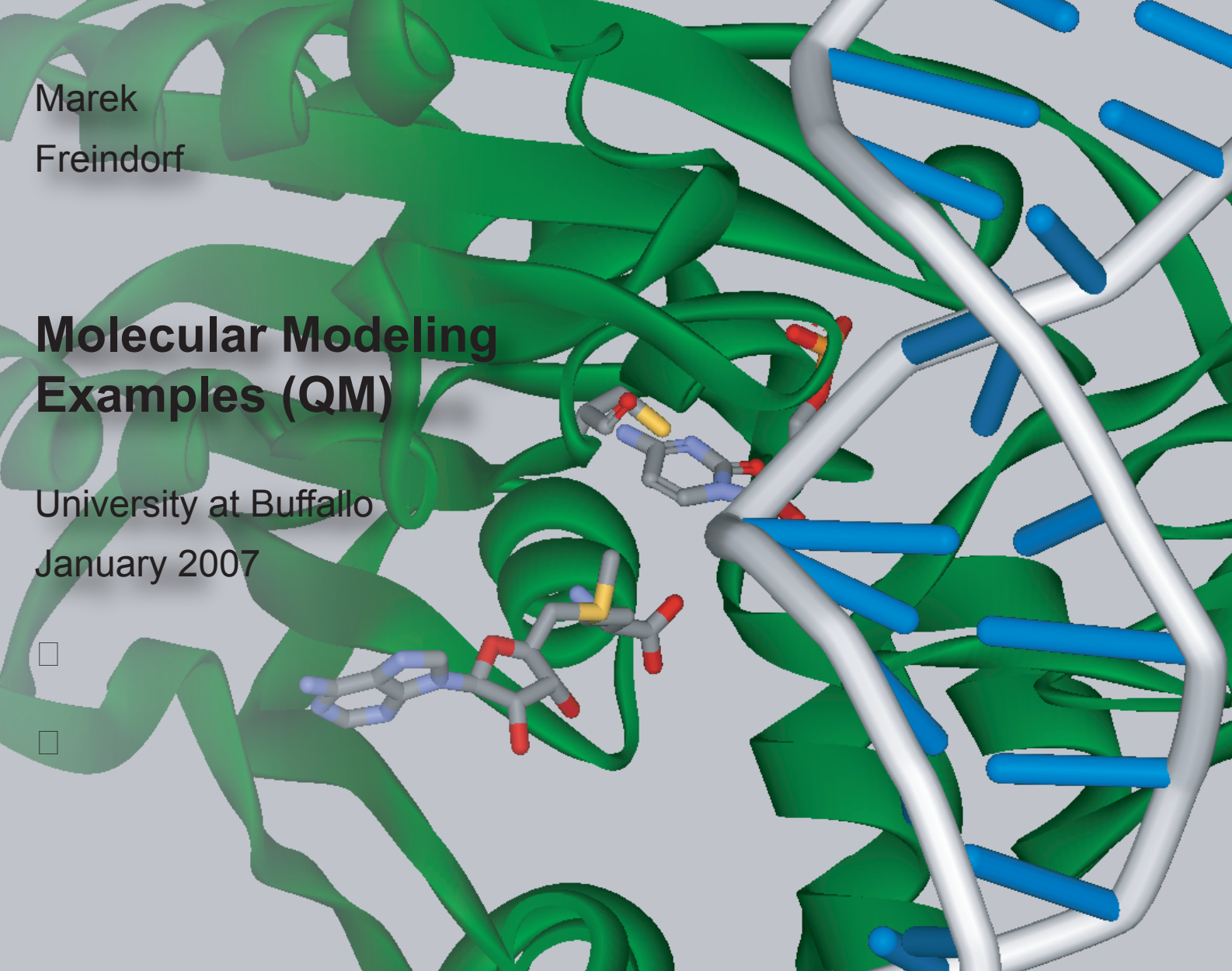
Marek
Freindorf

Molecular Modeling Examples (QM)

