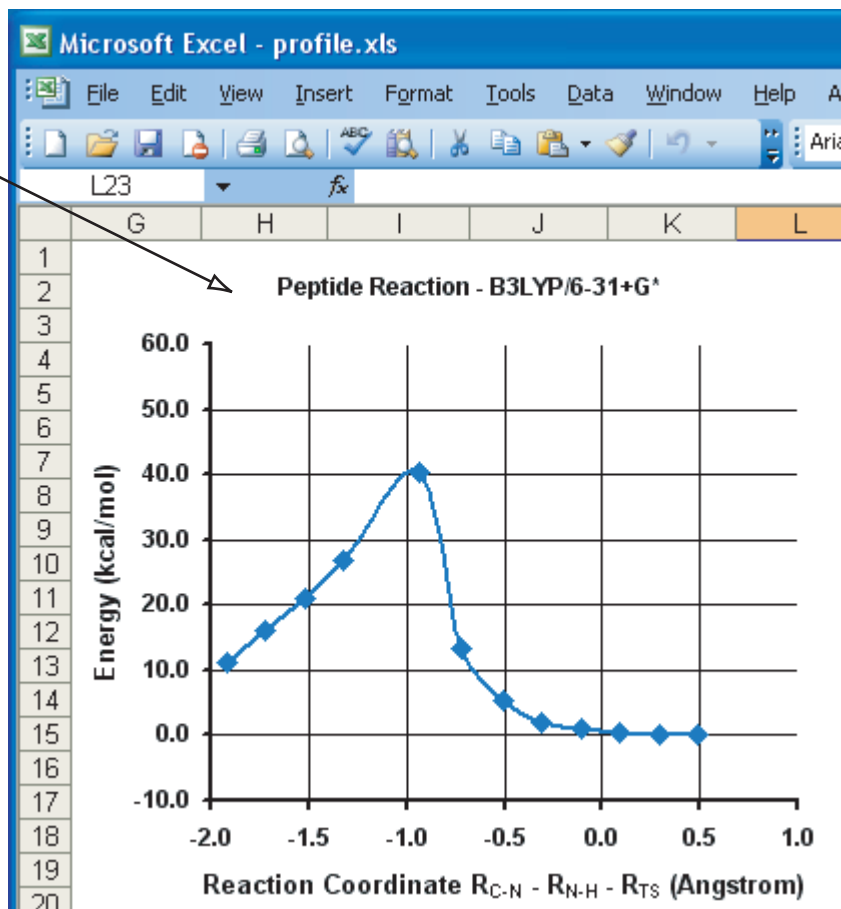
Reactants

Products

	A	B	C	D	E
1	R(NH)	R(CN)	R-Del	Energy	kcal/m
2	1.02	2.20	-1.92	-324.9458	11.32
3	1.02	2.00	-1.72	-324.9384	15.96
4	1.02	1.80	-1.52	-324.9304	20.96
5	1.02	1.60	-1.32	-324.9211	26.81
6	1.20	1.40	-0.94	-324.8993	40.47
7	1.40	1.38	-0.72	-324.9425	13.39
8	1.60	1.37	-0.51	-324.9551	5.44
9	1.80	1.37	-0.31	-324.9608	1.91
10	2.00	1.37	-0.11	-324.9621	1.09
11	2.20	1.37	0.09	-324.9632	0.36
12	2.40	1.37	0.29	-324.9634	0.28
13	2.60	1.37	0.49	-324.9638	0.00
14					
15				-324.9638	
16					

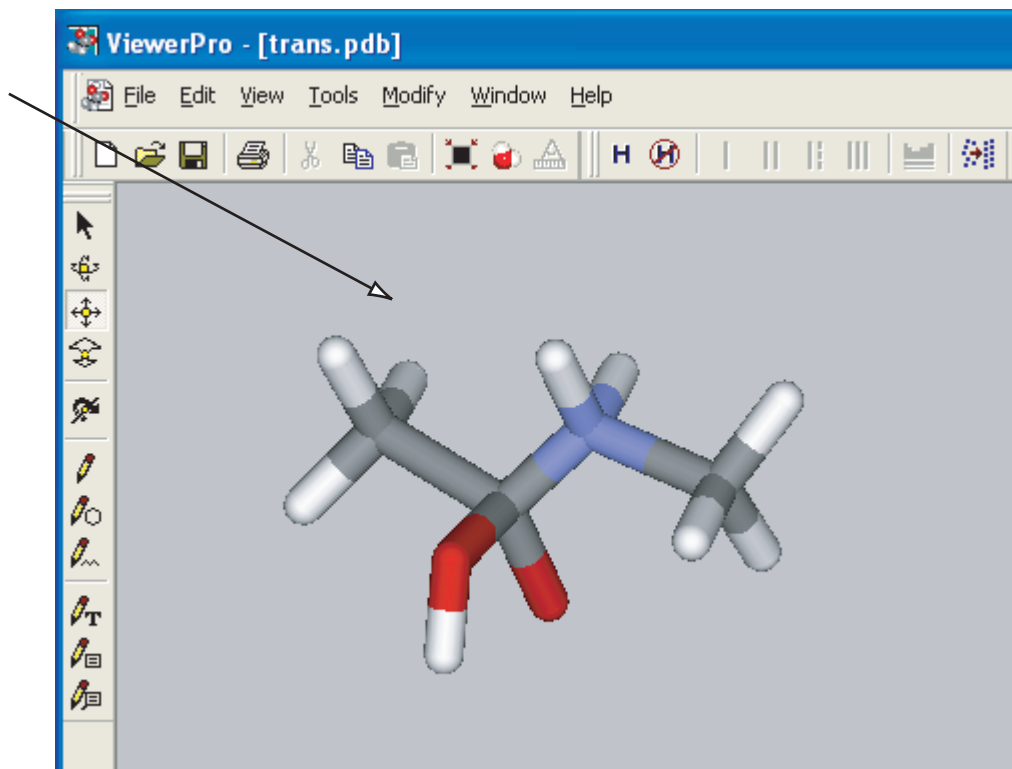
QM Reaction Profiles - Peptide Reaction

Reaction profile



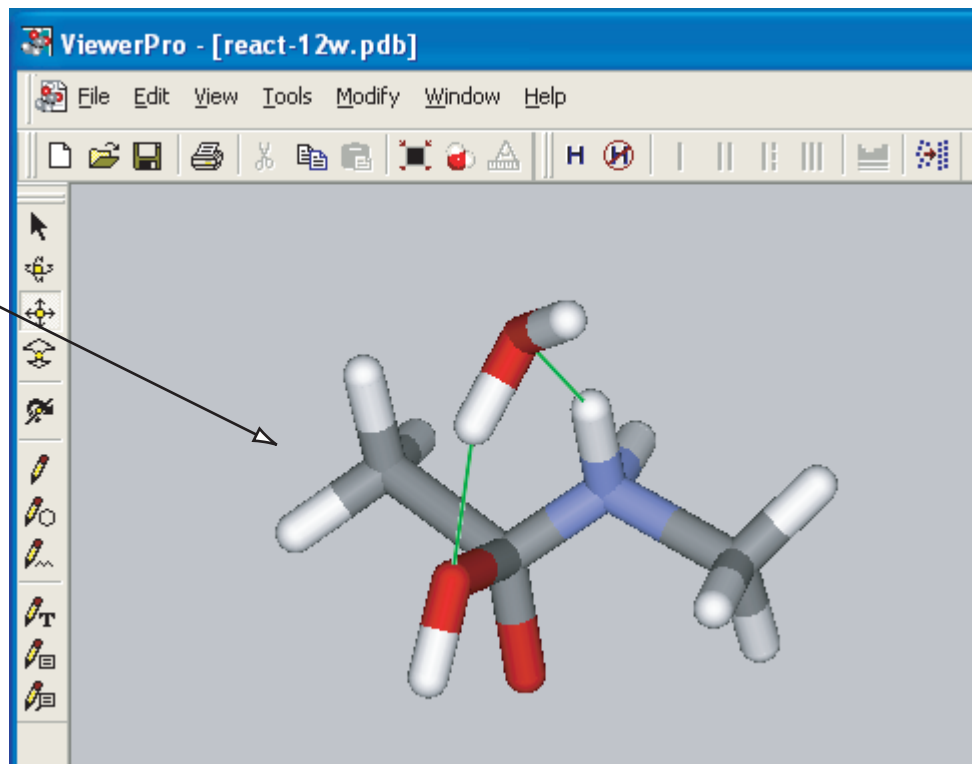
QM Reaction Profiles - Peptide Reaction

Transition state
structure of the
peptide reaction



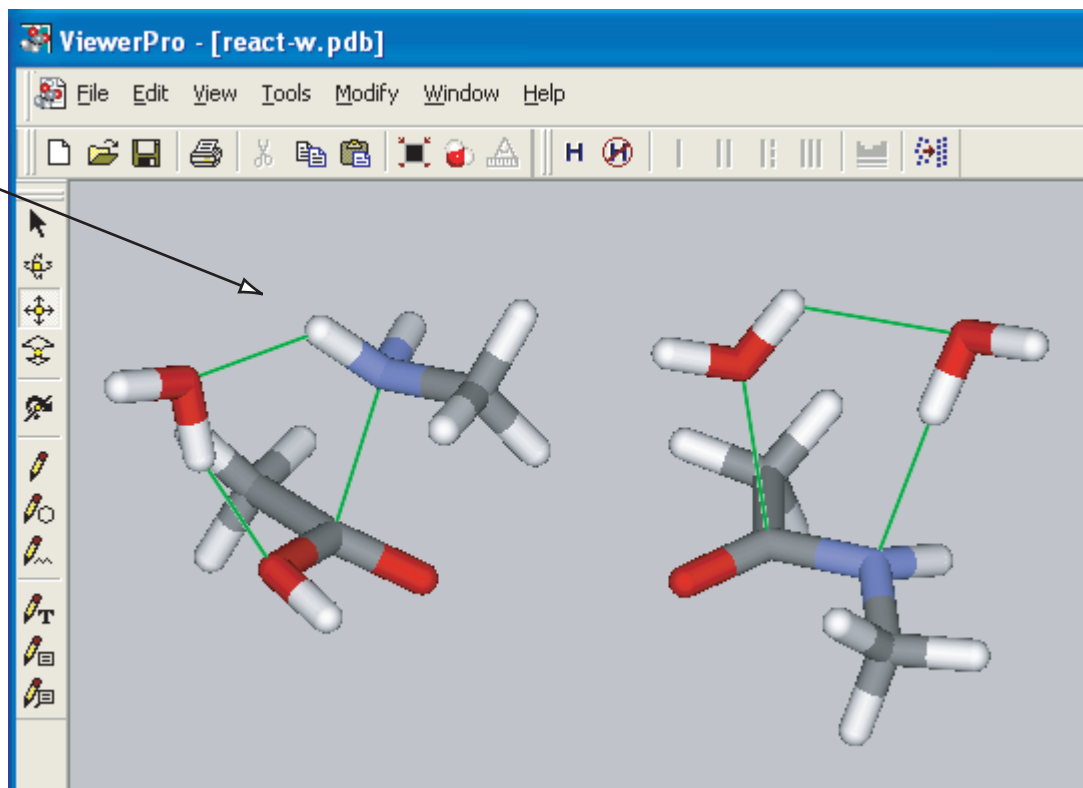
QM Reaction Profiles - Peptide Reaction

Transition state structure of the peptide reaction, which is stabilized by a water molecule



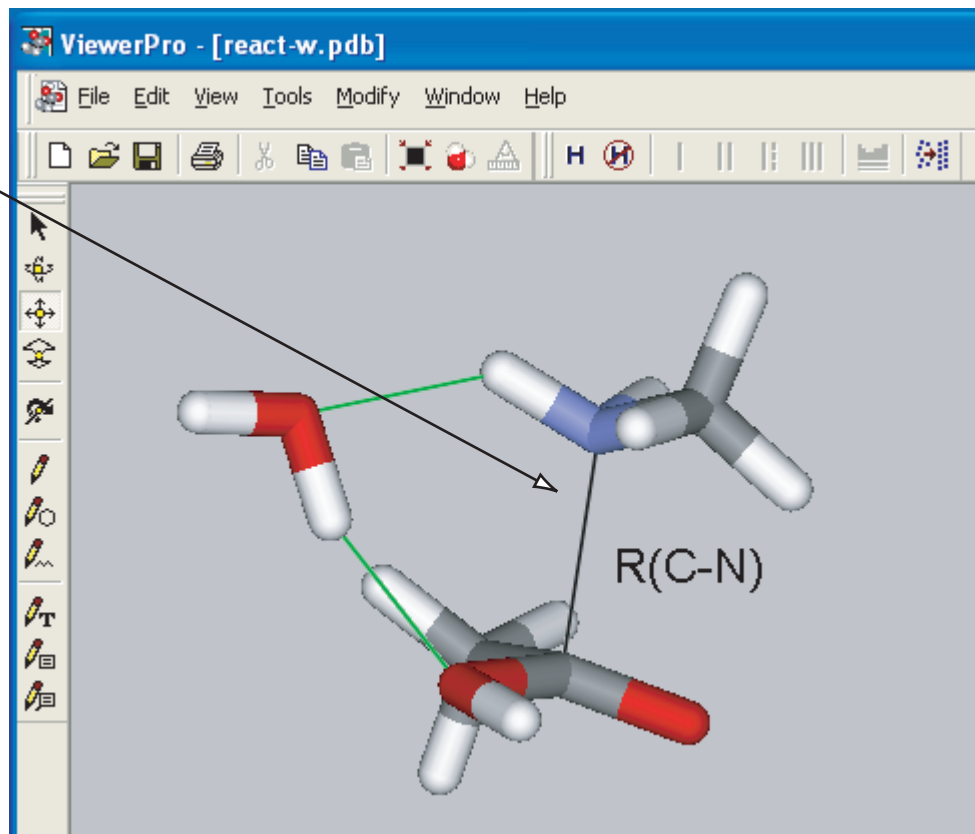
QM Reaction Profiles - Peptide Reaction

Reactants
and products
of the peptide
reaction in a
presence of a
water molecule



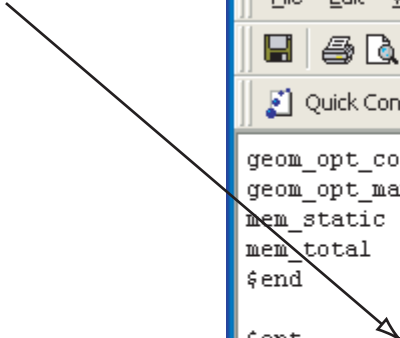
QM Reaction Profiles - Peptide Reaction

Reaction
coordinate for
reactants



QM Reaction Profiles - Peptide Reaction

Geometry optimization
with a constrained
distance



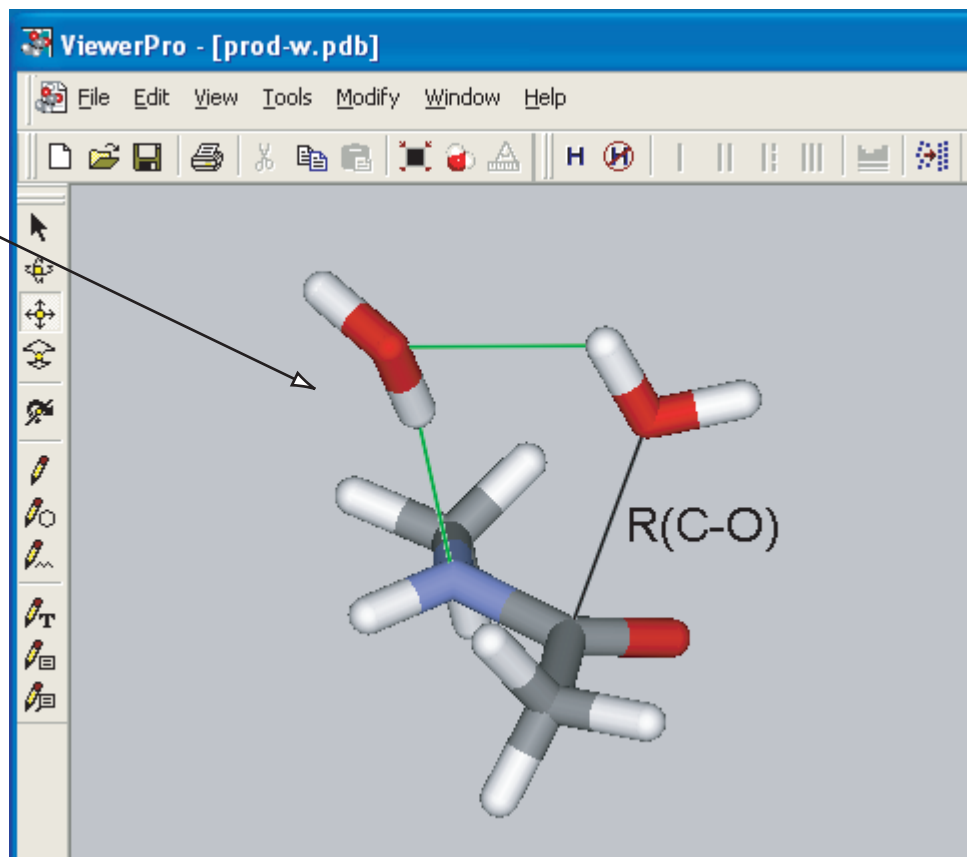
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
geom_opt_coords      0
geom_opt_max_cycles  200
mem_static           512
mem_total            2000
$end