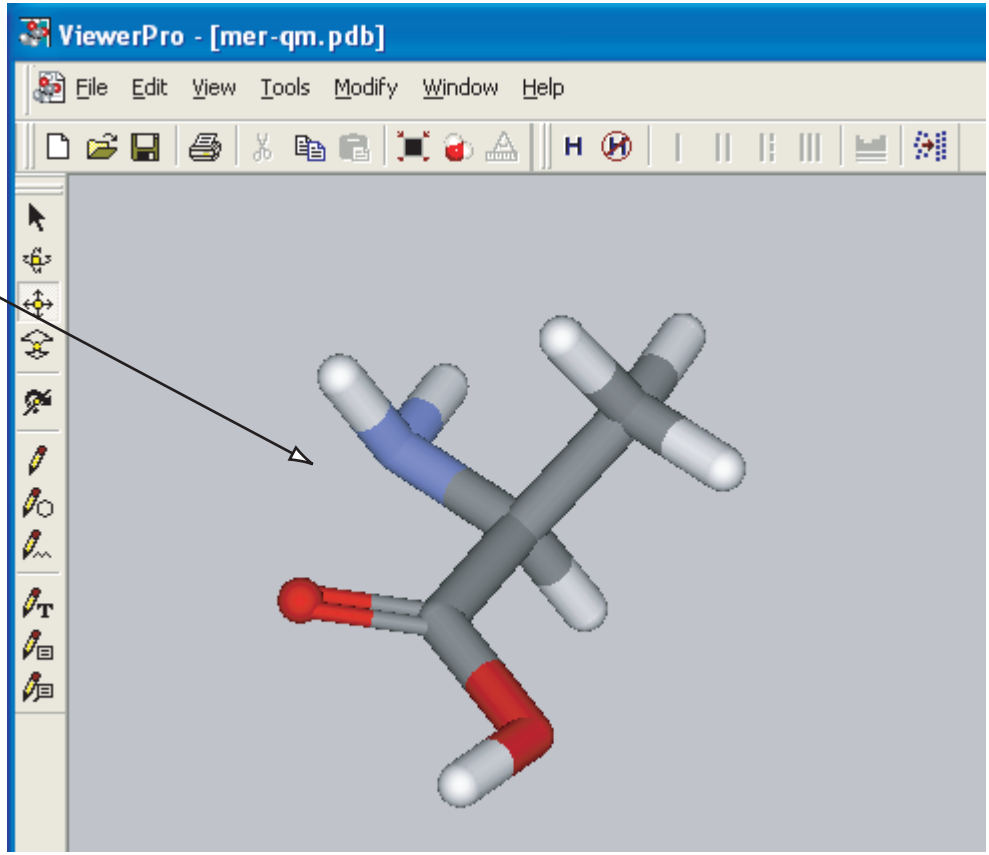
University at Buffalo

January 2007



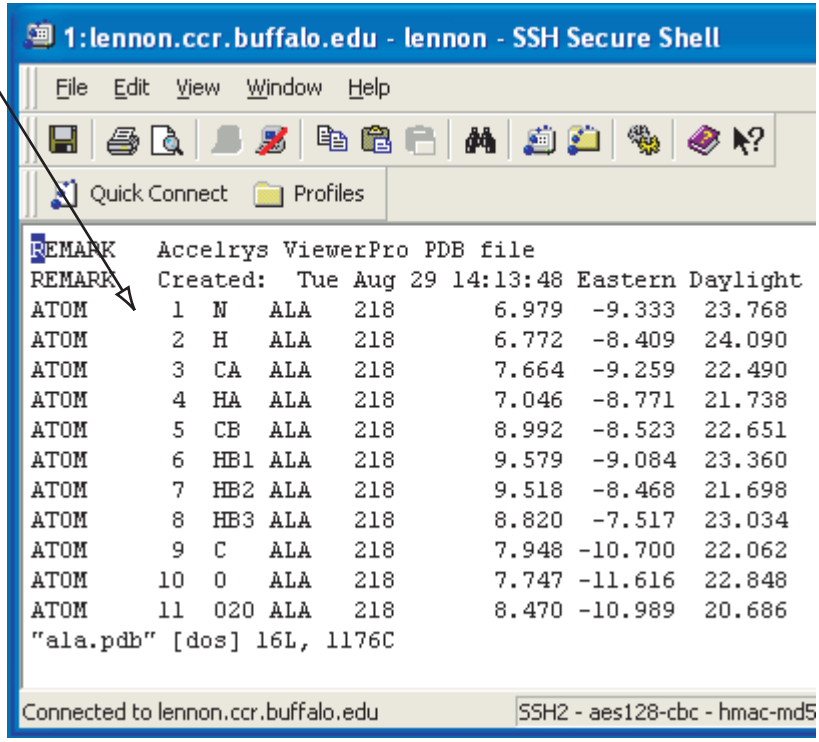
QM geometry optimization of alanine

Initial geometry of alanine



QM geometry optimization of alanine

A PDB file of alanine

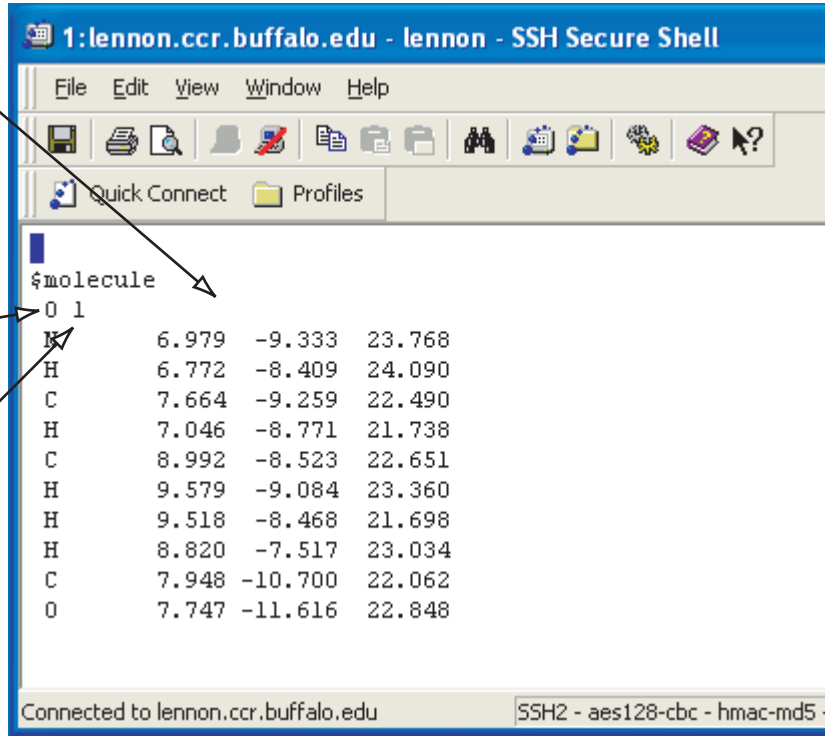


QM geometry optimization of alanine

Copy and paste the coordinates

Molecular charge

Multiplicity of the electronic wave function



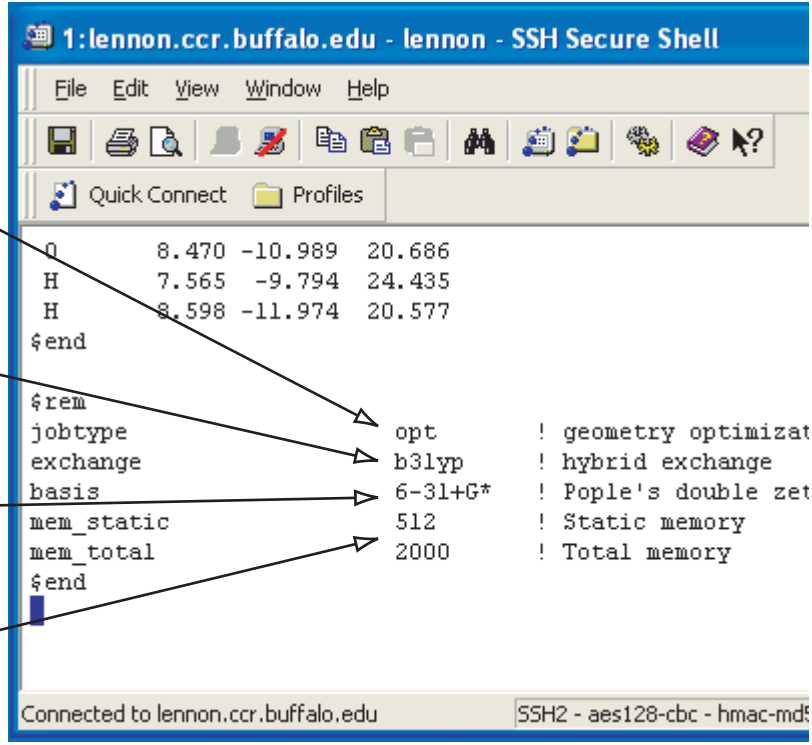
QM geometry optimization of alanine

Geometry optimization

Hamiltonian

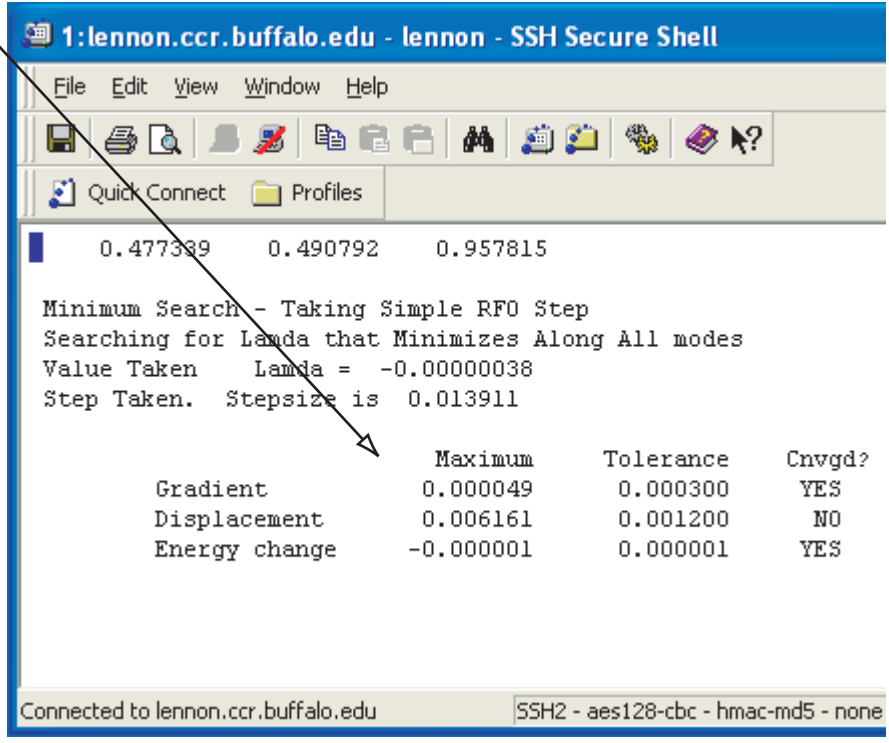
Basis set

Memory allocation



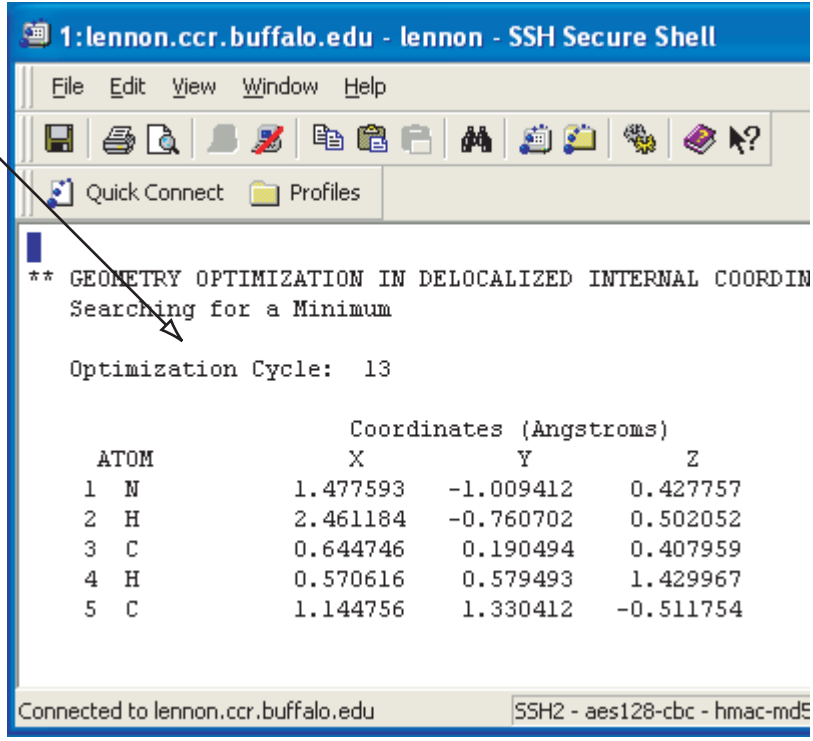
QM geometry optimization of alanine

Geometry optimized



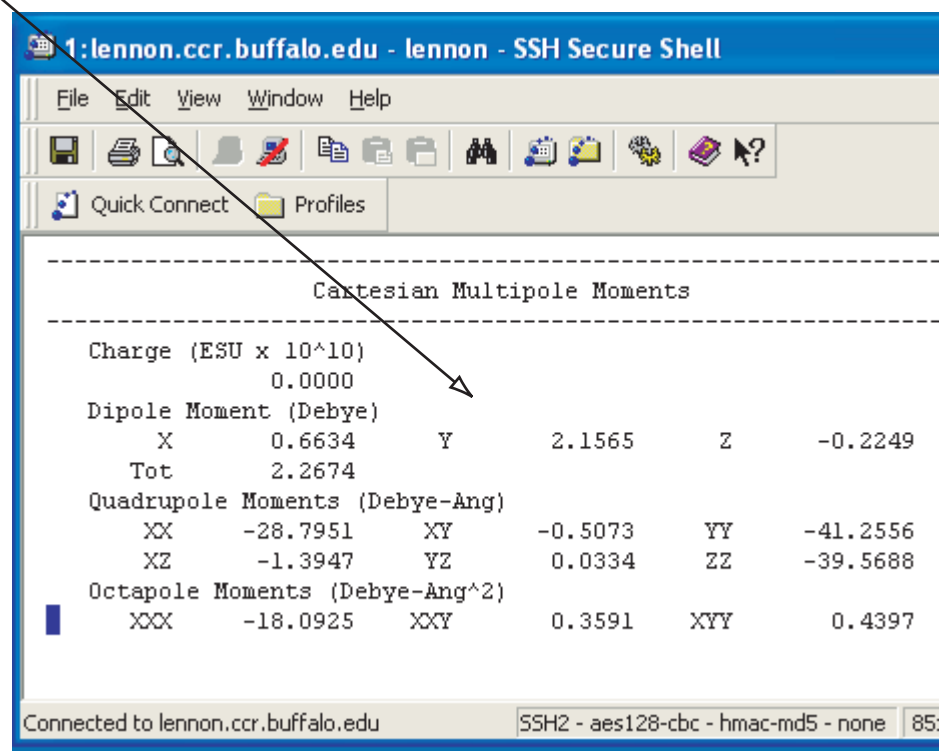
QM geometry optimization of alanine

Final geometry



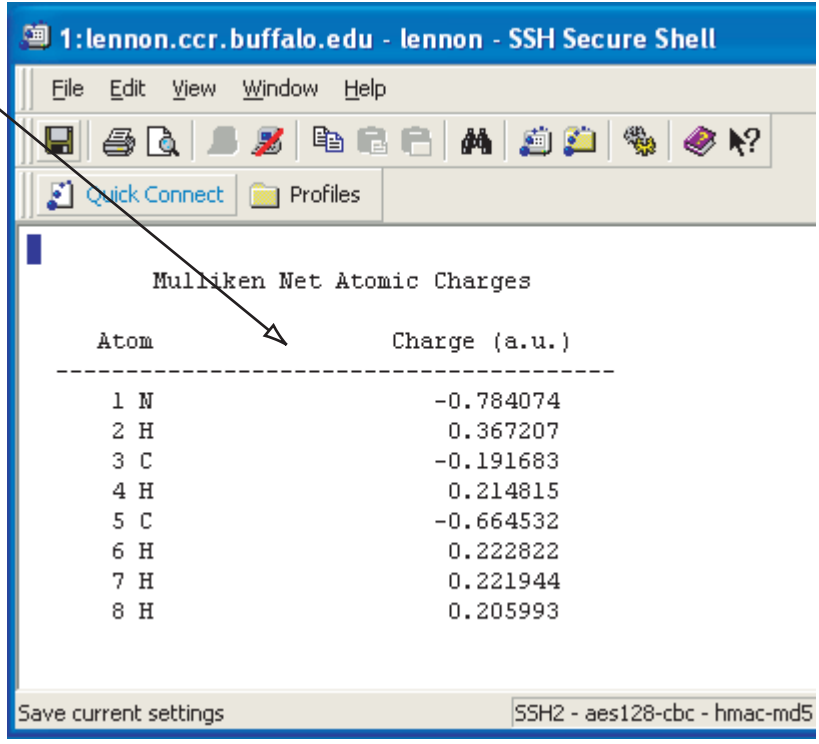
QM geometry optimization of alanine

Final dipol moment



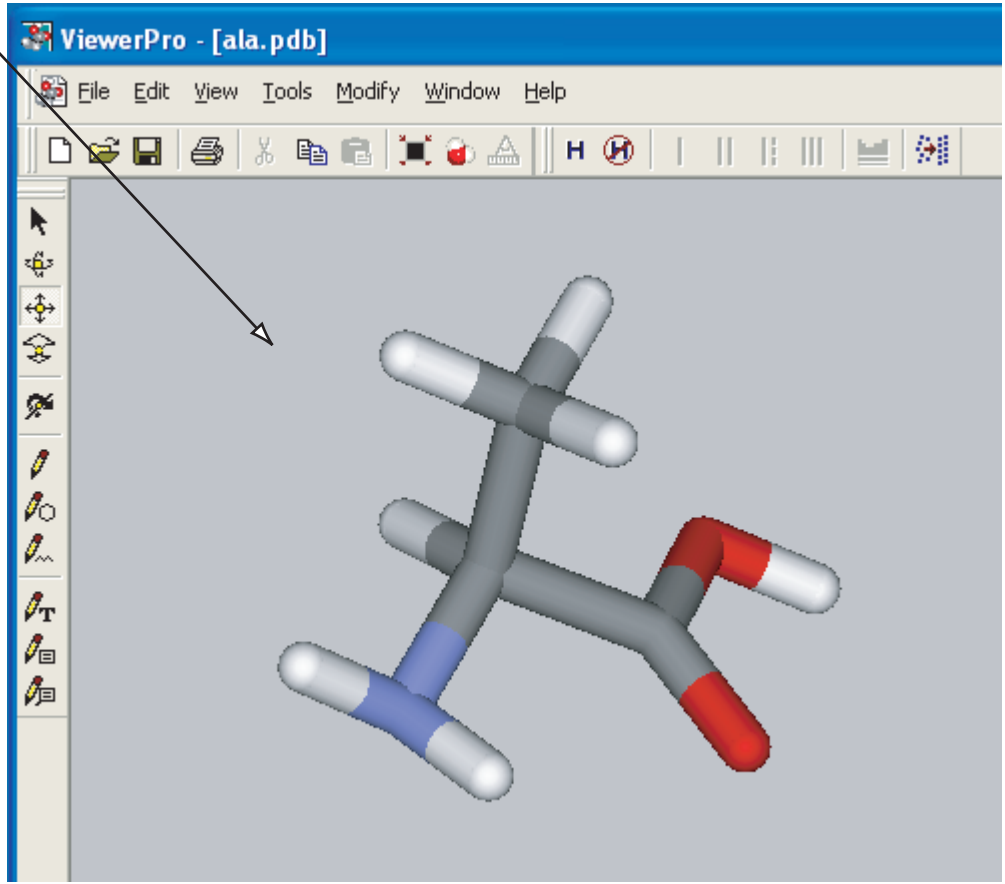
QM geometry optimization of alanine

Atomic charges



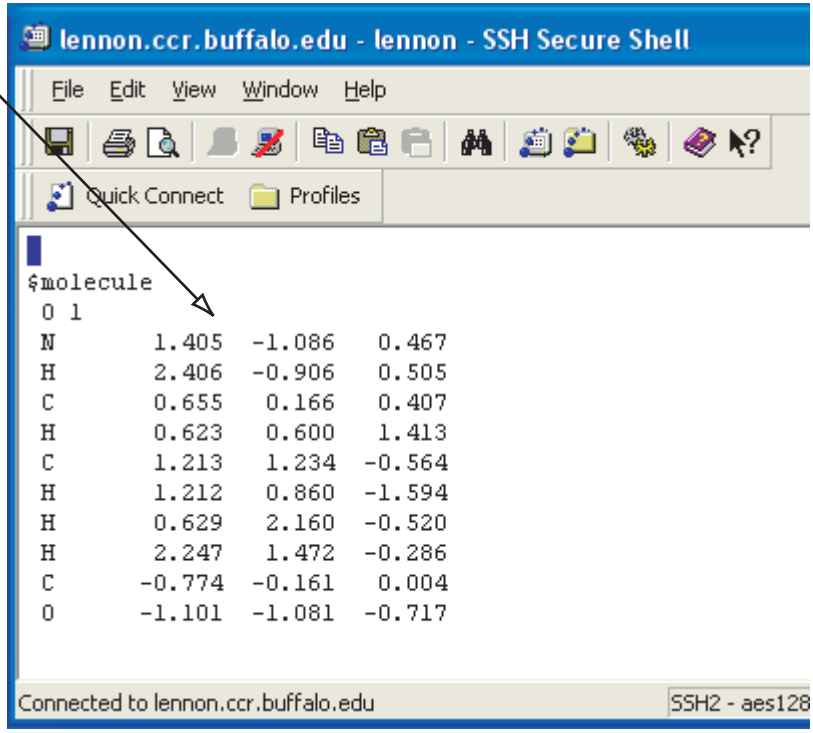
QM geometry optimization of alanine

Geometry optimized



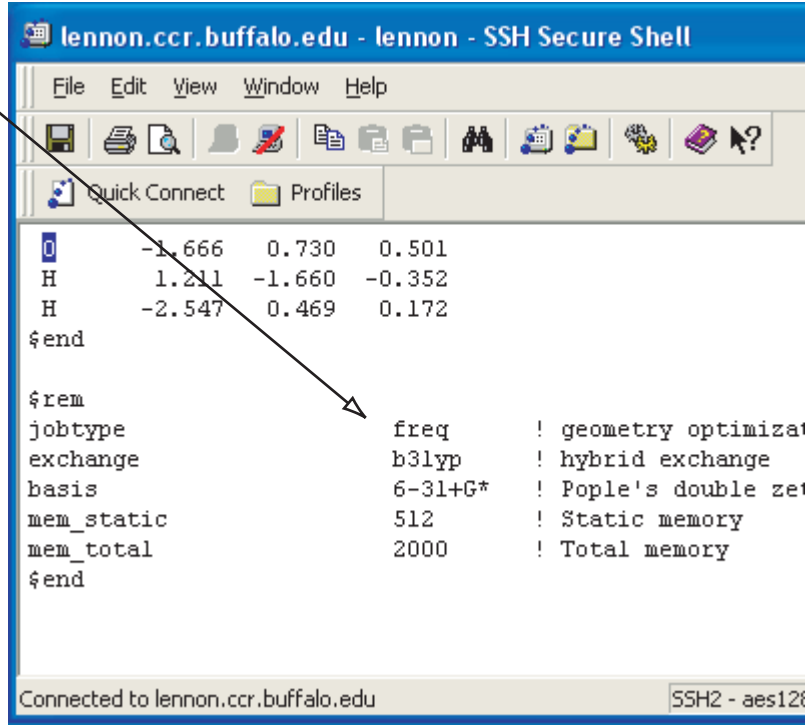
QM oscillations of alanine

Coordinates after
geometry optimization



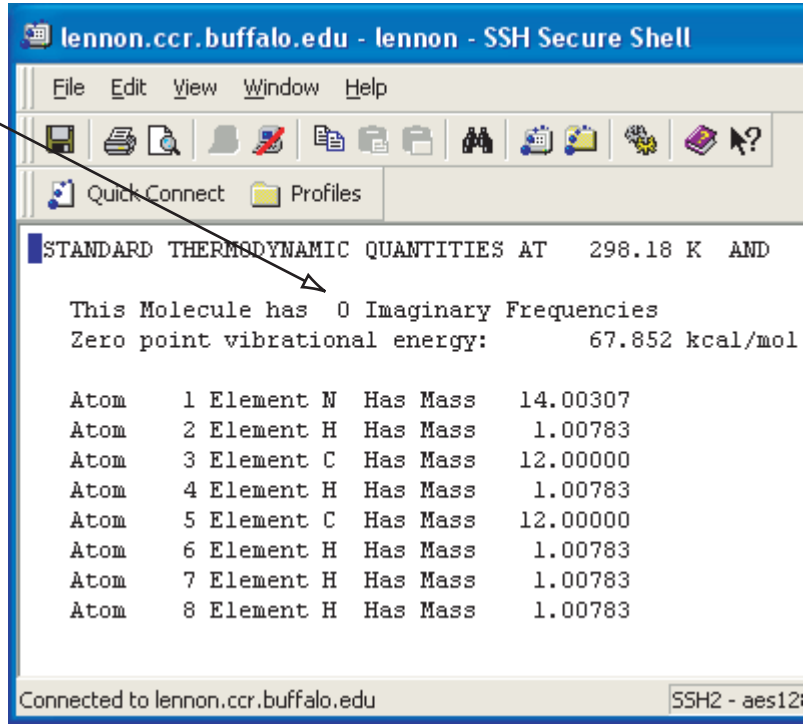
QM oscillations of alanine

Molecular oscillations calculations



QM oscillations of alanine

Results of oscillations calculations

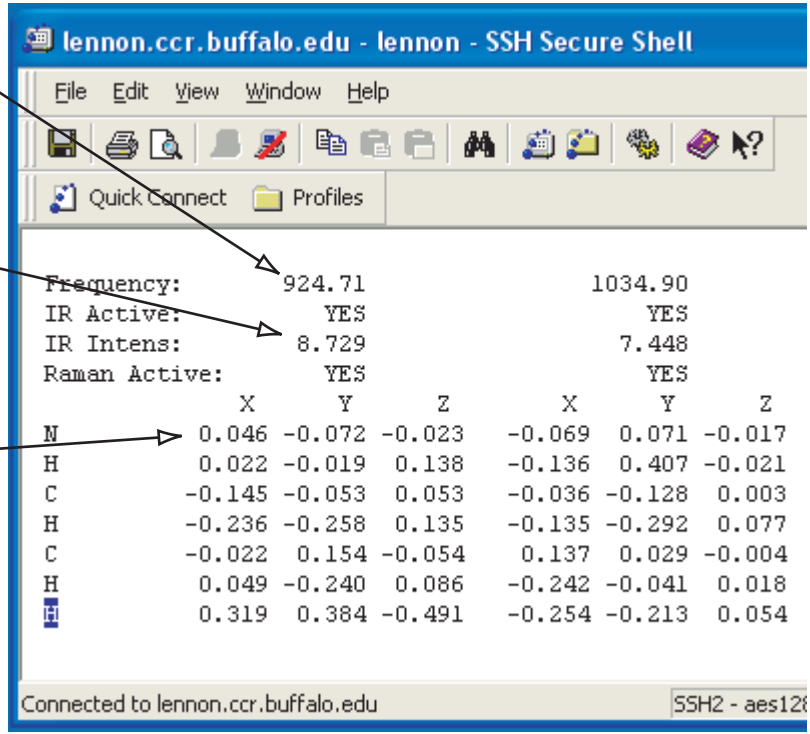


QM oscillations of alanine

Frequency

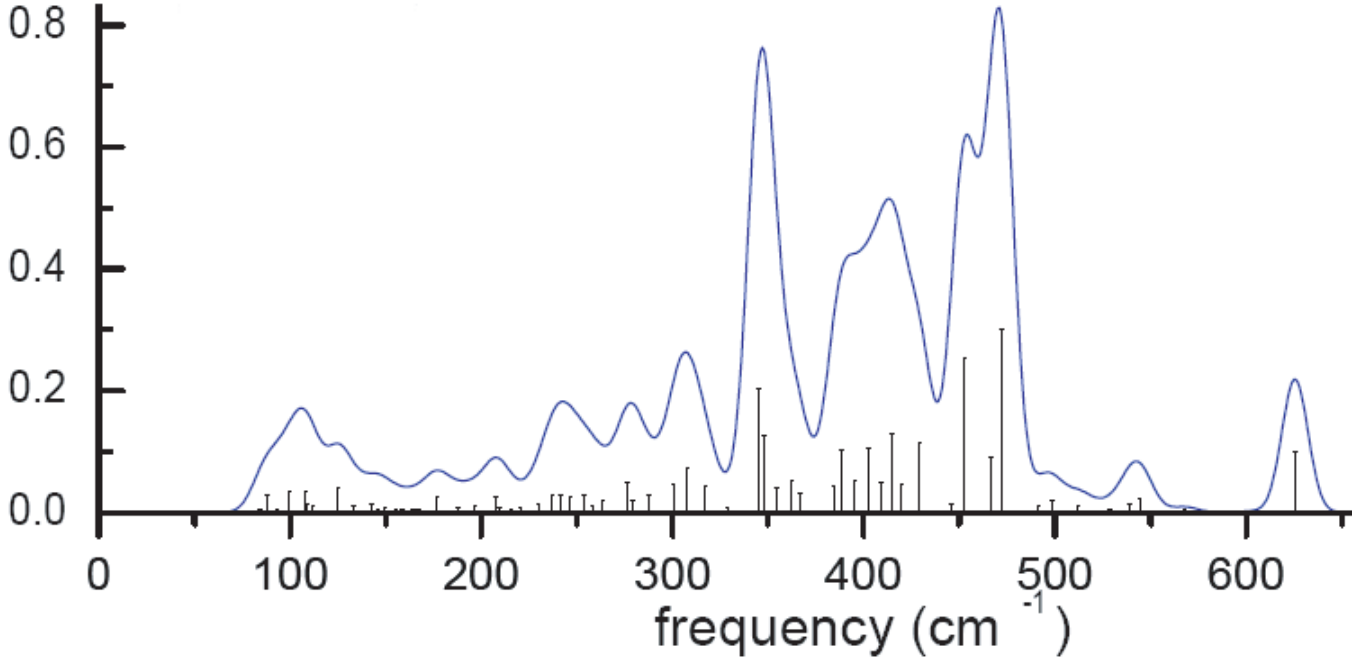
IR intensity

Atomic displacements



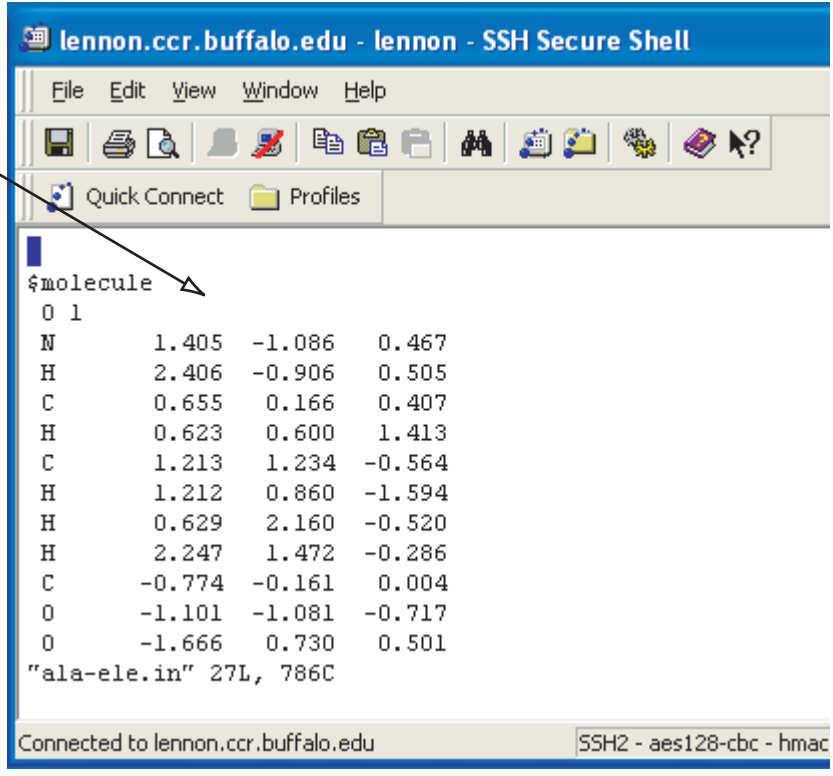
QM oscillations of alanine

IR intensity as a function
of oscillation frequency



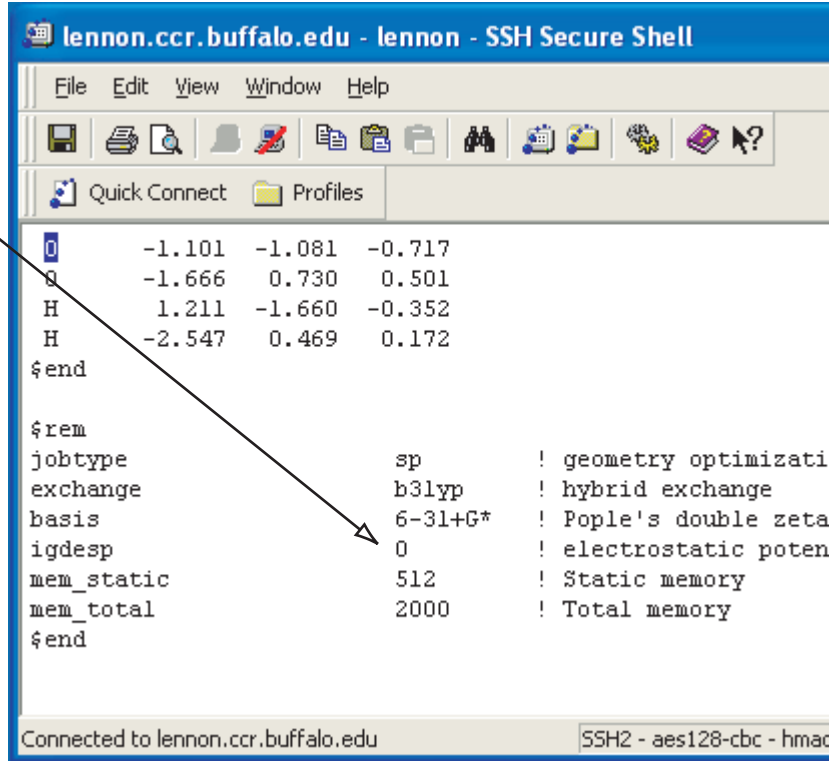
QM electrostatic potential of alanine

Copy and paste
optimal geometry



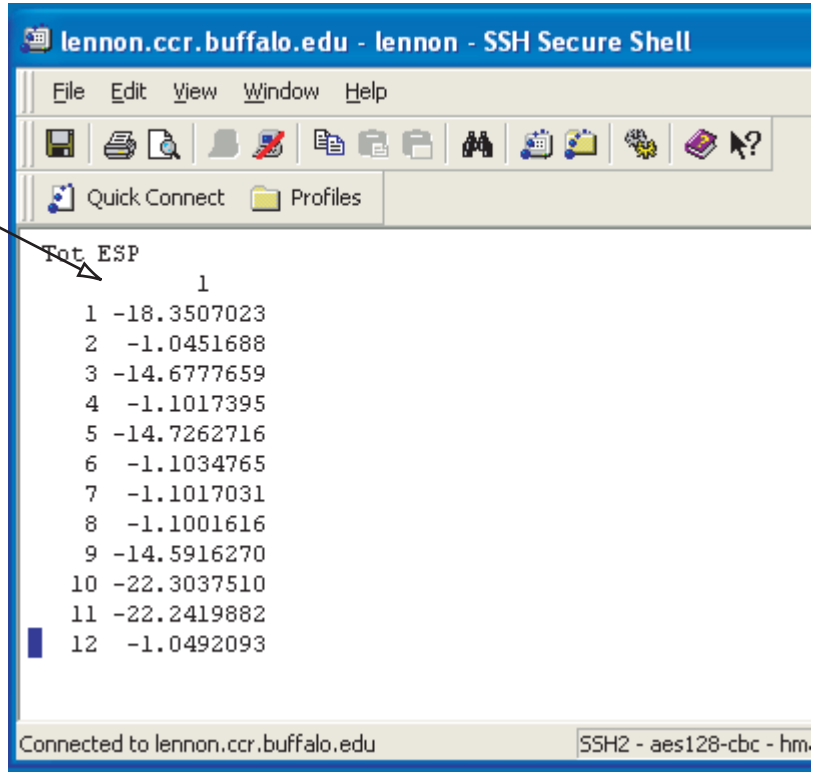
QM electrostatic potential of alanine

Electrostatic potential at the atomic positions



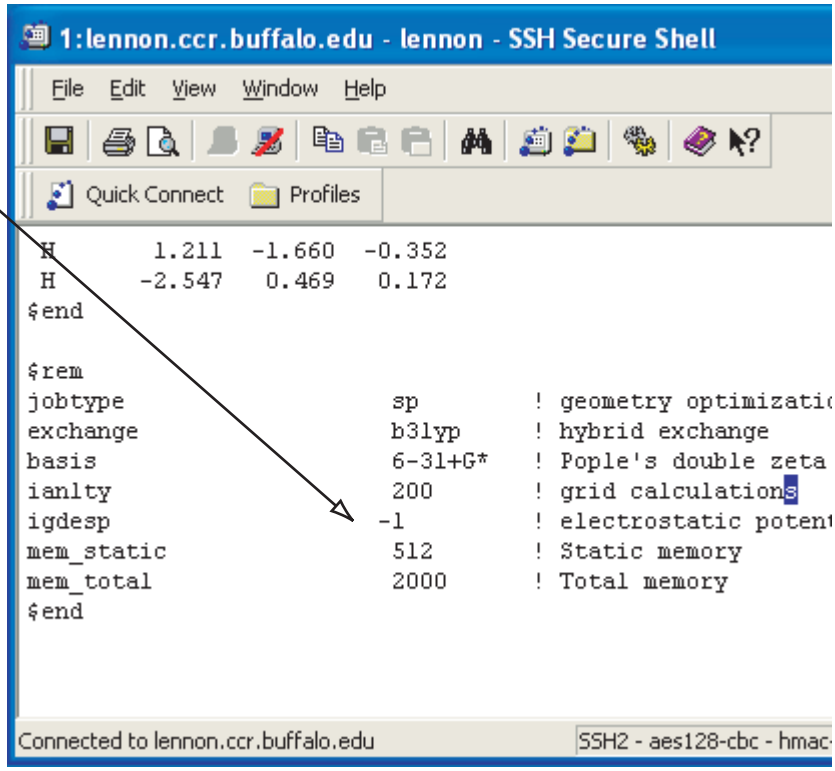
QM electrostatic potential of alanine

Final values of the electrostatic potential at the atomic positions



QM electrostatic potential of alanine

Electrostatic potential at the grid points

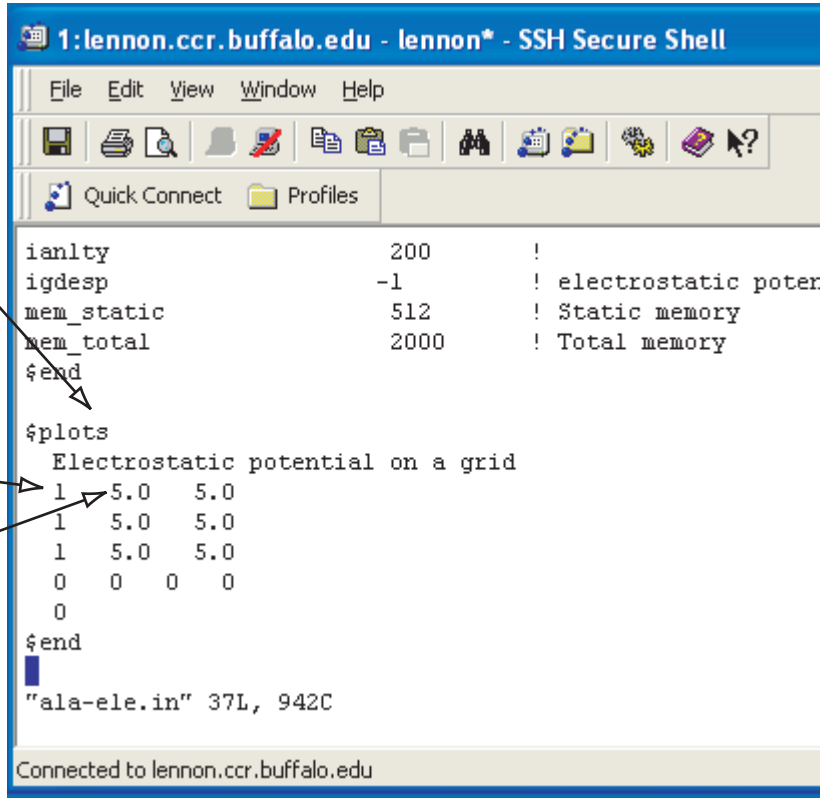


QM electrostatic potential of alanine

Definition of the grid points

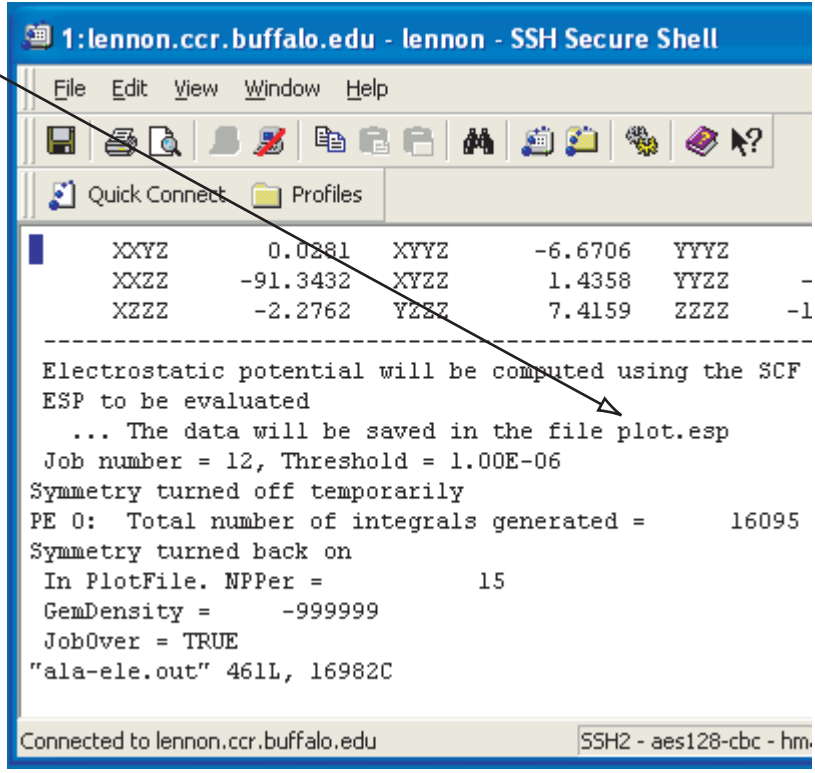
Number of grid points in the x direction

Minimum and maximum values



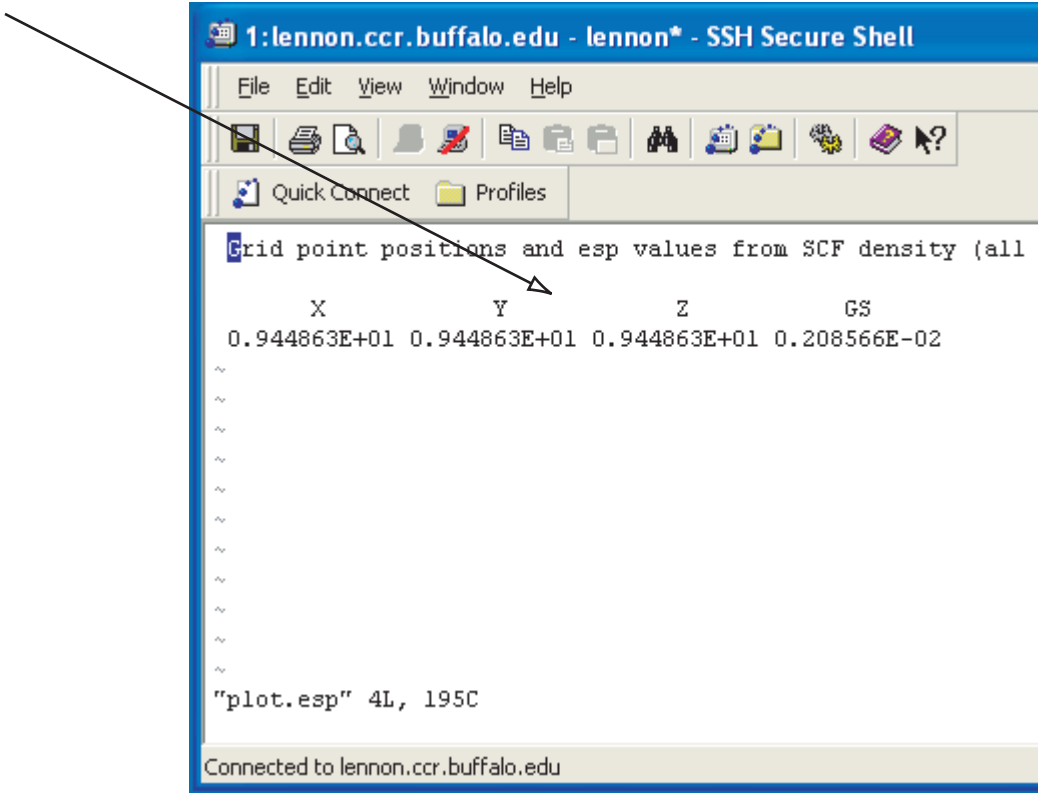
QM electrostatic potential of alanine

Results are written in the plot.esp file



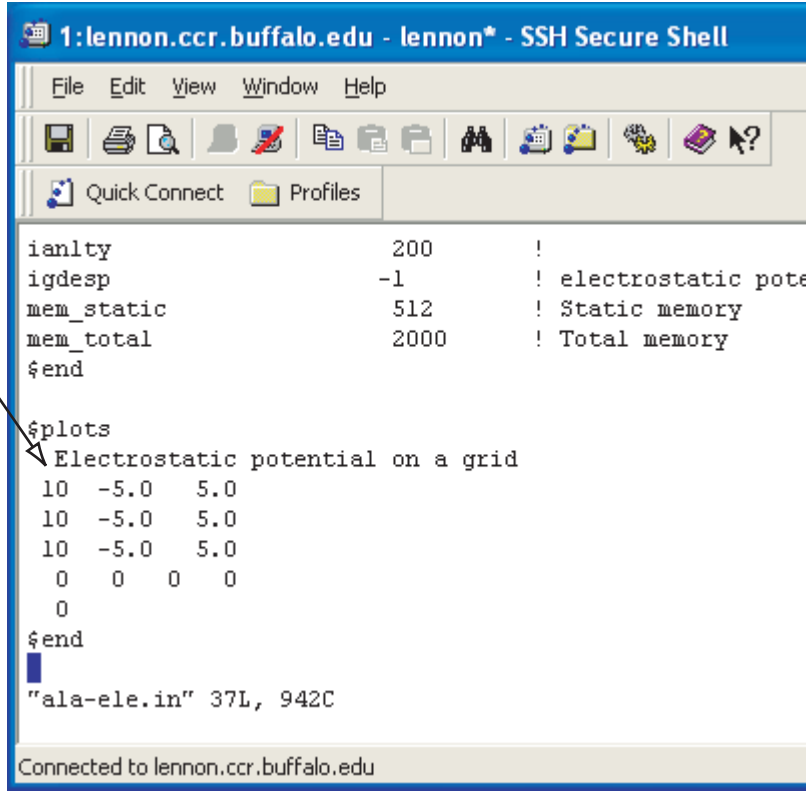
QM electrostatic potential of alanine

Electrostatic potential
at one points



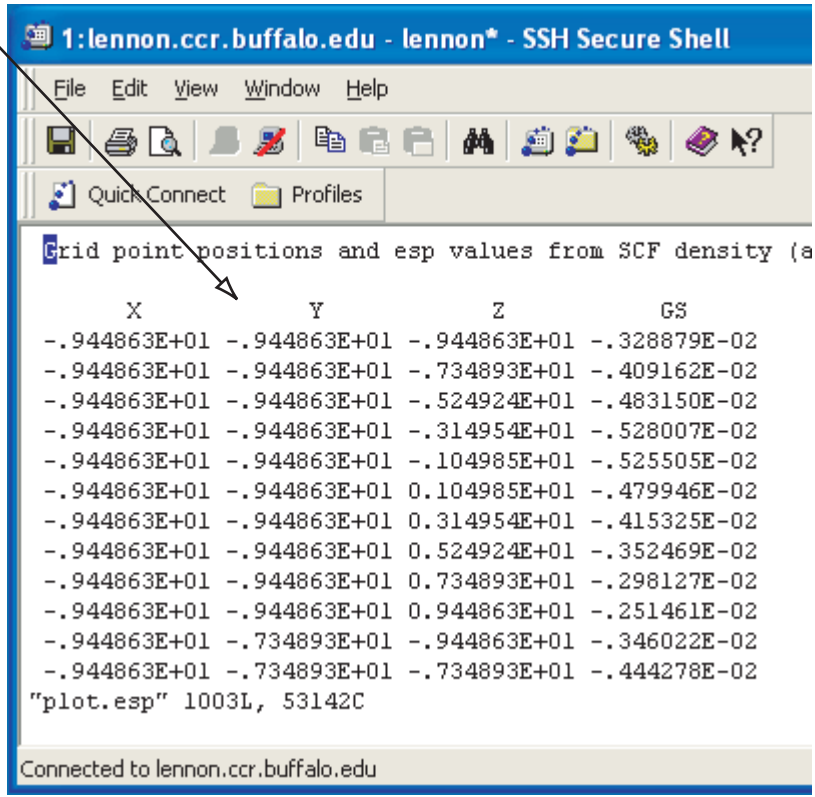
QM electrostatic potential of alanine

Three diemsional grid definition



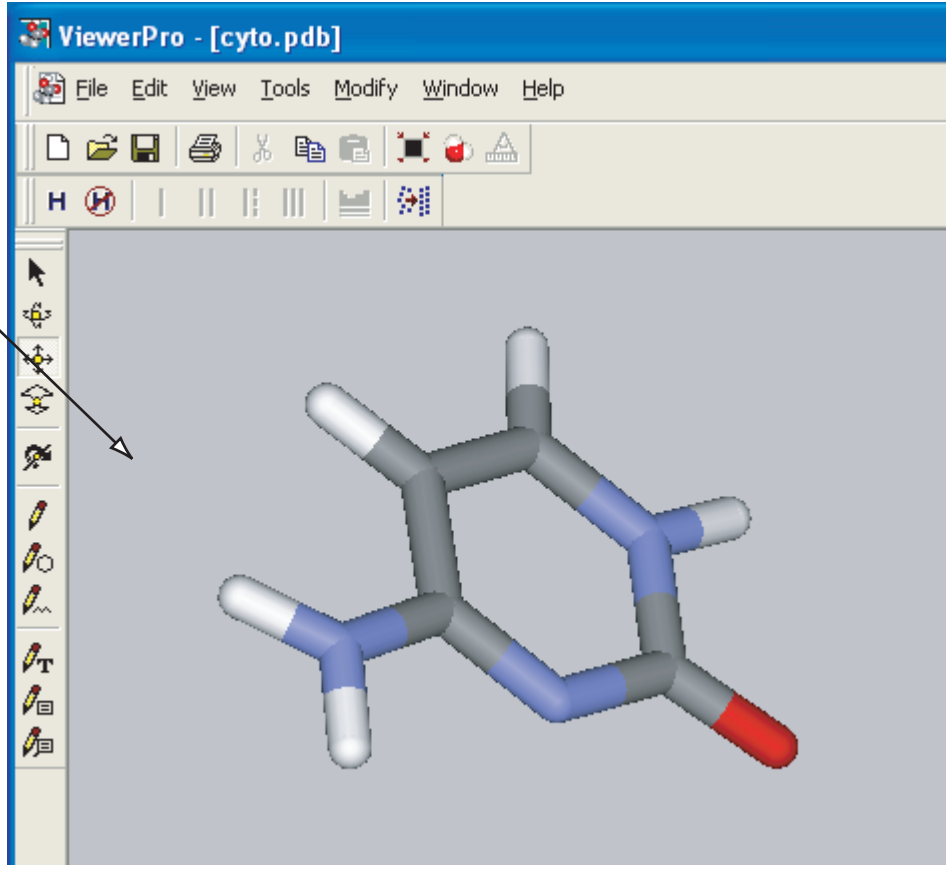
QM electrostatic potential of alanine

Results of electrostatic potential grid calculations



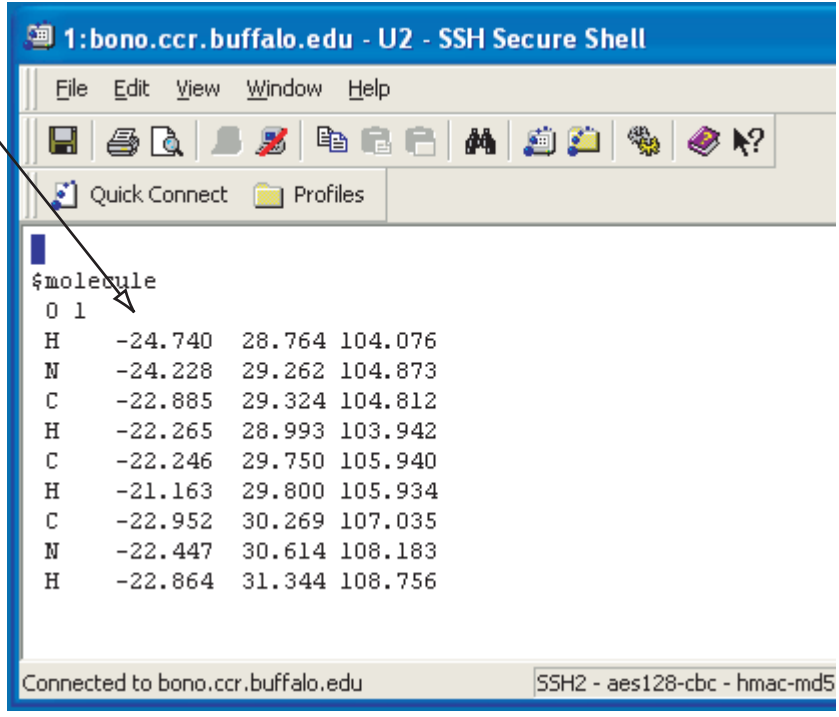
QM geometry optimization of cytosine

Initial geometry of cytosine



QM geometry optimization of cytosine

Initial geometry of cytosine



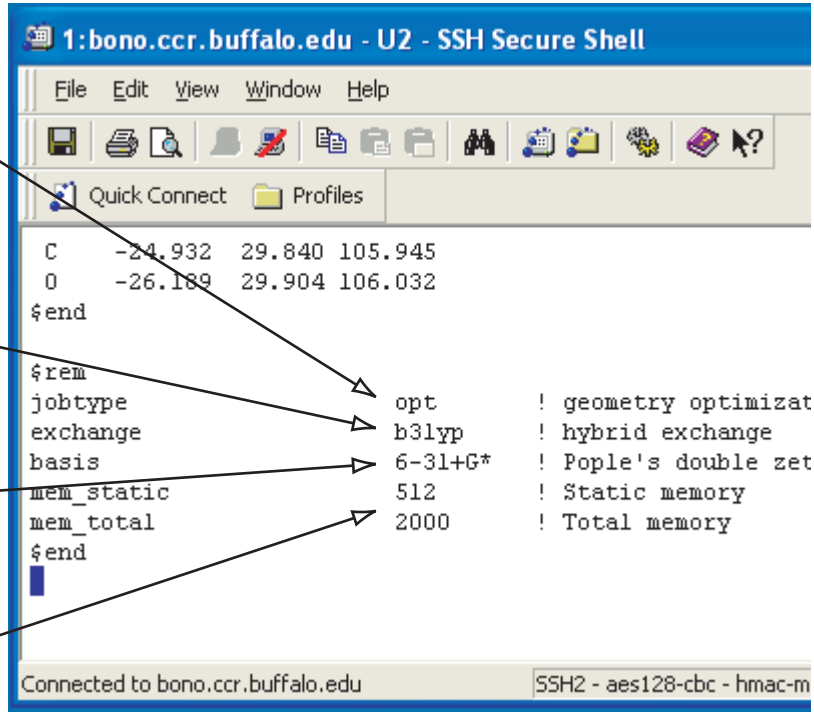
QM geometry optimization of cytosine

Geometry optimization

Hamiltionian

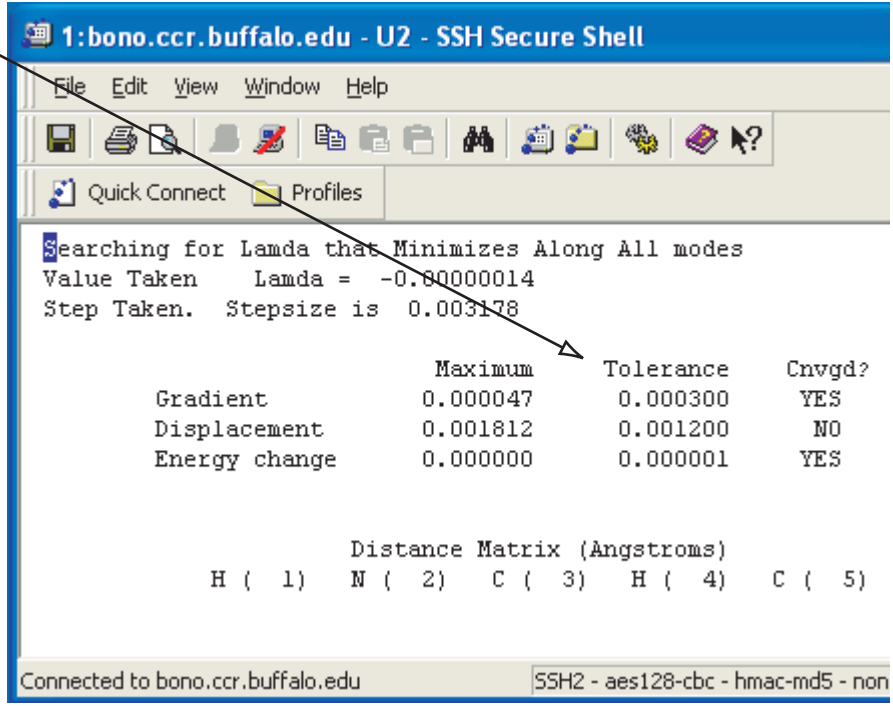
Basis set

Memory allocation



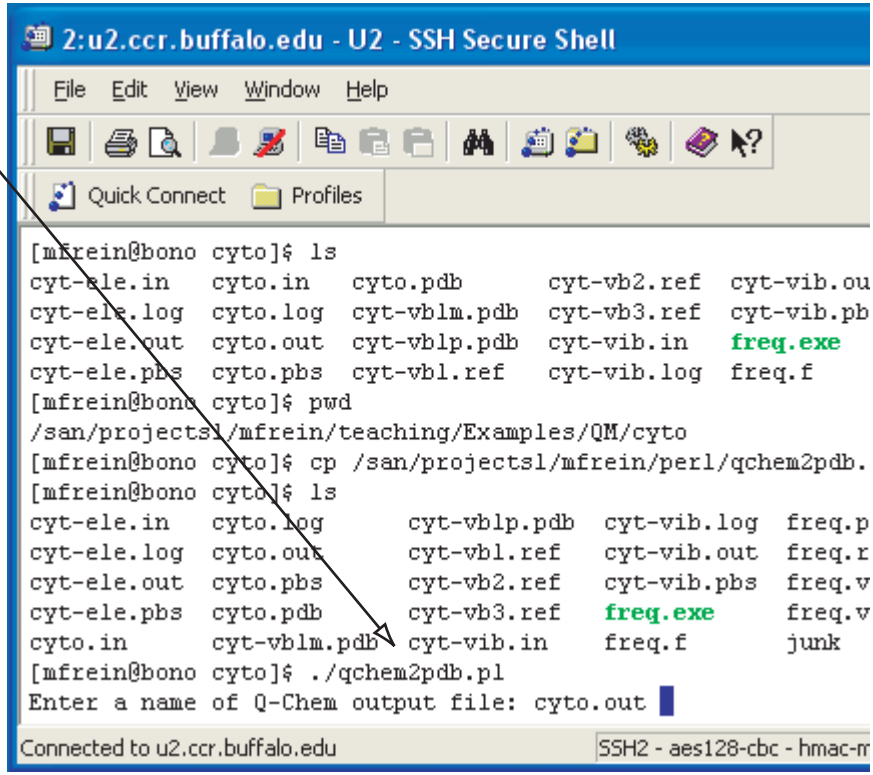
QM geometry optimization of cytosine

Geometry optimization
is converged



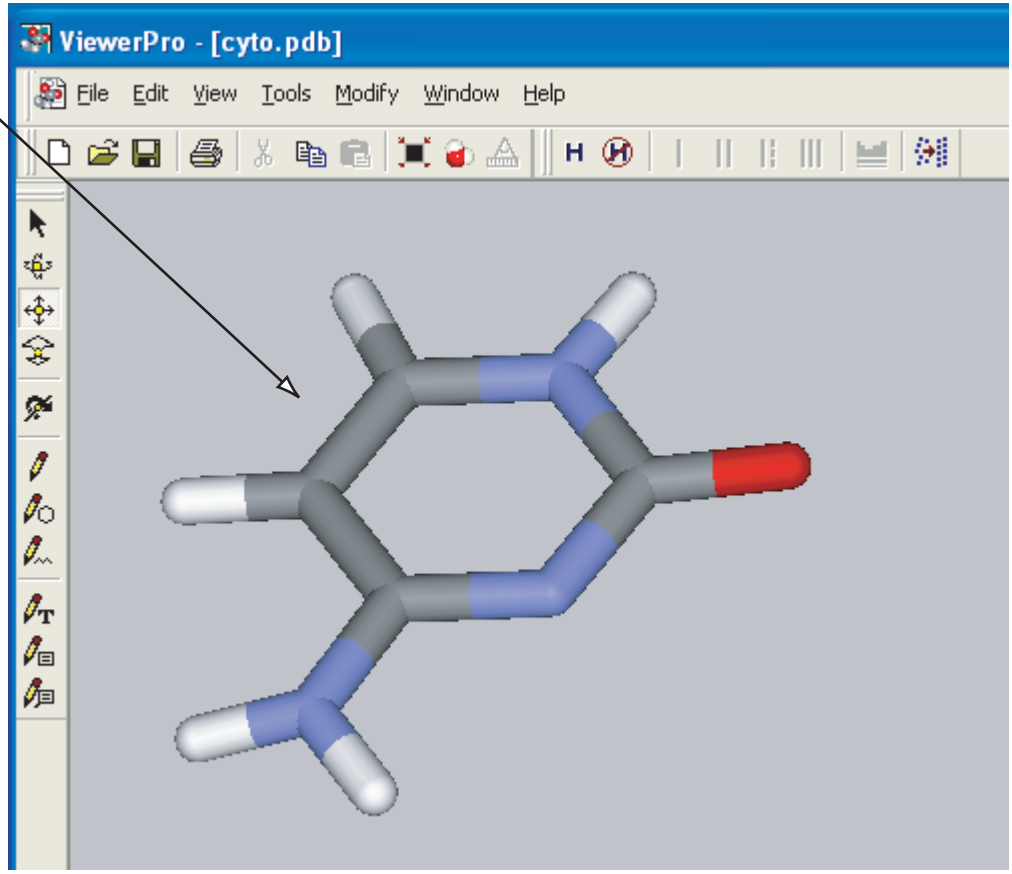
QM geometry optimization of cytosine

Converting qchem output into a PDB file



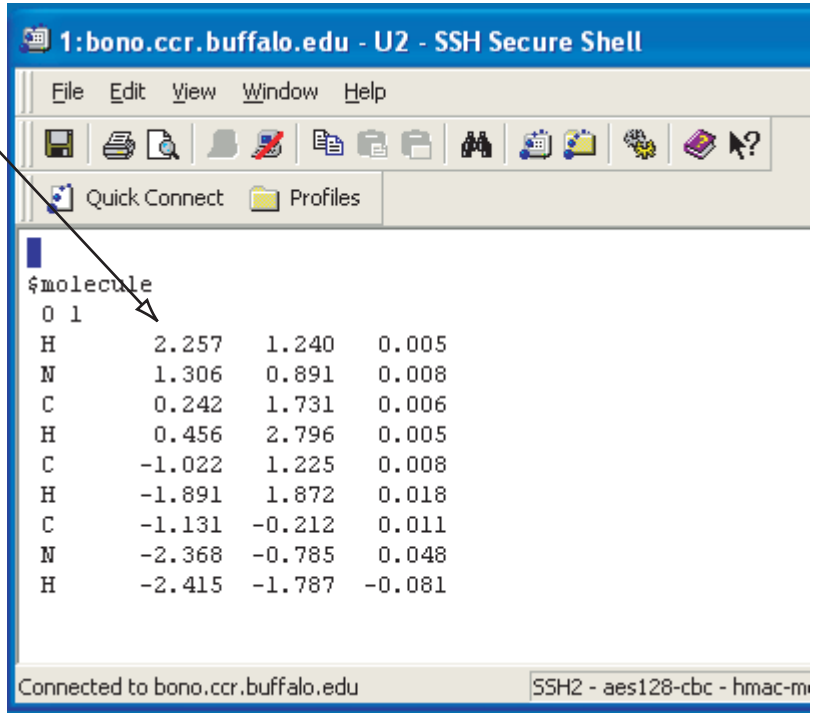
QM geometry optimization of cytosine

Final geometry of cytosine

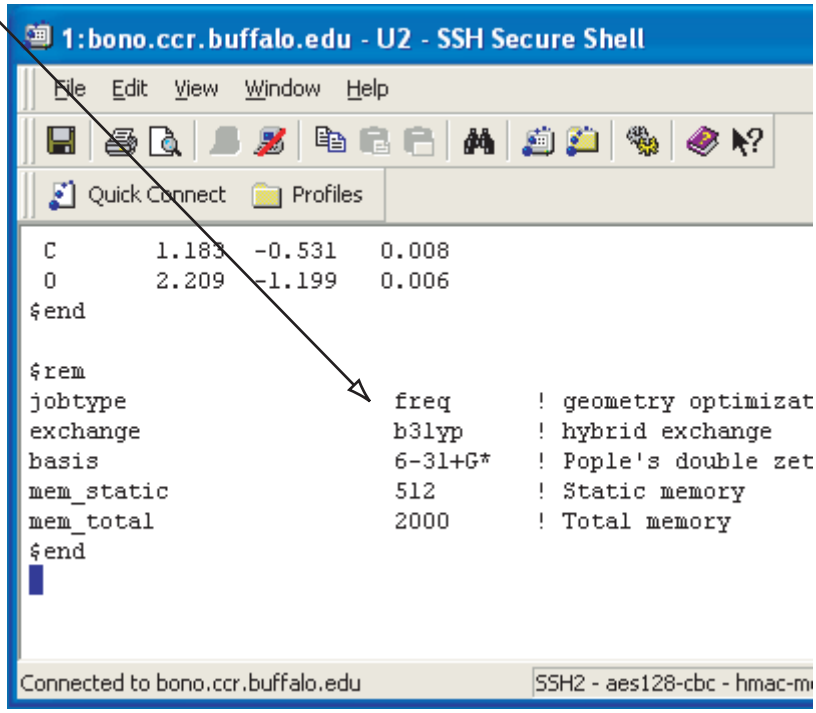


QM molecular oscillations of cytosine

Coordinates after
geometry optimization

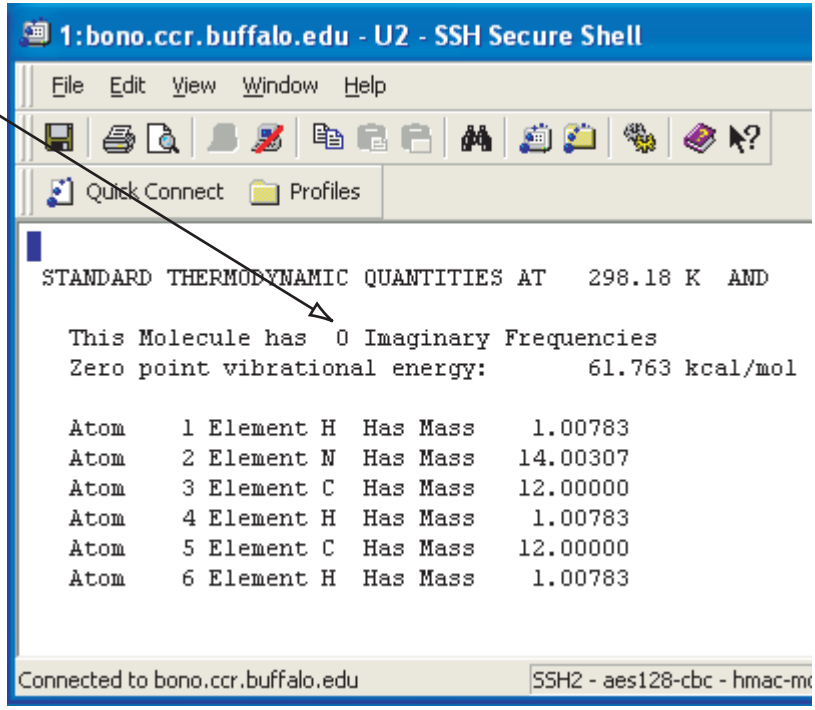


Frequency calculations



QM molecular oscillations of cytosine

Calculations are finished correctly

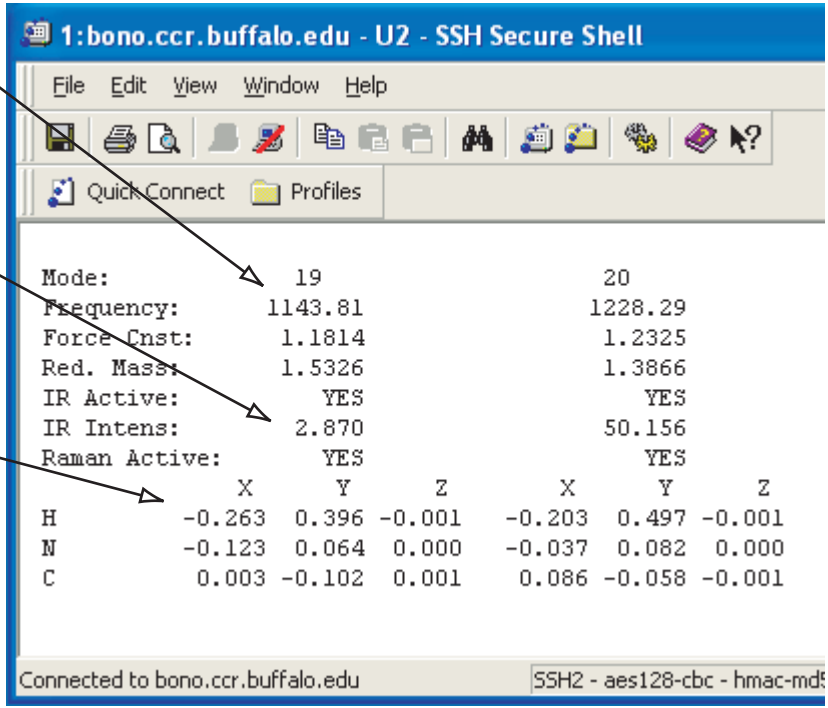


QM molecular oscillations of cytosine

Frequency (cm-1)