$opt
CONSTRAINT
stre 2 7 1.8
ENDCONSTRAINT
$end
█

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hm
```

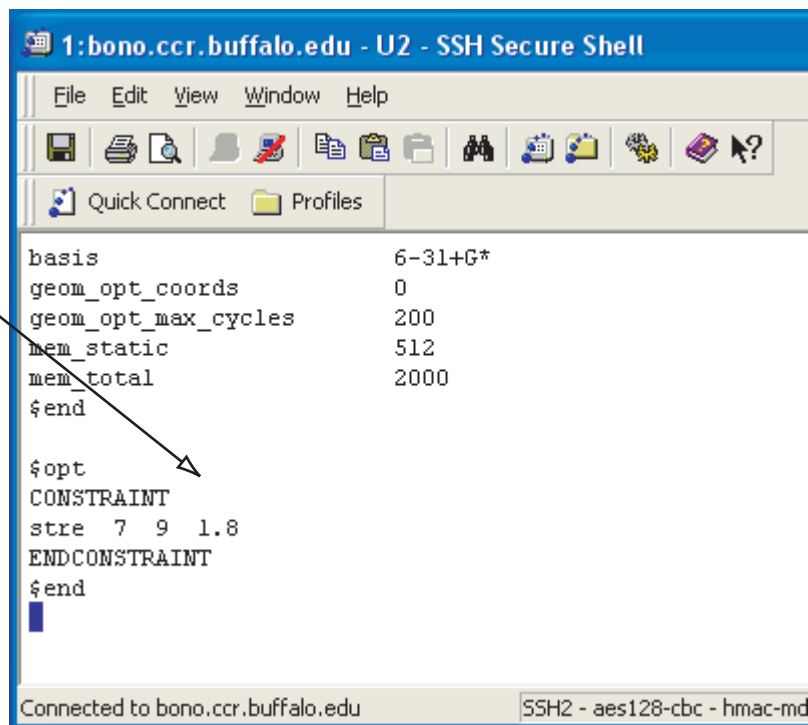

QM Reaction Profiles - Peptide Reaction

Reaction
coordinate for
products



QM Reaction Profiles - Peptide Reaction

Geometry
optimization with
a constrained
distance



The screenshot shows a terminal window titled "1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window contains the following Gaussian input text:

```
basis 6-31+G*
geom_opt_coords 0
geom_opt_max_cycles 200
mem_static 512
mem_total 2000
$end

$opt
CONSTRAINT
stre 7 9 1.8
ENDCONSTRAINT
$end
```

An arrow points from the text "Geometry optimization with a constrained distance" to the "CONSTRAINT" section of the input file.

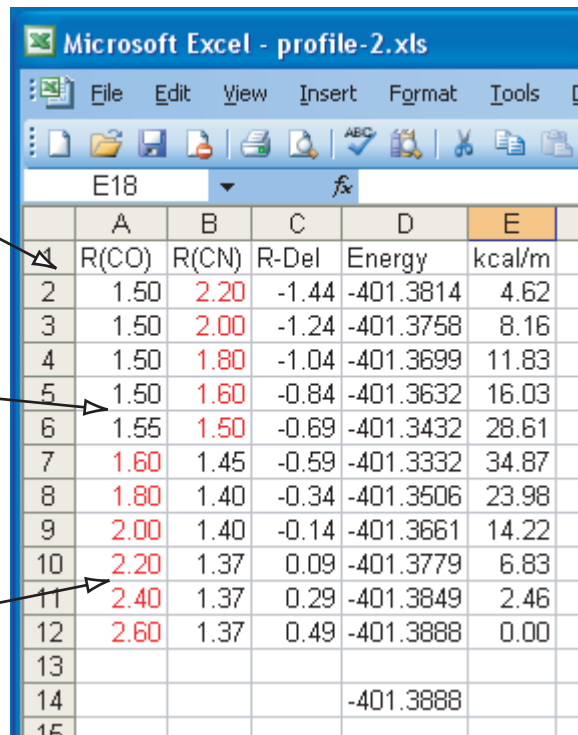
At the bottom of the terminal window, it says "Connected to bono.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-md".

QM Reaction Profiles - Peptide Reaction

Final results

Reactants

Products

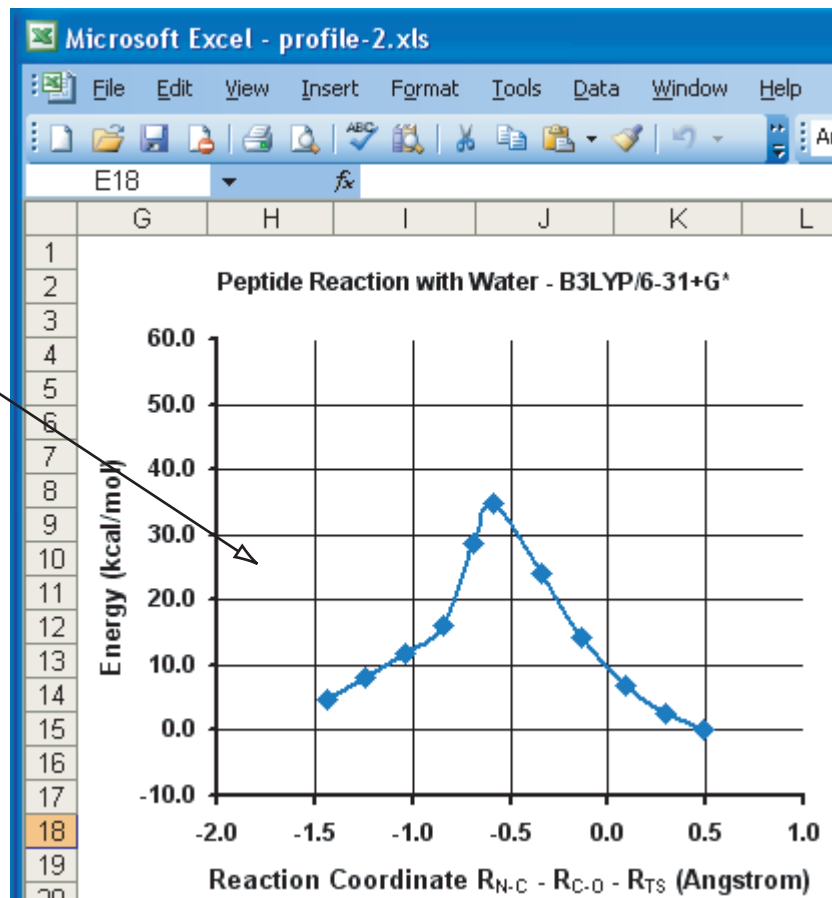


Microsoft Excel - profile-2.xls

	A	B	C	D	E
	R(CO)	R(CN)	R-Del	Energy	kcal/m
2	1.50	2.20	-1.44	-401.3814	4.62
3	1.50	2.00	-1.24	-401.3758	8.16
4	1.50	1.80	-1.04	-401.3699	11.83
5	1.50	1.60	-0.84	-401.3632	16.03
6	1.55	1.50	-0.69	-401.3432	28.61
7	1.60	1.45	-0.59	-401.3332	34.87
8	1.80	1.40	-0.34	-401.3506	23.98
9	2.00	1.40	-0.14	-401.3661	14.22
10	2.20	1.37	0.09	-401.3779	6.83
11	2.40	1.37	0.29	-401.3849	2.46
12	2.60	1.37	0.49	-401.3888	0.00
13					
14				-401.3888	
15					

QM Reaction Profiles - Peptide Reaction

Reaction profile of the peptide reaction with a presence of a water molecule



Definition of pKa



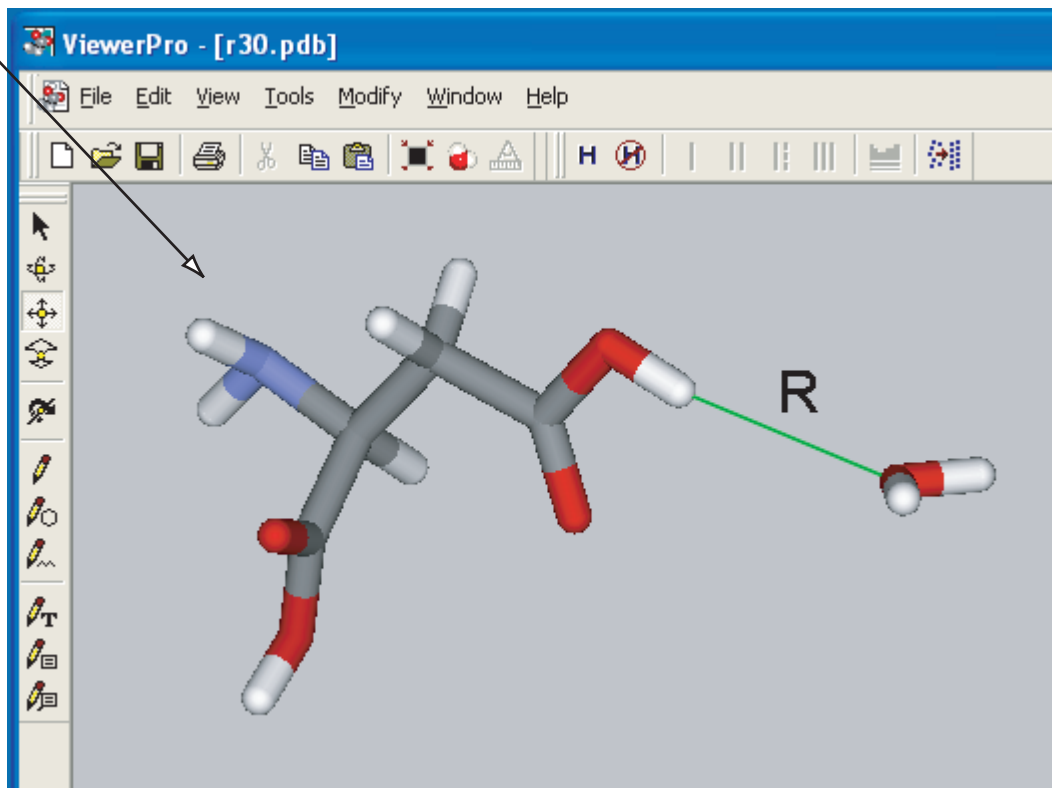
$$K_a = \frac{[H_3O^+][A^-]}{[HA]}$$

$$K_a = e^{-\frac{\Delta G}{RT}}$$

$$pK_a = -\text{Log}_{10} K_a$$

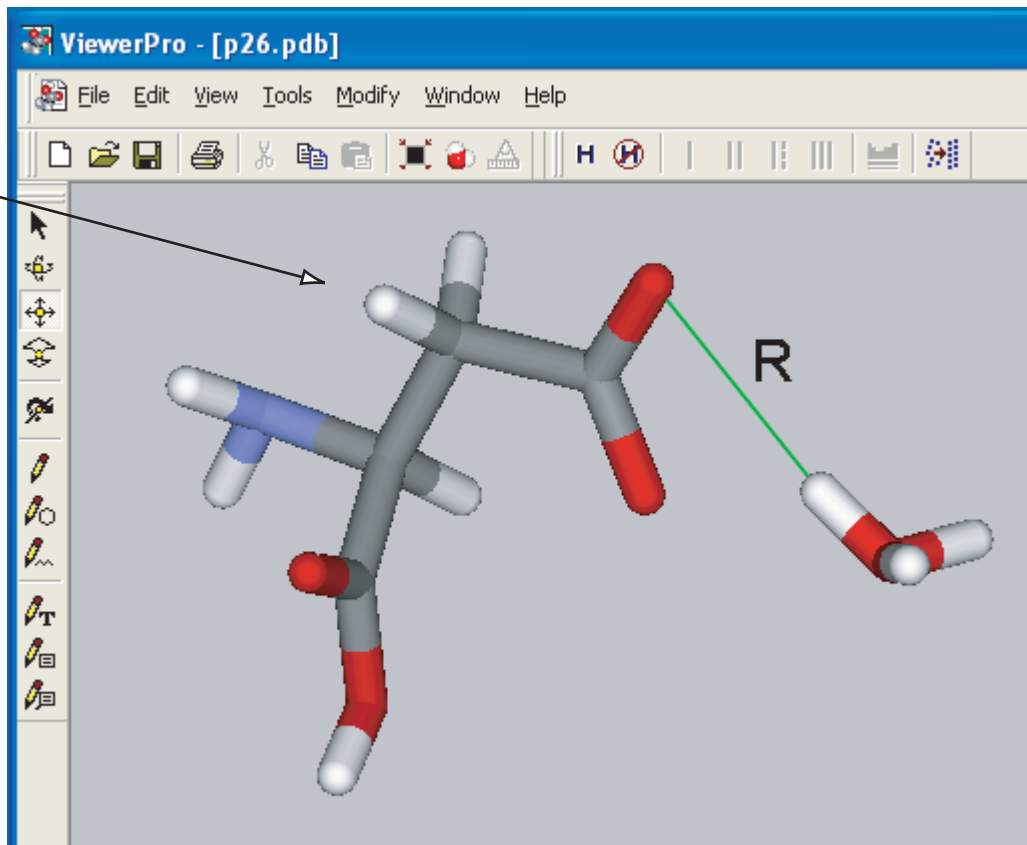
QM calculations of pKa in amino acids and base pairs

Reactants in the
deprotonation
reaction of
aspartic acid
with water



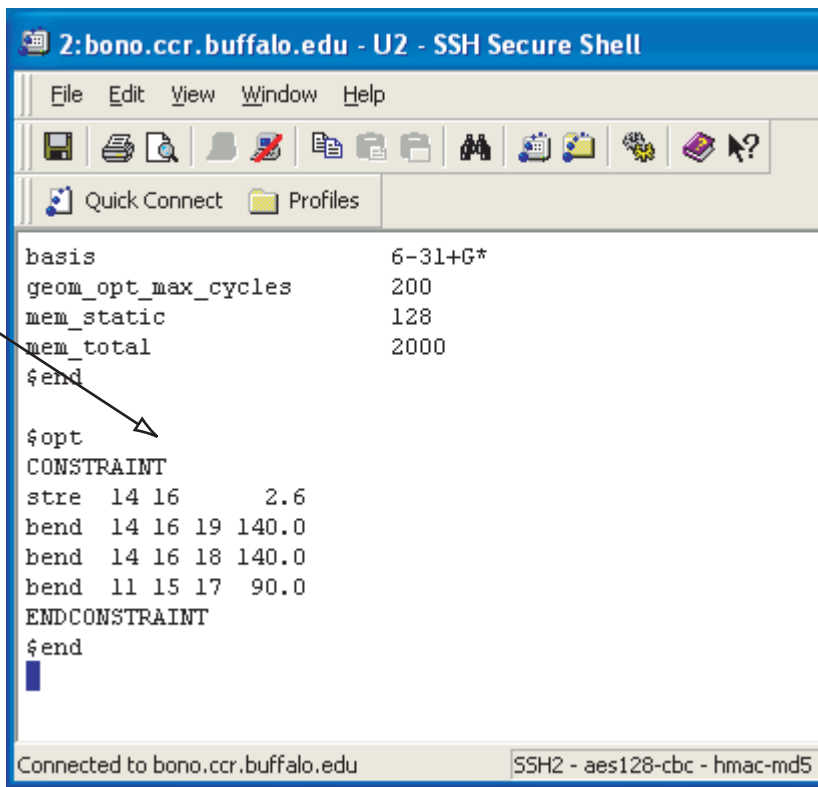
QM calculations of pKa in amino acids and base pairs

Products in the
deprotonation
reaction of
aspartic acid
with water



QM calculations of pKa in amino acids and base pairs

Geometry
optimization with
constrained distances
and angles



The screenshot shows an SSH terminal window titled "2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The terminal displays the following Gaussian input file content:

```
basis 6-31+G*
geom_opt_max_cycles 200
mem_static 128
mem_total 2000
$end

$opt
CONSTRAINT
stre 14 16 2.6
bend 14 16 19 140.0
bend 14 16 18 140.0
bend 11 15 17 90.0
ENDCONSTRAINT
$end
```

An arrow points from the text "Geometry optimization with constrained distances and angles" to the `$opt` section of the input file. The terminal window also shows a menu bar (File, Edit, View, Window, Help), a toolbar with various icons, and a status bar at the bottom indicating the connection to bono.ccr.buffalo.edu and the SSH2 encryption method (aes128-cbc - hmac-md5).

QM calculations of pKa in amino acids and base pairs

Final results

Reactants

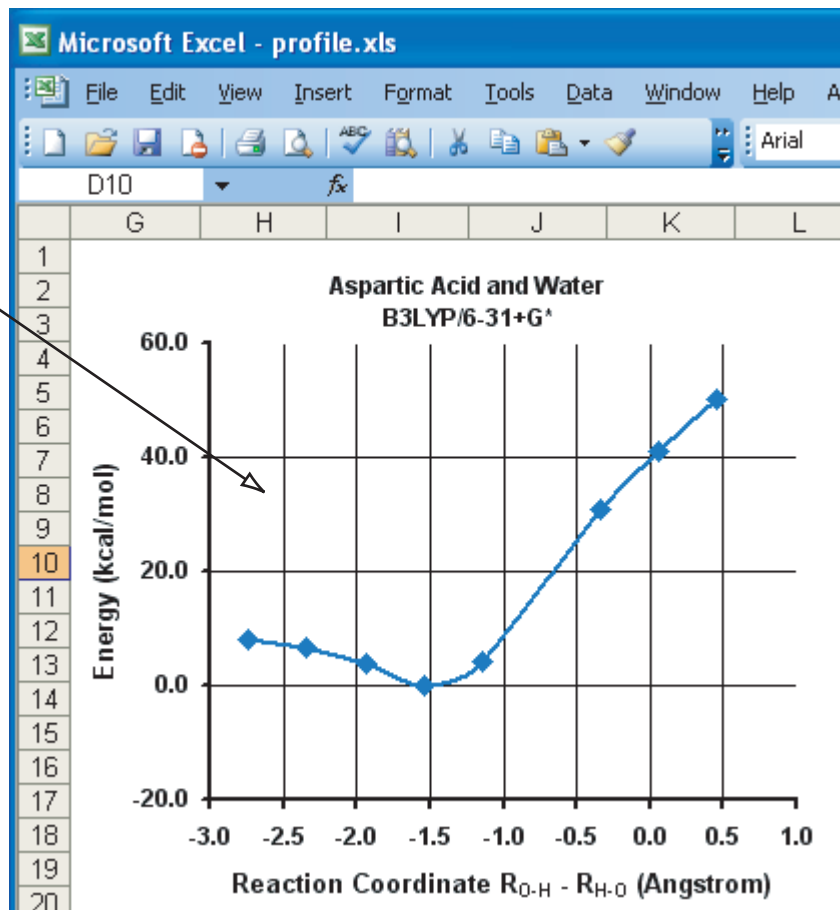
Products

Microsoft Excel - profile.xls

	A	B	C	D	E
1	R(OH)	R(HO)	R-Del	Energy	kcal/m
2	1.00	3.00	-2.74	-588.7598	7.93
3	1.00	2.60	-2.34	-588.7618	6.70
4	1.00	2.20	-1.94	-588.7664	3.77
5	1.00	1.80	-1.54	-588.7724	0.00
6	1.00	1.40	-1.14	-588.7660	4.04
7	1.40	1.00	-0.34	-588.7232	30.89
8	1.80	1.00	0.06	-588.7071	41.02
9	2.20	1.00	0.46	-588.6923	50.31
10				-588.7724	
11					
12					
13					

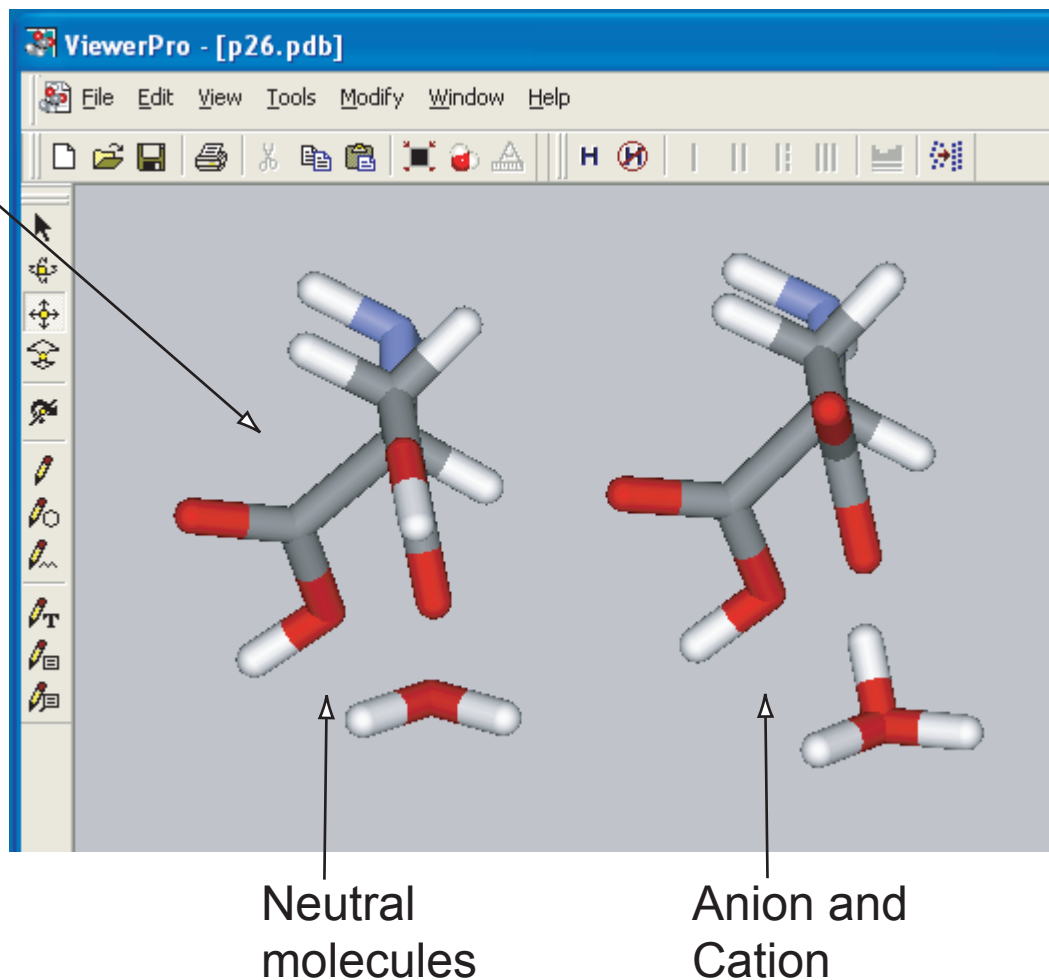
QM calculations of pKa in amino acids and base pairs

Potential energy surface of the deprotonation reaction



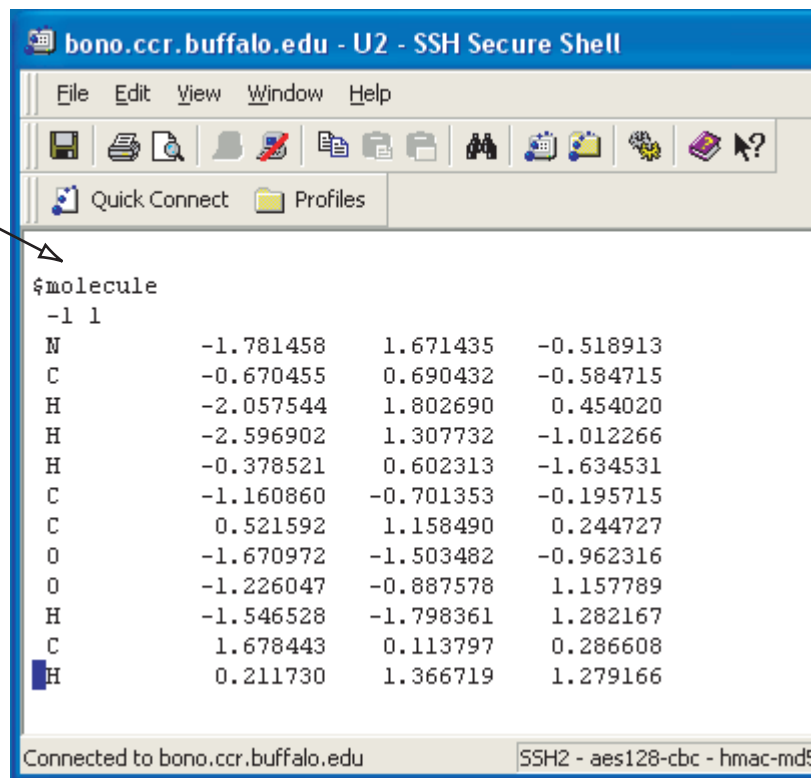
QM calculations of pKa in amino acids and base pairs

Separate calculations for all molecules used in the reaction



QM calculations of pKa in amino acids and base pairs

Calculations of
the anion in
the singlet
electronic state



The screenshot shows an SSH terminal window titled "bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window has a menu bar (File, Edit, View, Window, Help) and a toolbar with various icons. Below the toolbar, there are tabs for "Quick Connect" and "Profiles". The terminal content shows a prompt "\$molecule" followed by "-l 1" and a table of atomic coordinates. An arrow from the text "Calculations of the anion in the singlet electronic state" points to the terminal window.