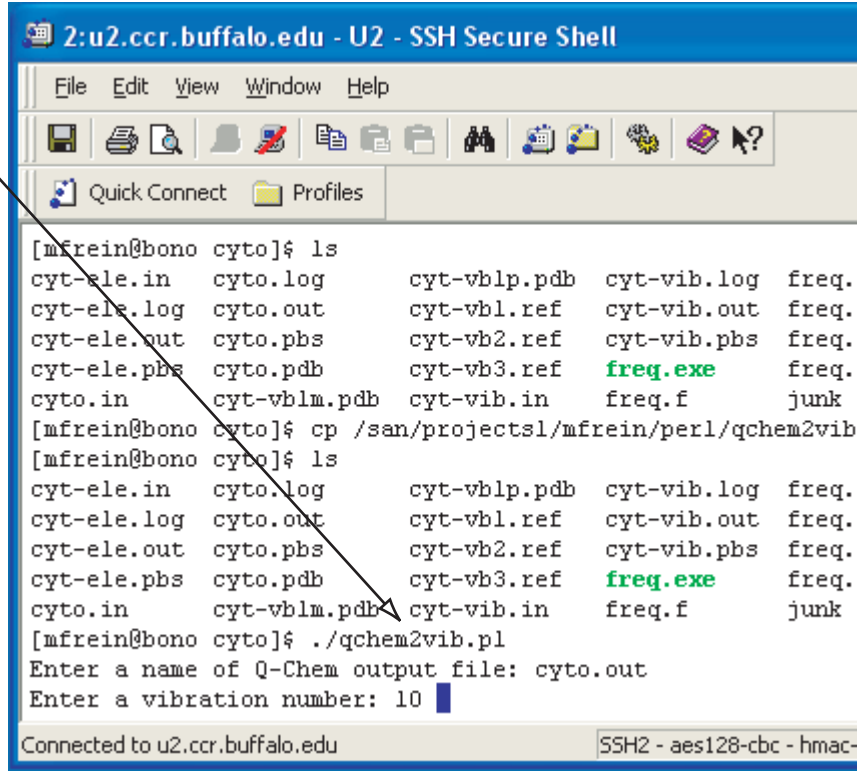
IR Intensity

Atomic displacements



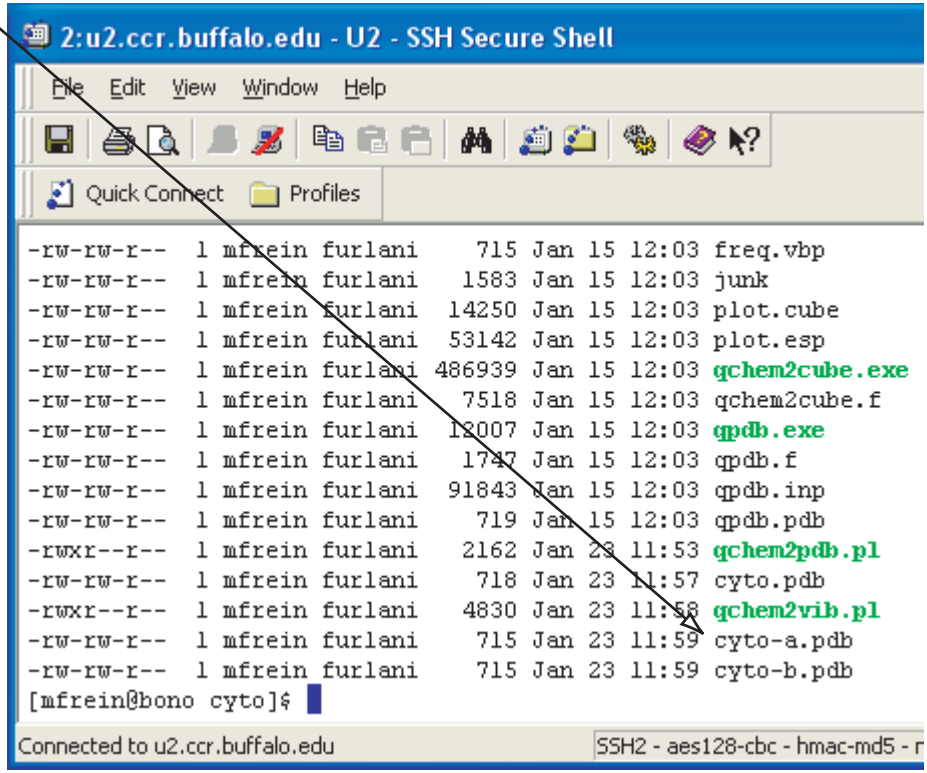
QM molecular oscillations of cytosine

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



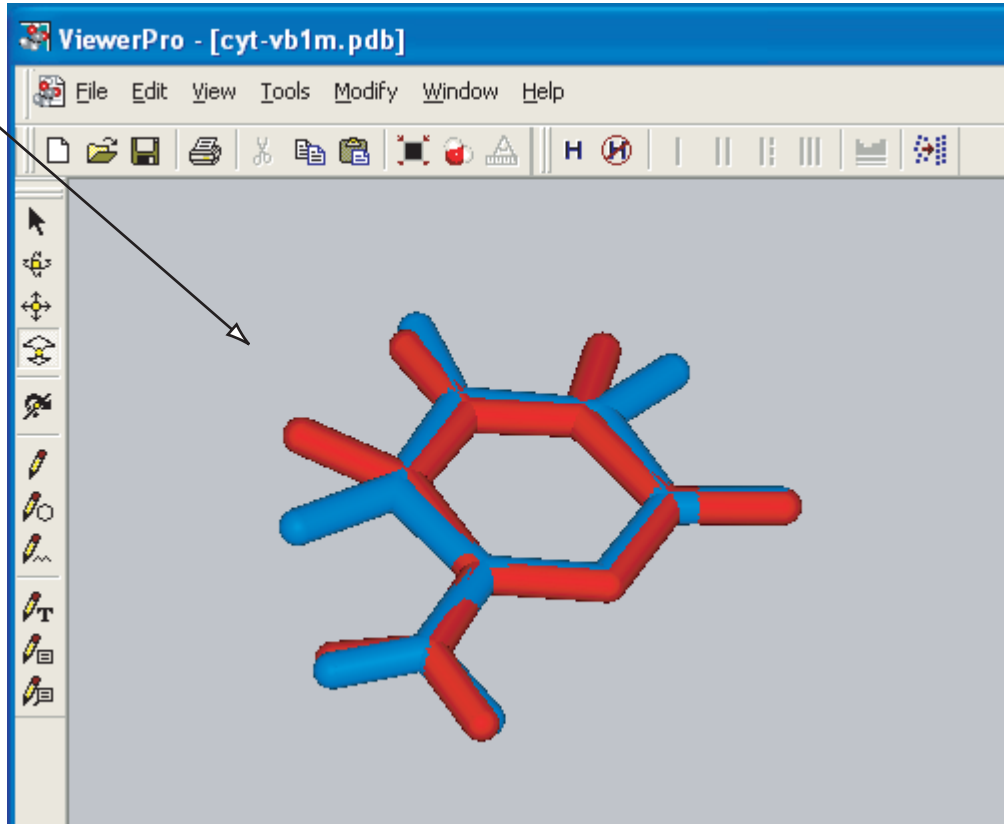
QM molecular oscillations of cytosine

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



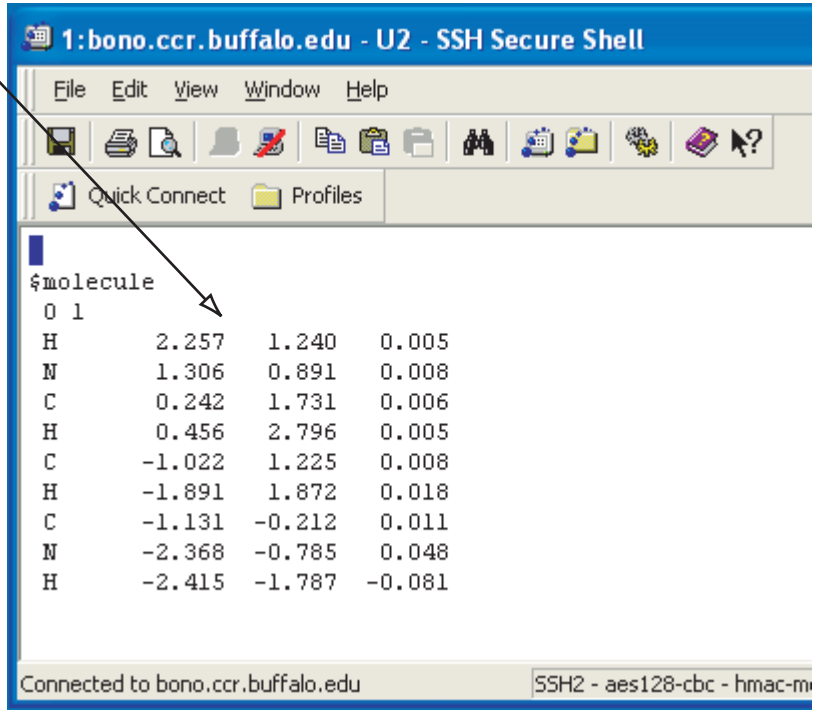
QM molecular oscillations of cytosine

Visualization of the molecular oscillation



QM electrostatic potential of cytosine

Optimal coordinates after geometry optimization

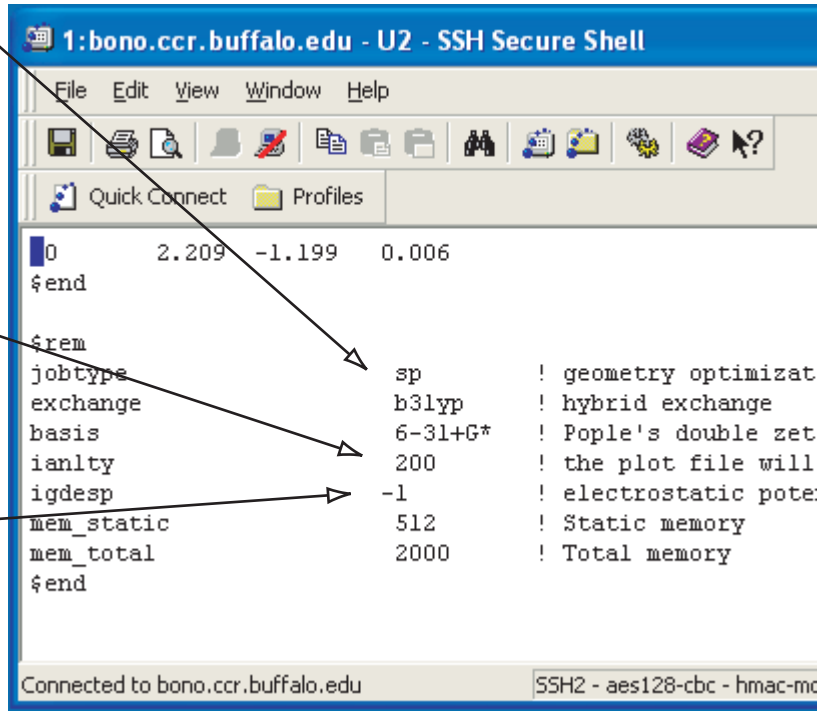


QM electrostatic potential of cytosine

Single point calculations
(no geometry optimization)

Generating the
plot file

Generating the
electrostatic
potential

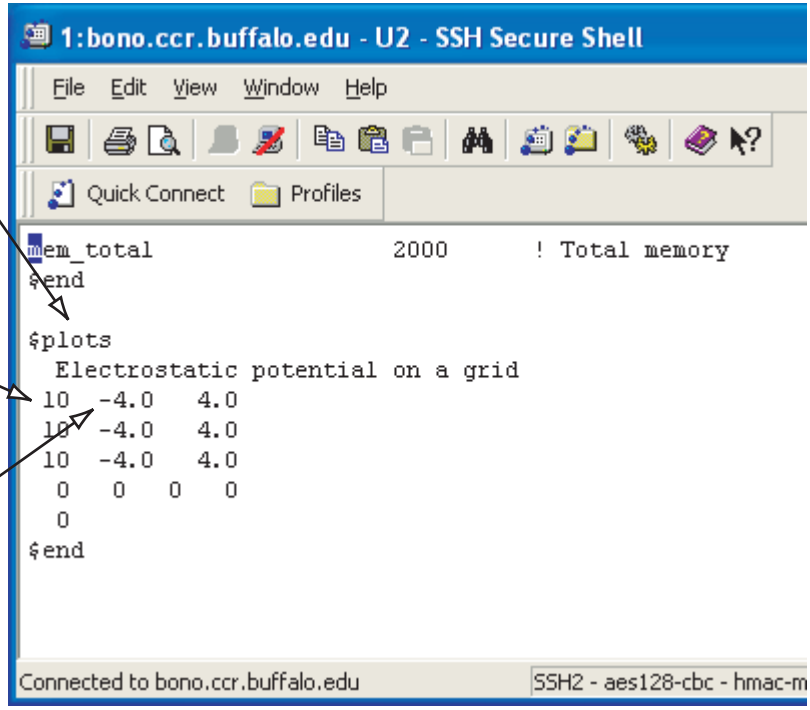


QM electrostatic potential of cytosine

Details of the plot calculations

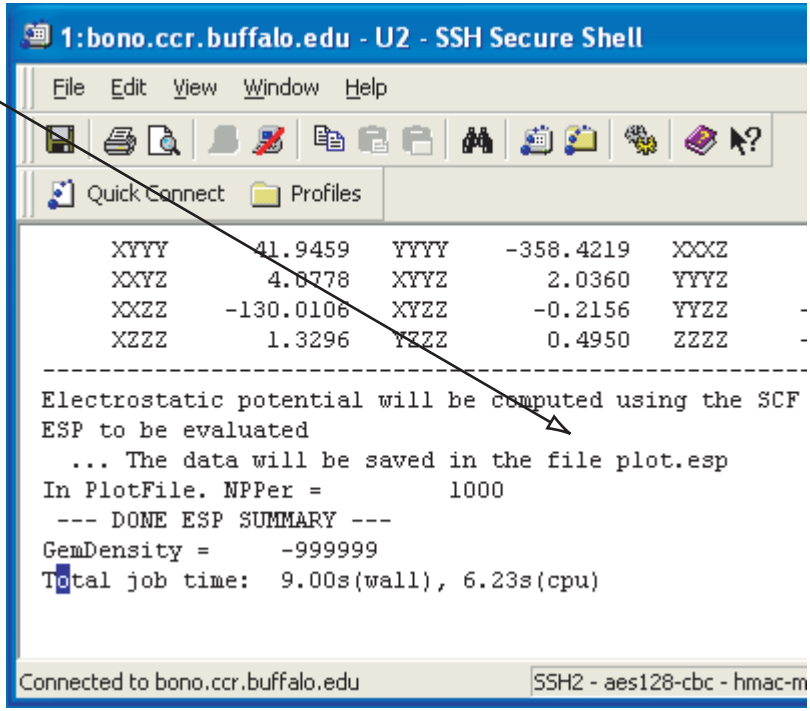
Number of points in the x direction

Minimum and maximum values of the grid in the x direction



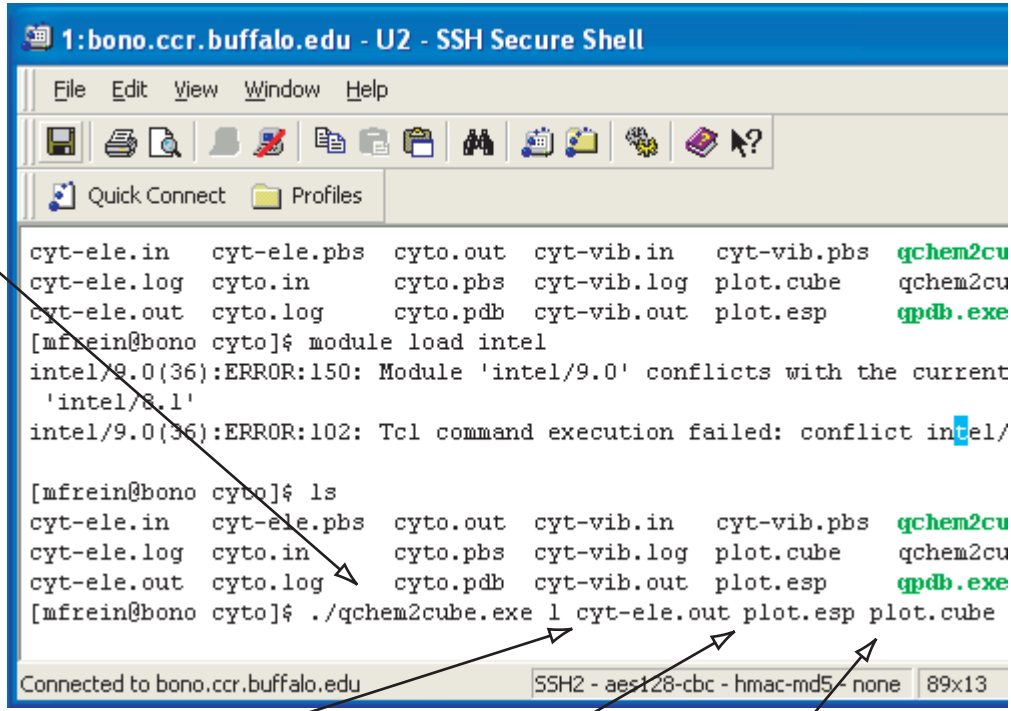
QM electrostatic potential of cytosine

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



QM electrostatic potential of cytosine

Executing the converting program



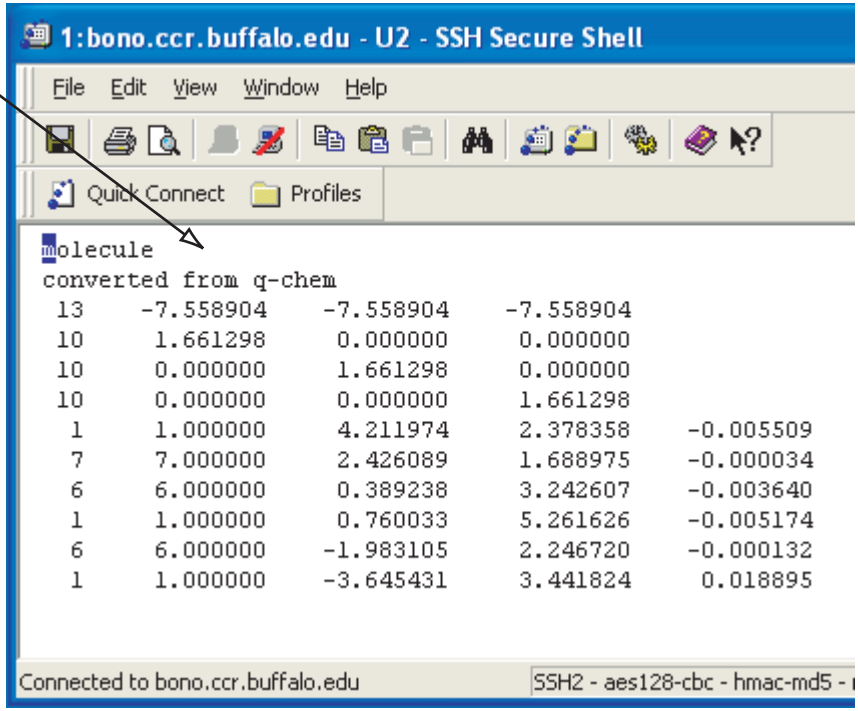
Output from qchem

Plot file from qchem

Cube file

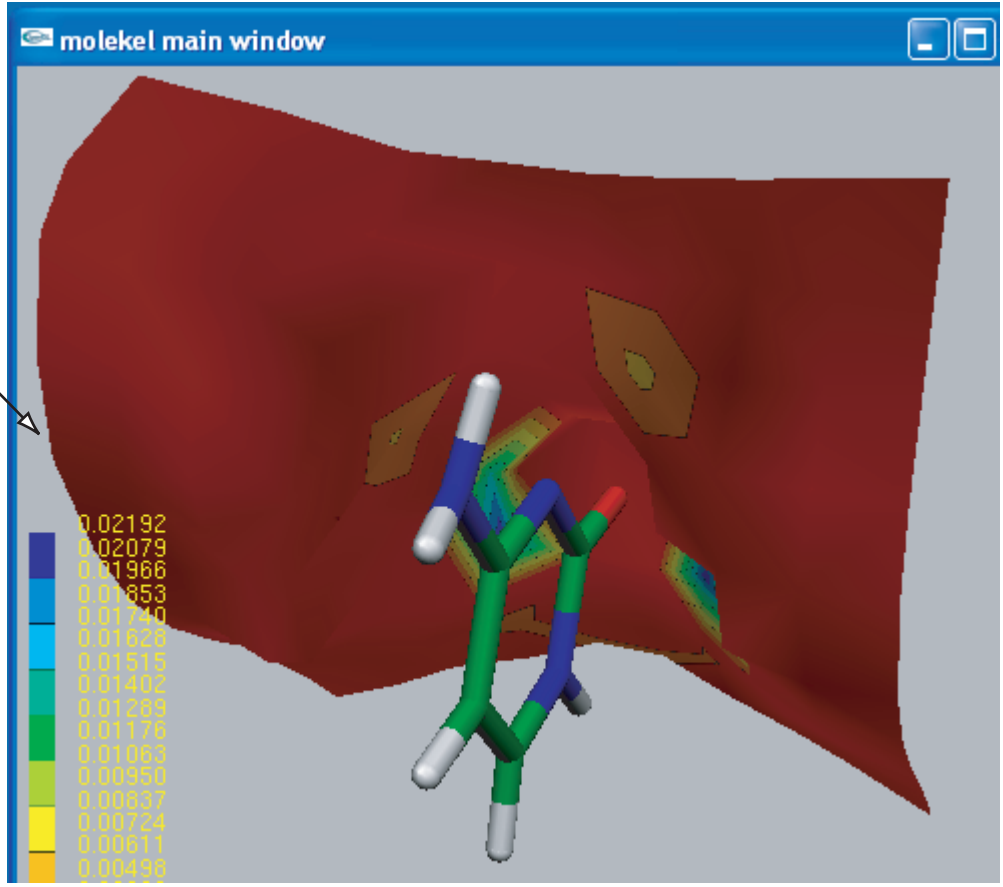
QM electrostatic potential of cytosine

Cube file



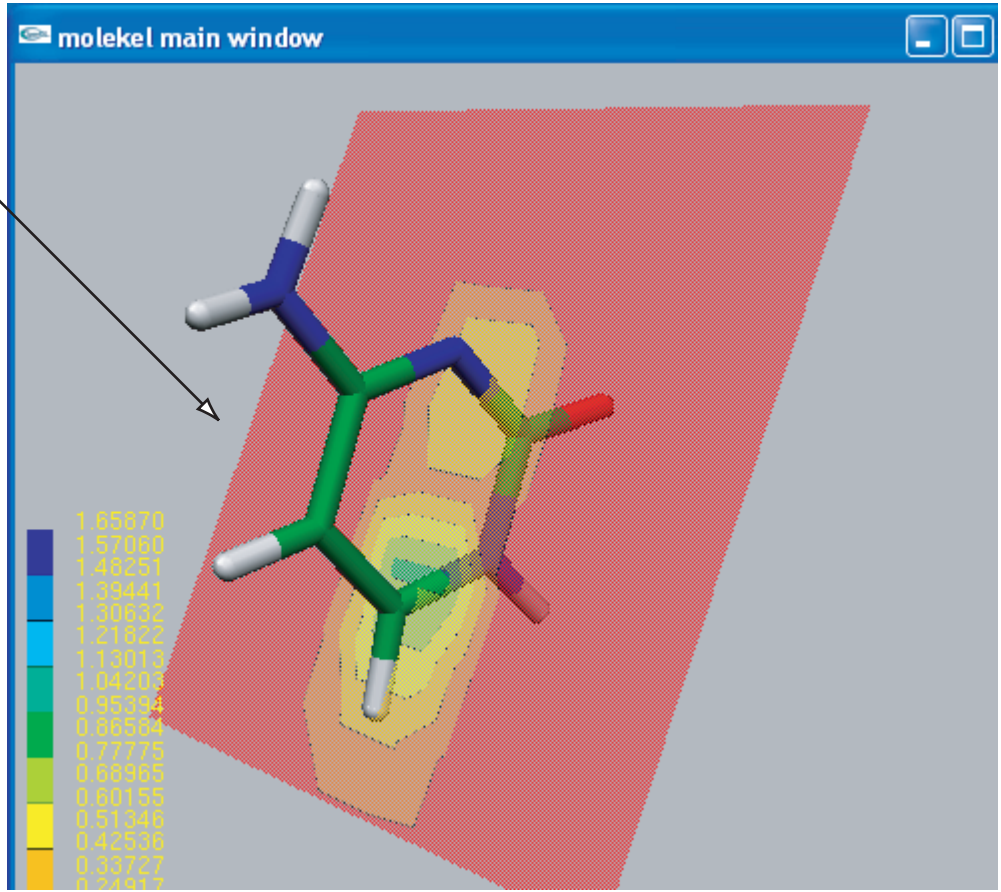
QM electrostatic potential of cytosine

Visualization of the electrostatic potential using the Molekel program



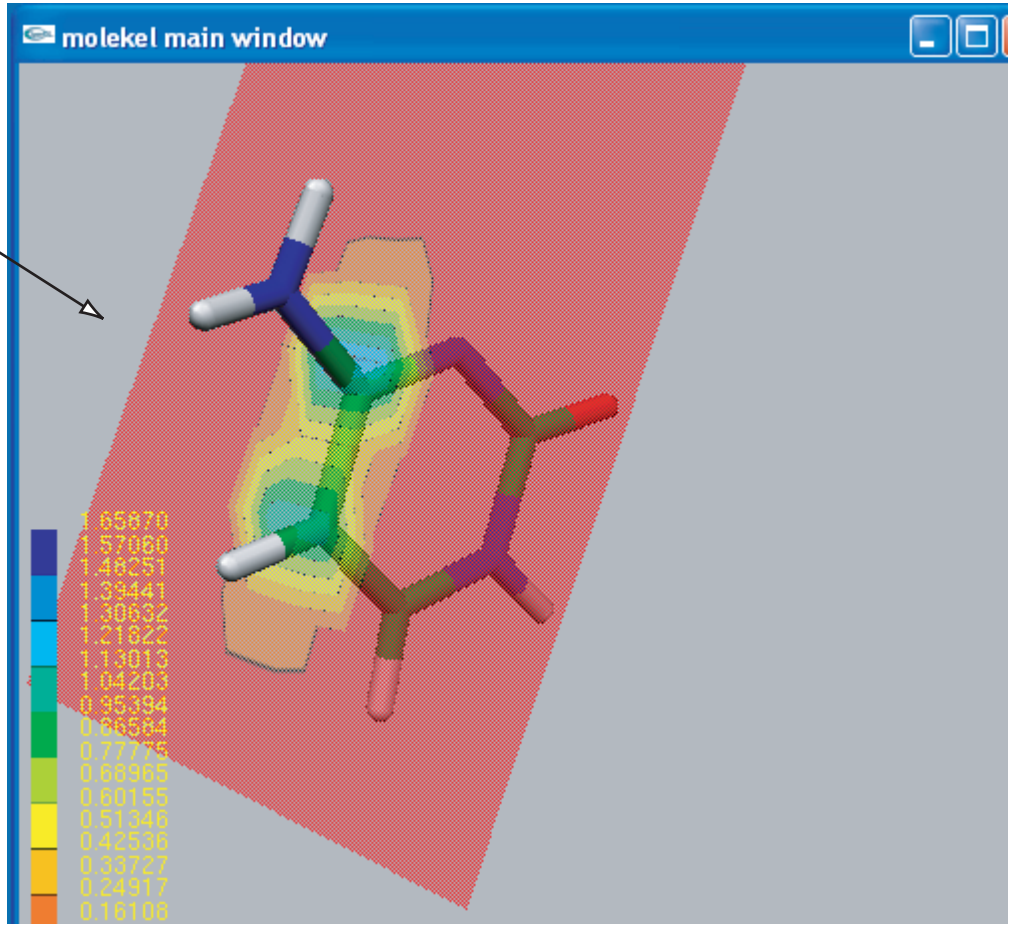
QM electrostatic potential of cytosine

Plane cut through the electrostatic potential



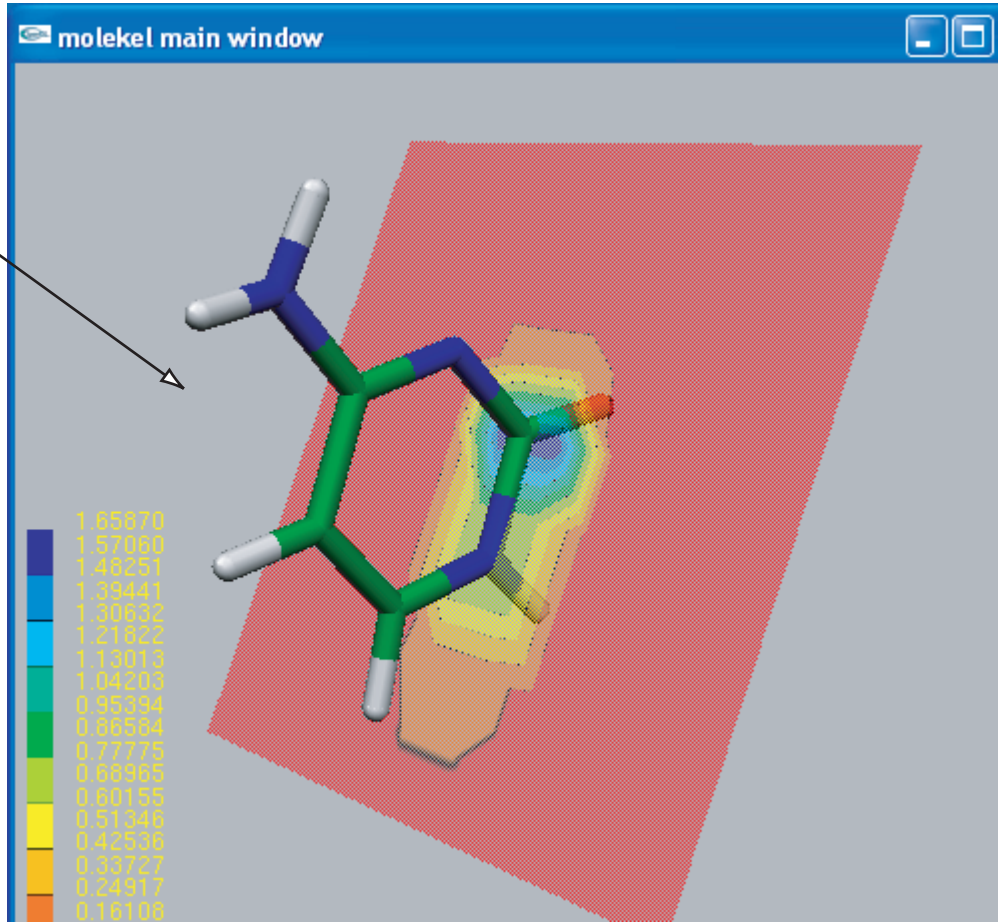
QM electrostatic potential of cytosine

Plane cut through the electrostatic potential



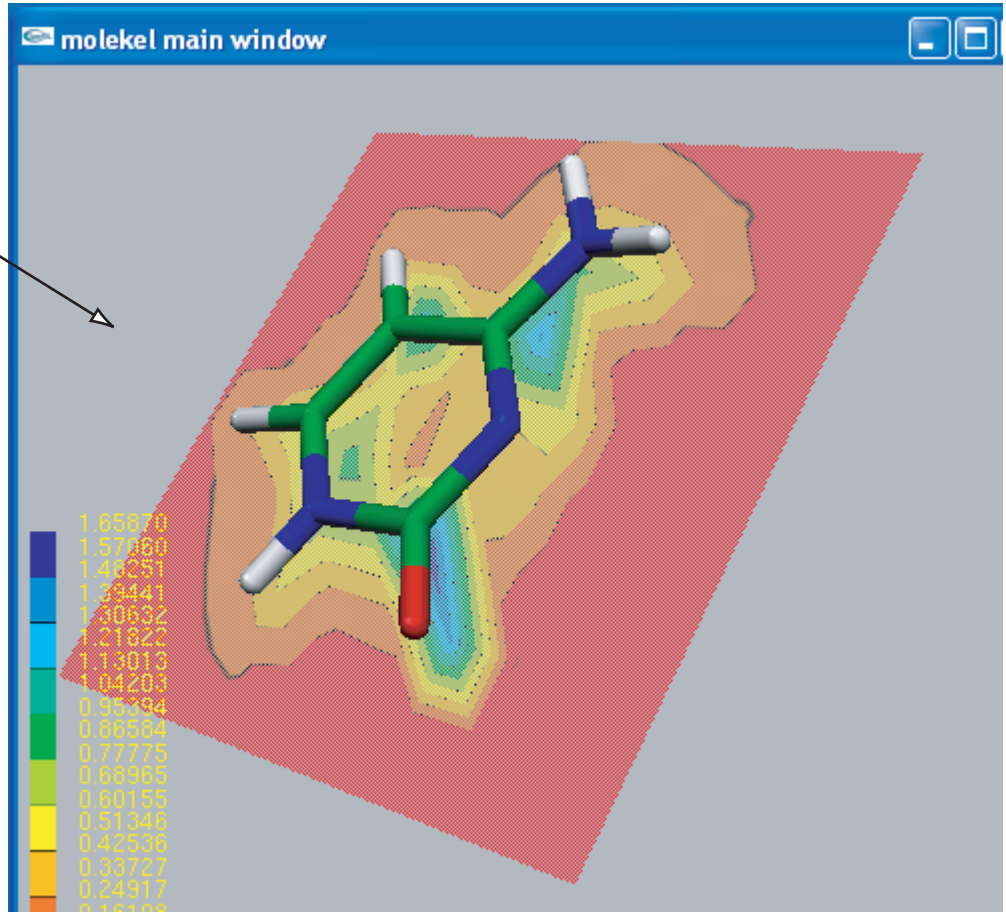
QM electrostatic potential of cytosine

Plane cut through the electrostatic potential



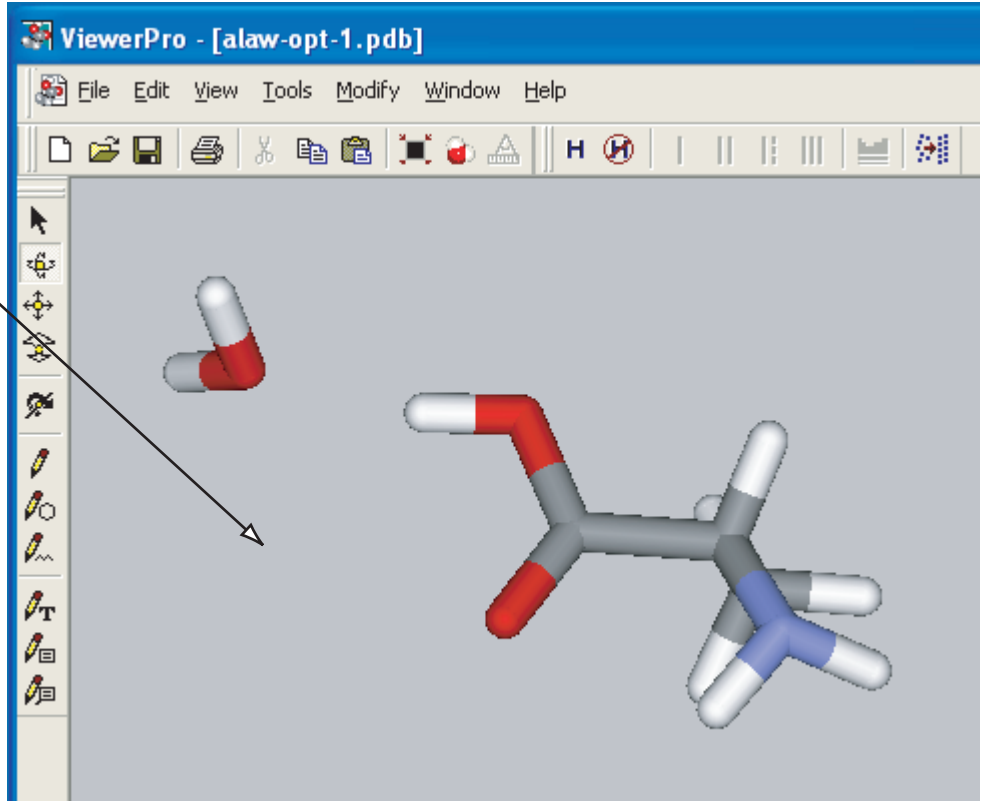
QM electrostatic potential of cytosine

Plane cut through the electrostatic potential



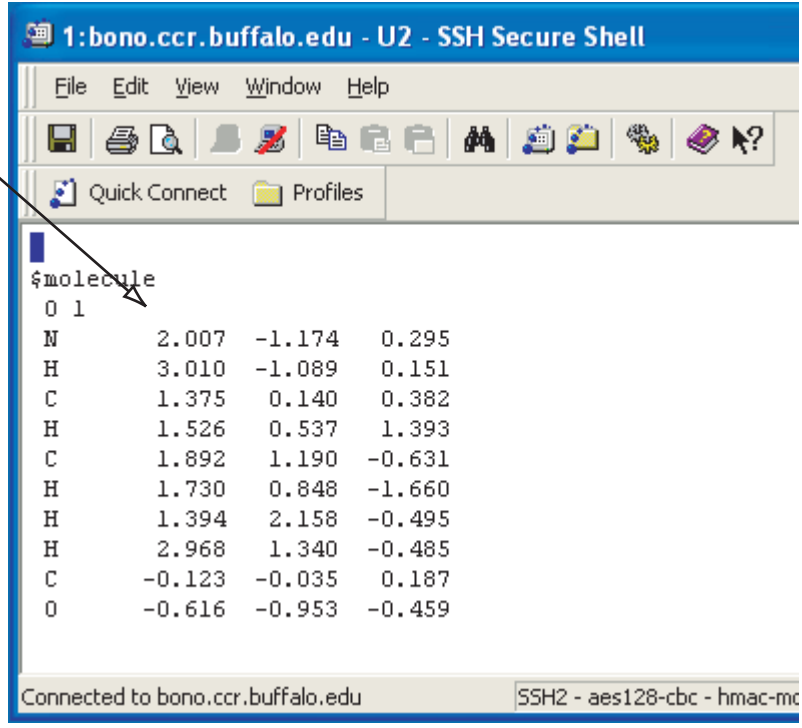
QM geometry optimization of alanine and water