```
$molecule
-l 1
N      -1.781458    1.671435   -0.518913
C      -0.670455    0.690432   -0.584715
H      -2.057544    1.802690    0.454020
H      -2.596902    1.307732   -1.012266
H      -0.378521    0.602313   -1.634531
C      -1.160860   -0.701353   -0.195715
C       0.521592    1.158490    0.244727
O      -1.670972   -1.503482   -0.962316
O      -1.226047   -0.887578    1.157789
H      -1.546528   -1.798361    1.282167
C       1.678443    0.113797    0.286608
H       0.211730    1.366719    1.279166
```

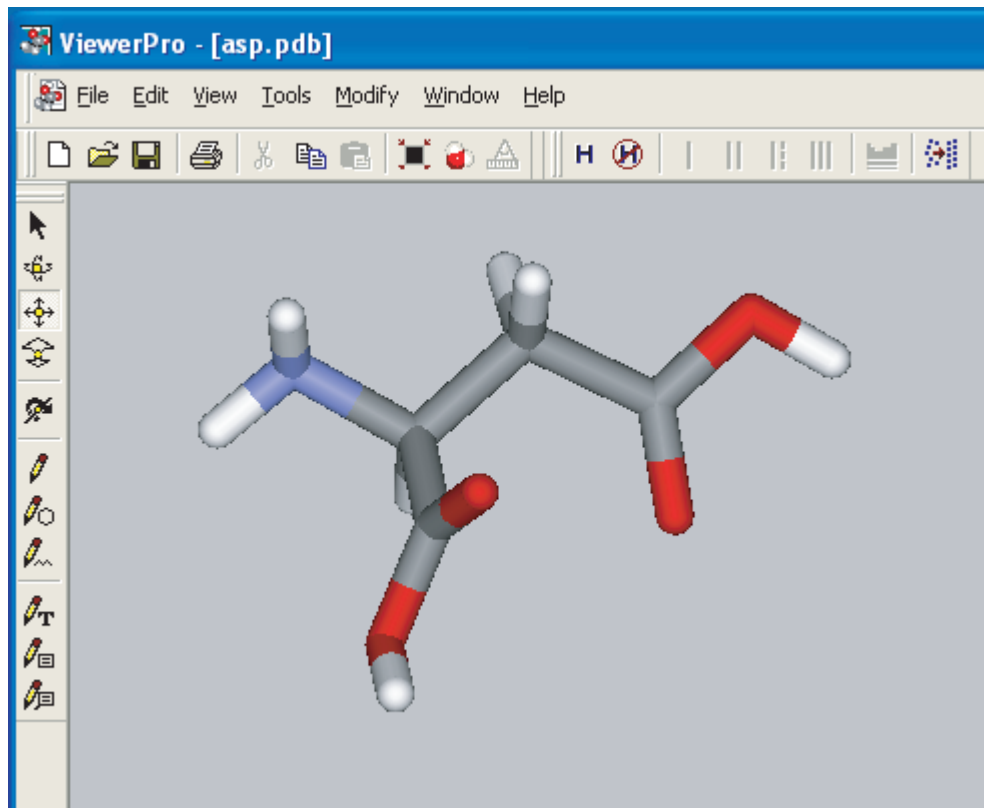
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5

QM calculations of pKa in amino acids and base pairs

Aspartic Acid

Deprotonation
energy:

$$E = 173 \text{ kcal/mol}$$

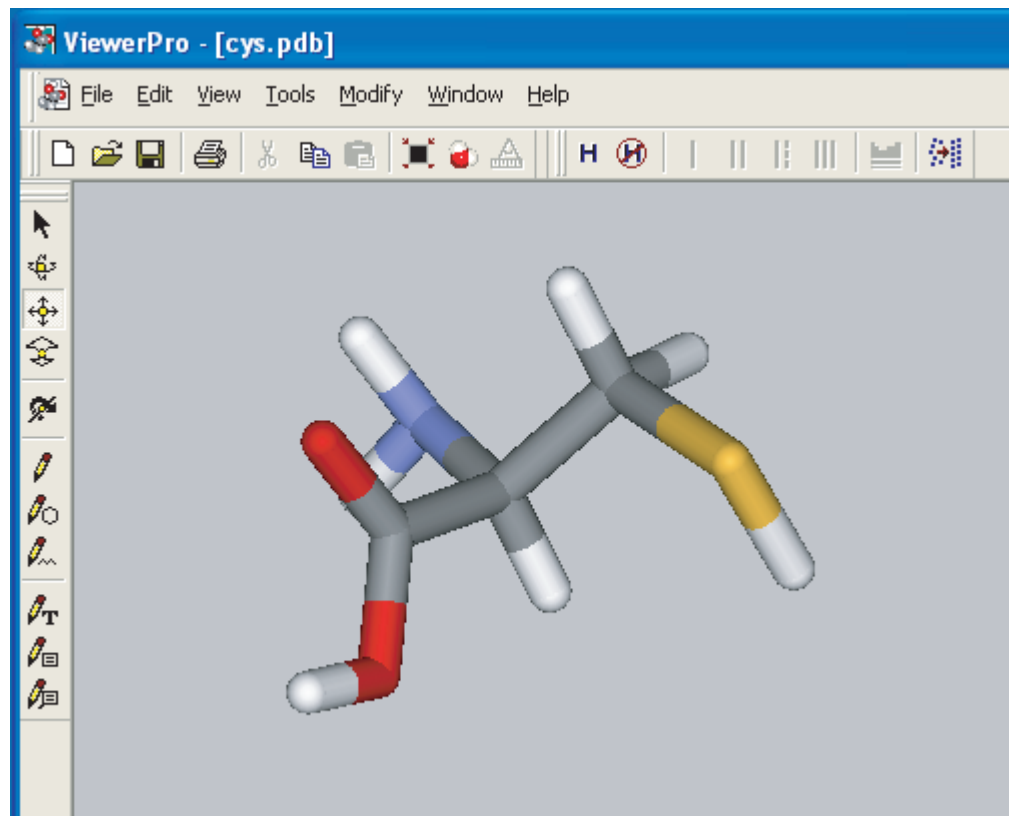


QM calculations of pKa in amino acids and base pairs

Cysteine

Deprotonation
energy:

$$E = 181 \text{ kcal/mol}$$

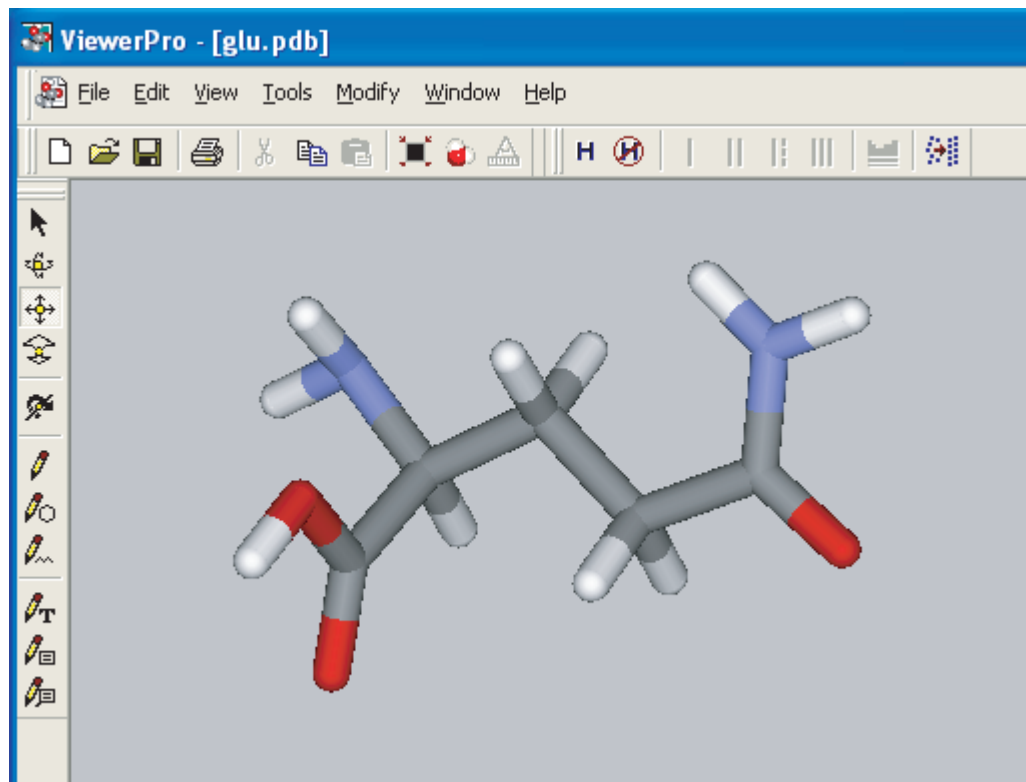


QM calculations of pKa in amino acids and base pairs

Glutamic Acid

Deprotonation
energy:

$$E = 199 \text{ kcal/mol}$$

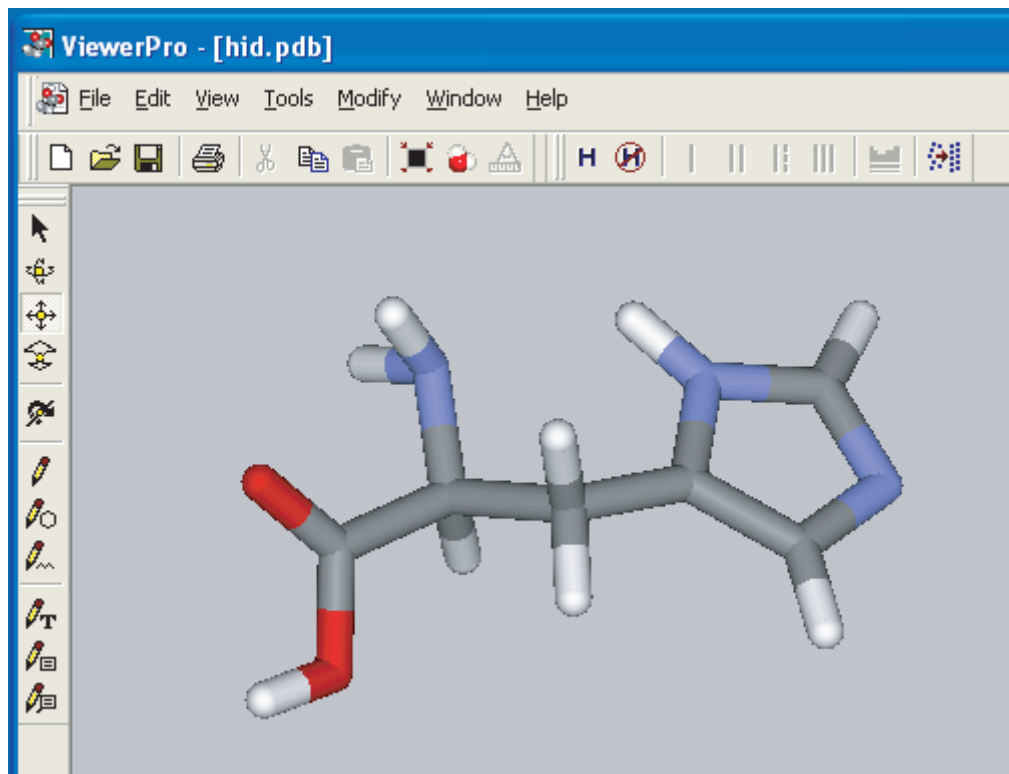


QM calculations of pKa in amino acids and base pairs

Histidine (δ)

Deprotonation
energy:

$E = 181 \text{ kcal/mol}$

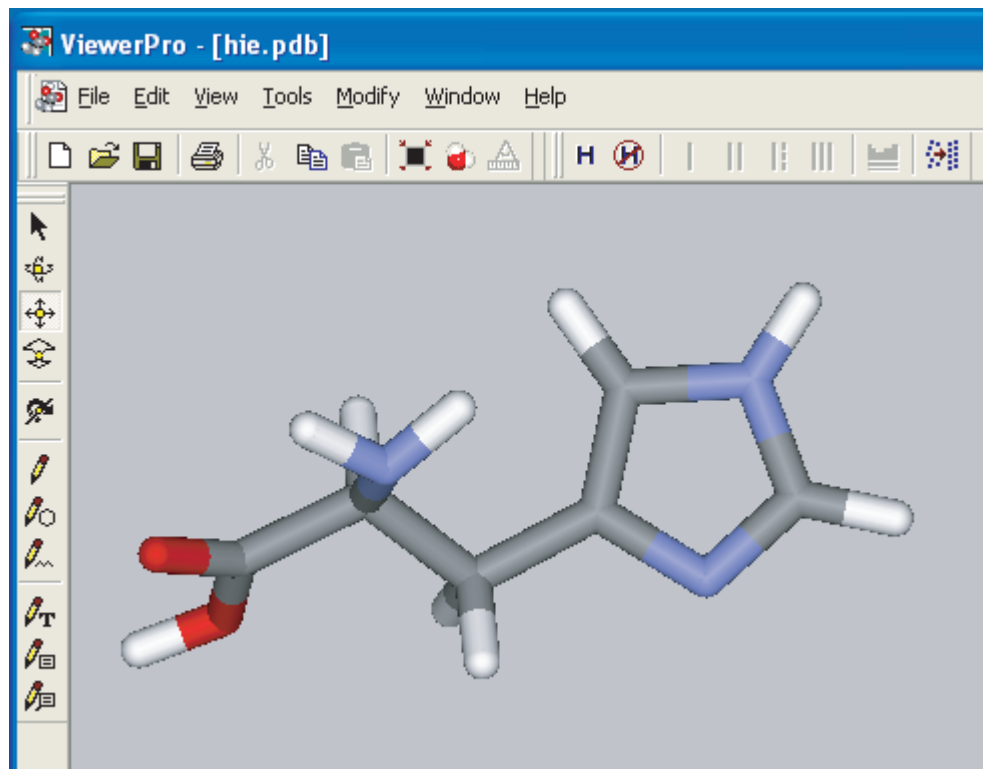


QM calculations of pKa in amino acids and base pairs

Histidine (ϵ)

Deprotonation
energy:

$E = 175 \text{ kcal/mol}$

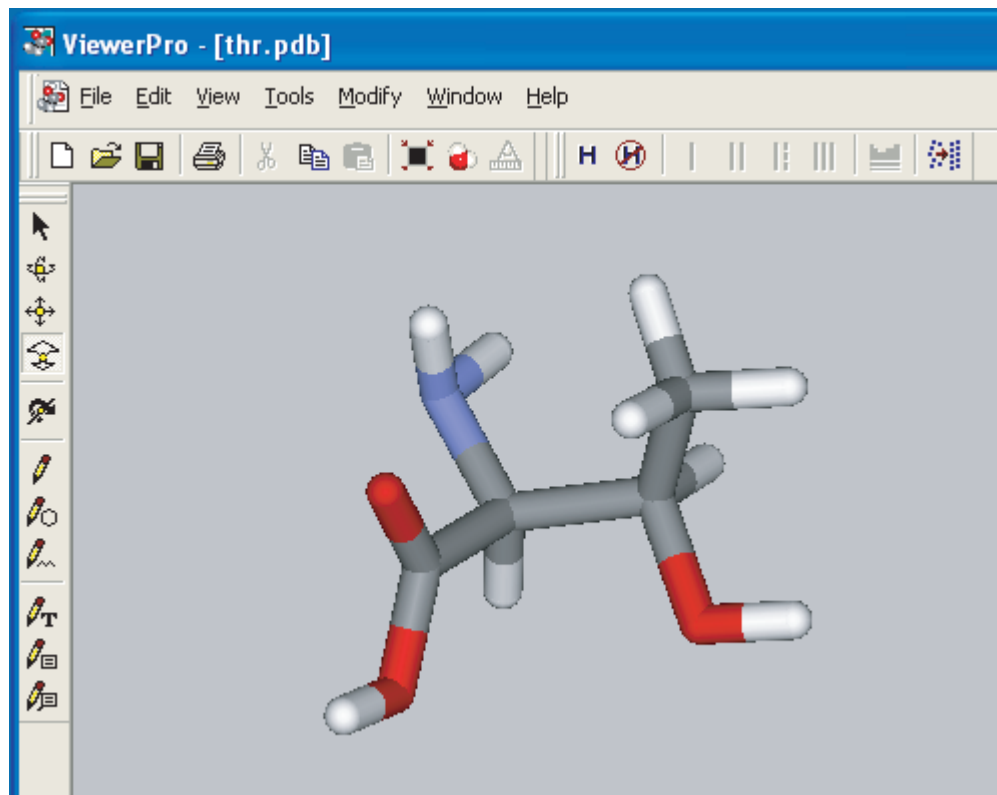


QM calculations of pKa in amino acids and base pairs

Threonine

Deprotonation
energy:

$E = 196 \text{ kcal/mol}$

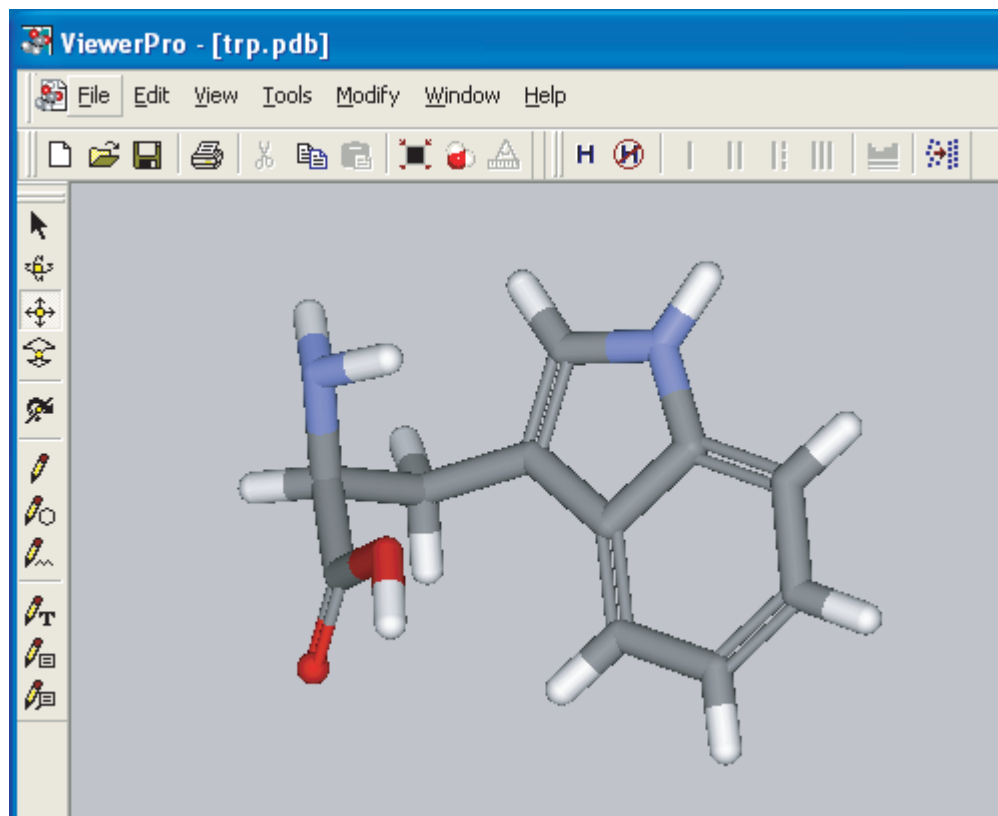