Initial geometry of an alanine and water dimer



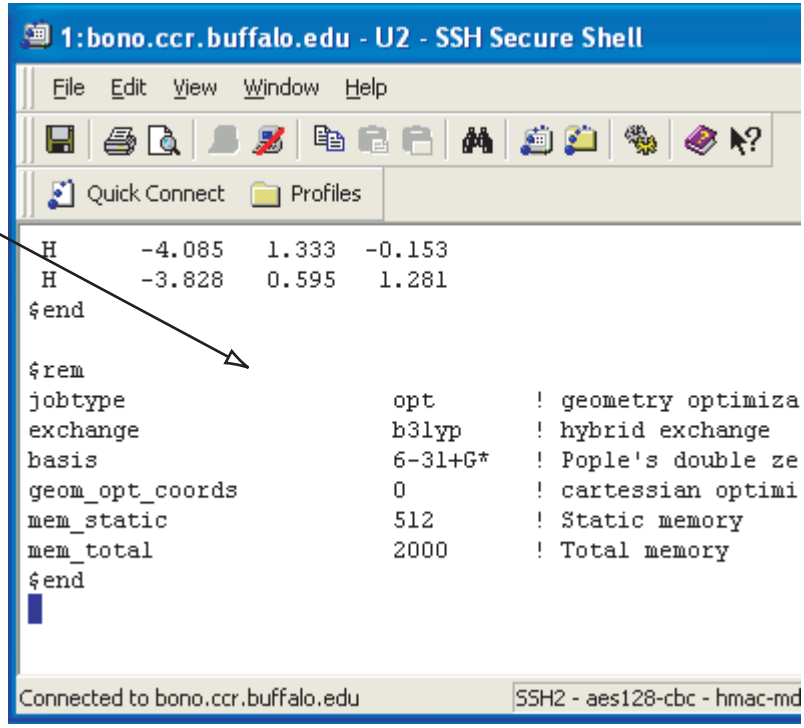
QM geometry optimization of alanine and water

Initial coordinates of the dimer



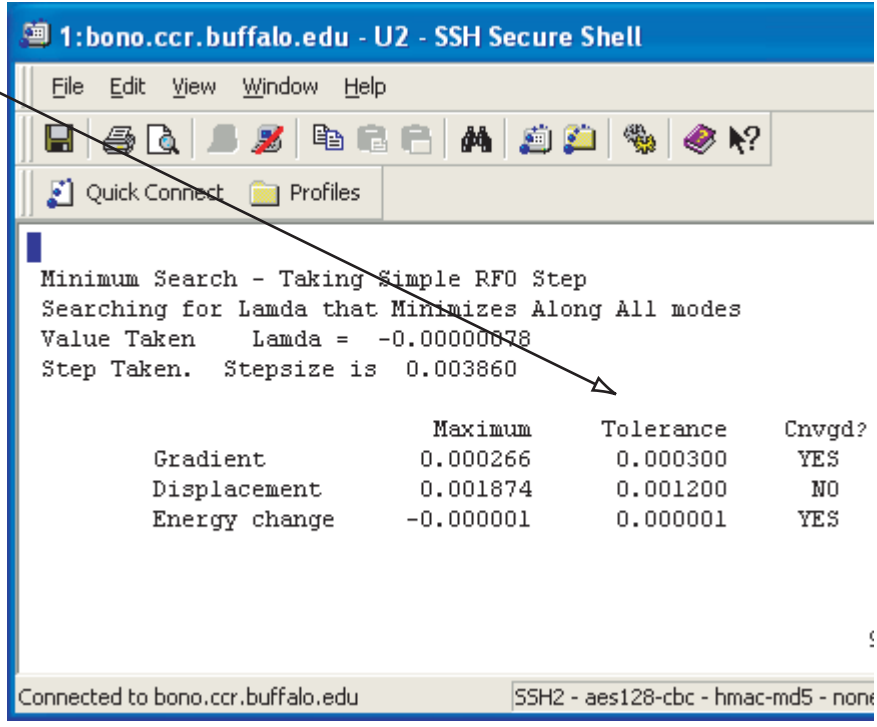
QM geometry optimization of alanine and water

Geometry optimization using cartessian coordinates



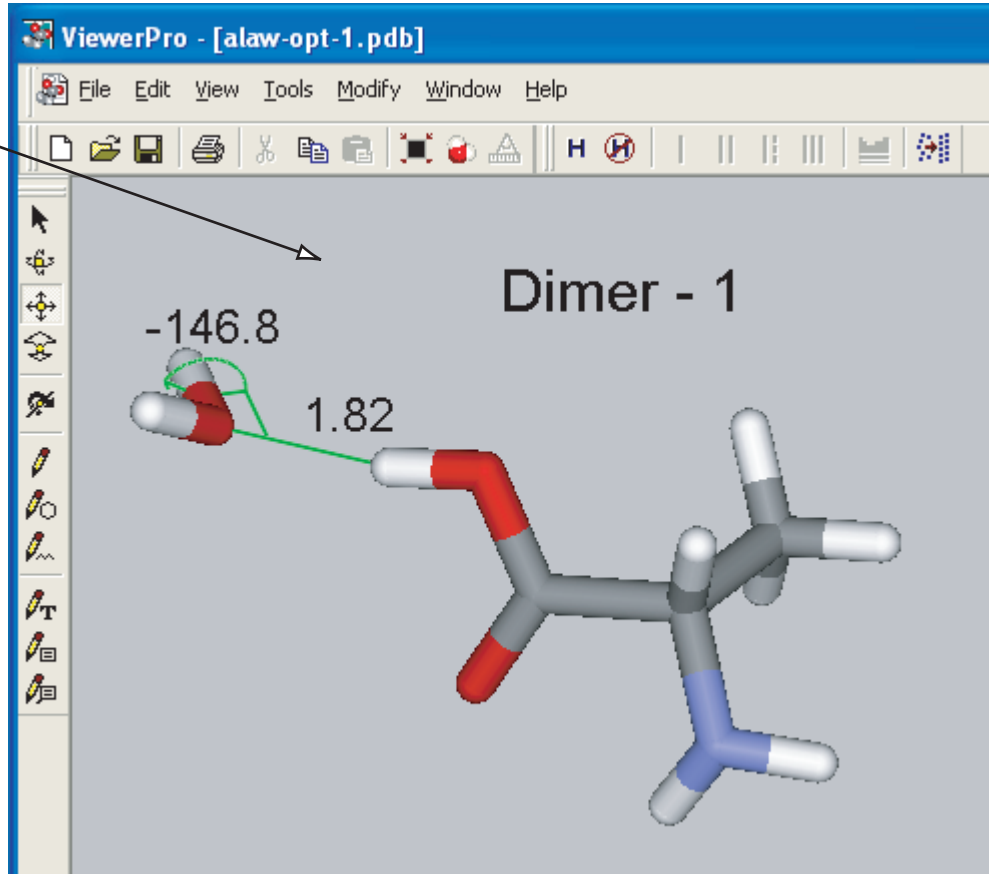
QM geometry optimization of alanine and water

Optimization converged



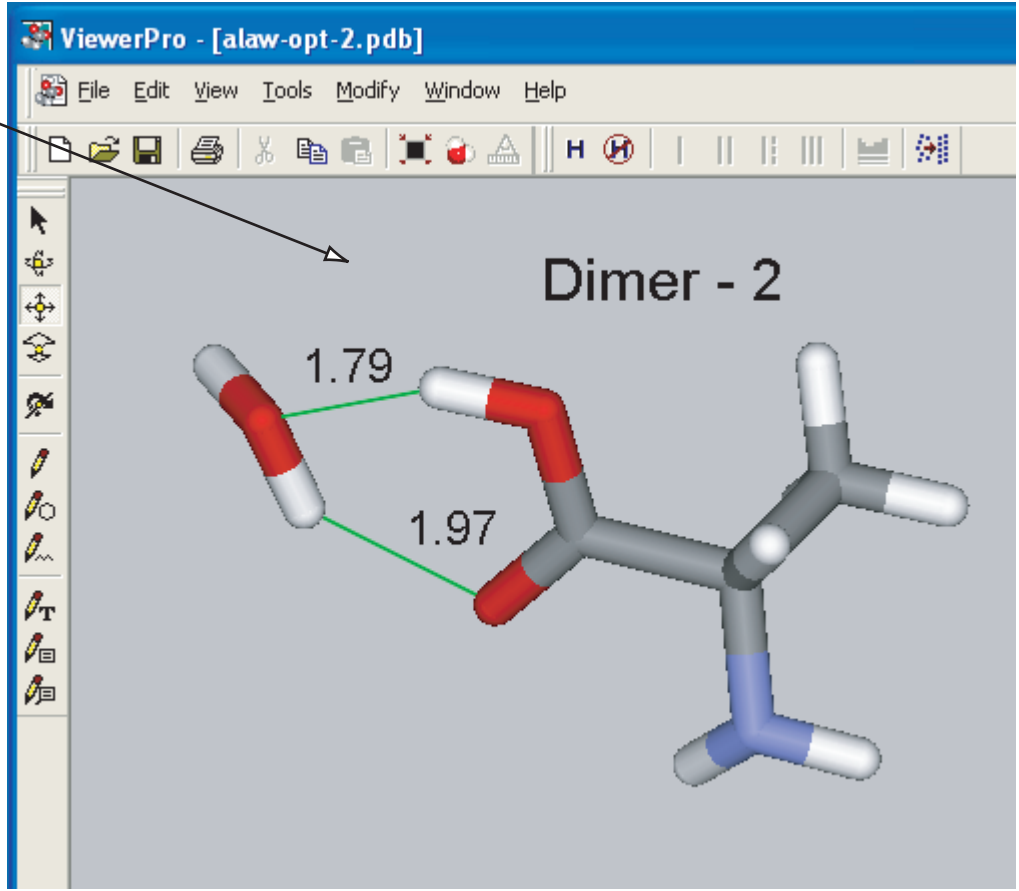
QM geometry optimization of alanine and water

Geometrical parameters of the dimer -1



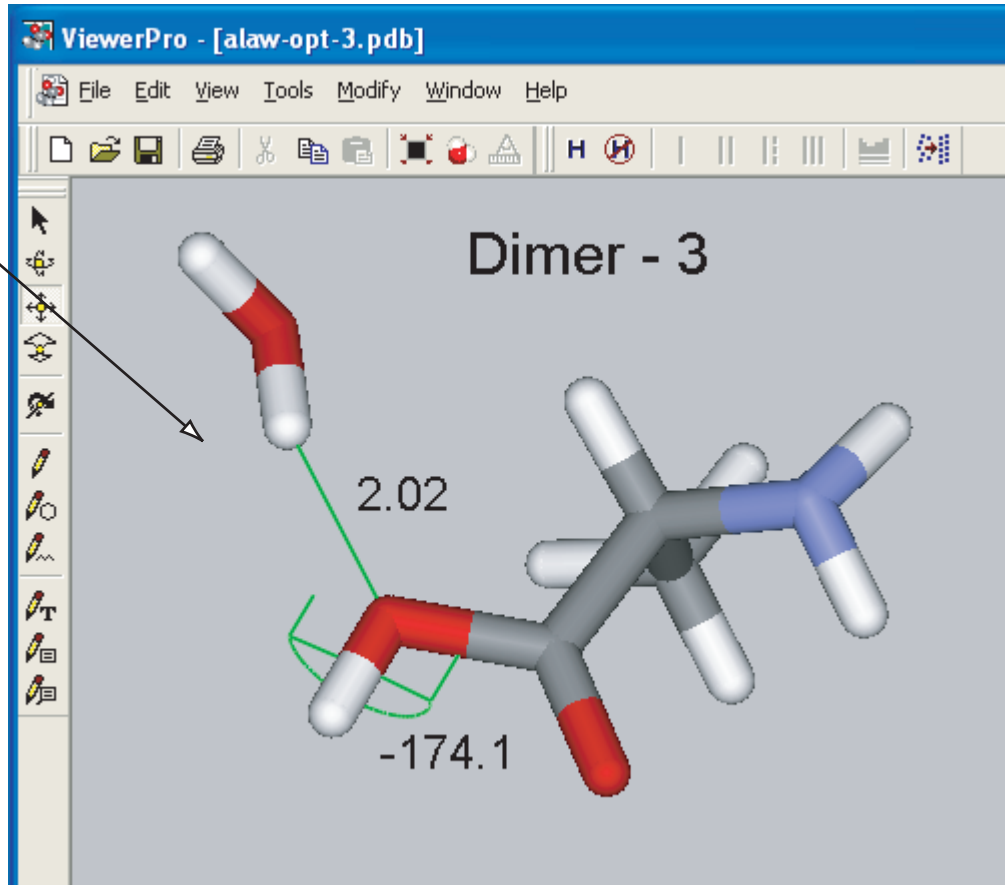
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 2



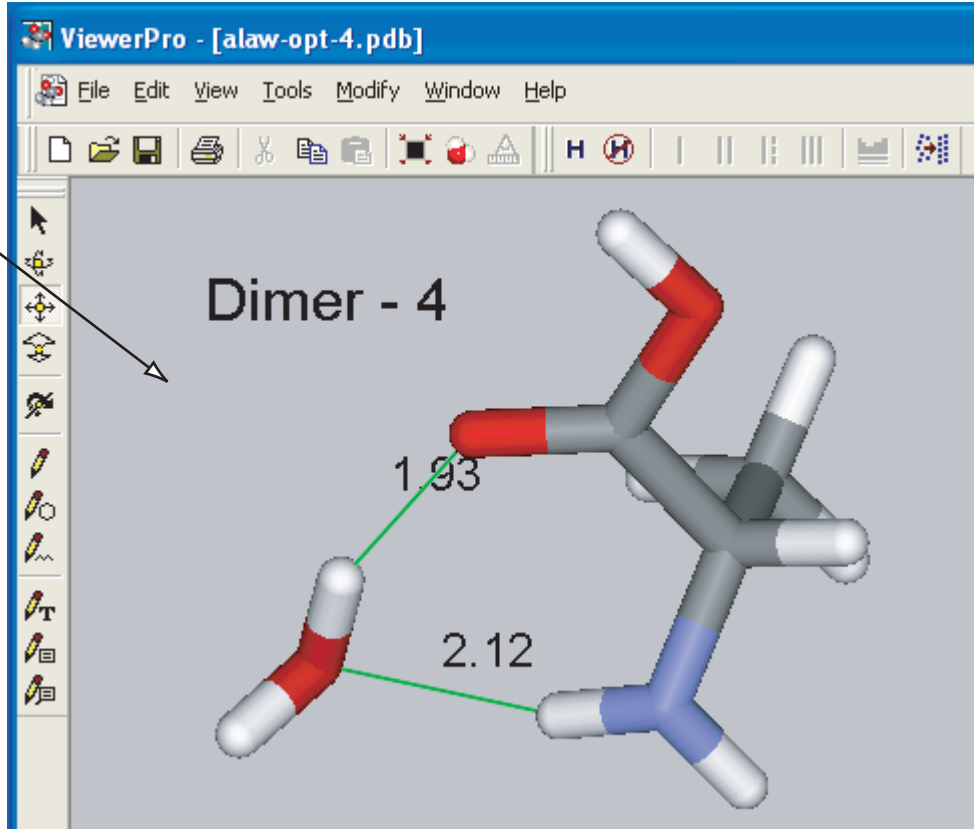
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 3



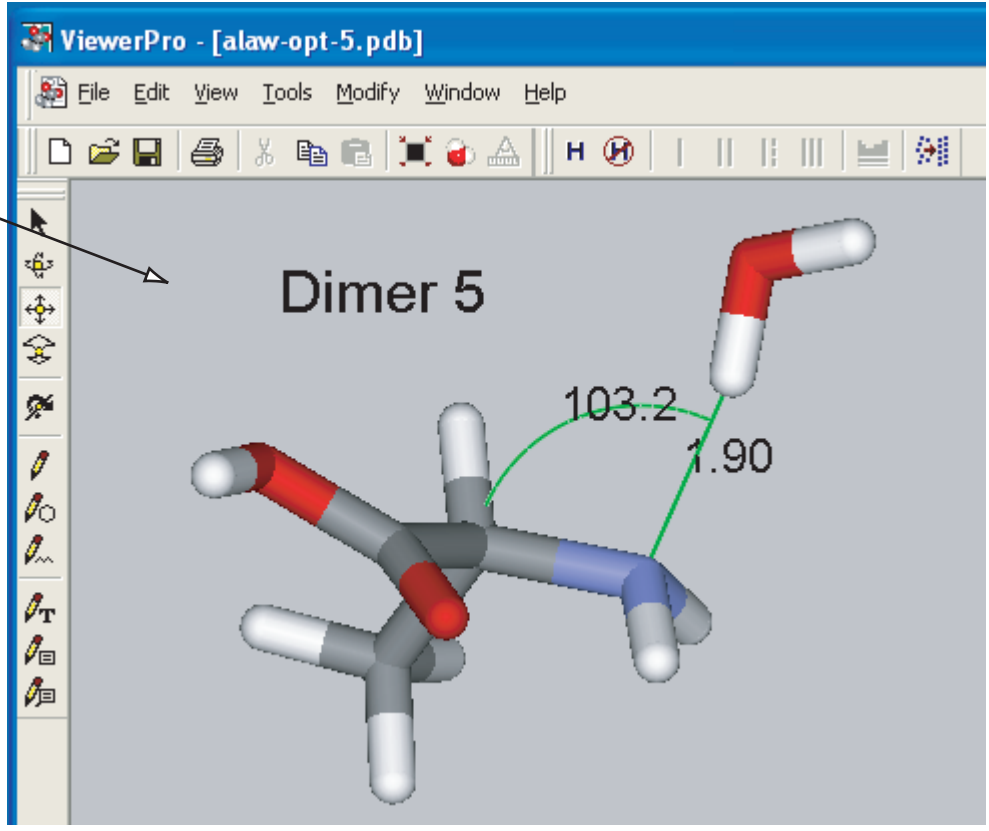
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 4



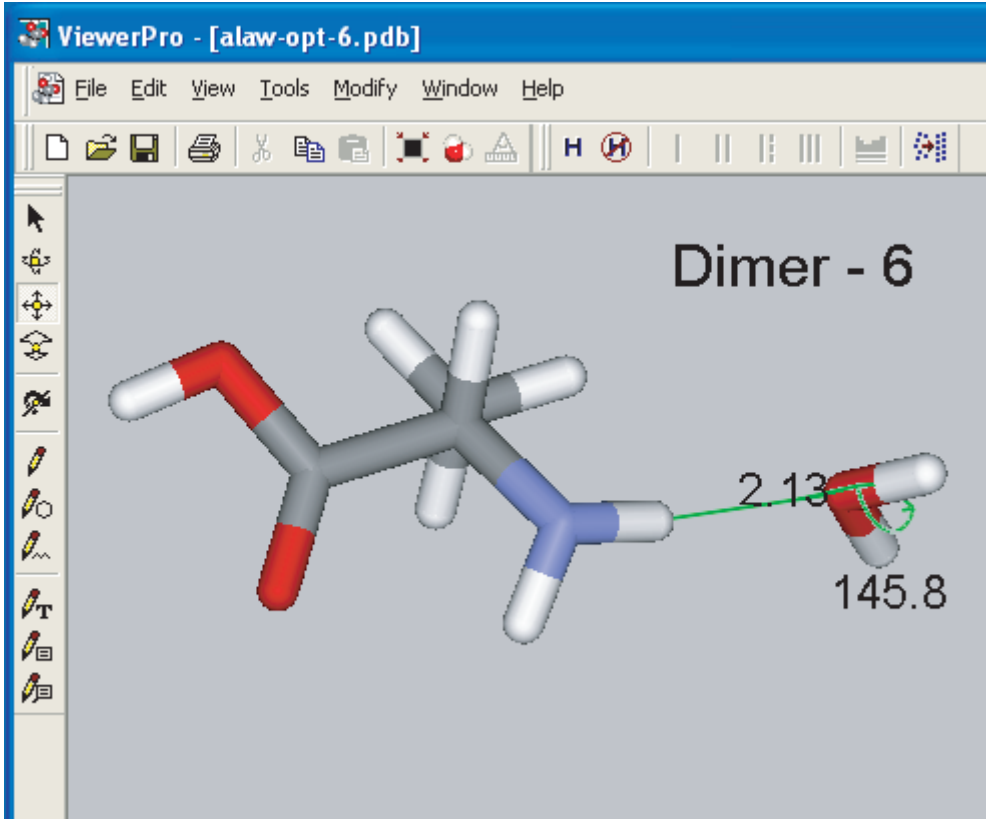
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 5



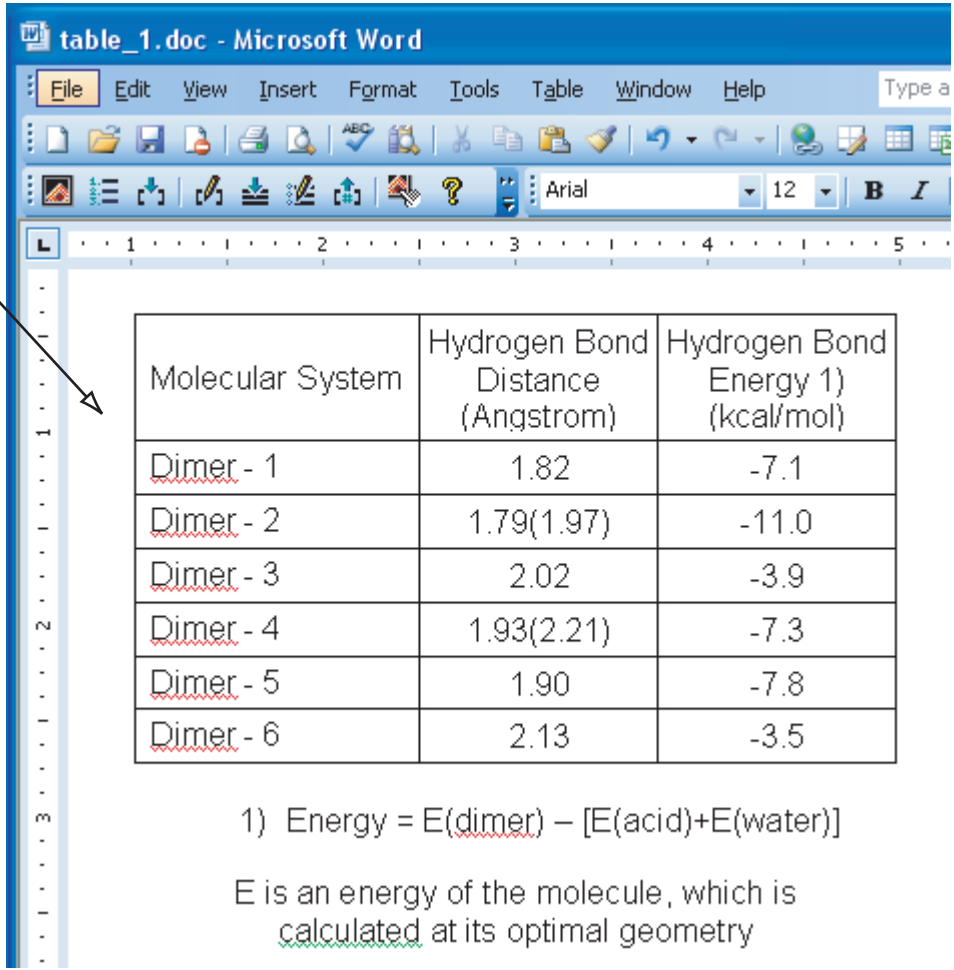
QM geometry optimization of alanine and water

Geometrical parameters of the dimer - 6



QM geometry optimization of alanine and water

Results of the calculations



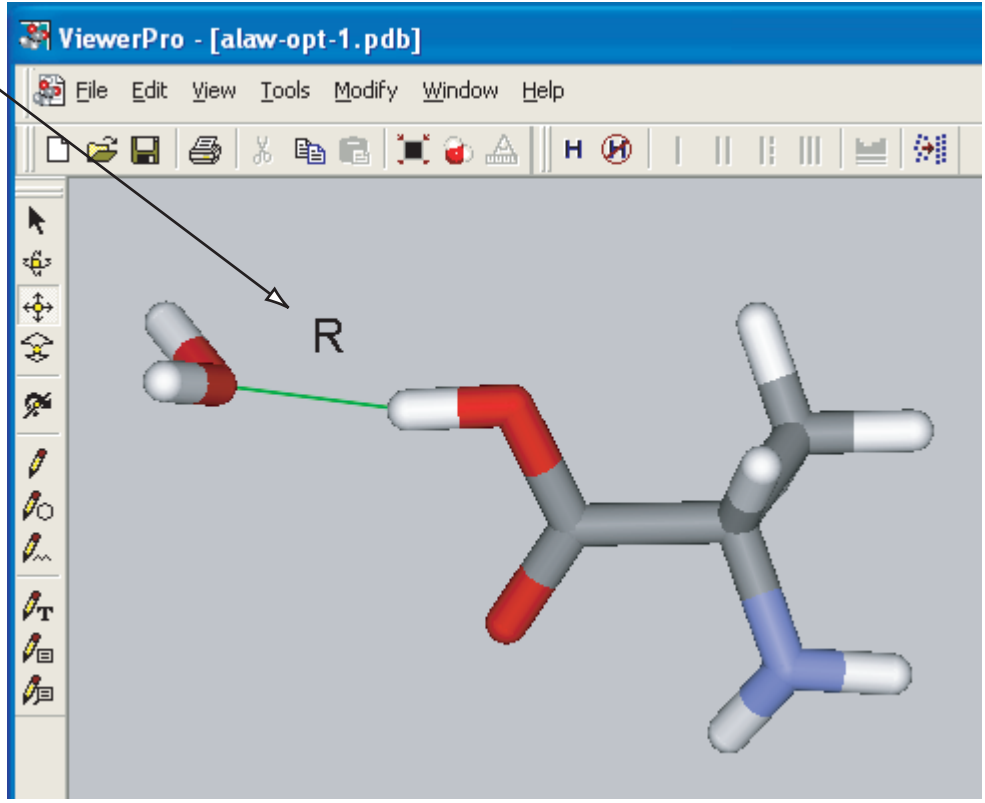
Molecular System	Hydrogen Bond Distance (Angstrom)	Hydrogen Bond Energy 1) (kcal/mol)
Dimer - 1	1.82	-7.1
Dimer - 2	1.79(1.97)	-11.0
Dimer - 3	2.02	-3.9
Dimer - 4	1.93(2.21)	-7.3
Dimer - 5	1.90	-7.8
Dimer - 6	2.13	-3.5

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

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

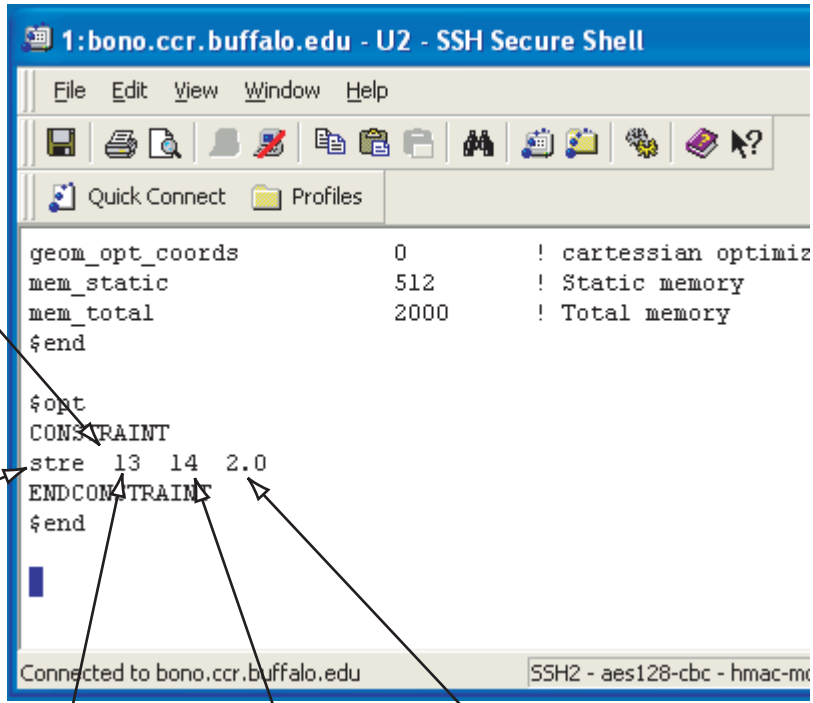
QM energy of alanine-water dimer

Intermolecular
distance R



QM energy of alanine-water dimer

Geometry optimization with a constrained distance

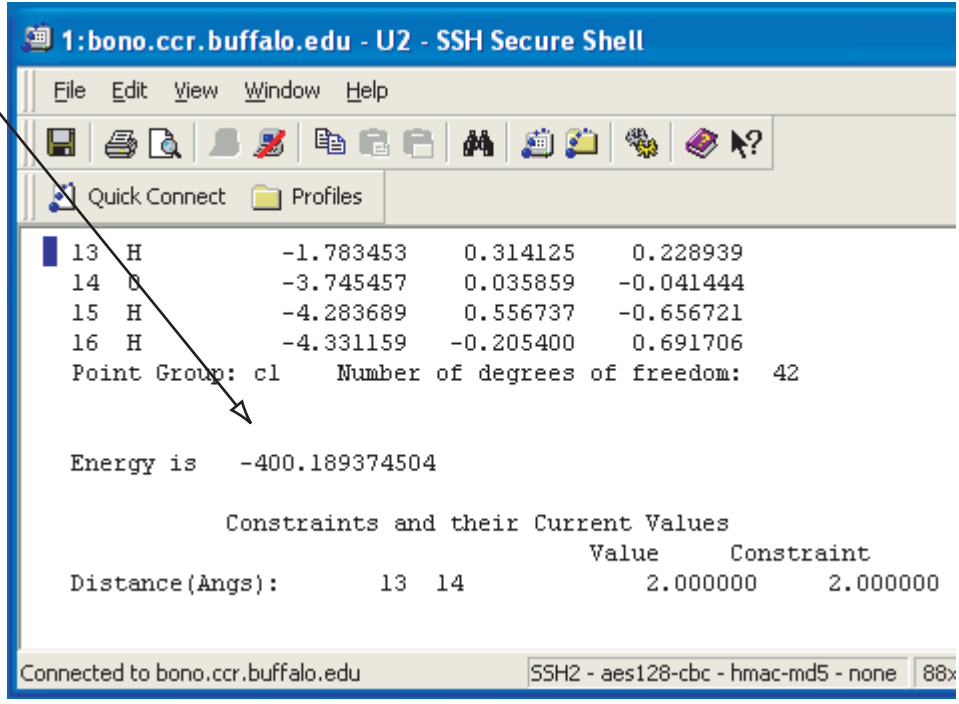


Distance

Atom #1 Atom #2 Value

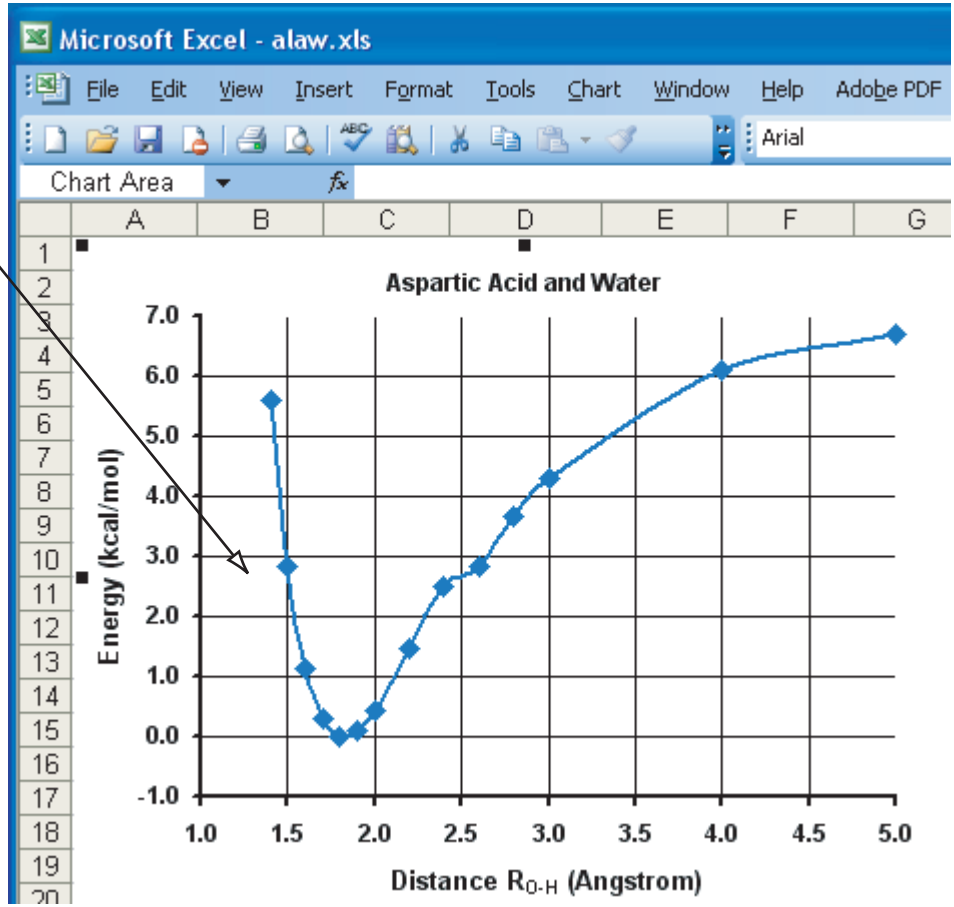
QM energy of alanine-water dimer

Final energy for a constrained distance



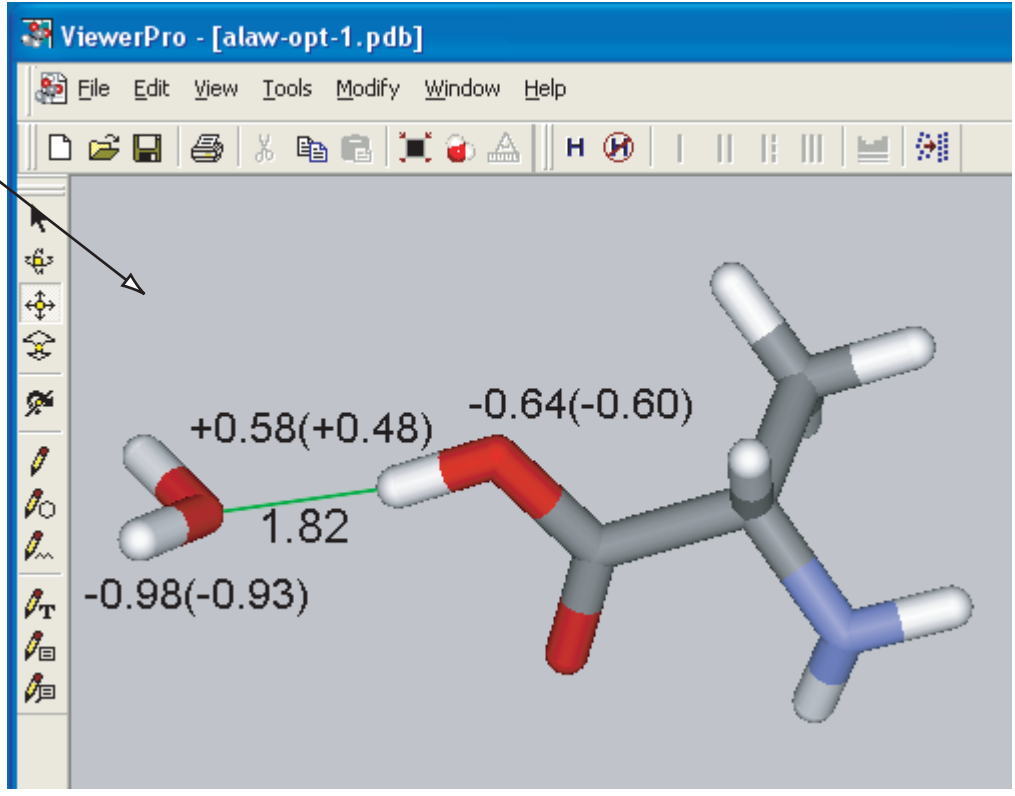
QM energy of alanine-water dimer

Final energy for a constrained distance



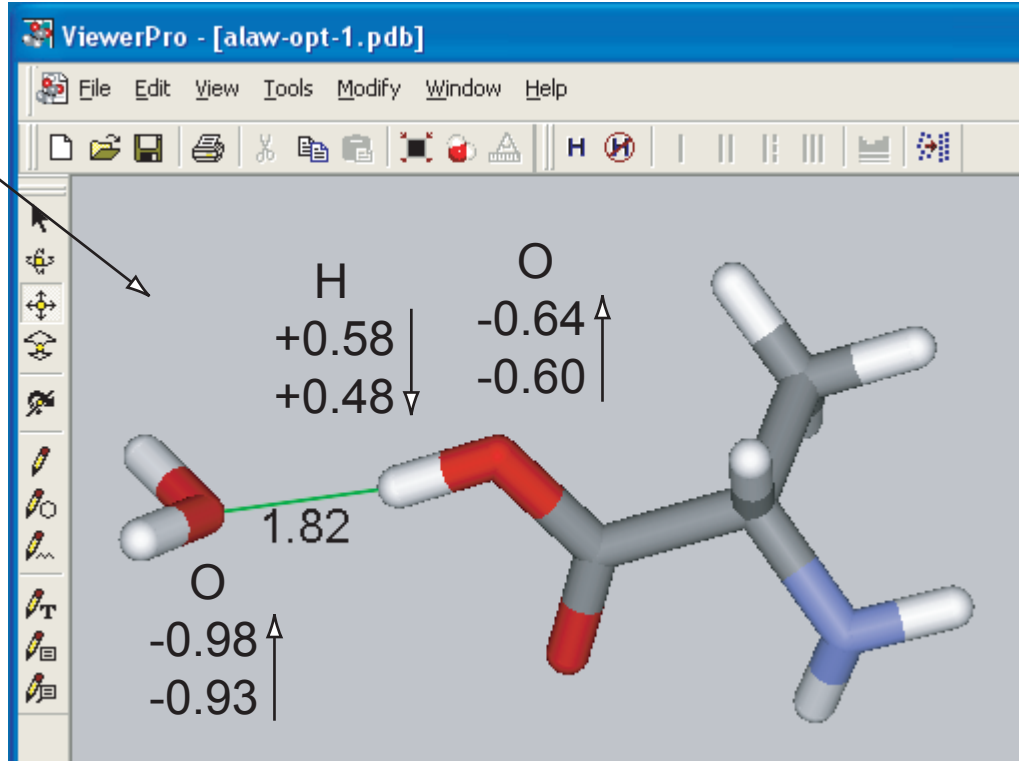
QM properties of alanine-water dimer

Atomic charges
before and after
hydrogen bonding



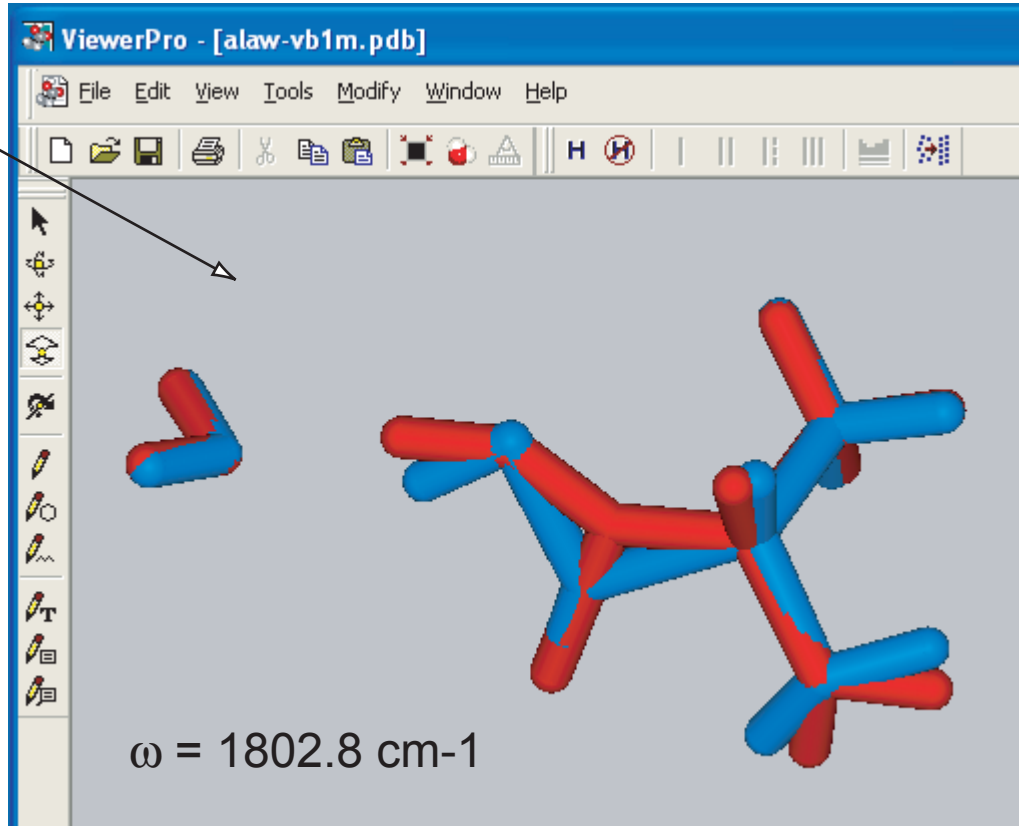
QM properties of alanine-water dimer

Atomic charges
before and after
hydrogen bonding



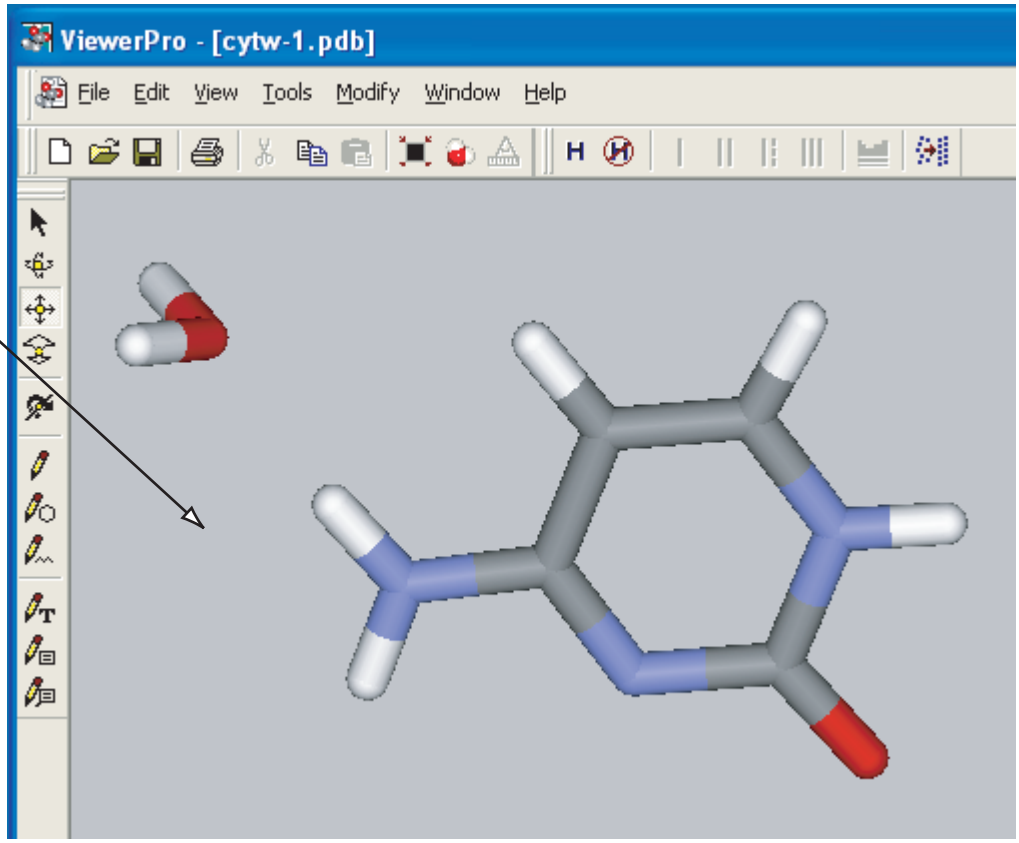
QM properties of alanine-water dimer

Vibration involving the hydrogen move



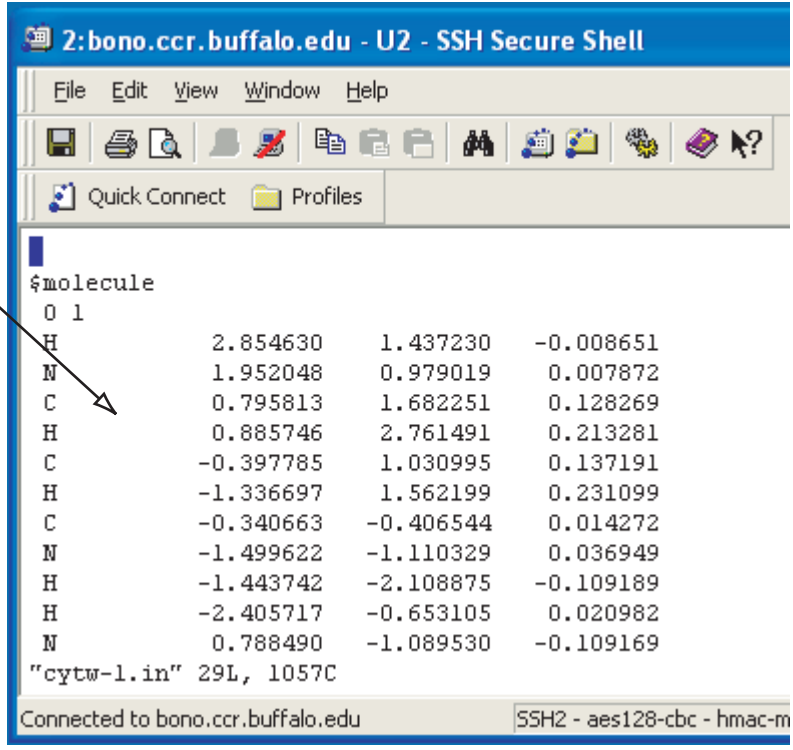
QM geometry optimization of cytosine and water

Initial geometry of the cytosine and water dimer



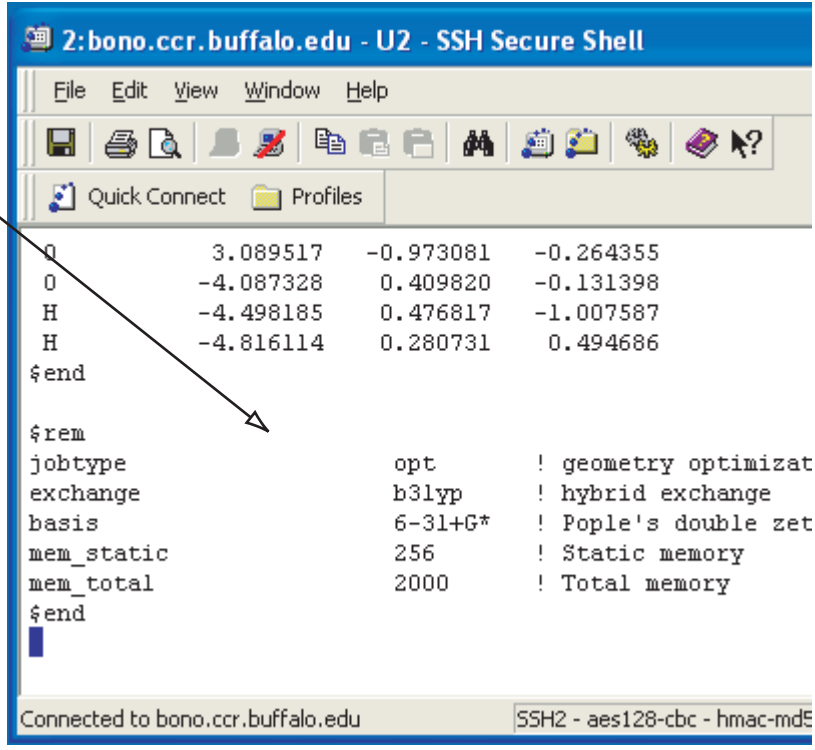
QM geometry optimization of cytosine and water

Initial geometry of the cytosine and water dimer



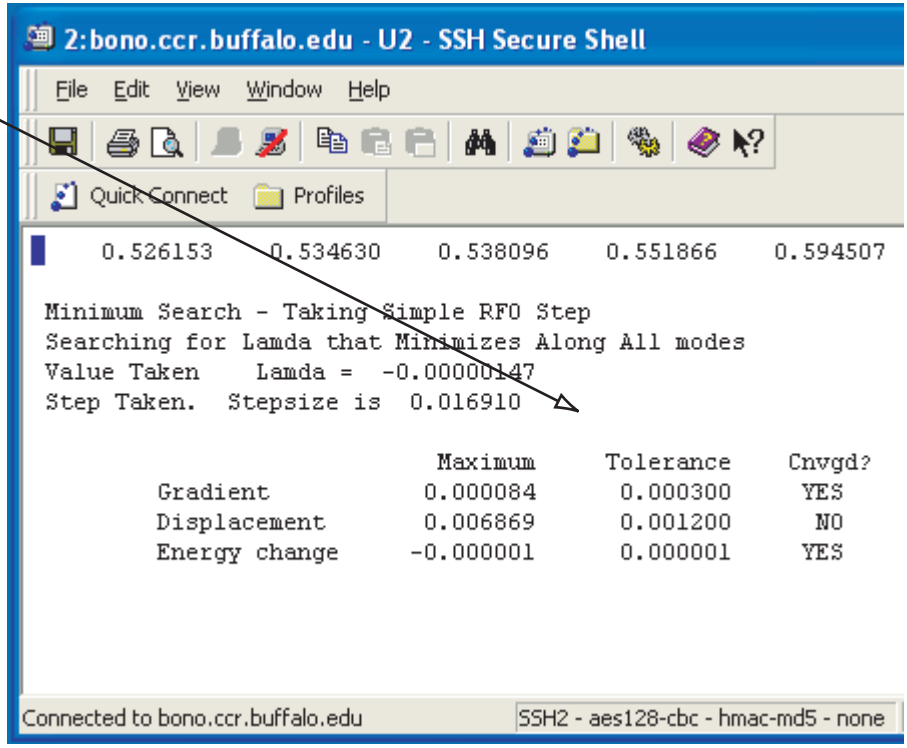
QM geometry optimization of cytosine and water

Geometry optimization



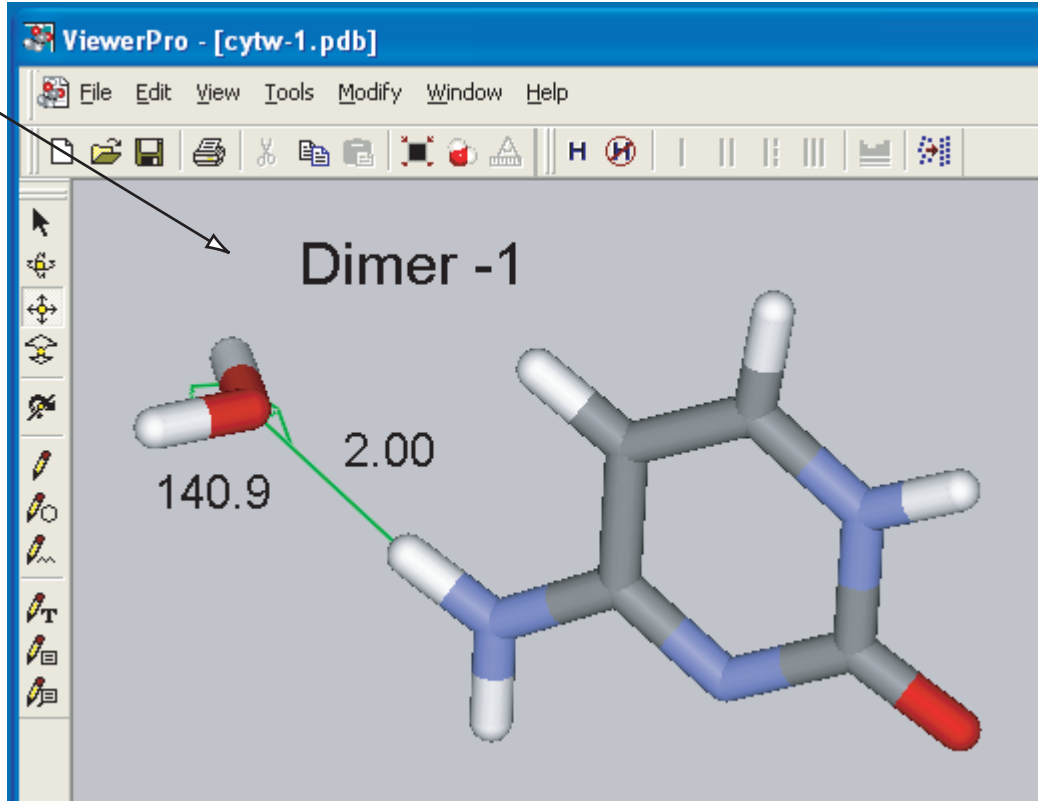
QM geometry optimization of cytosine and water

Optimization converged



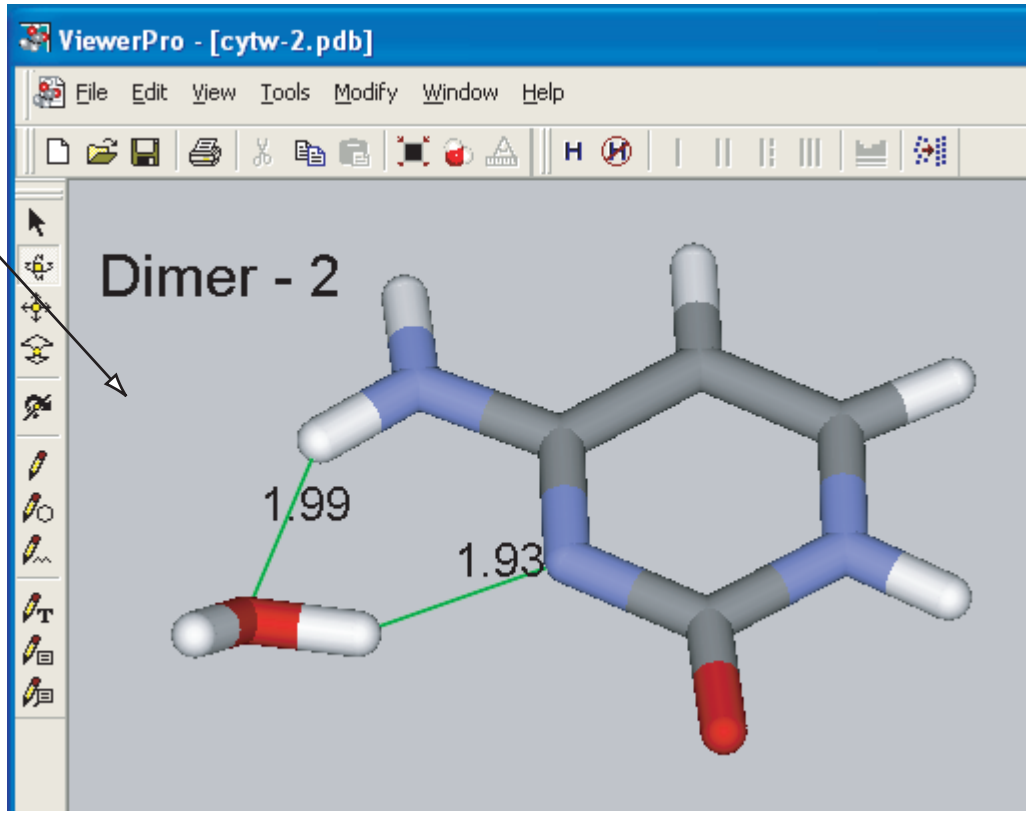
QM geometry optimization of cytosine and water

Final geometry
of Dimer -1

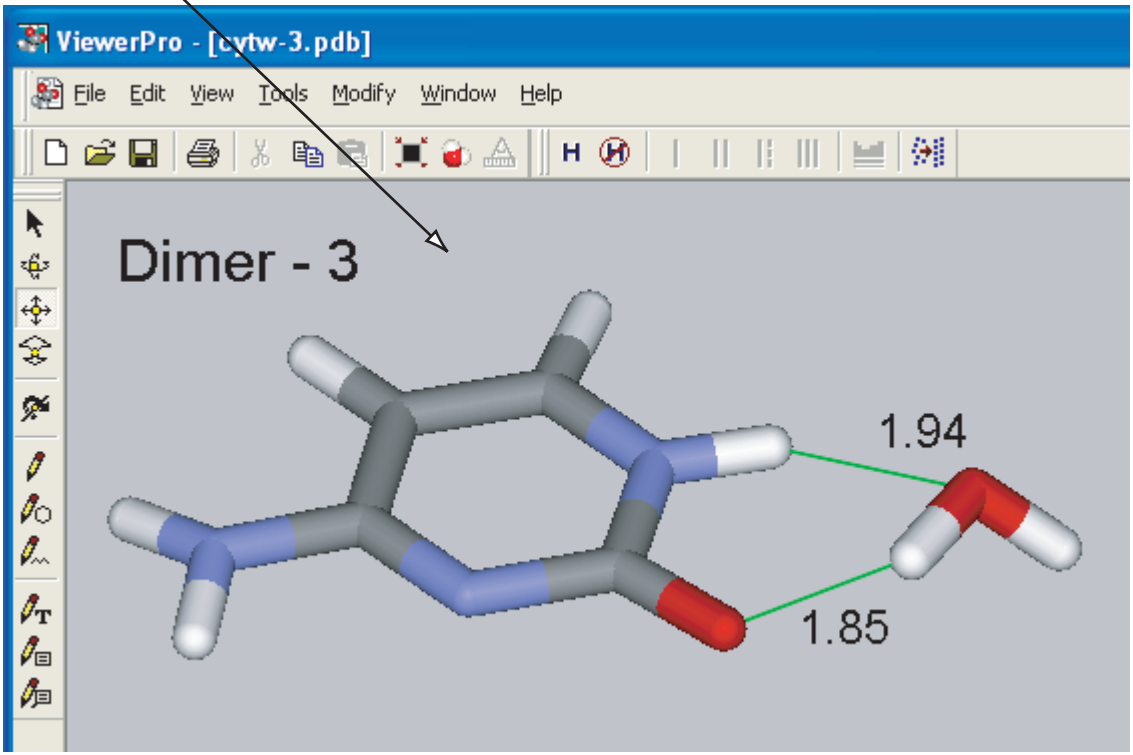


QM geometry optimization of cytosine and water

Final geometry
of Dimer -2

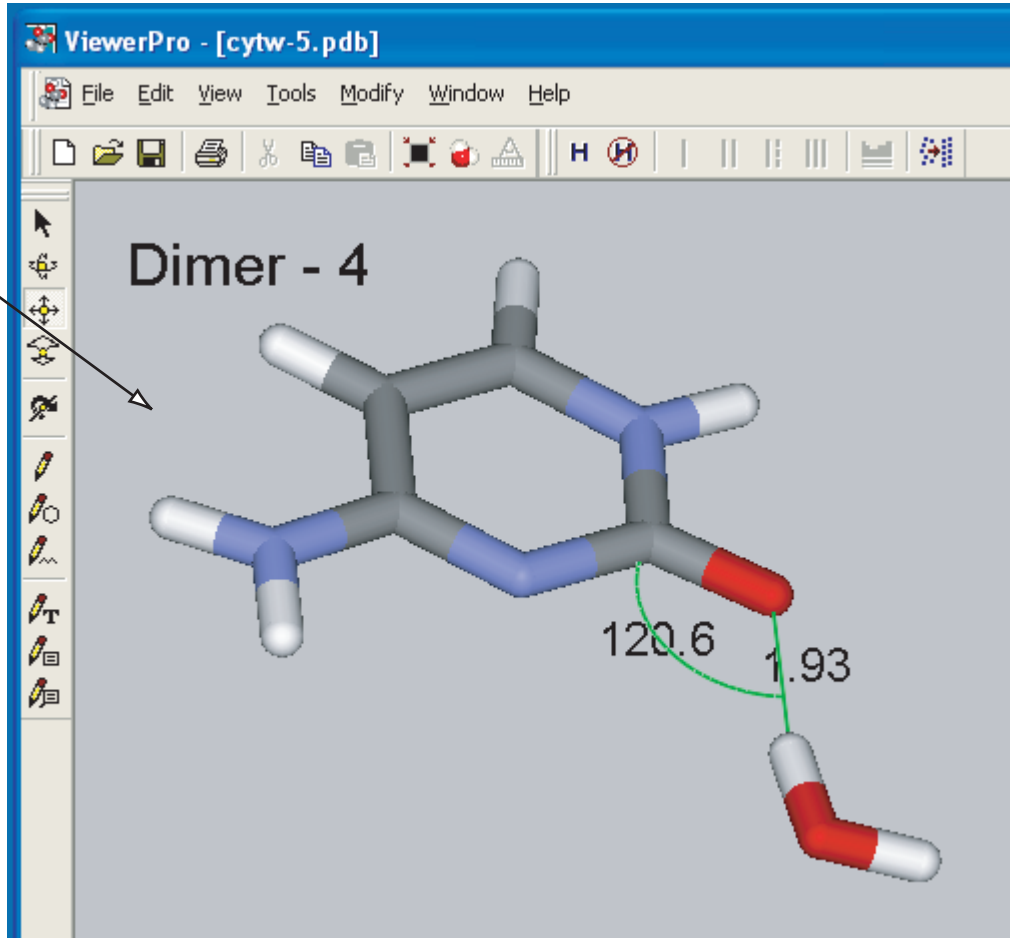


Final geometry
of Dimer - 3



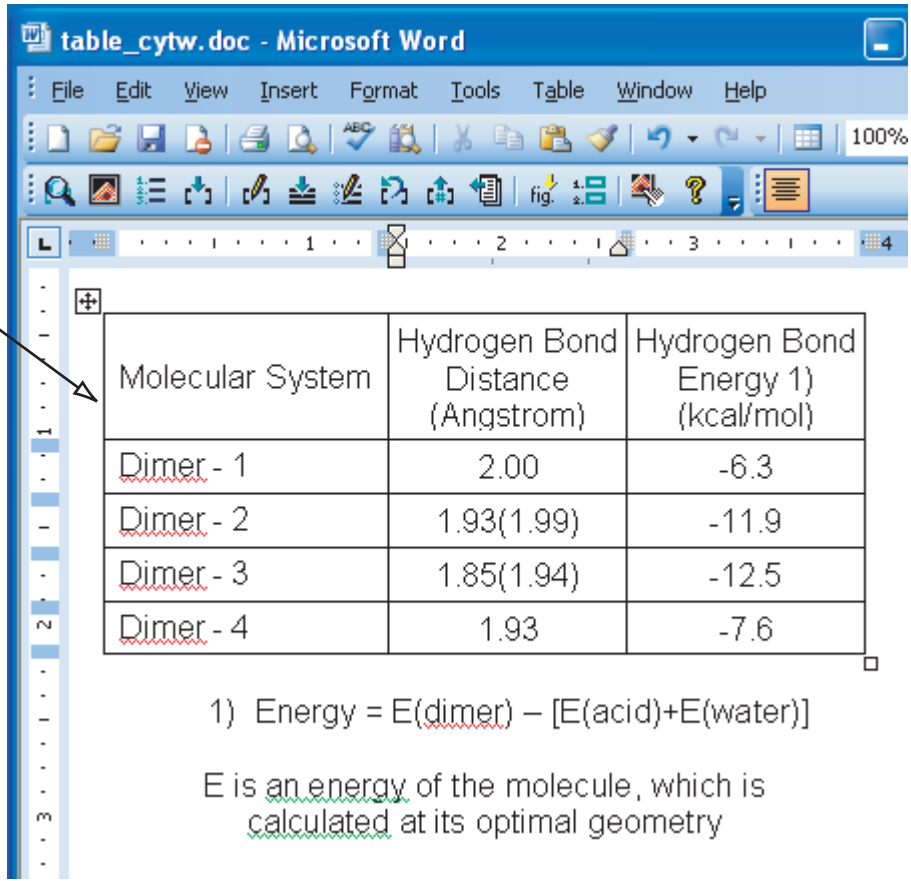
QM geometry optimization of cytosine and water

Final geometry of Dimer - 4



QM geometry optimization of cytosine and water

Final results



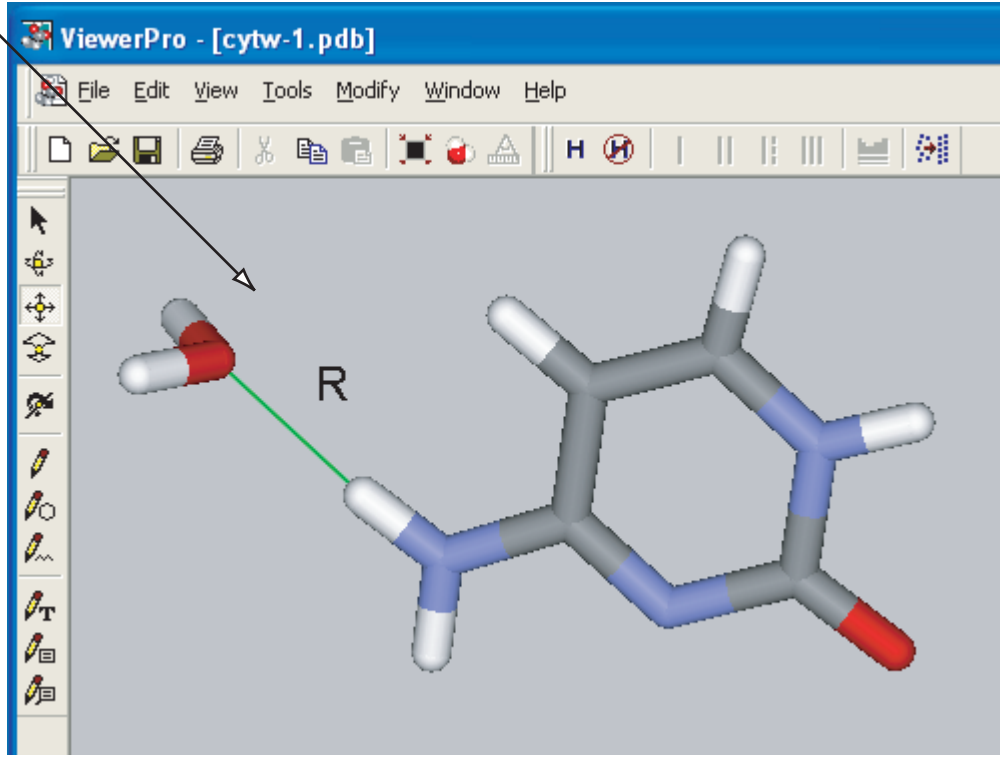
Molecular System	Hydrogen Bond Distance (Angstrom)	Hydrogen Bond Energy 1) (kcal/mol)
Dimer - 1	2.00	-6.3
Dimer - 2	1.93(1.99)	-11.9
Dimer - 3	1.85(1.94)	-12.5
Dimer - 4	1.93	-7.6