QM calculations of pKa in amino acids and base pairs

Tryptophan

Deprotonation
energy:

$E = 180 \text{ kcal/mol}$

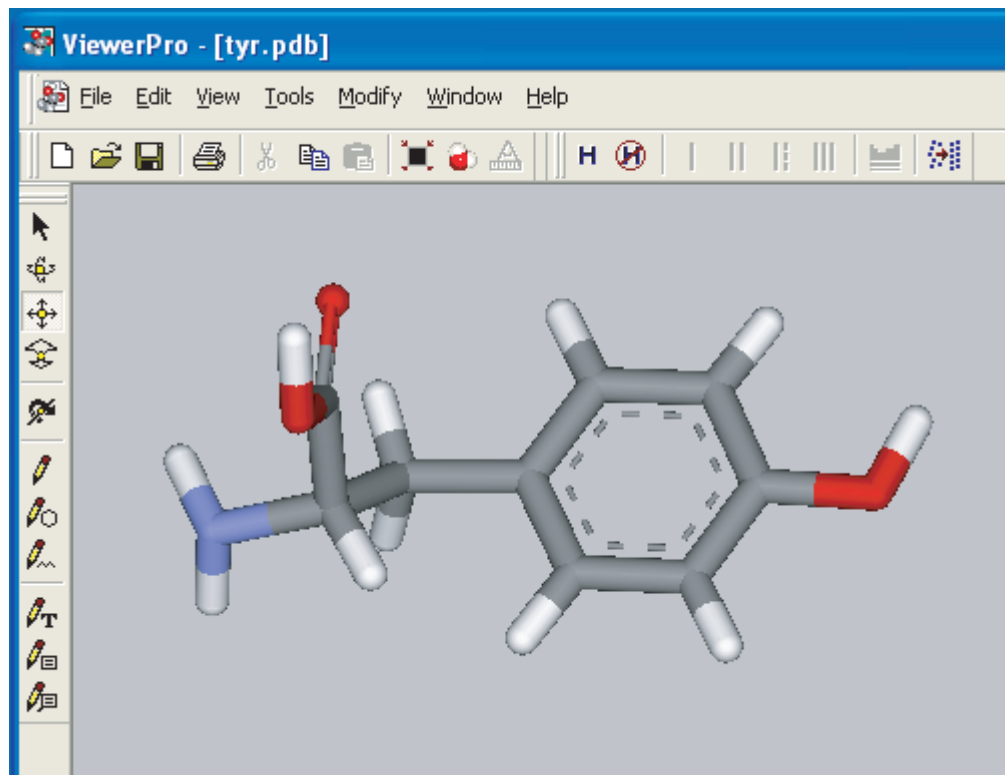


QM calculations of pKa in amino acids and base pairs

Tyrosine

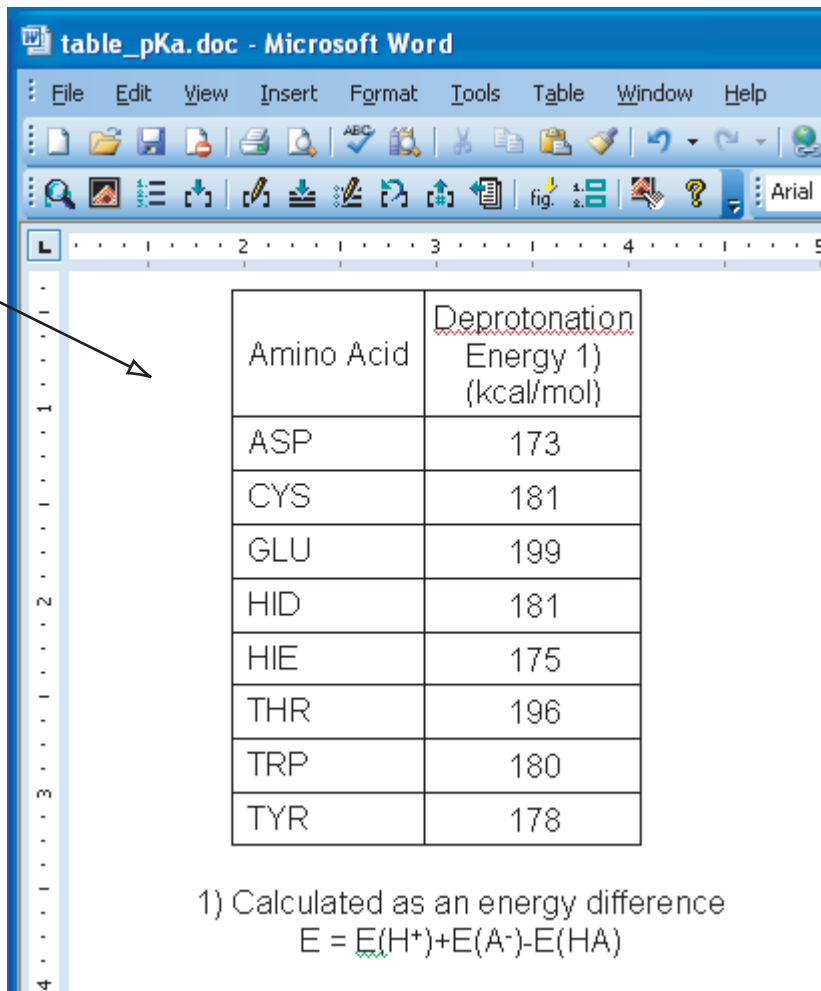
Deprotonation
energy:

$E = 178 \text{ kcal/mol}$



QM calculations of pKa in amino acids and base pairs

Final results

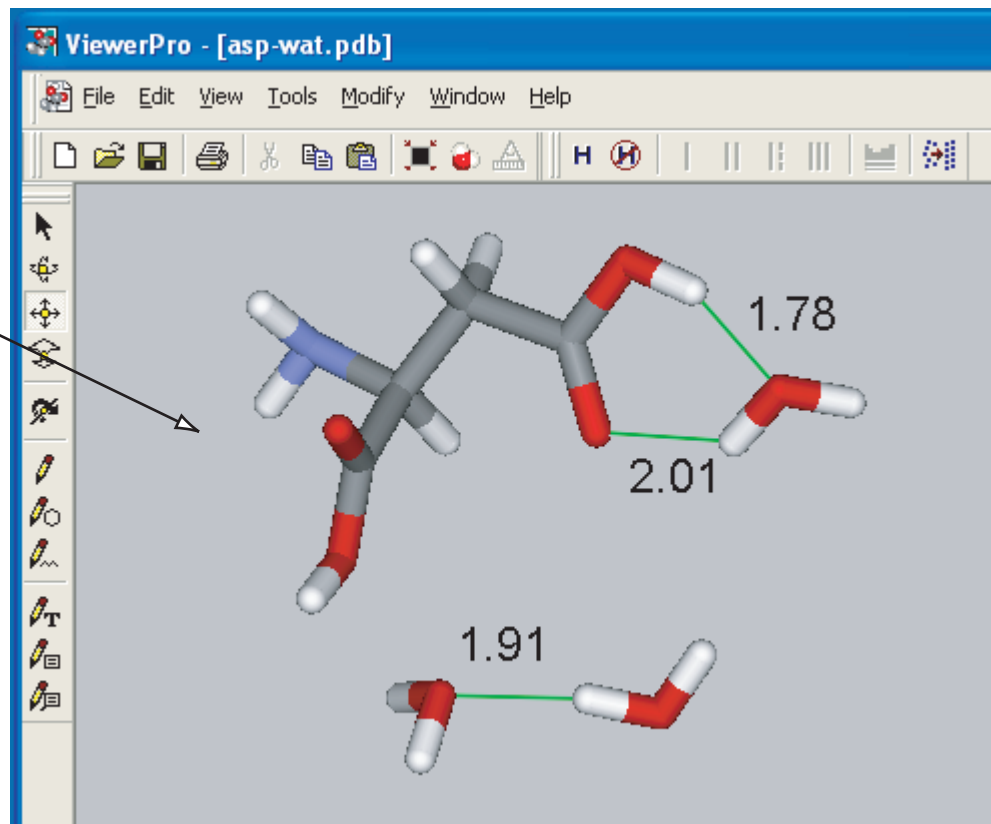


Amino Acid	Deprotonation Energy 1) (kcal/mol)
ASP	173
CYS	181
GLU	199
HID	181
HIE	175
THR	196
TRP	180
TYR	178

1) Calculated as an energy difference
 $E = E(H^+) + E(A^-) - E(HA)$

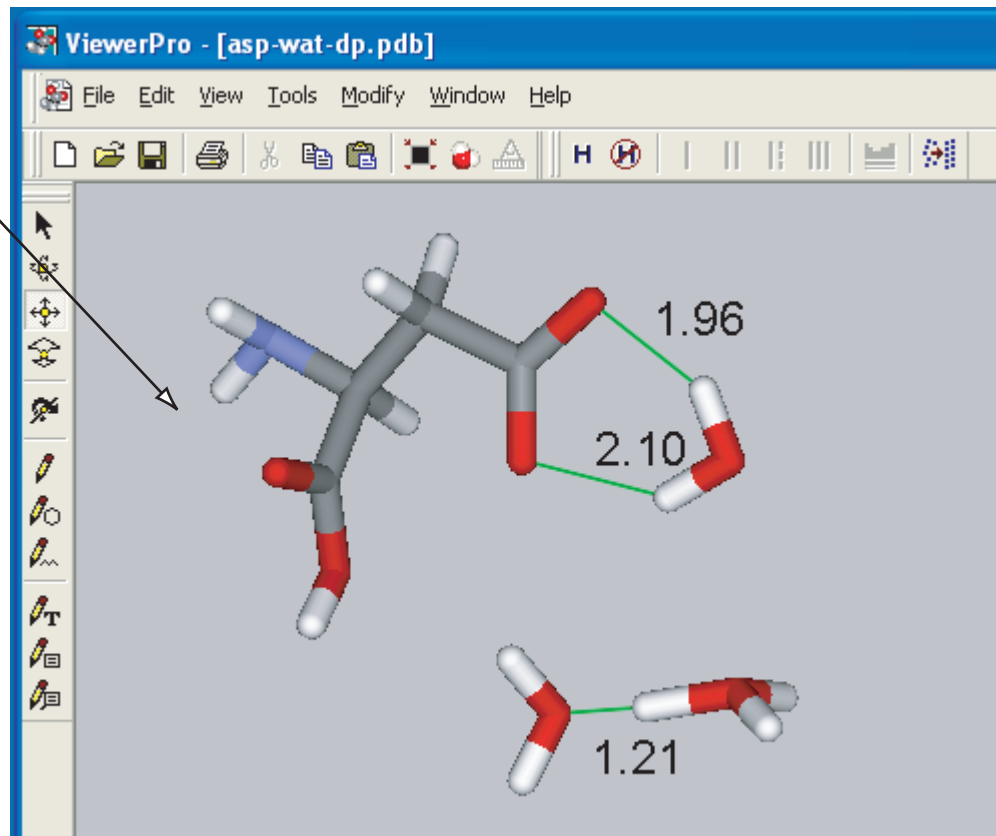
QM calculations of pKa in amino acids and base pairs

Stabilization of
neutral aspartic
acid and water by
two water
molecules



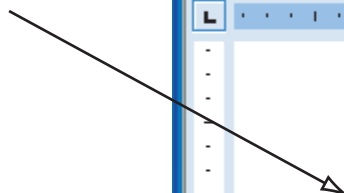
QM calculations of pKa in amino acids and base pairs

Stabilization of
ionic aspartic acid
and water by two
water molecules



QM calculations of pKa in amino acids and base pairs

Deprotonation energy
of acetic acid
stabilized by a water
molecule



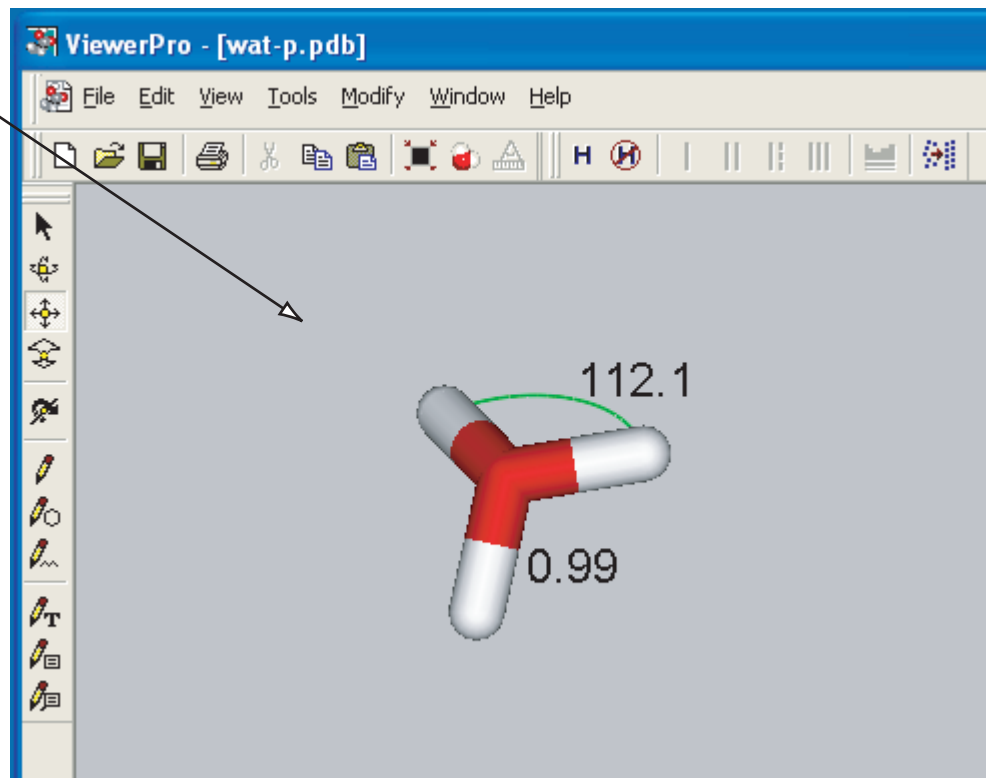
table_pKa-1.doc - Microsoft Word

Amino Acid	Deprotonation Energy 1) (kcal/mol)
ASP	173
ASP-WAT	135

1) Calculated as an energy difference
 $E = E(H^+) + E(A^-) - E(HA)$

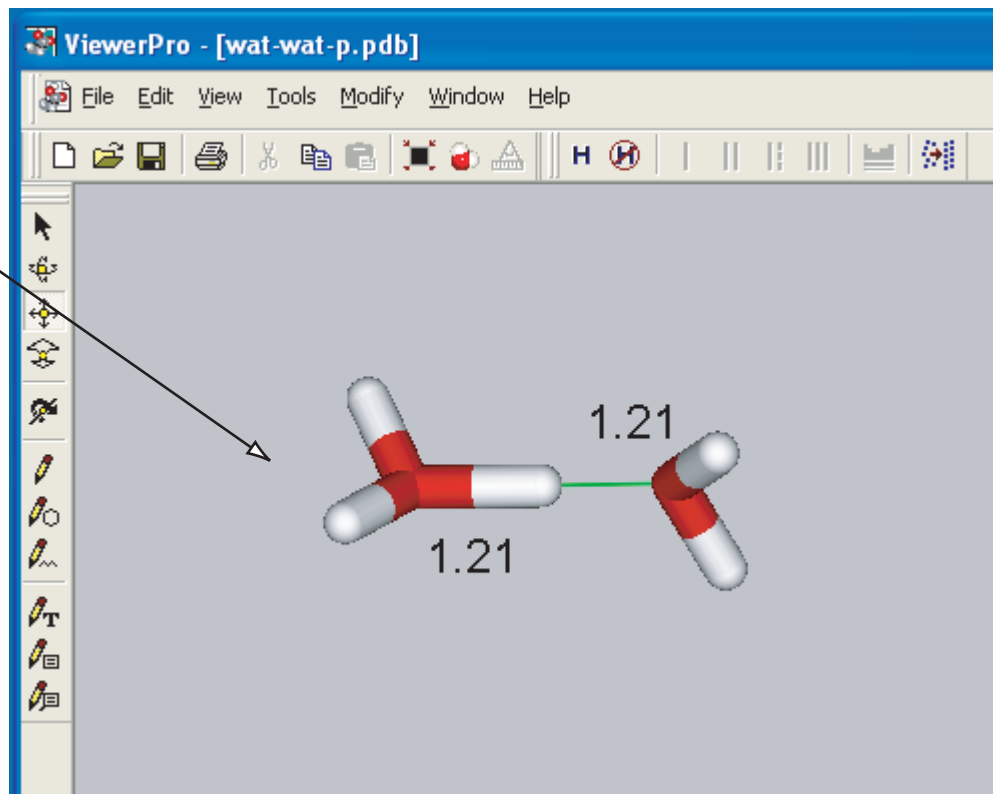
QM calculations of hydronium ion

Optimal geometry
of hydronium ion



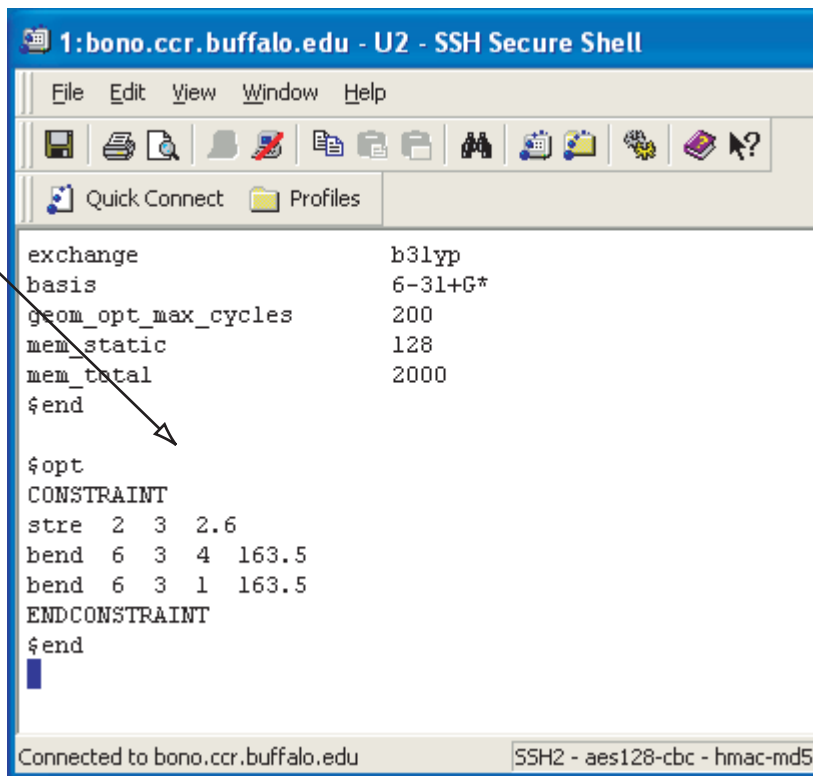
QM calculations of hydronium ion

Optimal geometry
of a dimer of
hydronium ion
and a water
molecule



QM calculations of hydronium ion