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

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

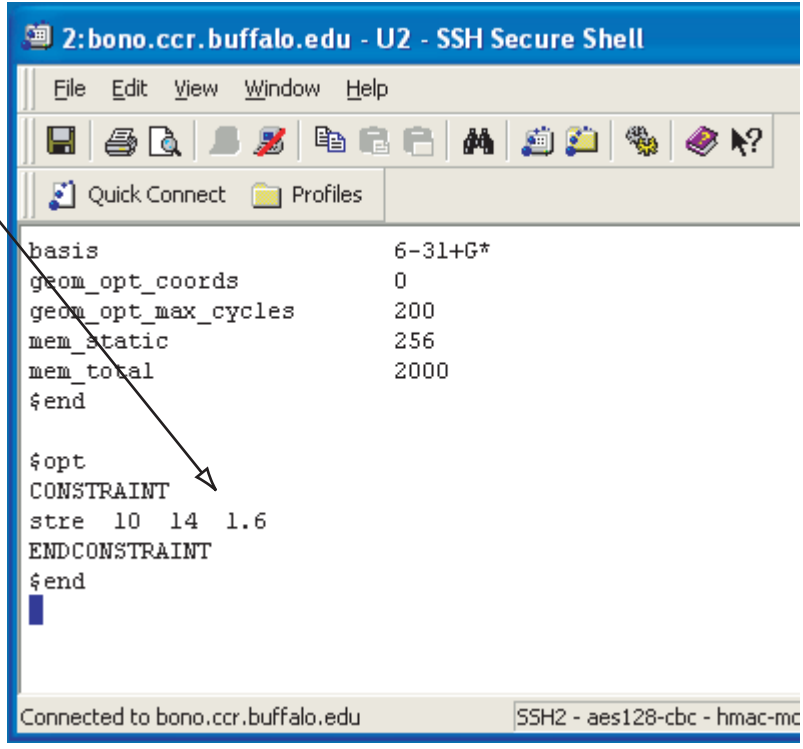
QM geometry optimization of cytosine and water

Calculations with a
constrained distance



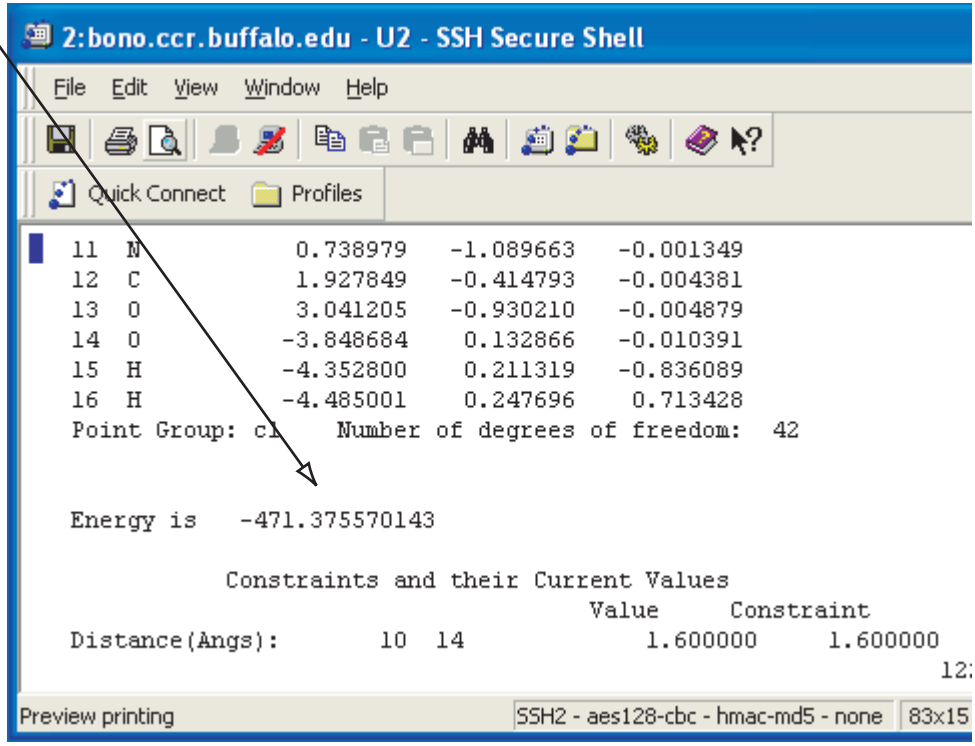
QM geometry optimization of cytosine and water

Constrained distance between two atoms



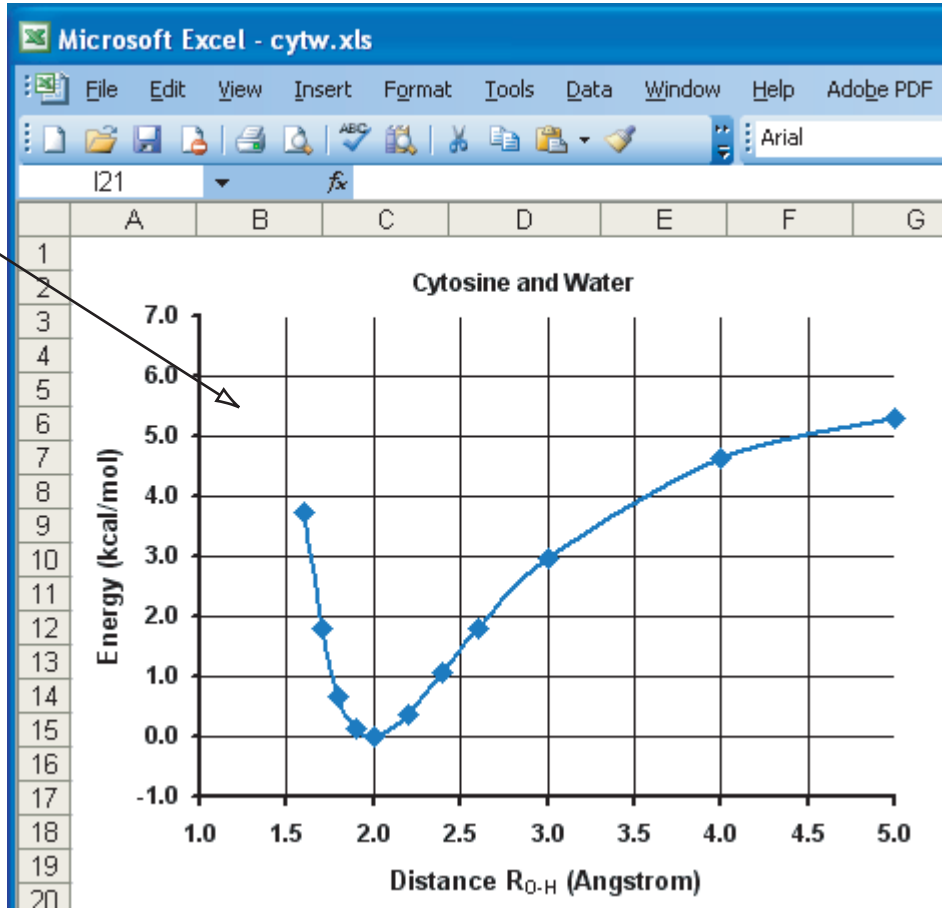
QM geometry optimization of cytosine and water

Final energy with a constrained distance

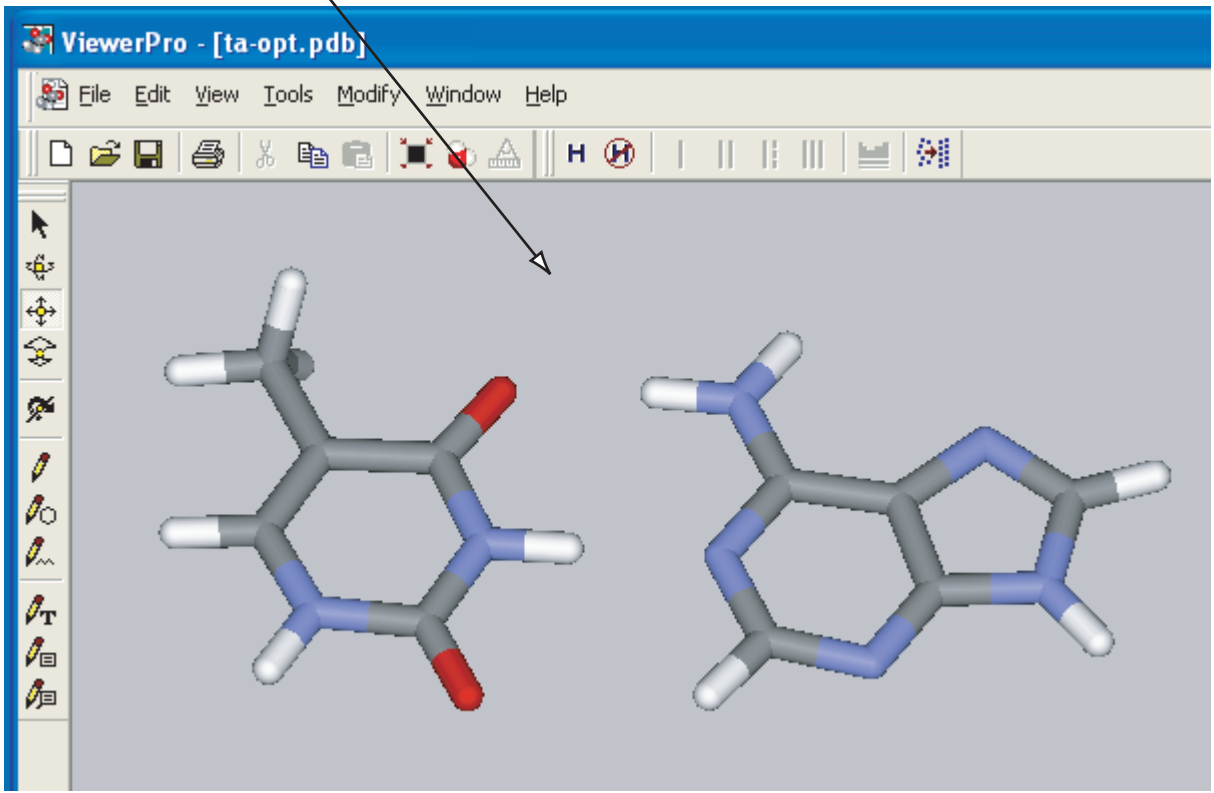


QM geometry optimization of cytosine and water

Energy as a function of a constrained distance

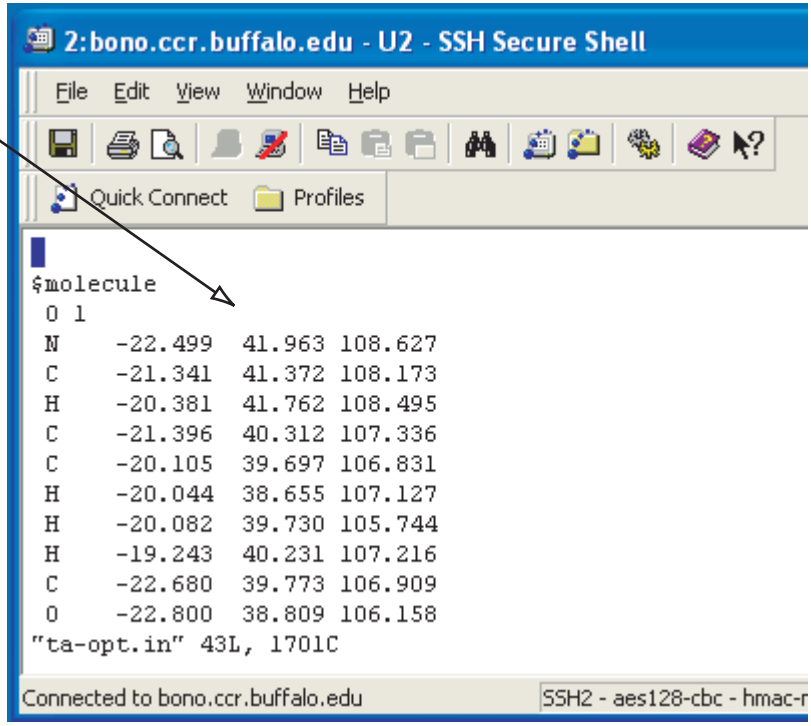


Initial geometry of Thymine
and Adenine dimer

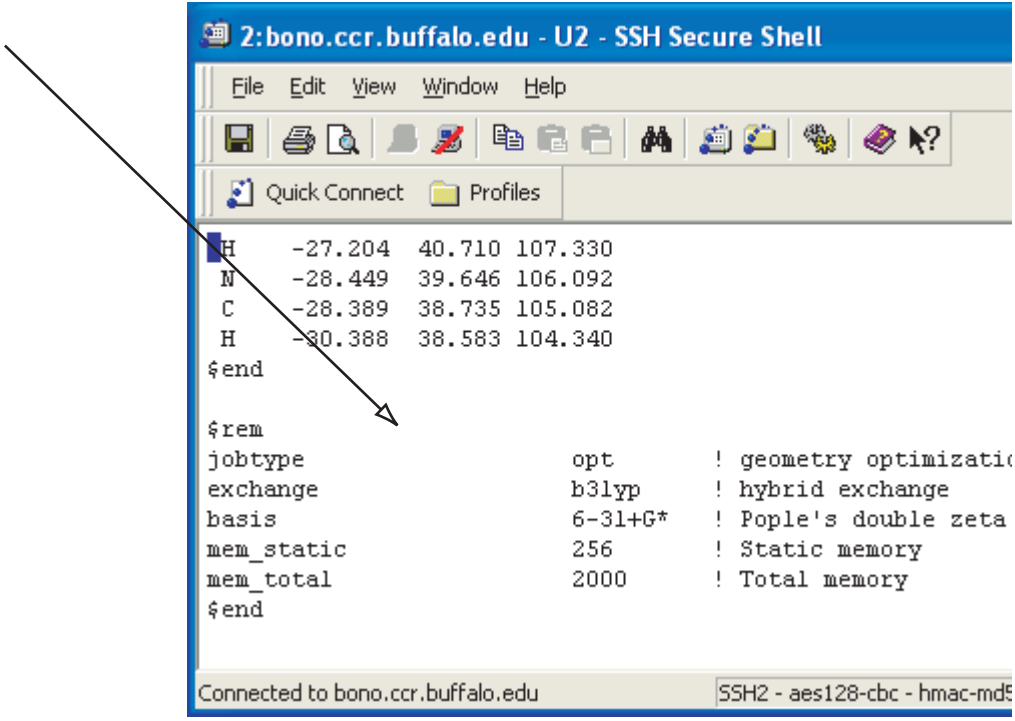


QM proton transfer in Thymine and Adenine dimer

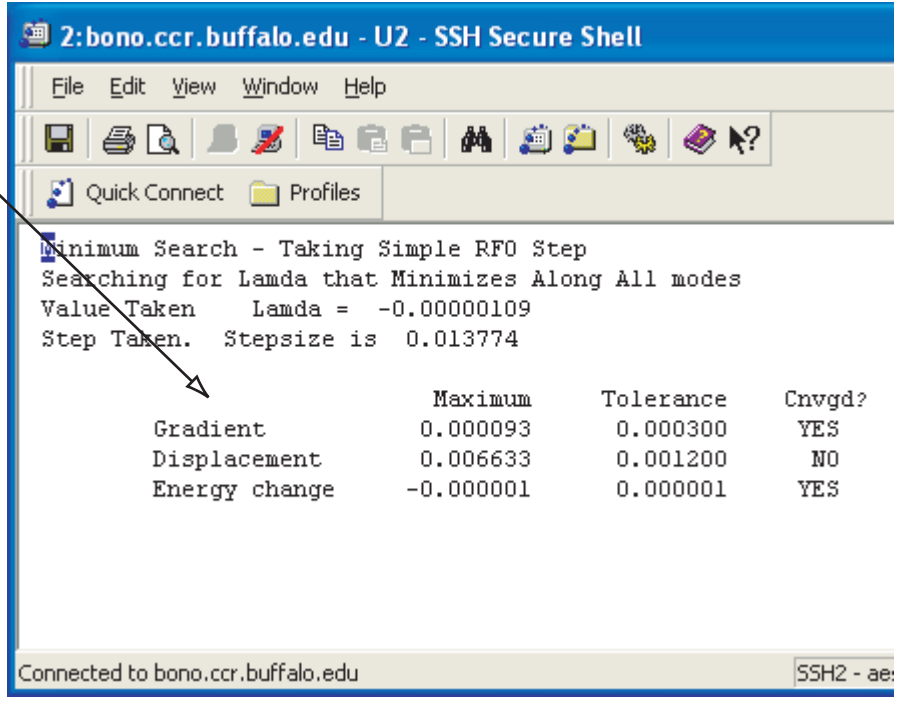
Initial geometry of the dimer taken from an experimental PDB file



Geometry optimization
of the dimer

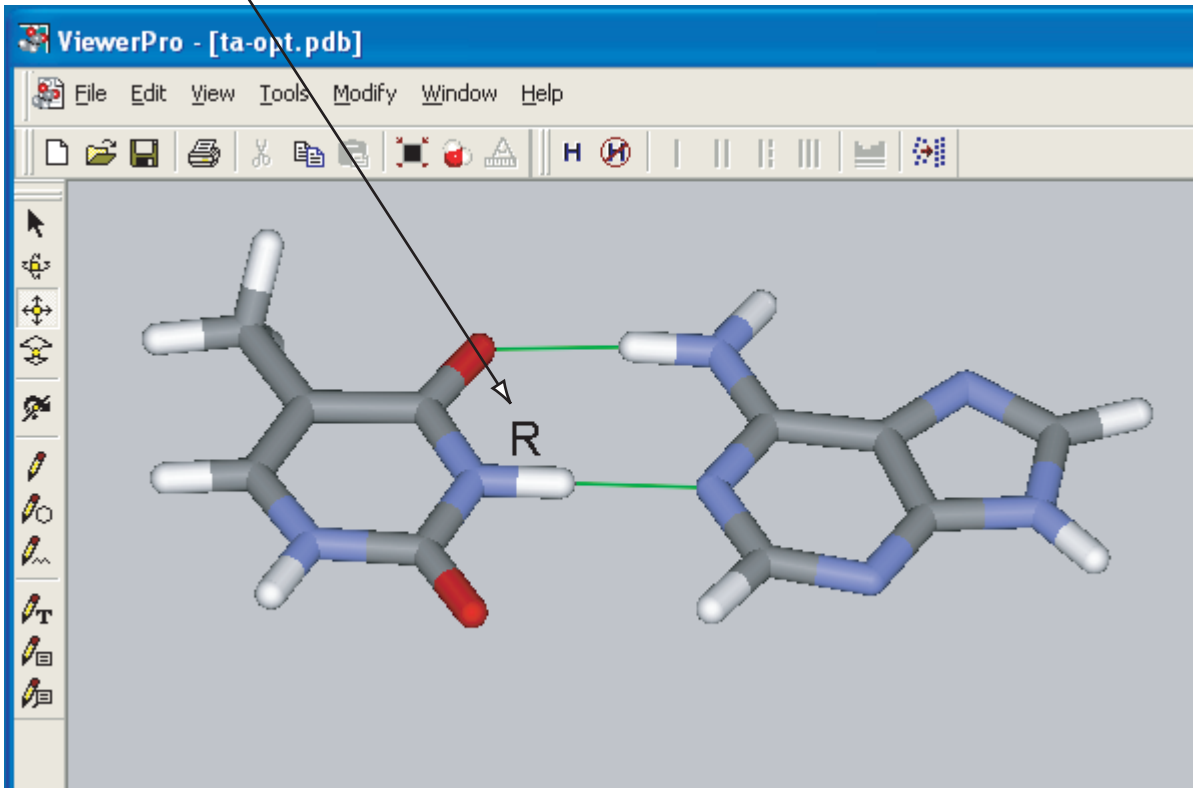


Optimization converged



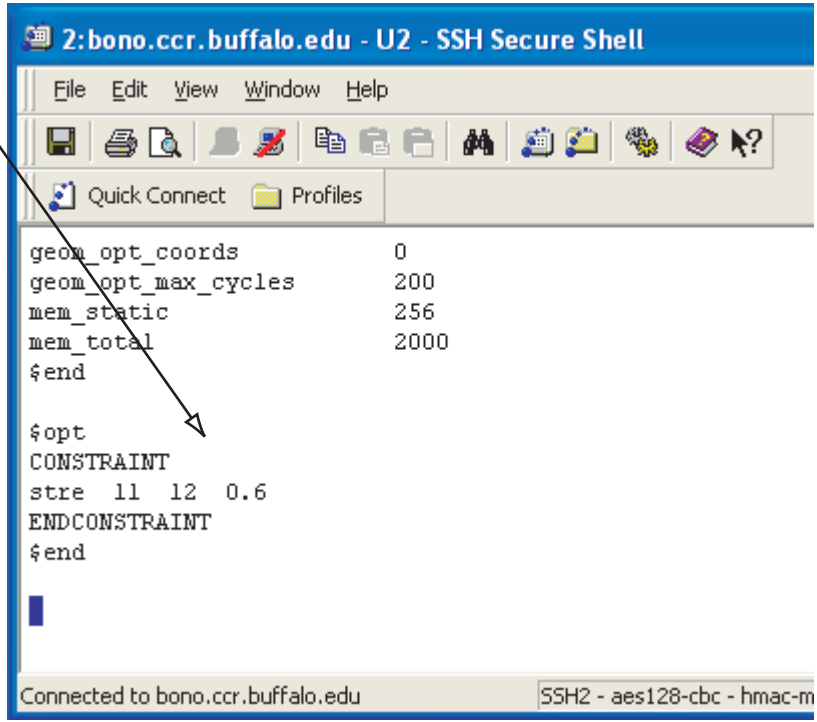
QM proton transfer in Thymine and Adenine dimer

A series of calculations for
the constrained R value

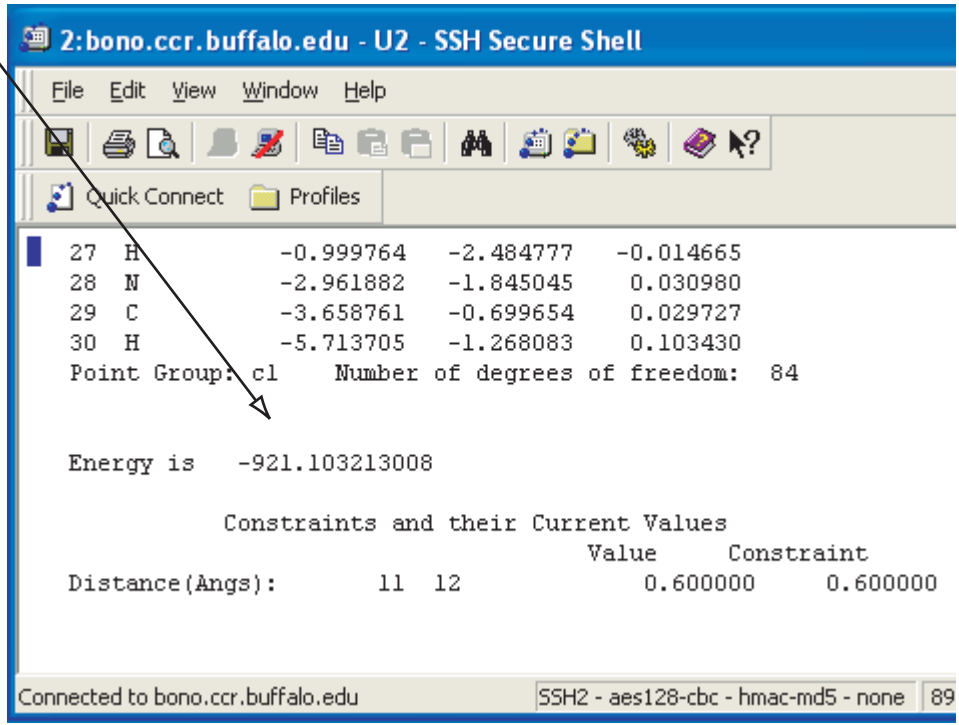


QM proton transfer in Thymine and Adenine dimer

A constrained distance between two atoms

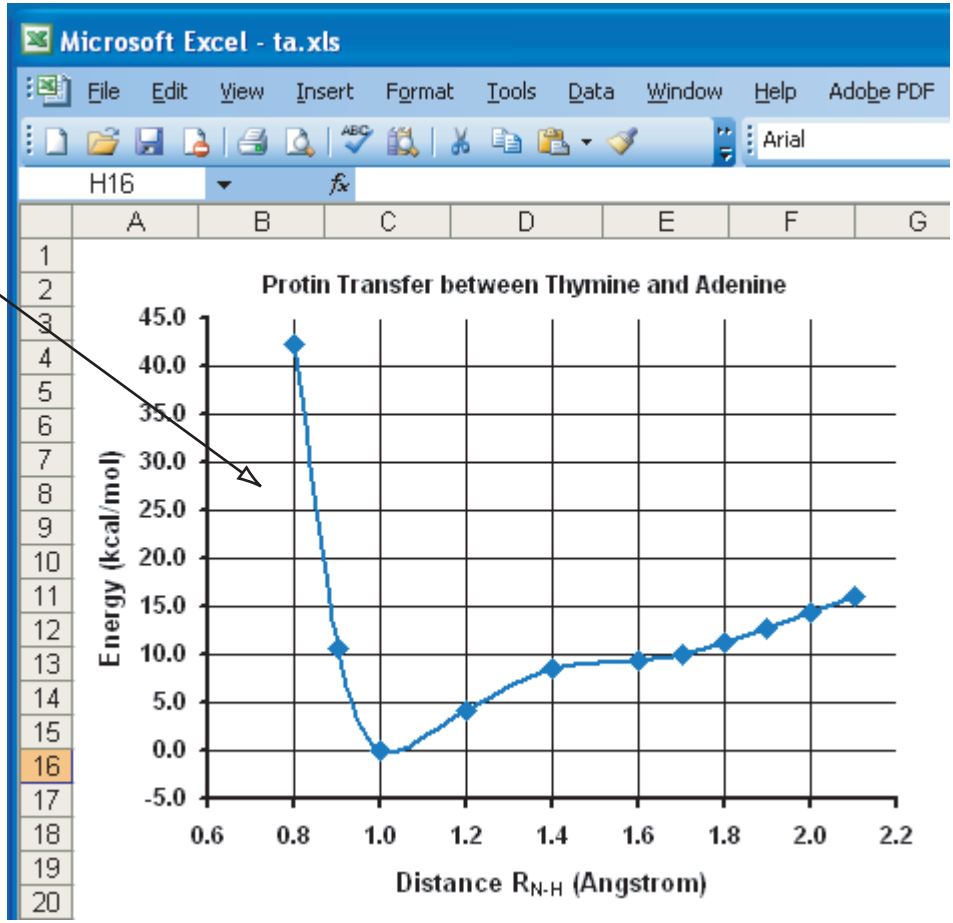


Final energy for a constrained distance



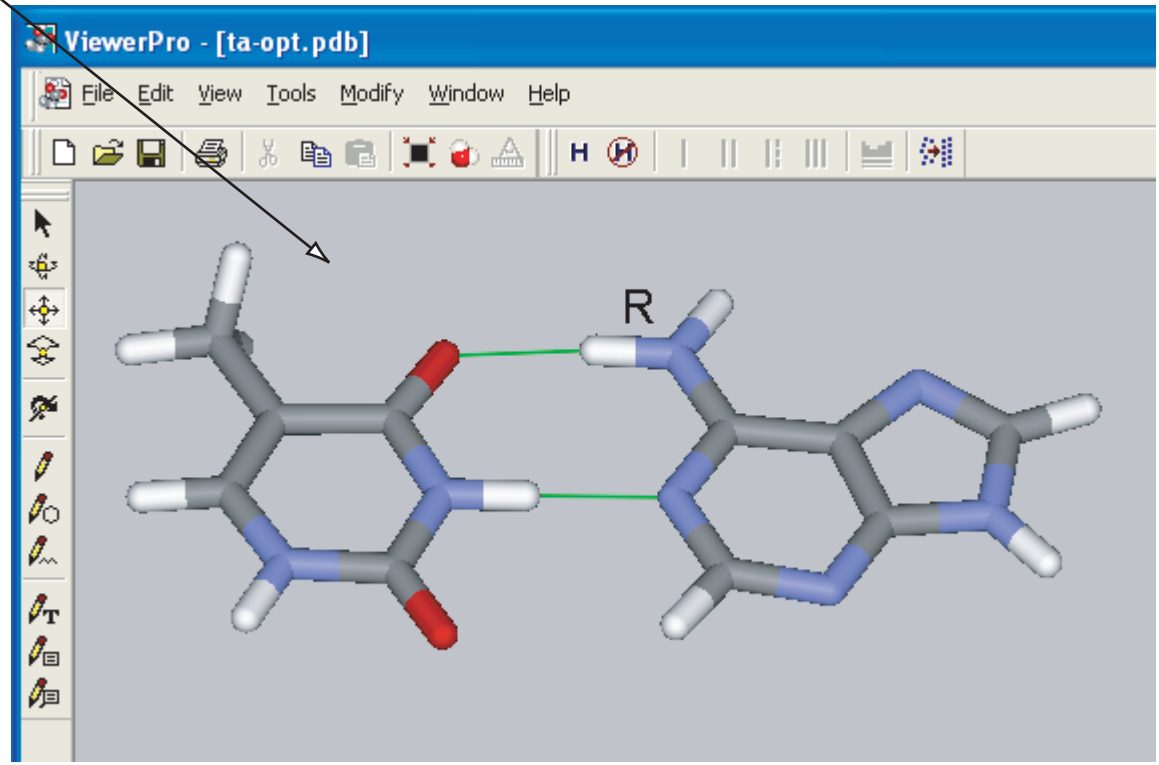
QM proton transfer in Thymine and Adenine dimer

The energy as a function of the R(N-H) distance



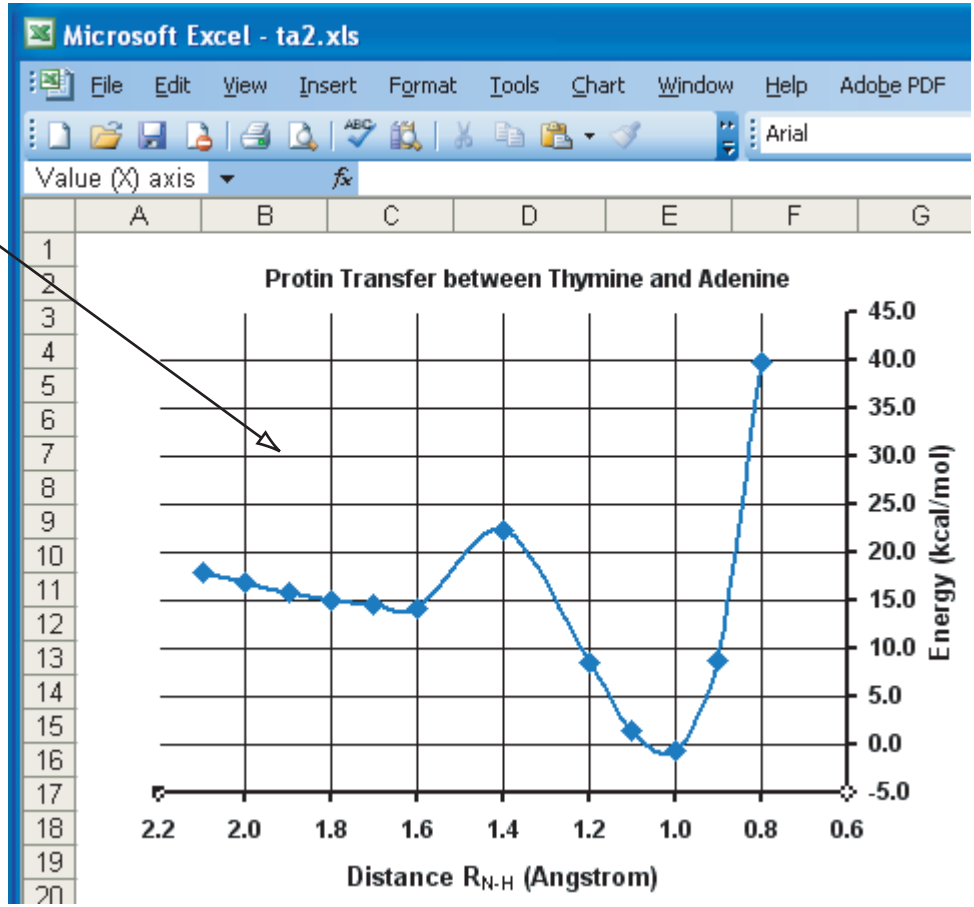
QM proton transfer in Thymine and Adenine dimer

A constrained
interatomic distance



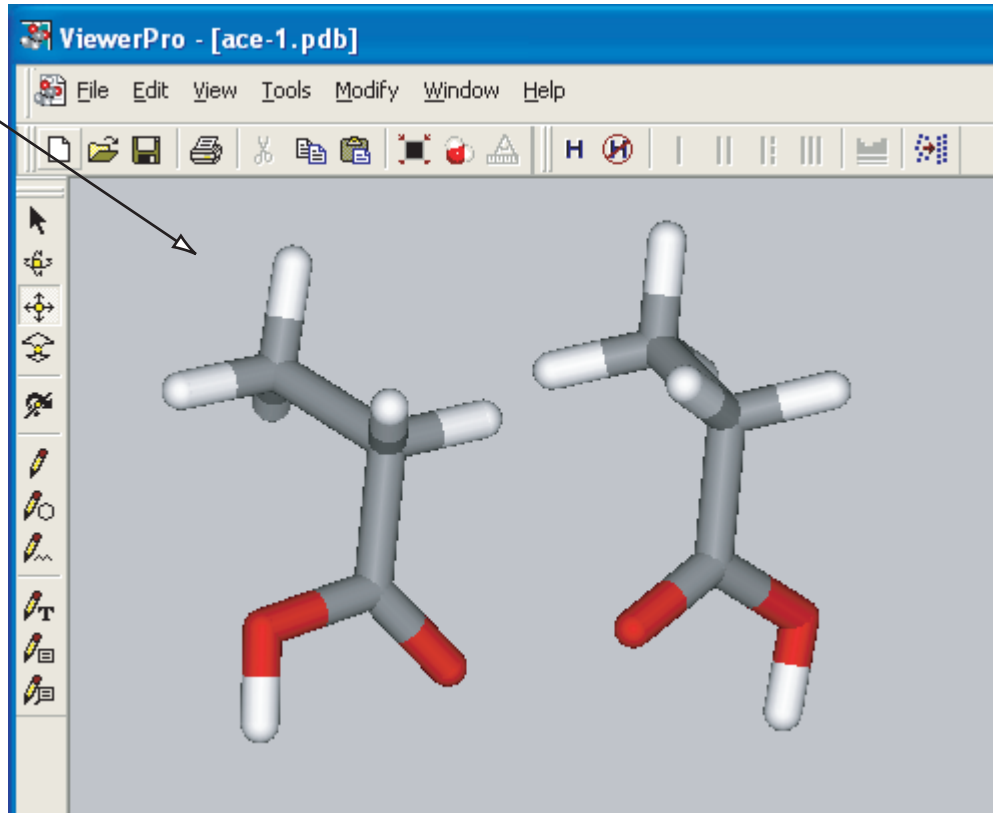
QM proton transfer in Thymine and Adenine dimer

The energy as a function of the R(N-H) distance



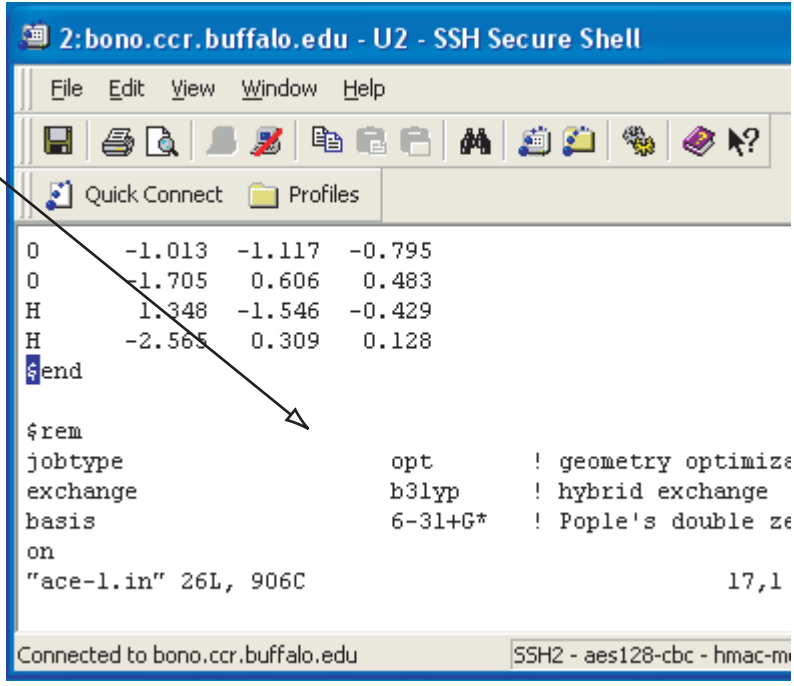
QM tautomerization - Alanine

Two tautomers of alanine



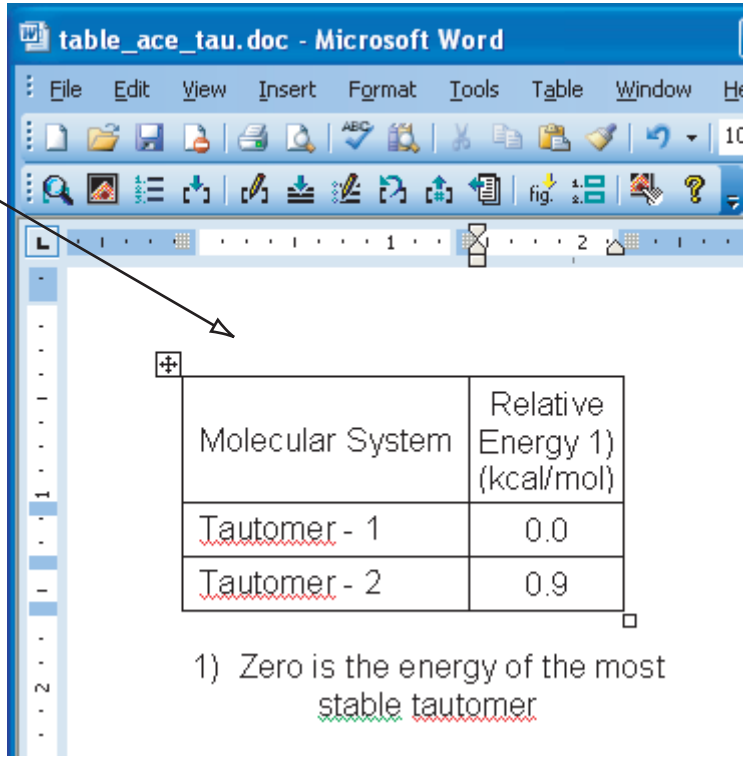
QM tautomerization - Alanine

Geometry optimization



QM tautomerization - Alanine

Final results

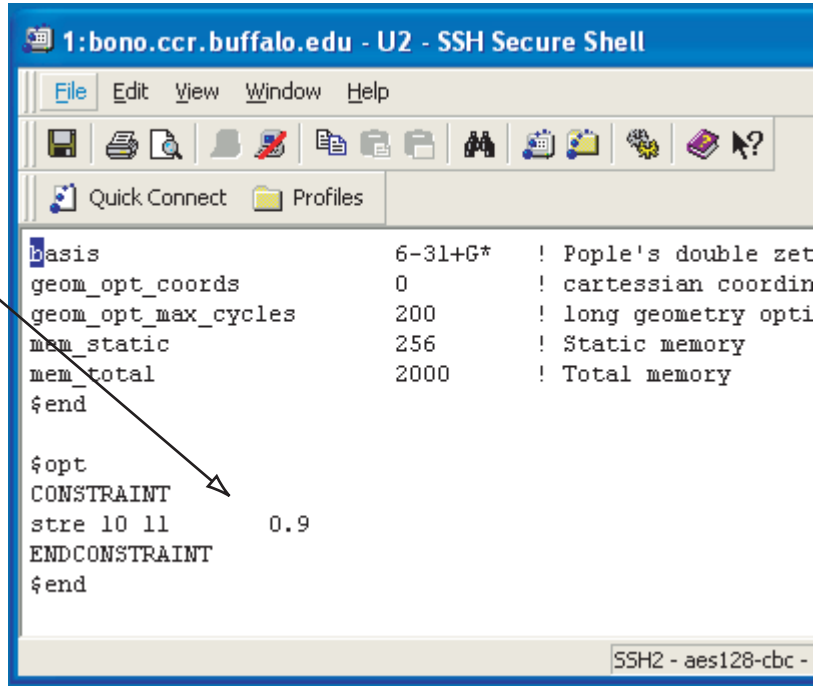


Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - 1	0.0
Tautomer - 2	0.9

1) Zero is the energy of the most stable tautomer

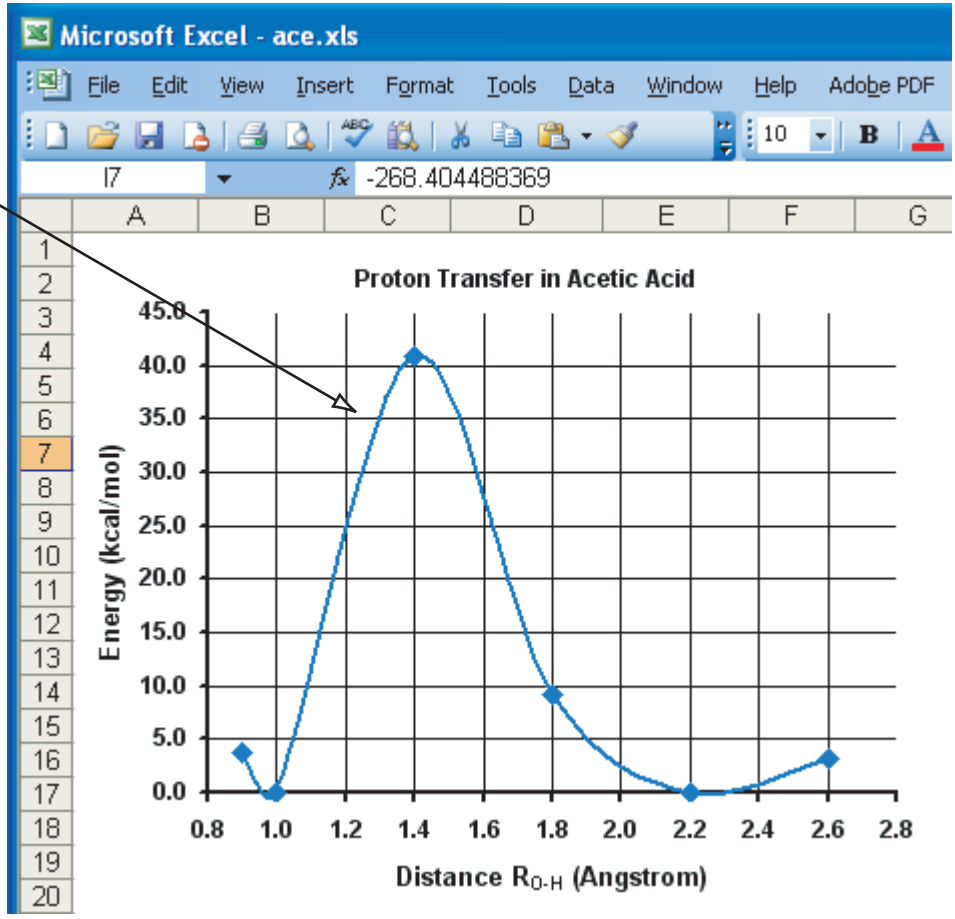
QM tautomerization - Alanine

Geometry optimization with a constrained distance



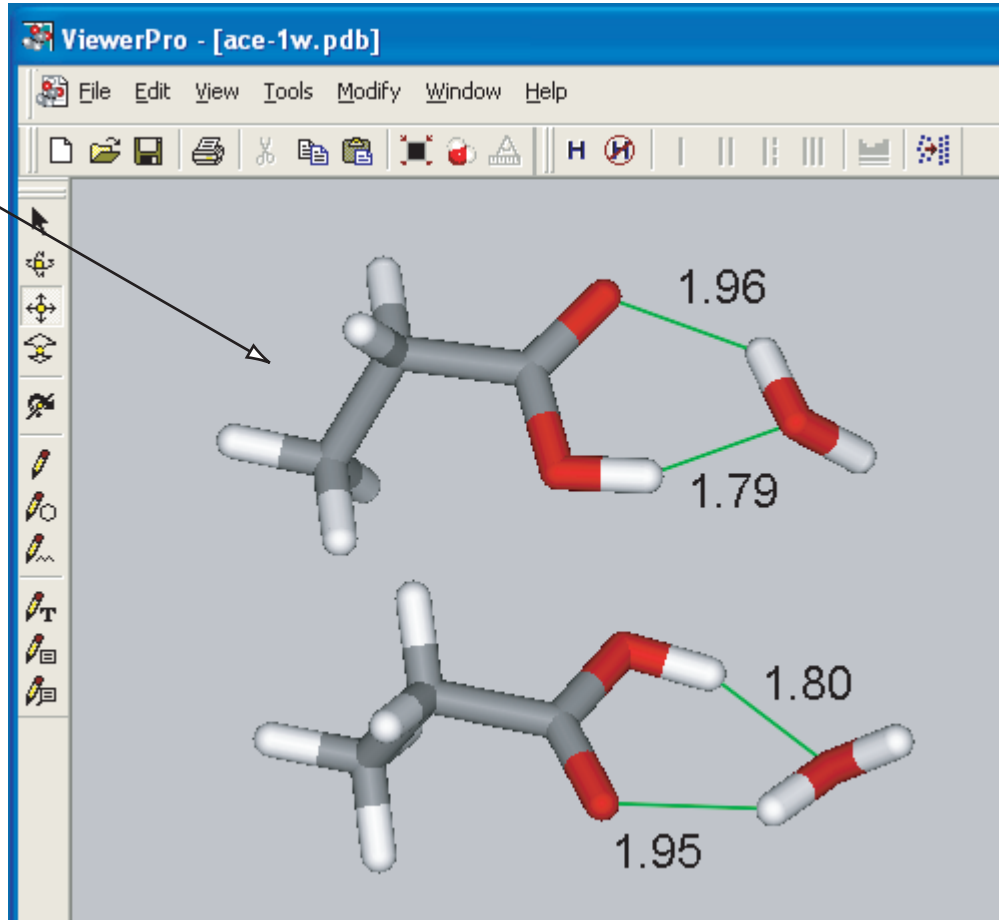
QM tautomerization - Alanine

Final results



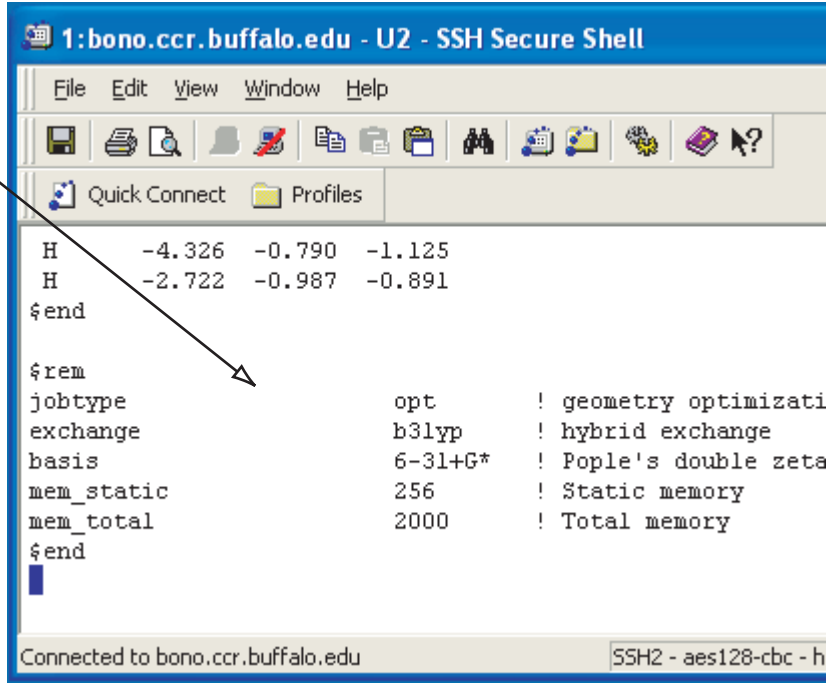
QM tautomerization - Alanine

Alanine and water dimers



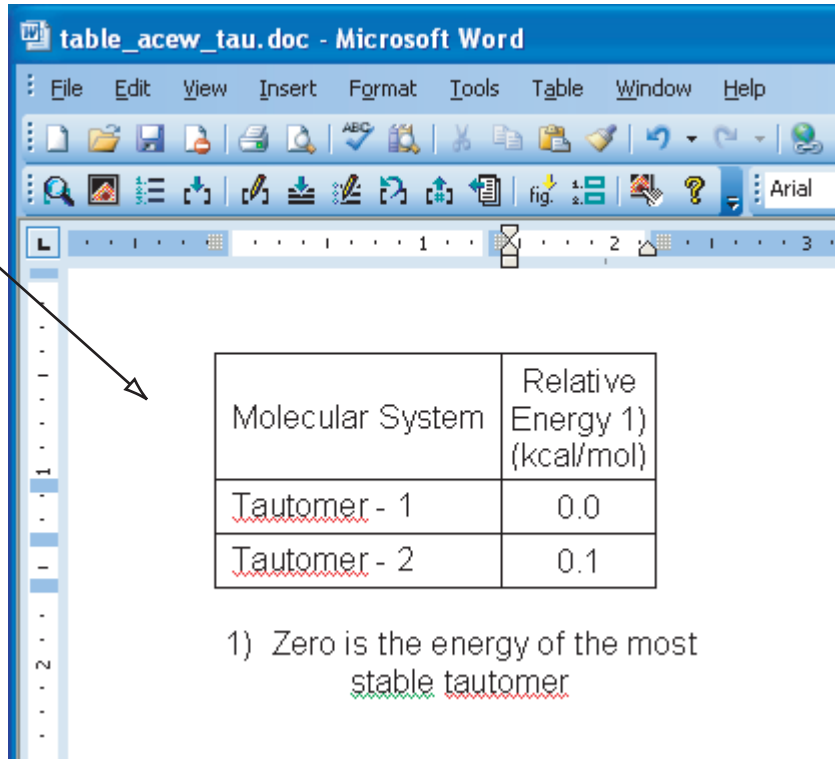
QM tautomerization - Alanine

Geometry optimization



QM tautomerization - Alanine

Final results

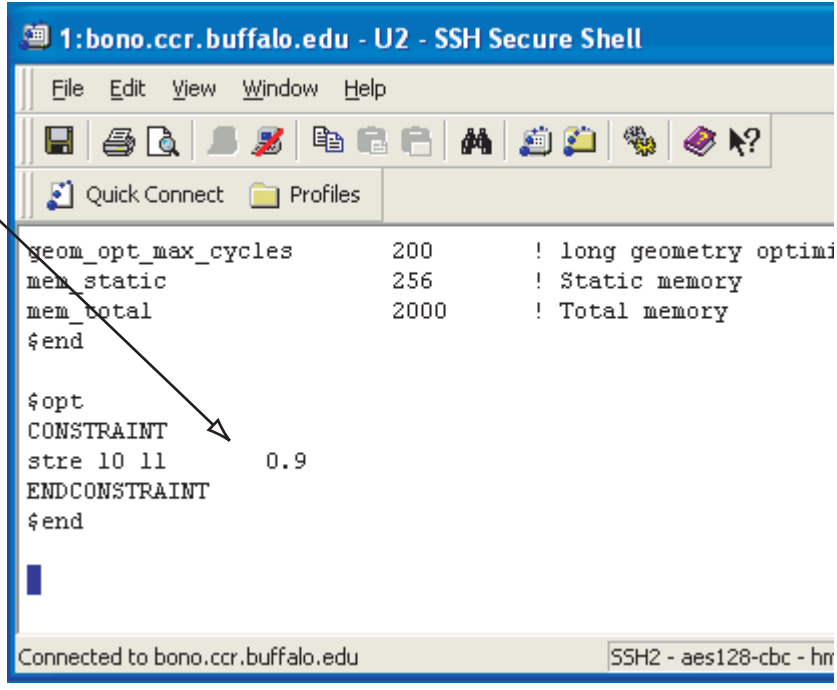


Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - 1	0.0
Tautomer - 2	0.1

1) Zero is the energy of the most stable tautomer

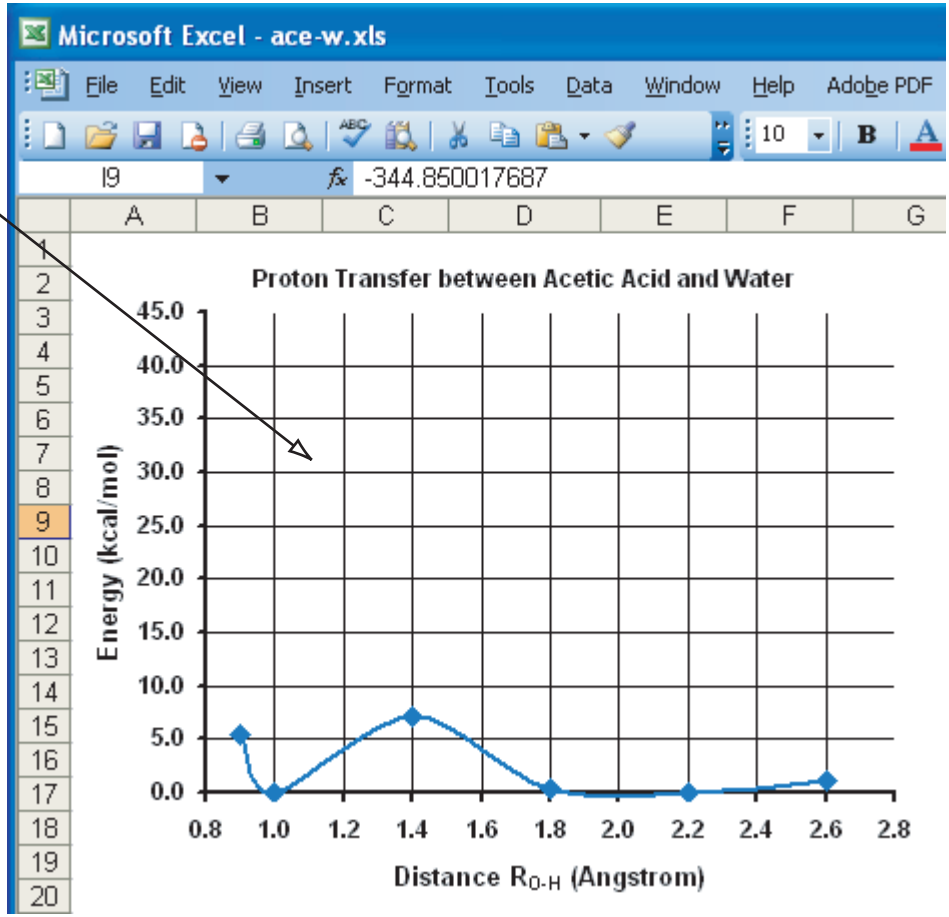
QM tautomerization - Alanine

Calculations with a constrained distance



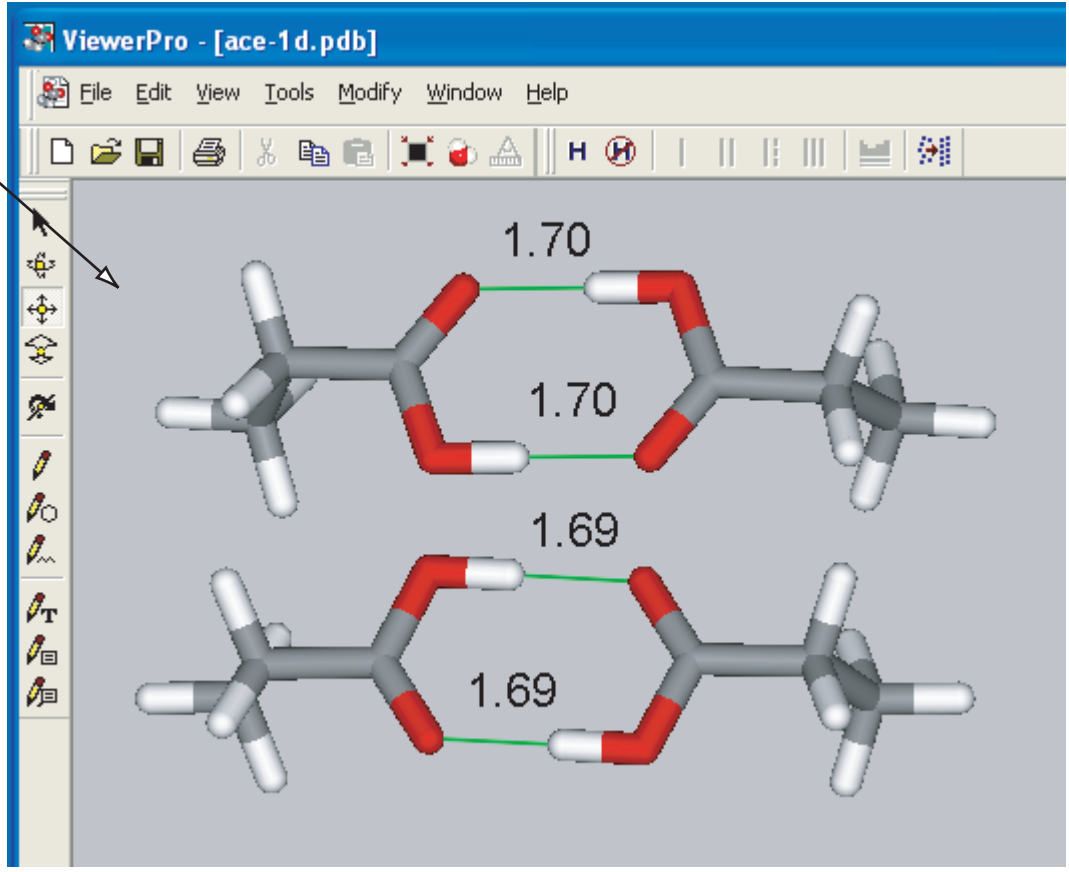
QM tautomerization - Alanine

Energy of the proton transfer



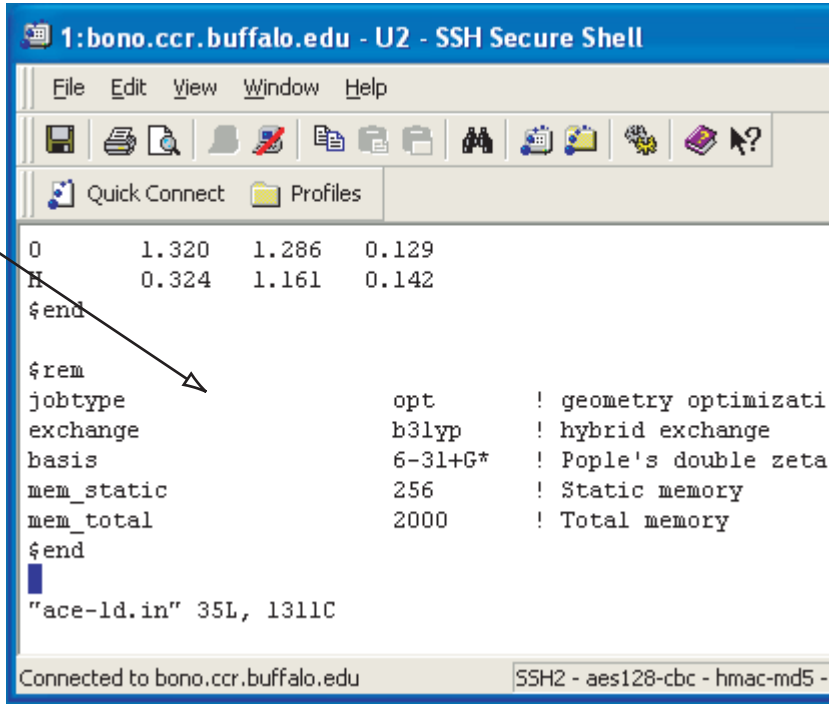
QM tautomerization - Alanine

Alanine dimers



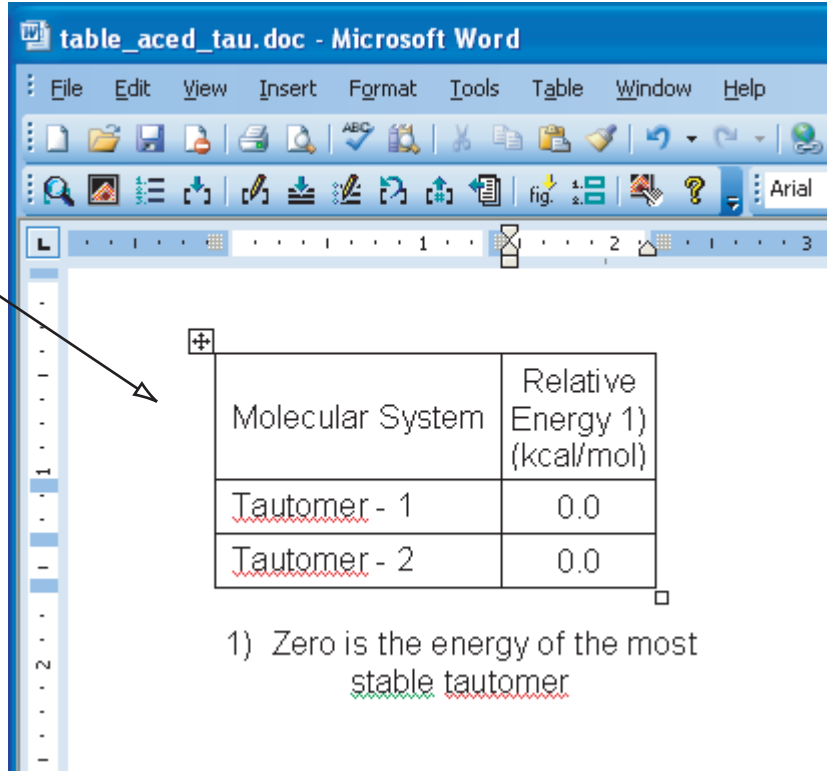
QM tautomerization - Alanine

Geometry optimization



QM tautomerization - Alanine

Final results

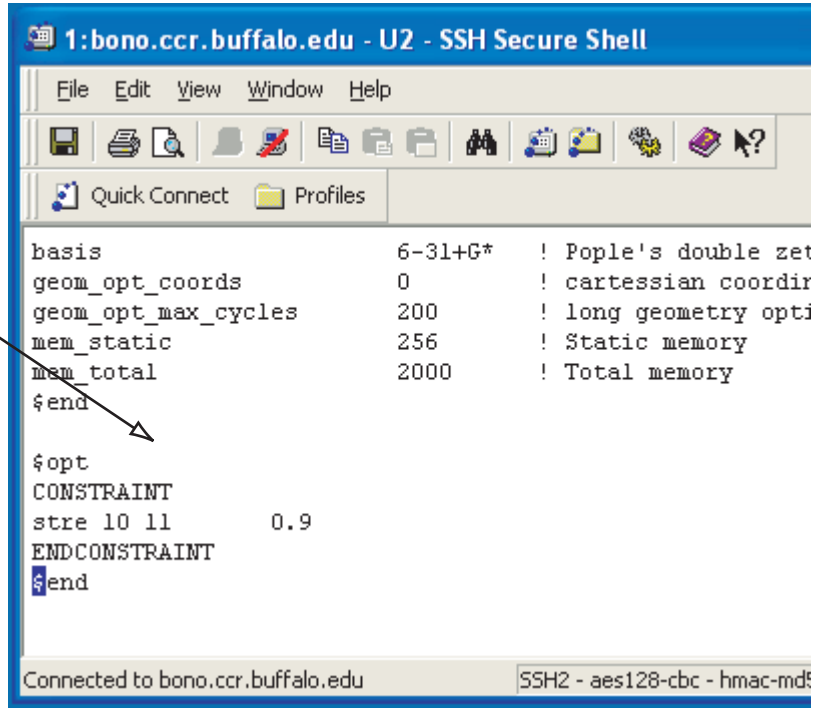


Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - 1	0.0
Tautomer - 2	0.0

1) Zero is the energy of the most stable tautomer

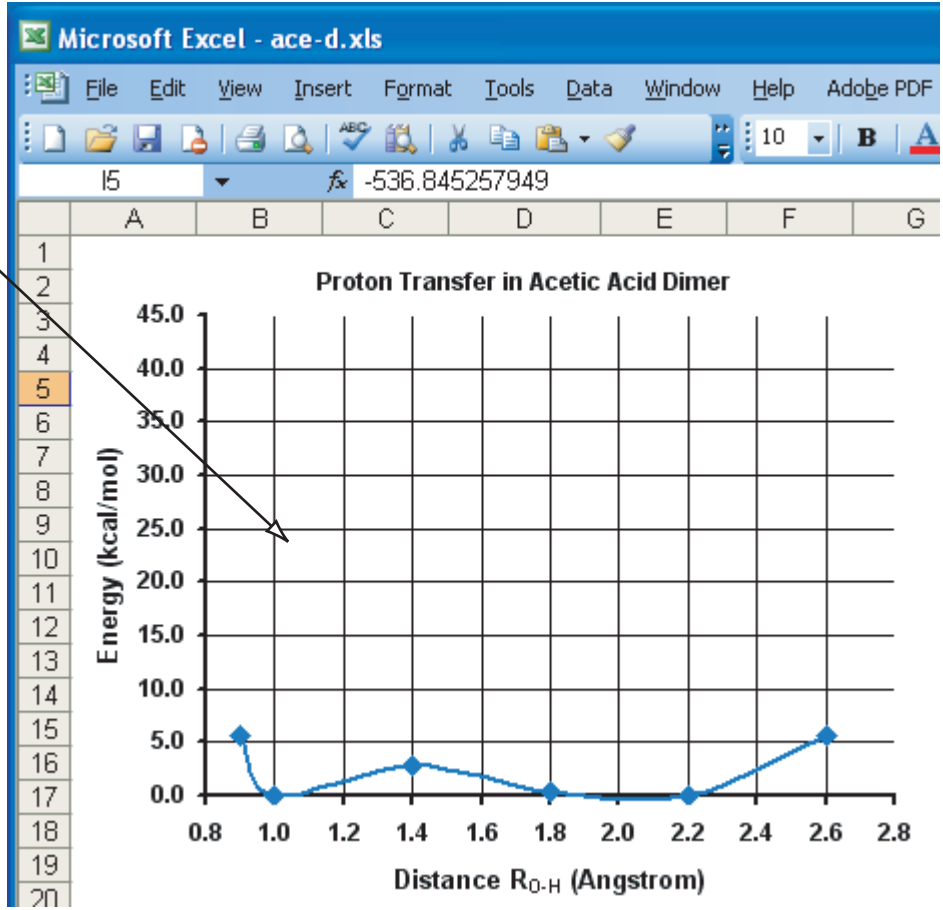
QM tautomerization - Alanine

Geometry optimization with a constrained distance



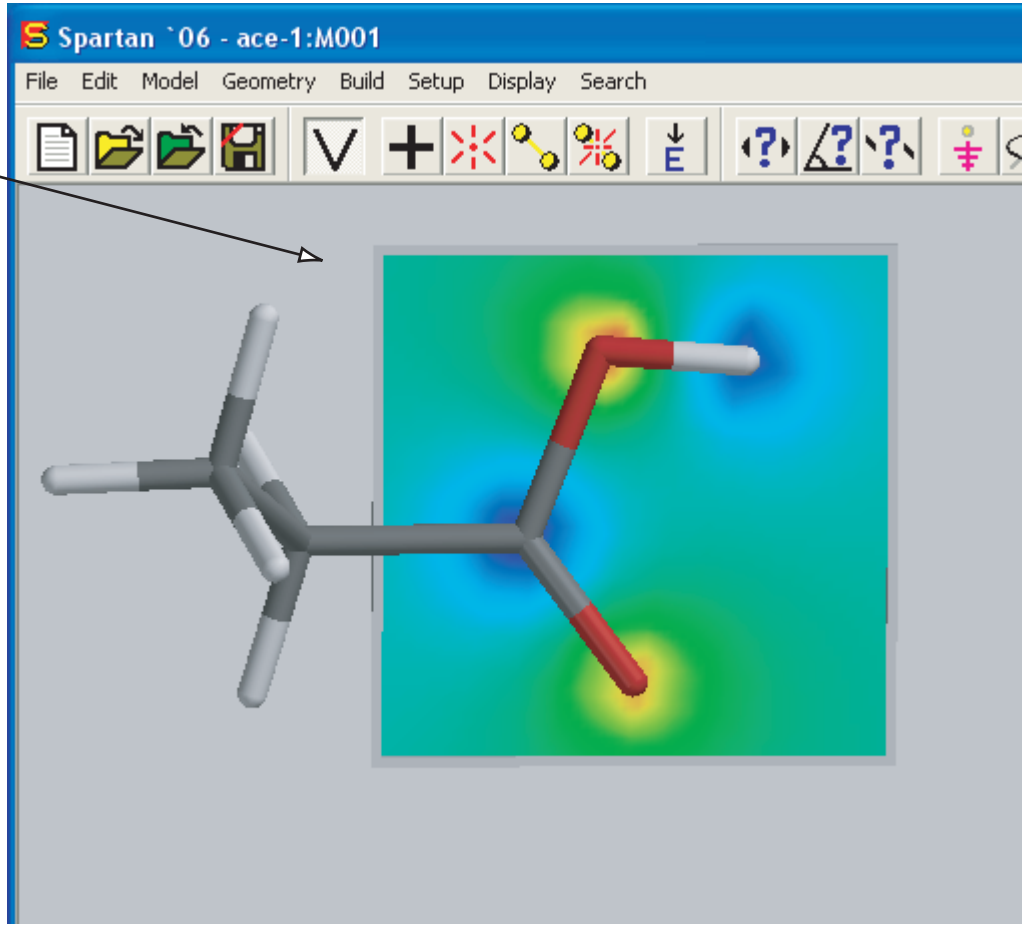
QM tautomerization - Alanine

Energy of proton transfer in the dimer



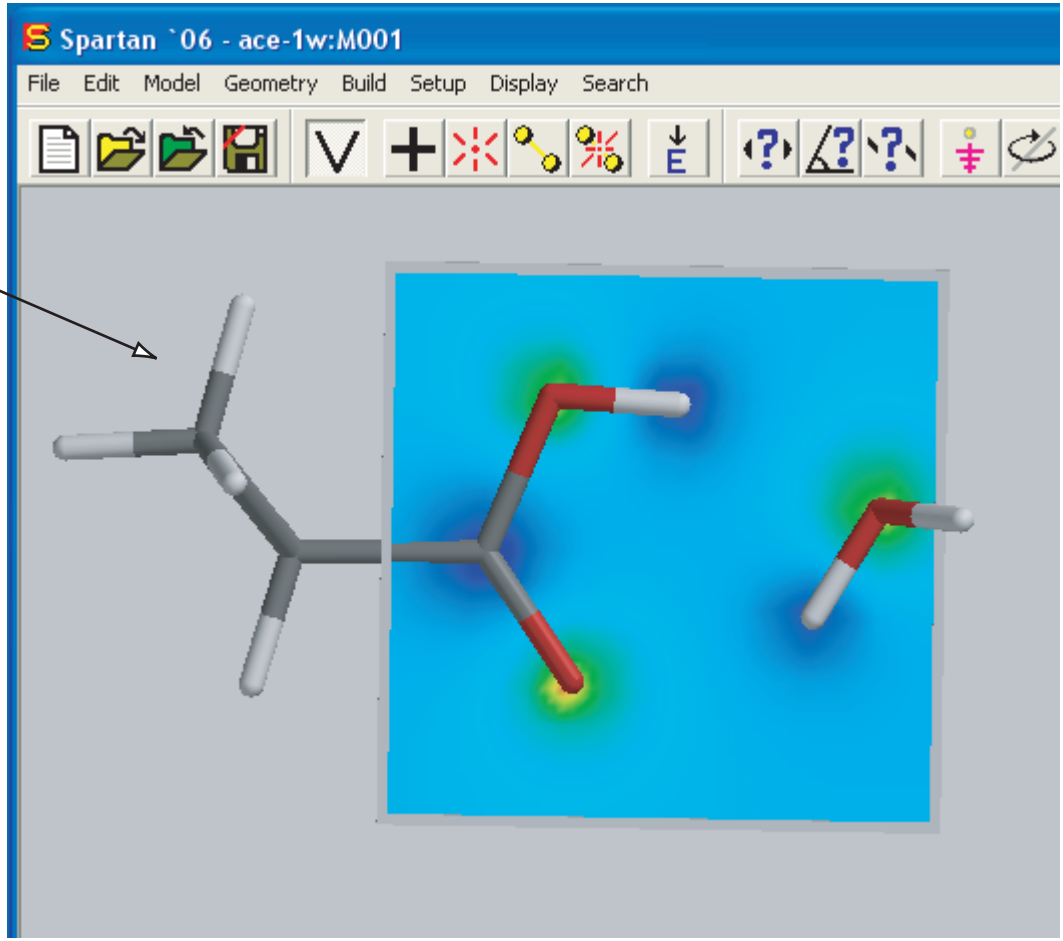
QM tautomerization - Alanine

Electrostatic potential