Geometry optimization
with a constrained
distance and angles



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

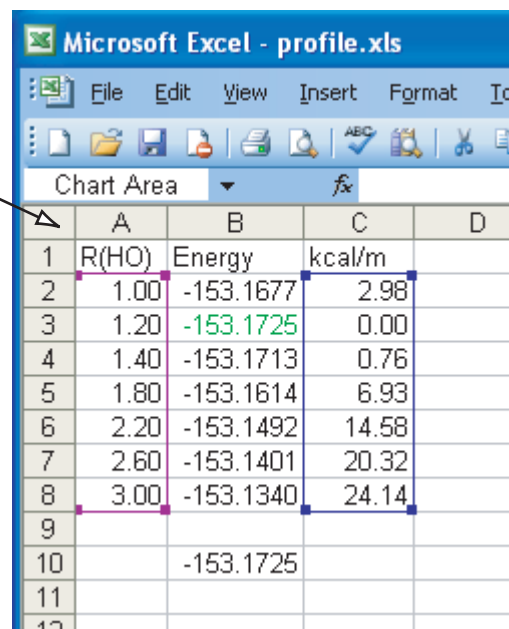
exchange                b3lyp
basis                   6-31+G*
geom_opt_max_cycles     200
mem_static              128
mem_total               2000
$end

$opt
CONSTRAINT
stre  2  3  2.6
bend  6  3  4  163.5
bend  6  3  1  163.5
ENDCONSTRAINT
$end
█

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```

QM calculations of hydronium ion

Results of the
calculation



Microsoft Excel - profile.xls

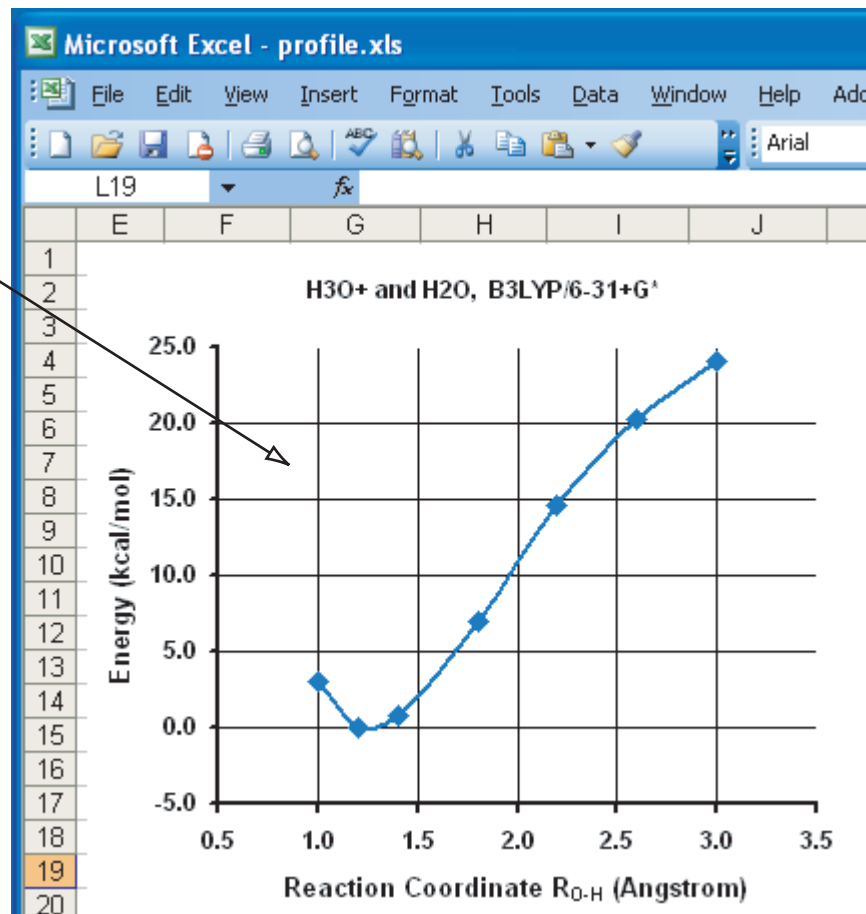
File Edit View Insert Format Io

Chart Area

	A	B	C	D
1	R(HO)	Energy	kcal/m	
2	1.00	-153.1677	2.98	
3	1.20	-153.1725	0.00	
4	1.40	-153.1713	0.76	
5	1.80	-153.1614	6.93	
6	2.20	-153.1492	14.58	
7	2.60	-153.1401	20.32	
8	3.00	-153.1340	24.14	
9				
10		-153.1725		
11				
12				

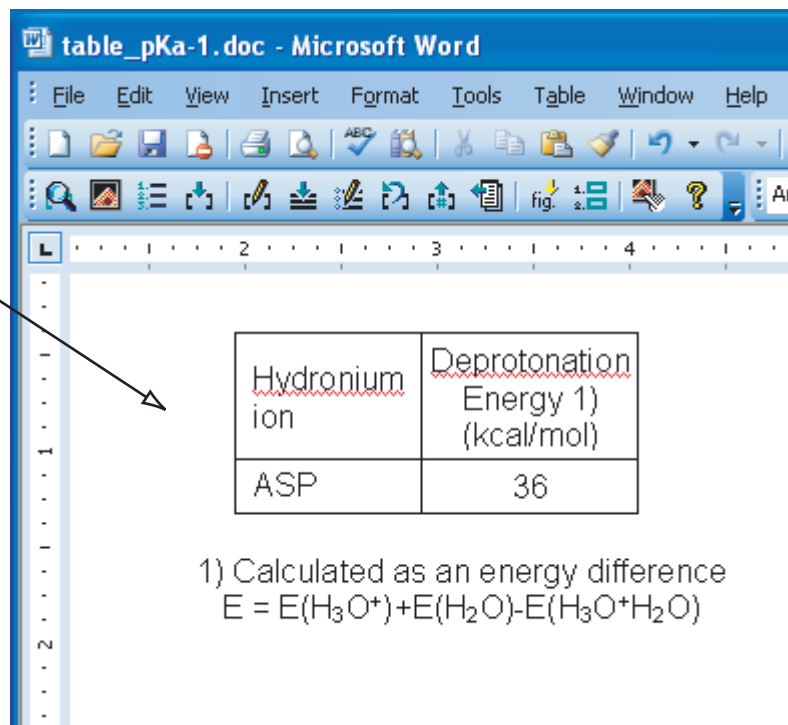
QM calculations of hydronium ion

Potential energy surface of the deprotonation reaction of hydronium ion



QM calculations of hydronium ion

Deprotonation energy
of hydronium ion
calculated in a
presence of a water
molecule



The screenshot shows a Microsoft Word document with a table containing the following data:

Hydronium ion	Deprotonation Energy 1) (kcal/mol)
ASP	36

1) Calculated as an energy difference
 $E = E(\text{H}_3\text{O}^+) + E(\text{H}_2\text{O}) - E(\text{H}_3\text{O}^+ \cdot \text{H}_2\text{O})$

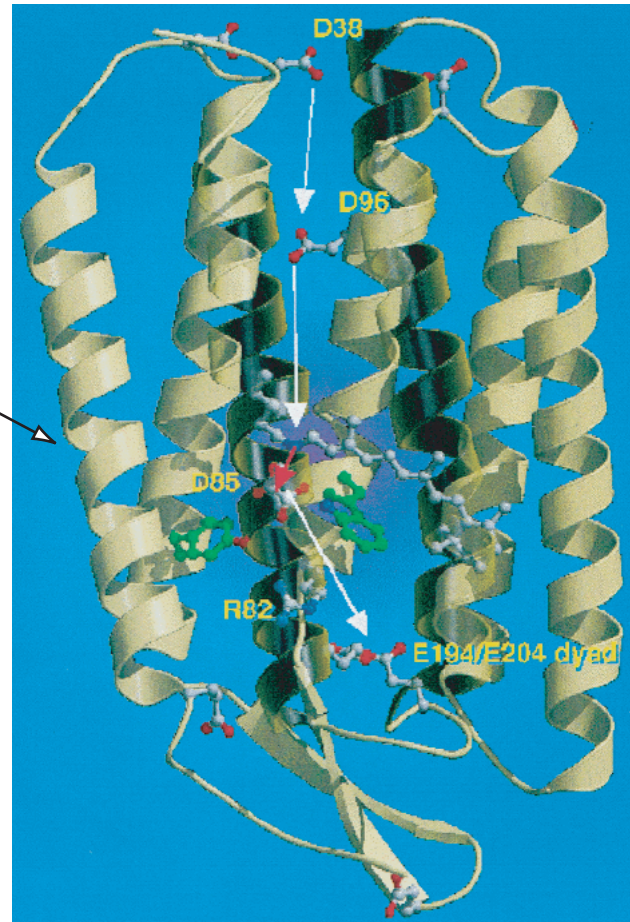
Schrodinger equation

$$H\Psi = E\Psi$$

Ground electronic state $\longrightarrow \Psi_g \quad E_g$

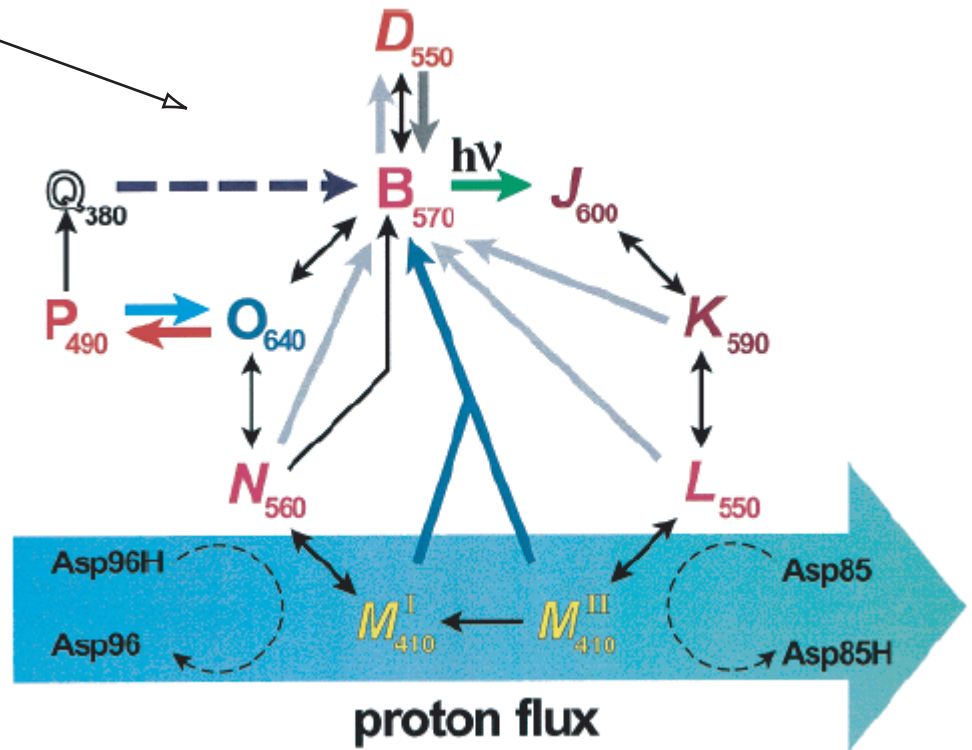
Excited electronic state $\longrightarrow \Psi_e \quad E_e$

Bacteriorhodopsin



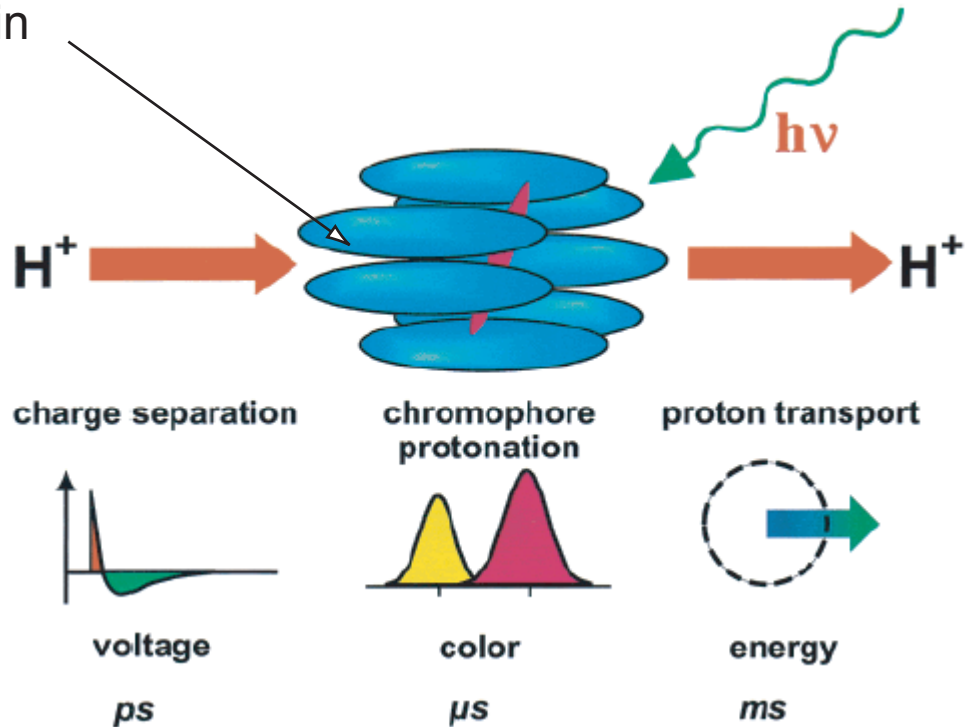
QM calculations of excited electronic states

The reaction cycle of bacteriorhodopsin



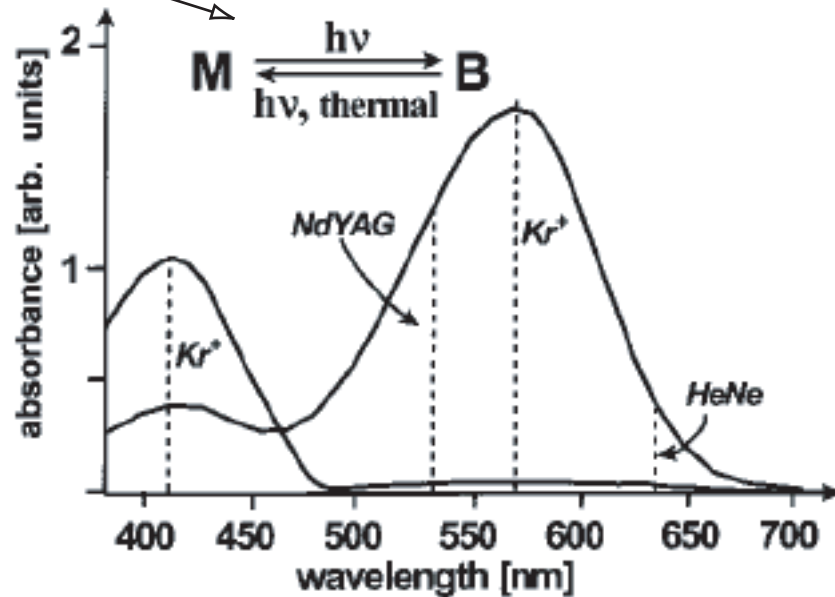
QM calculations of excited electronic states

Molecular function of
bacteriorhodopsin



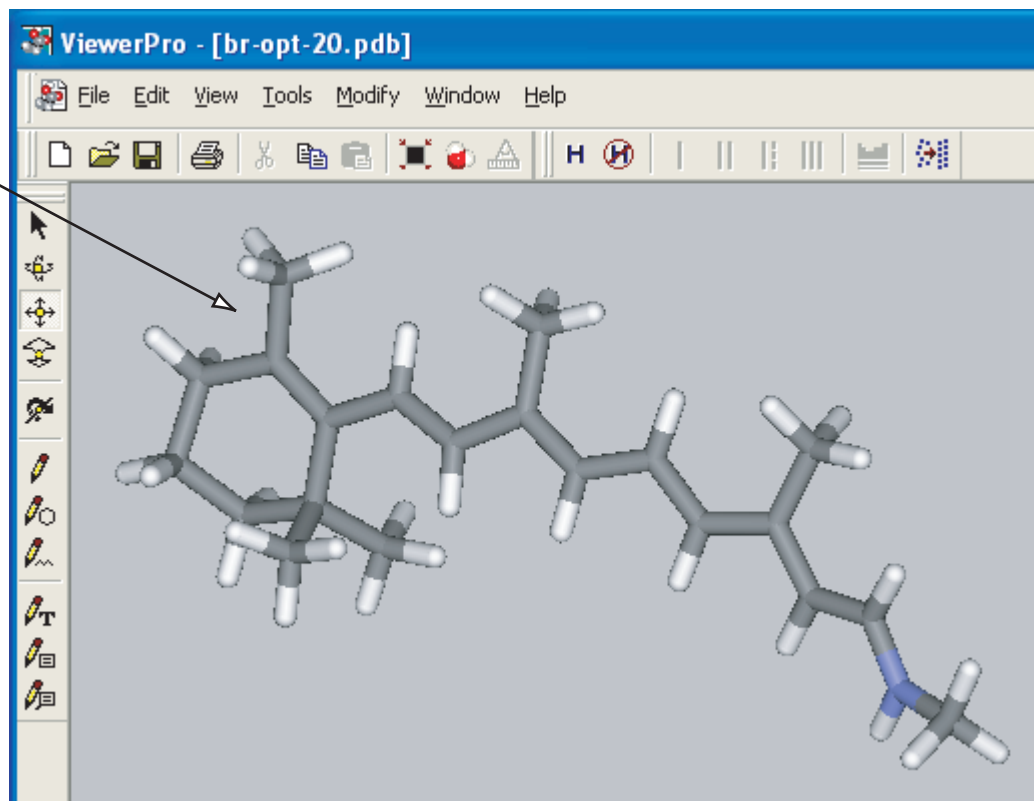
QM calculations of excited electronic states

Experimental UV
spectrum of bR



QM calculations of excited electronic states

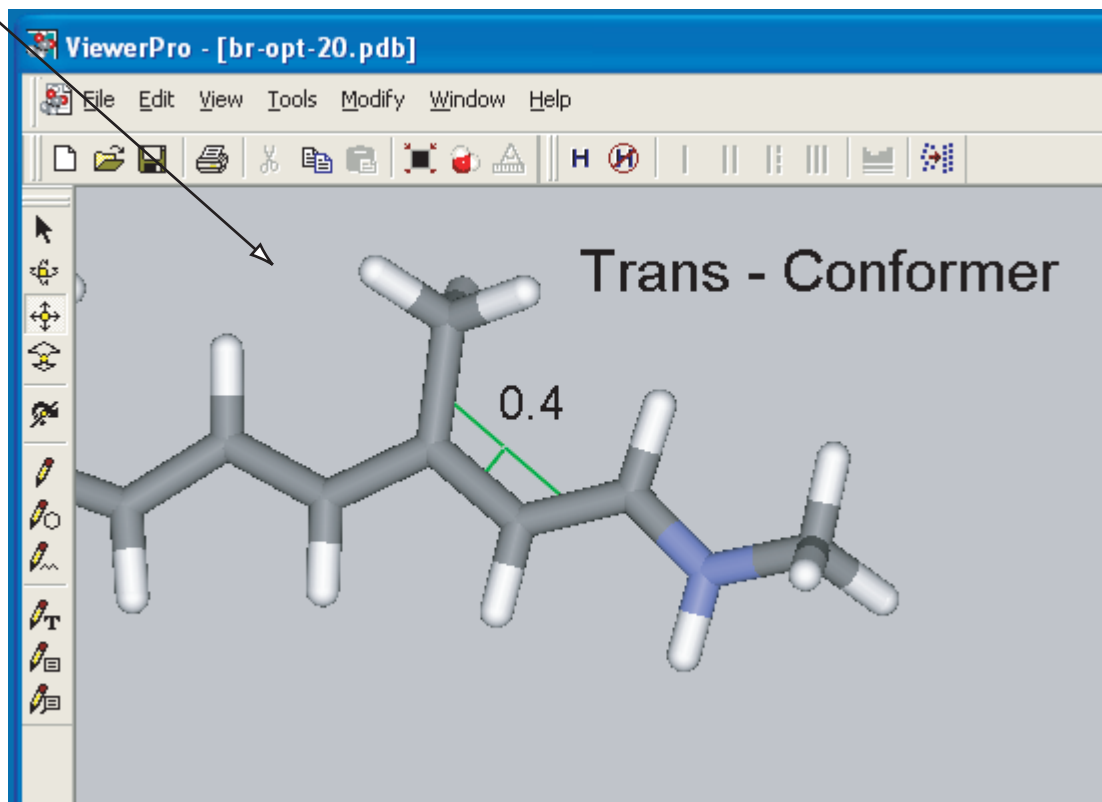
The active site of bacteriorhodopsin



QM calculations of excited electronic states

The trans conformer
of retinal

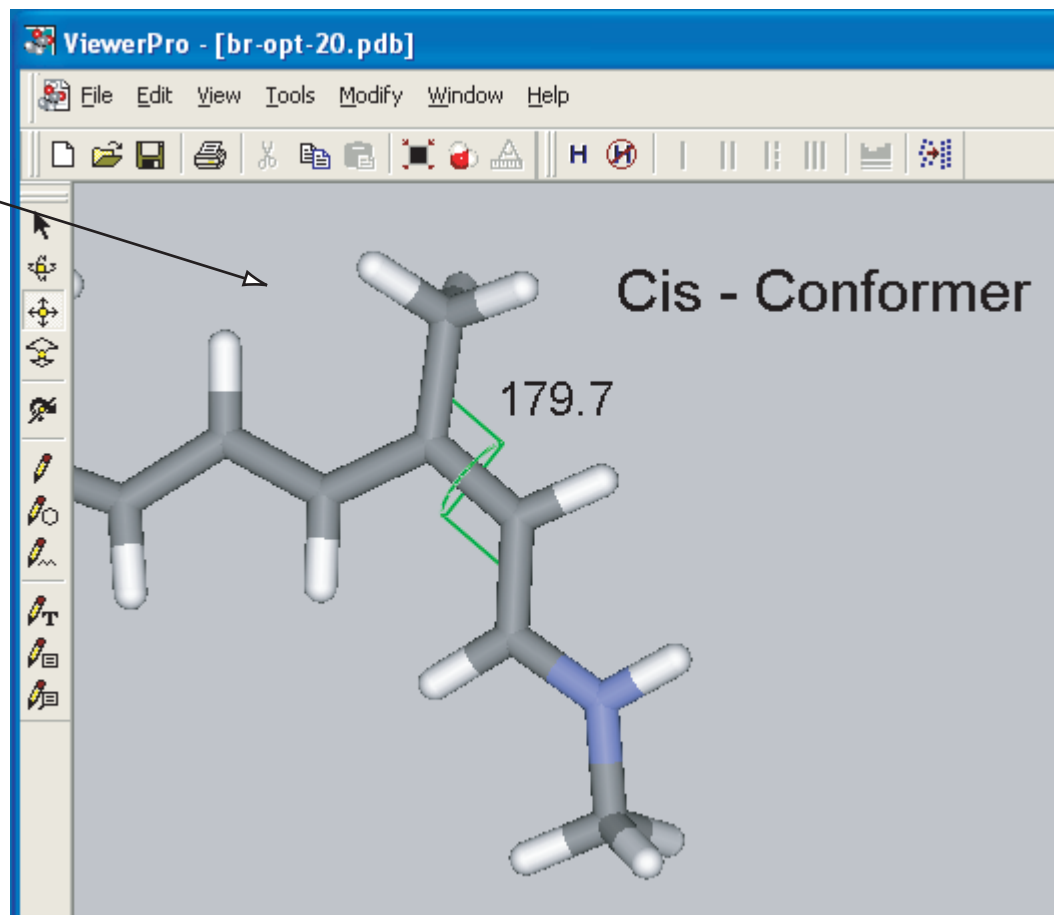
$E = 570 \text{ nm}$
(17500 cm^{-1})



QM calculations of excited electronic states

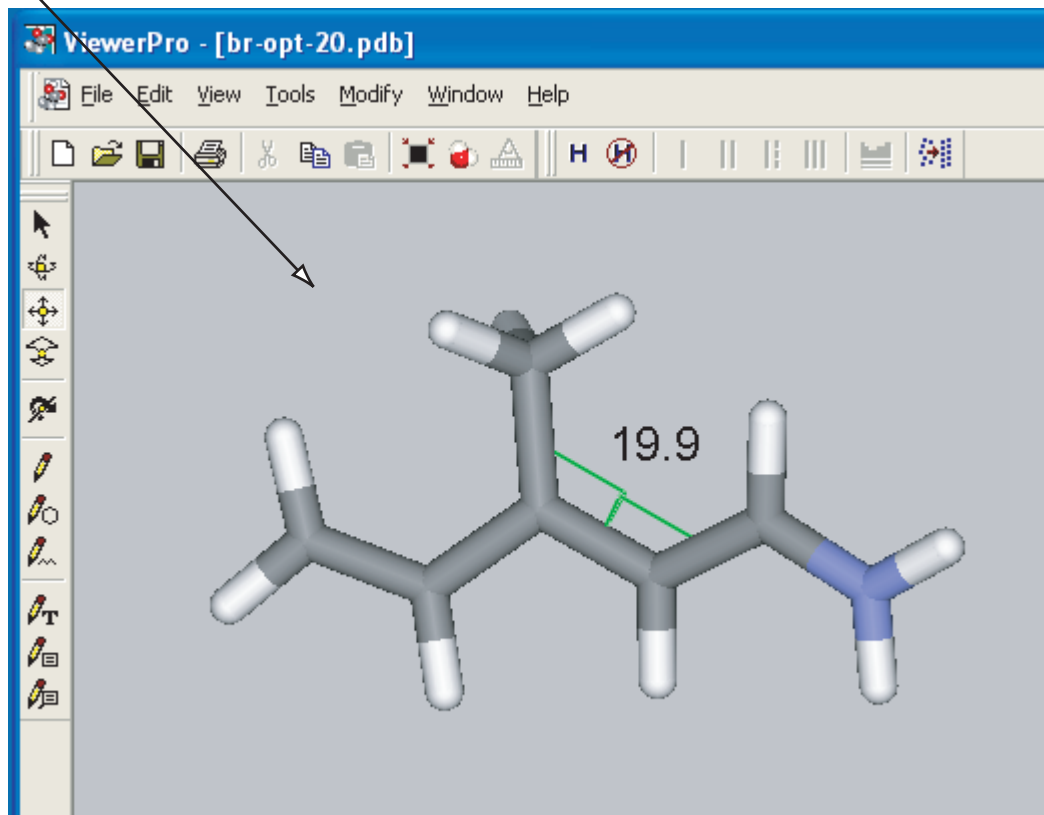
The cis conformer of retinal

E = 410 nm
(24400 cm⁻¹)



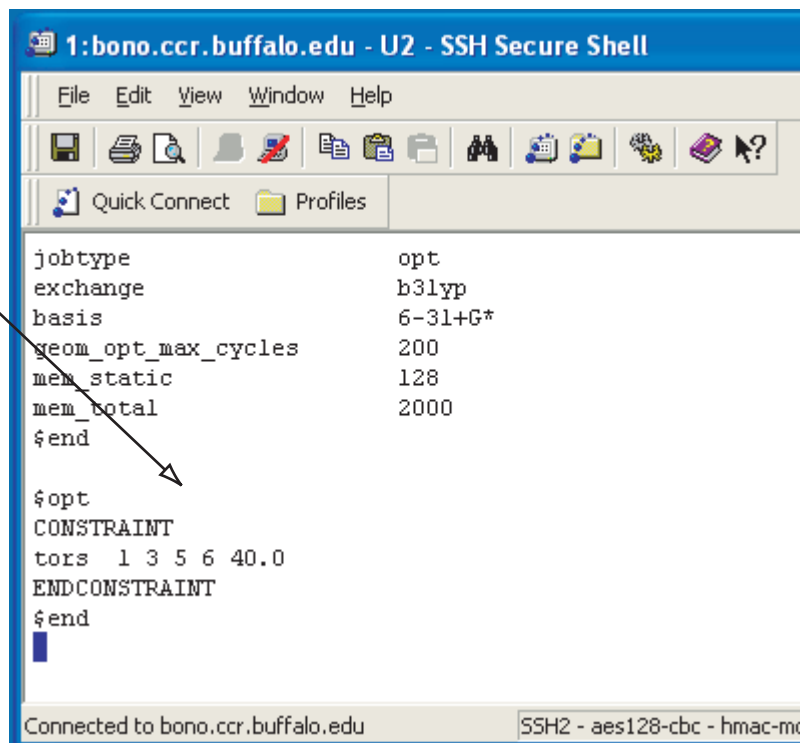
QM calculations of excited electronic states

A small computational
model of retinal



QM calculations of excited electronic states

Geometry optimization
of retinal with a
constrained dihedral
angle



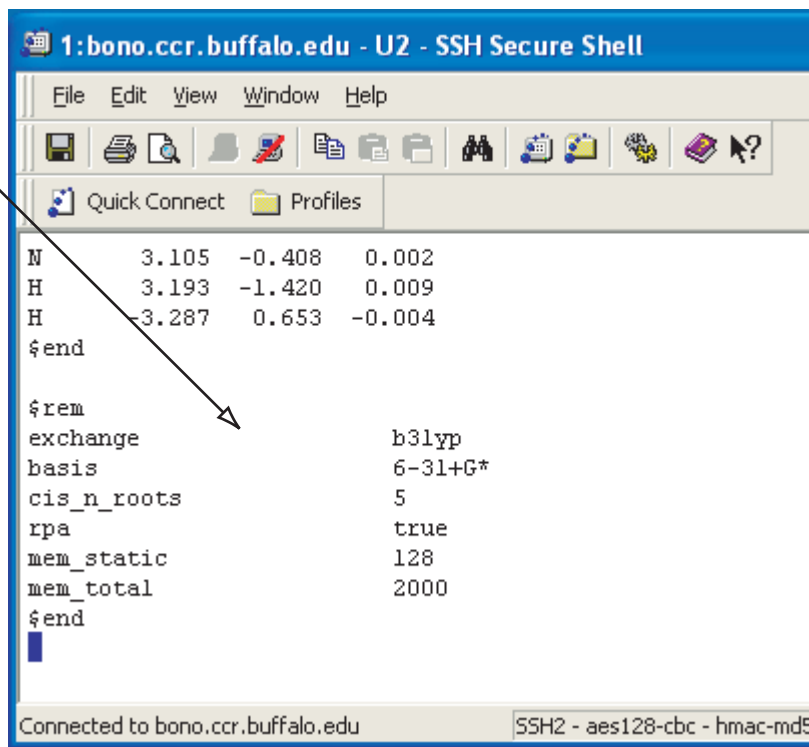
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
jobtype                opt
exchange               b3lyp
basis                  6-31+G*
geom_opt_max_cycles    200
mem_static             128
mem_total              2000
$end

$opt
CONSTRAINT
tors 1 3 5 6 40.0
ENDCONSTRAINT
$end
█

Connected to bono.ccr.buffalo.edu      SSH2 - aes128-cbc - hmac-mc
```


QM calculations of excited electronic states

Calculations of five
excited electronic
states of retinal model
using TD-DFT



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
N      3.105  -0.408   0.002
H      3.193  -1.420   0.009
H     -3.287   0.653  -0.004
$end

$rem
exchange                b3lyp
basis                   6-31+G*
cis_n_roots              5
rpa                      true
mem_static              128
mem_total               2000
$end
█

Connected to bono.ccr.buffalo.edu      SSH2 - aes128-cbc - hmac-md5
```

QM calculations of excited electronic states

Results of the calculations for the ground electronic state, the excited singlet and triplet

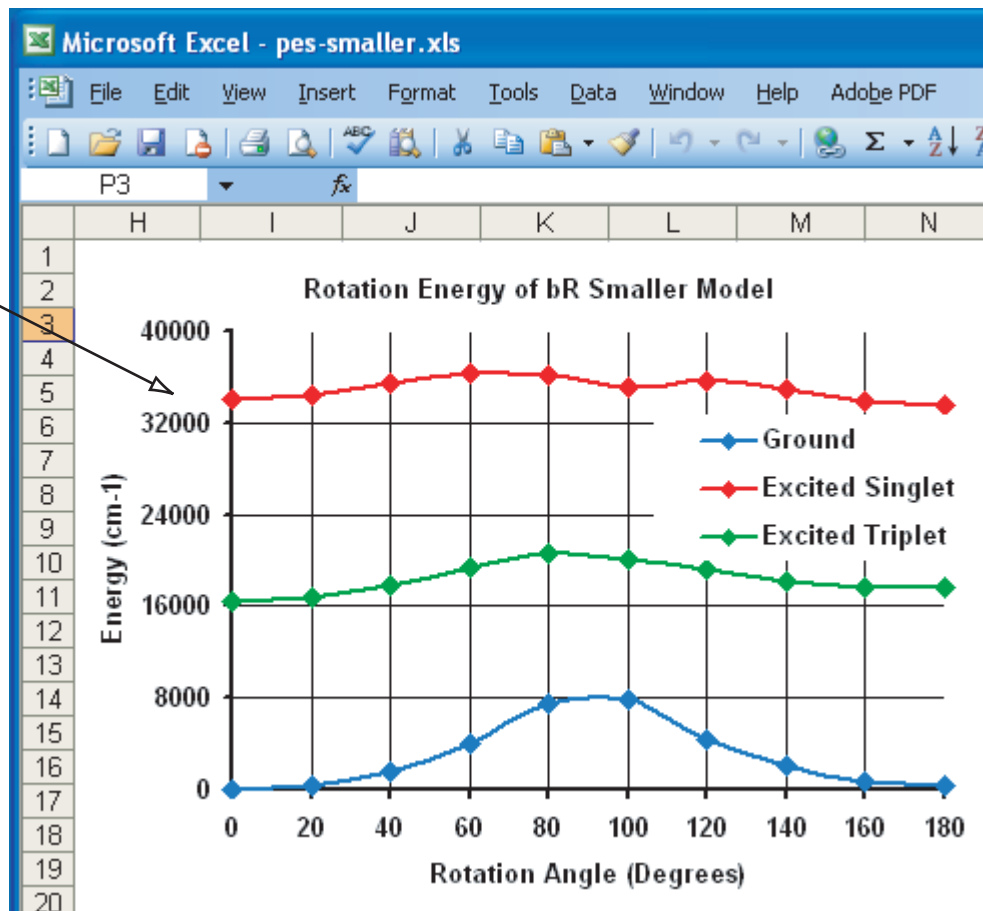
Microsoft Excel - pes-smaller.xls

Chart 5

	A	B	C	D	E	F	G
1		Singlet		Singlet		Triplet	
2		Ground	Ground	Excited	Excited	Excited	Excited
3		au	cm-1	au	cm-1	au	cm-1
4	0	-289.15282	0	-288.99781	34021	-289.07807	16406
5	20	-289.15100	400	-288.99614	34386	-289.07628	16797
6	40	-289.14540	1628	-288.99162	35379	-289.07141	17866
7	60	-289.13468	3980	-288.98693	36408	-289.06438	19410
8	80	-289.11891	7441	-288.98780	36216	-289.05861	20676
9	100	-289.11704	7853	-288.99300	35076	-289.06151	20041
10	120	-289.13264	4428	-288.99028	35673	-289.06552	19160
11	140	-289.14343	2060	-288.99373	34915	-289.06990	18198
12	160	-289.14928	776	-288.99834	33905	-289.07221	17692
13	180	-289.15098	404	-289.00002	33534	-289.07279	17564
14							
15		-289.15282					
16							

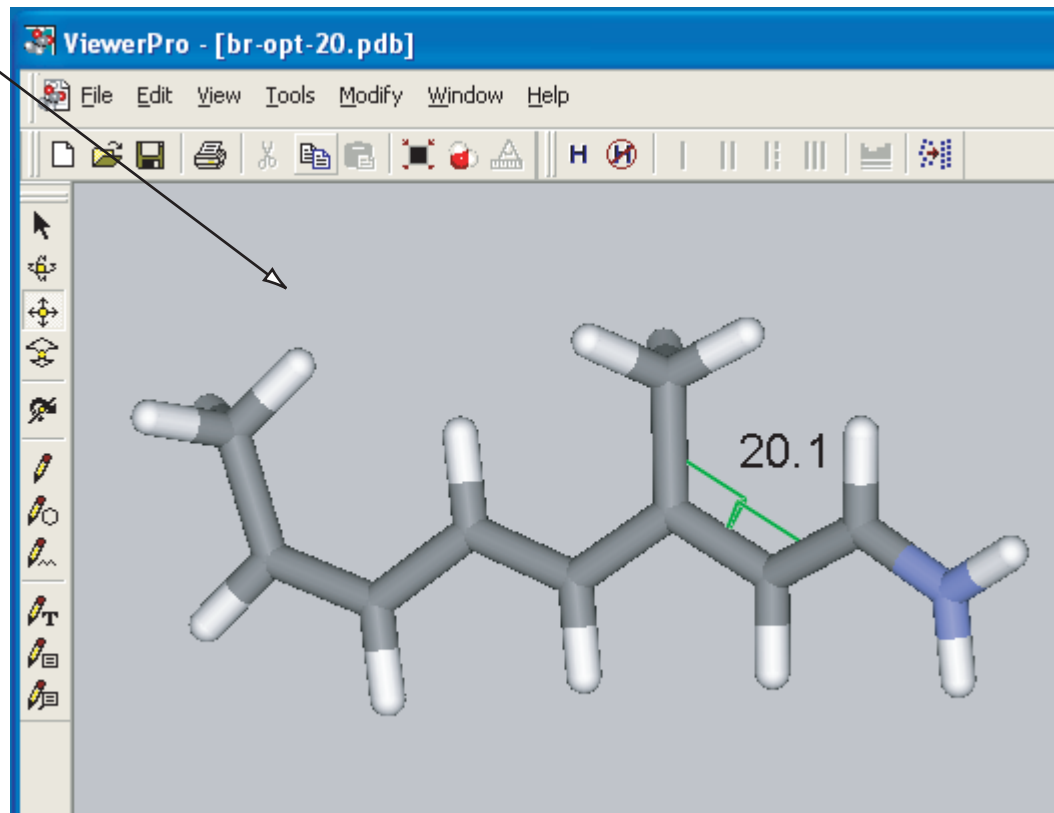
QM calculations of excited electronic states

Results of the calculations for the ground electronic state, the excited singlet and triplet



QM calculations of excited electronic states

The bigger model of
retinal



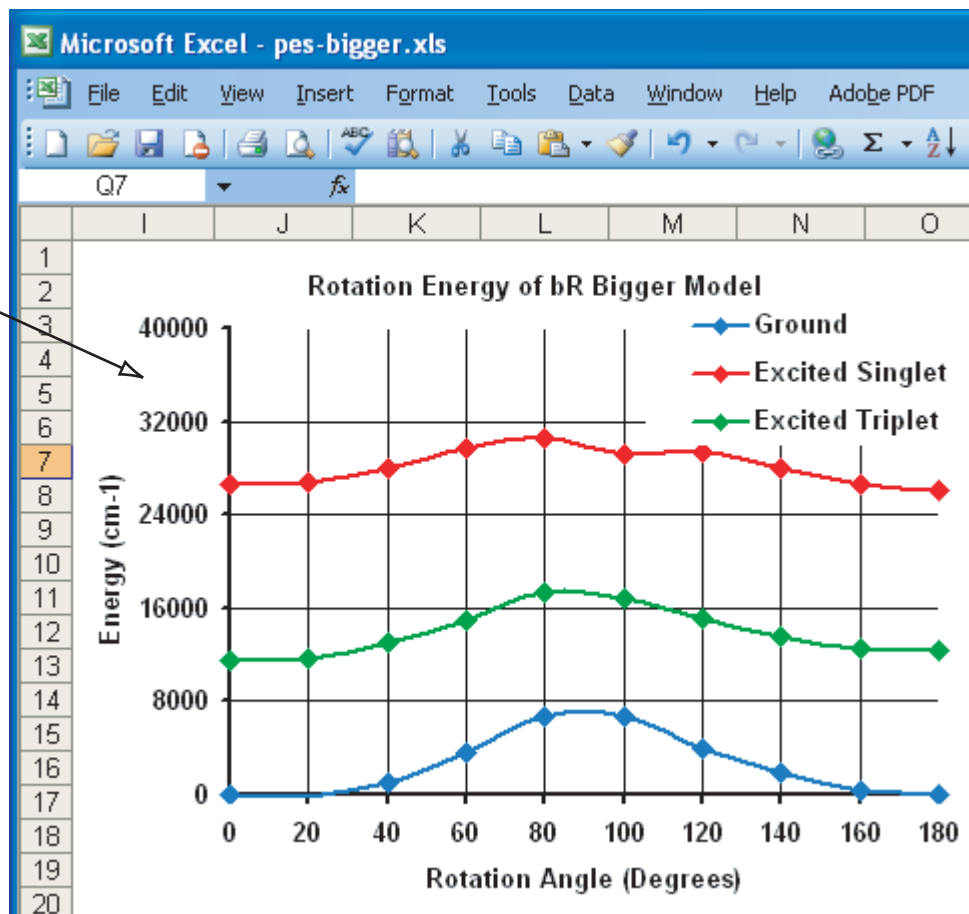
QM calculations of excited electronic states

Results of the calculations for the ground electronic state, the excited singlet and triplet

	A	B	C	D	E	F	G
1		Singlet		Singlet		Triplet	
2		Ground	Ground	Excited	Excited	Excited	Excited
3		au	cm-1	au	cm-1	au	cm-1
4	0	-405.89254	0	-405.77133	26601	-405.84042	11437
5	20	-405.89315	-135	-405.77063	26754	-405.83911	11724
6	40	-405.88786	1027	-405.76473	28051	-405.83317	13029
7	60	-405.87609	3609	-405.75748	29640	-405.82430	14976
8	80	-405.86234	6628	-405.75334	30549	-405.81384	17271
9	100	-405.86181	6744	-405.75933	29235	-405.81613	16770
10	120	-405.87481	3890	-405.75847	29425	-405.82401	15040
11	140	-405.88391	1894	-405.76477	28041	-405.83076	13557
12	160	-405.89117	300	-405.77162	26538	-405.83537	12545
13	180	-405.89225	62	-405.77330	26170	-405.83627	12349
14							
15		-405.89254					
16							

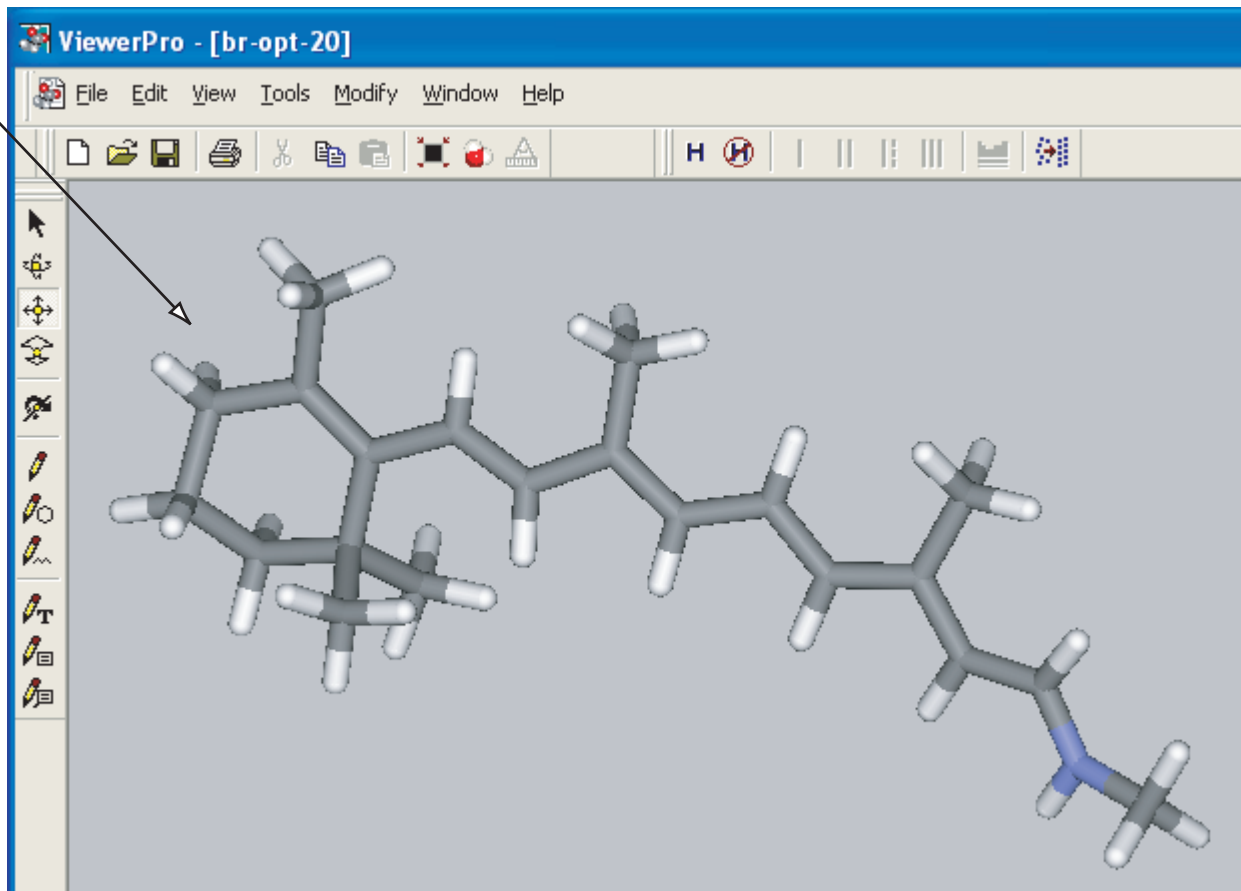
QM calculations of excited electronic states

Results of the calculations for the ground electronic state, the excited singlet and triplet



QM calculations of excited electronic states

The full model of
retinal



The results of the calculations

Page 18

QM calculations of excited electronic states

Energies of the
ground electronic
state, the first
excited singlet and
triple