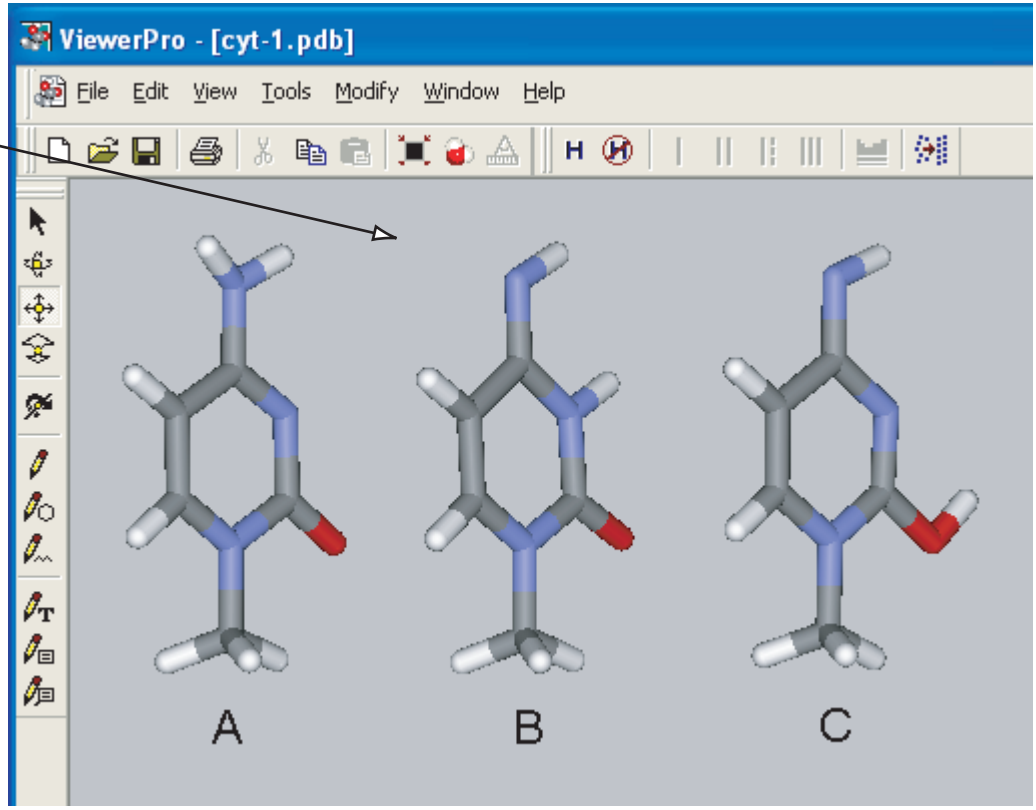
QM tautomerization - Alanine

Electrostatic potential of hydrogen bonded dimer



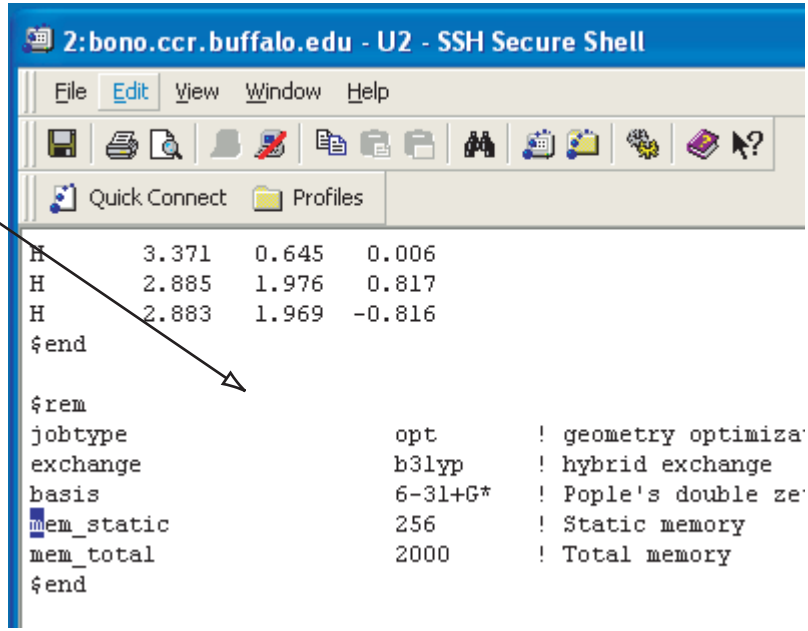
QM tautomerization - Cytosine

Geometry optimization of three cytosine tautomers



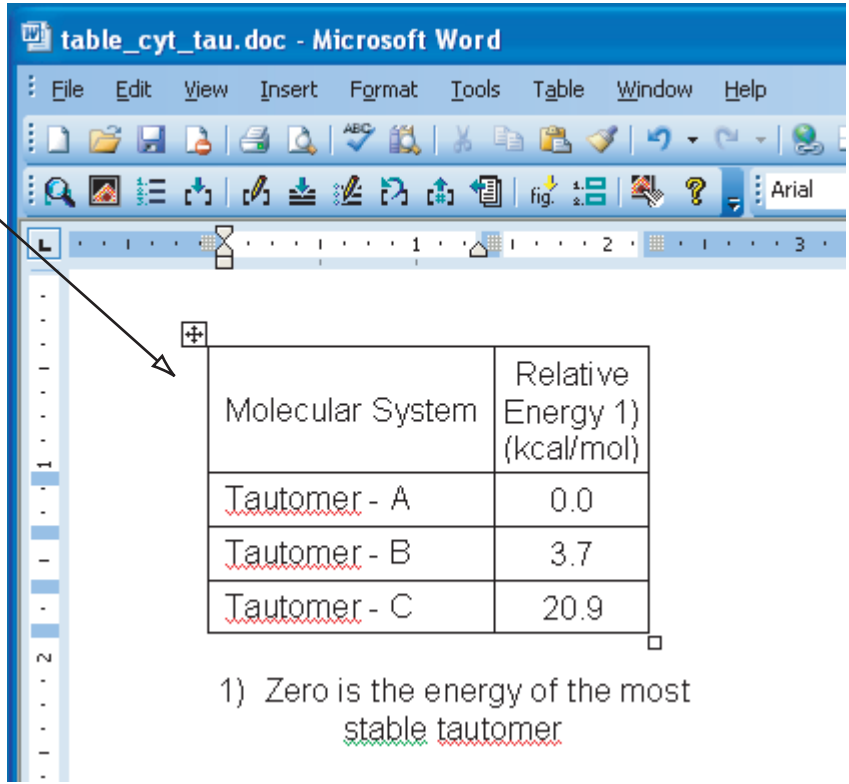
QM tautomerization - Cytosine

Geometry optimization of three cytosine tautomers



QM tautomerization - Cytosine

Final results of the calculations

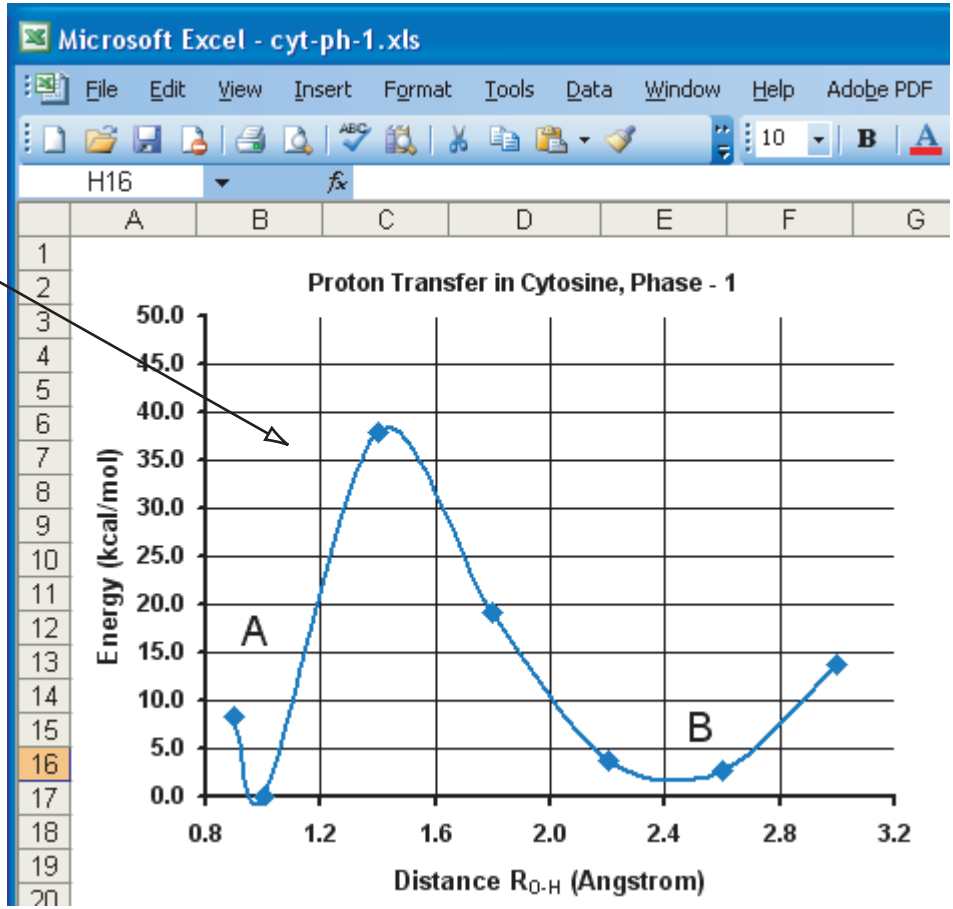


Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - A	0.0
Tautomer - B	3.7
Tautomer - C	20.9

1) Zero is the energy of the most stable tautomer

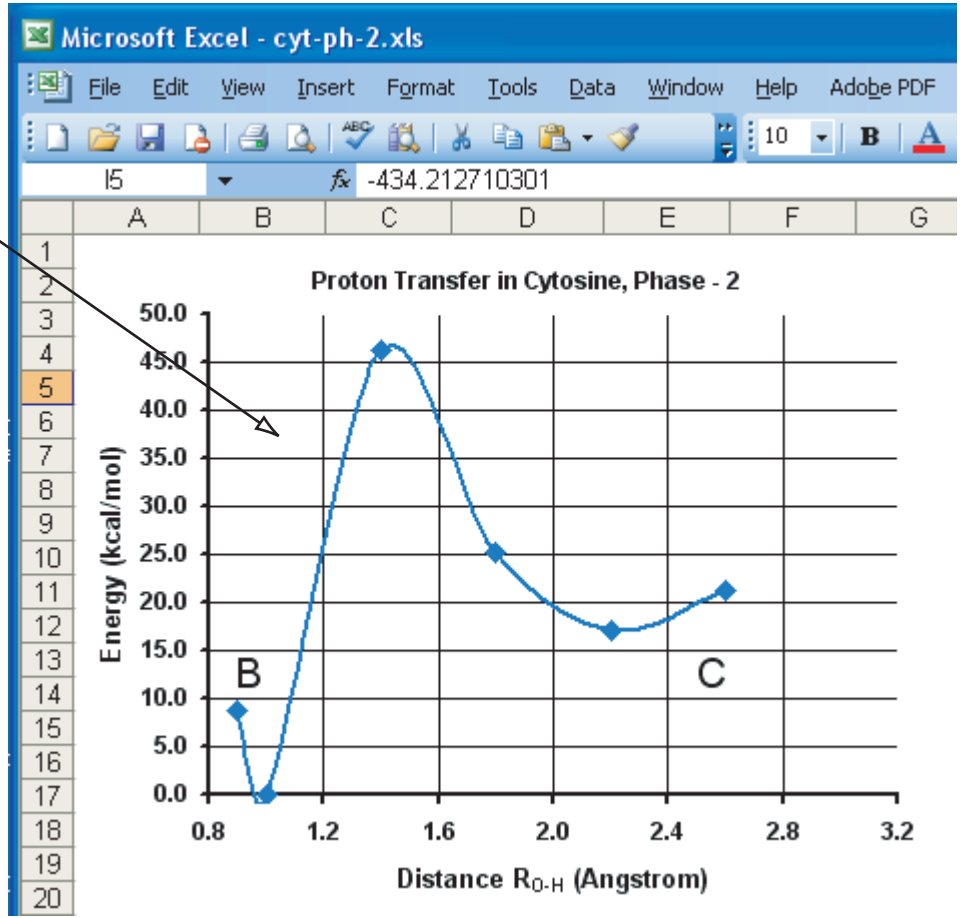
QM tautomerization - Cytosine

Energy of the first phase of proton transfer



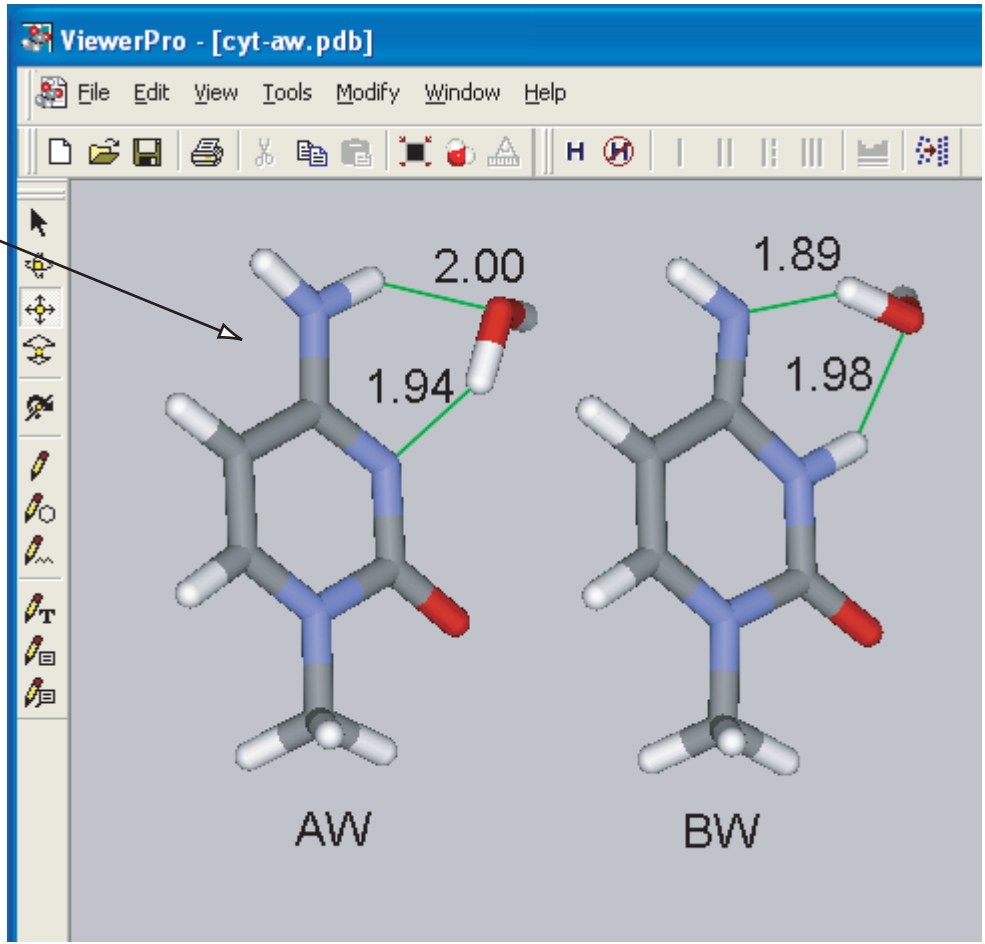
QM tautomerization - Cytosine

Energy of the second phase of proton transfer



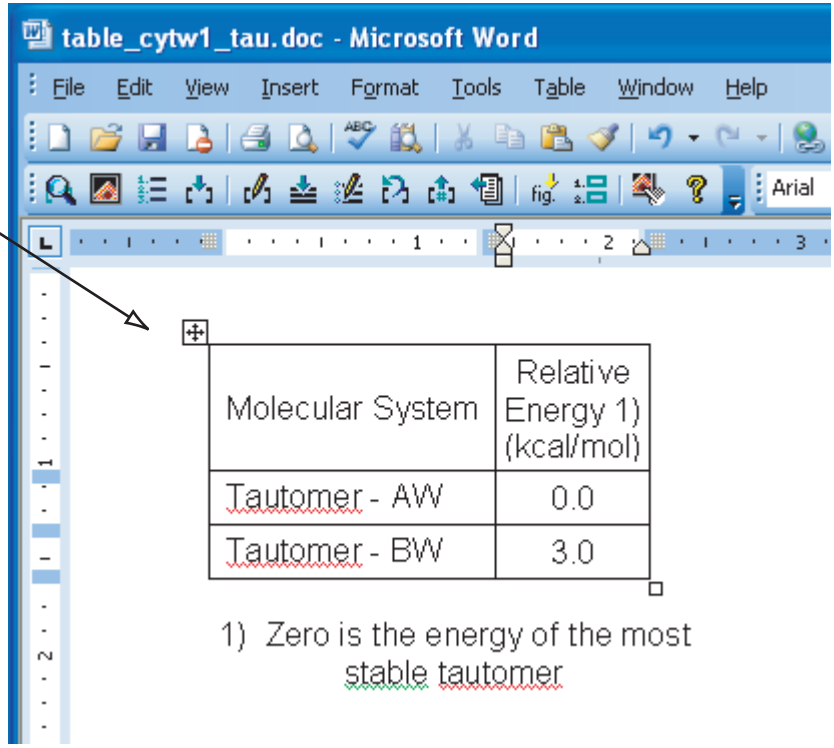
QM tautomerization - Cytosine

Two tautomers of the cysteine and water dimer



QM tautomerization - Cytosine

Energies of the calculated dimers

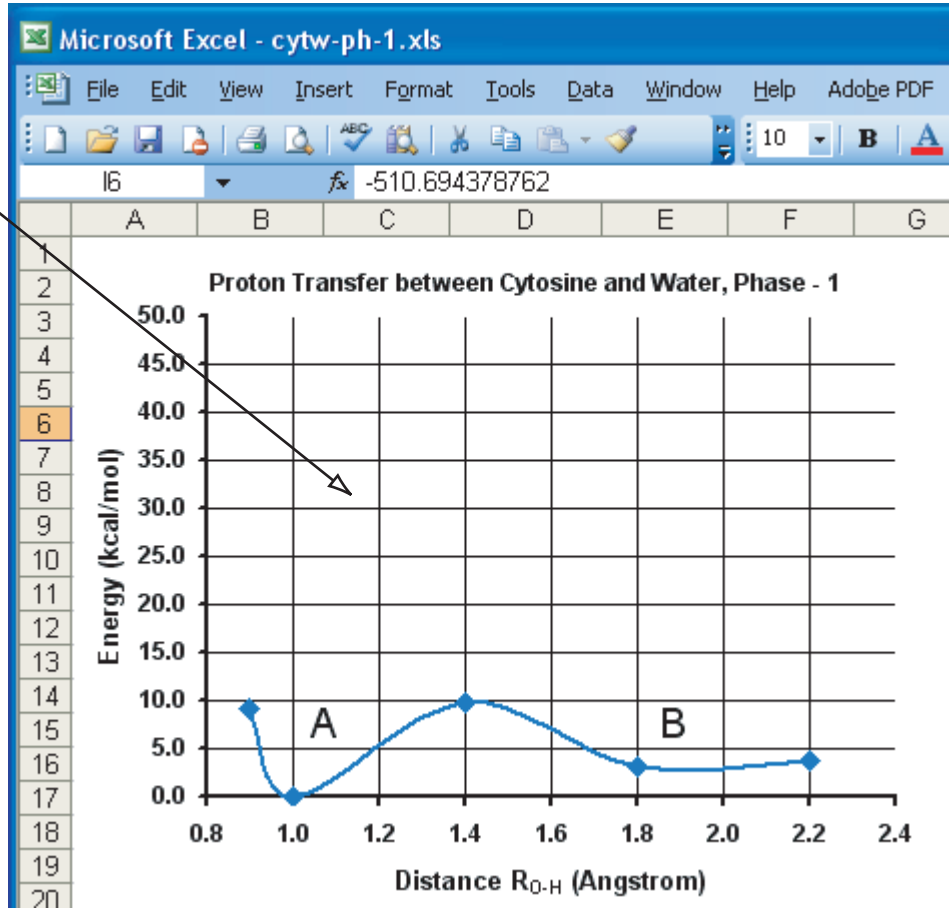


Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - AW	0.0
Tautomer - BW	3.0

1) Zero is the energy of the most stable tautomer

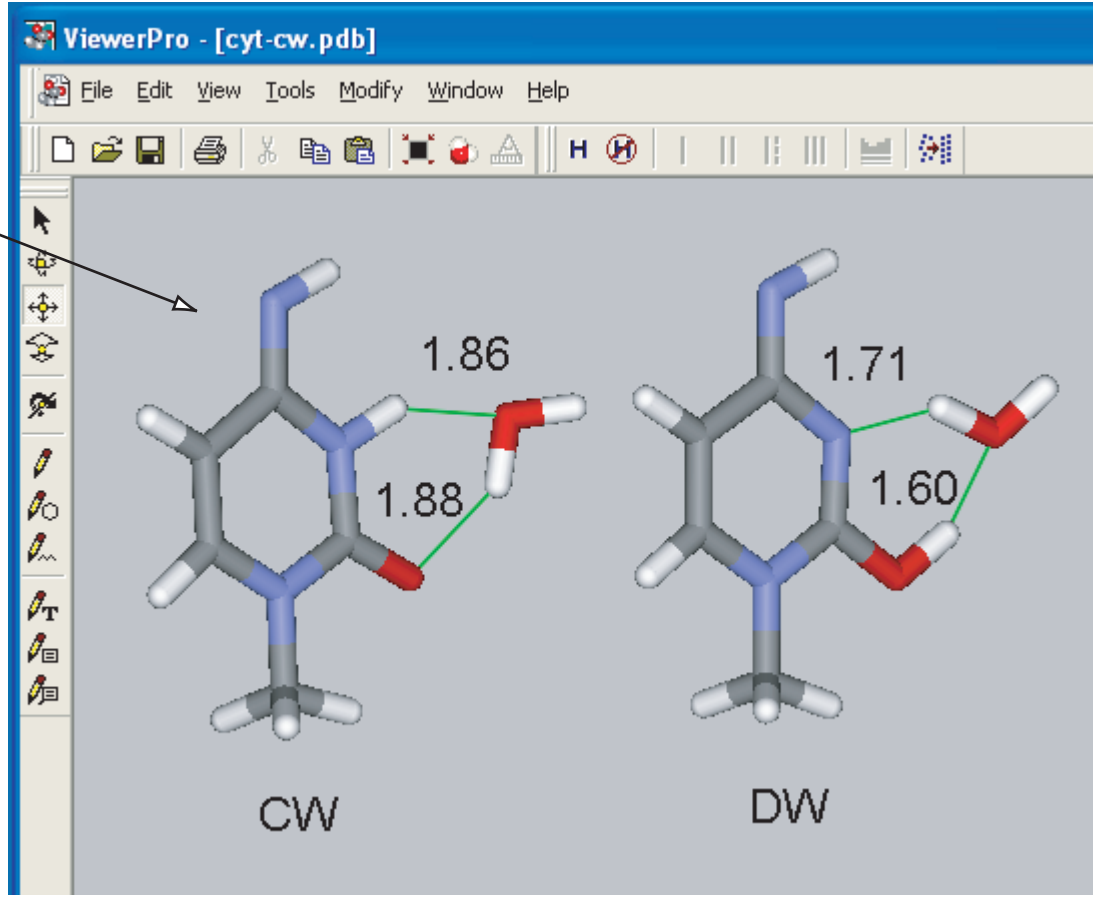
QM tautomerization - Cytosine

Energy of proton transfer



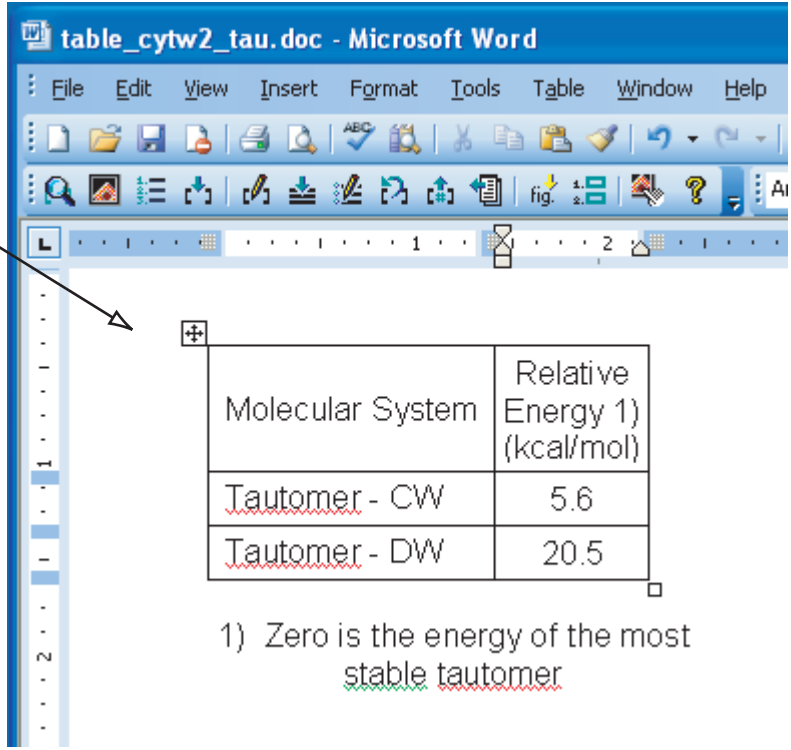
QM tautomerization - Cytosine

Two tautomers of the cysteine water dimer



QM tautomerization - Cytosine

Results of the calculations

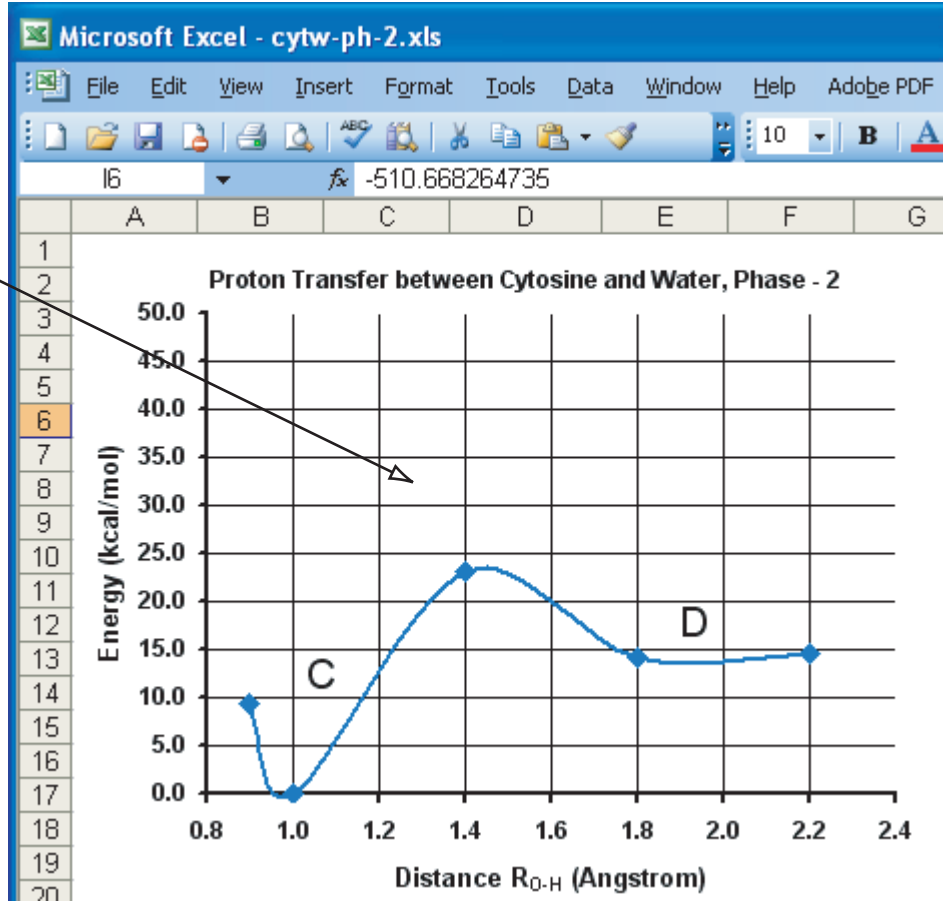


Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - CW	5.6
Tautomer - DW	20.5

1) Zero is the energy of the most stable tautomer

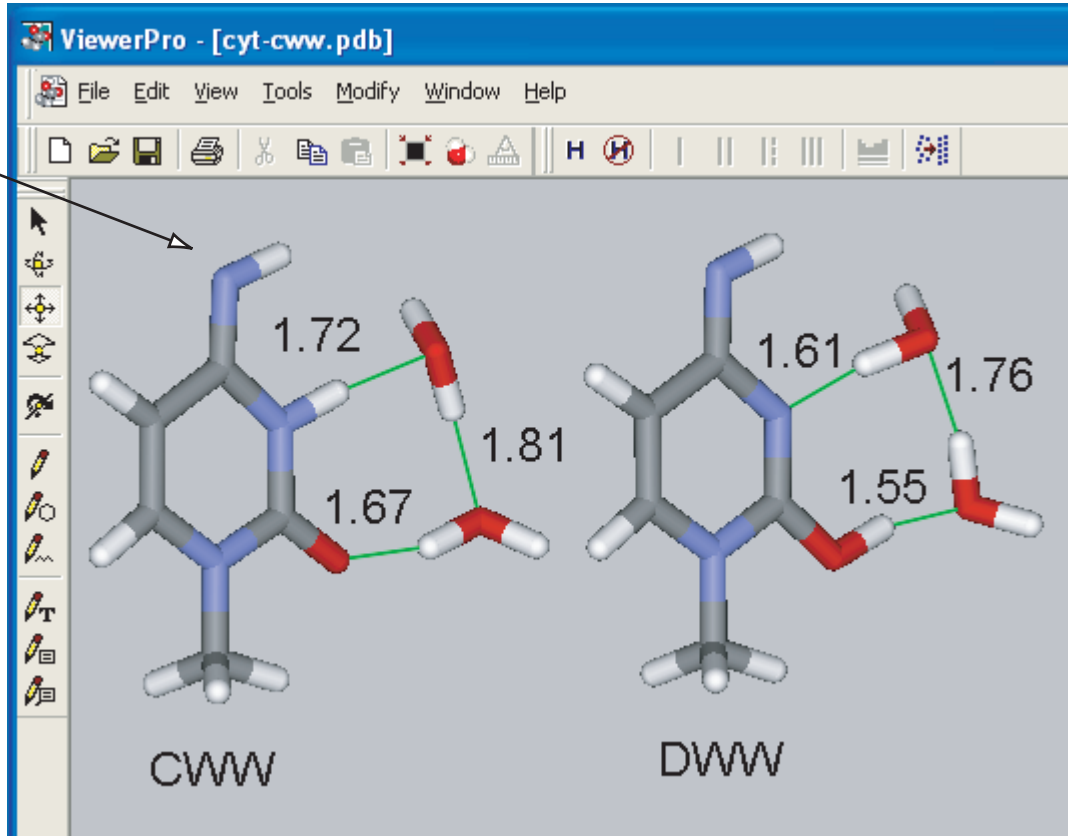
QM tautomerization - Cytosine

Energy of proton transfer between tautomers of the dimer



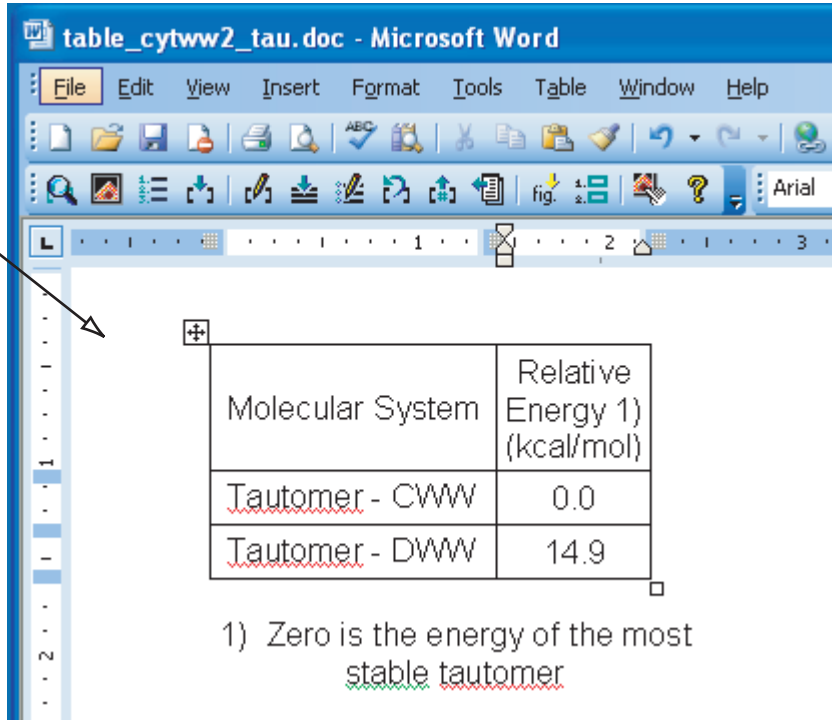
QM tautomerization - Cytosine

Two tautomers of a cysteine water trimer



QM tautomerization - Cytosine

Results of the calculations

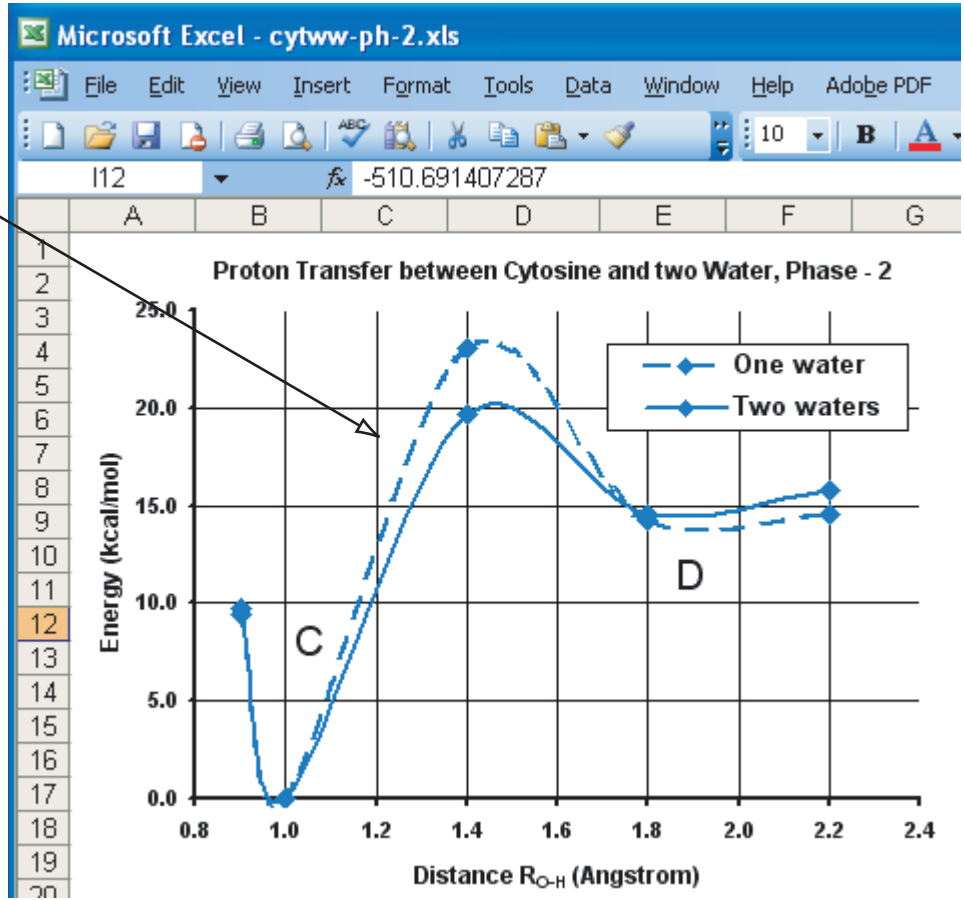


Molecular System	Relative Energy 1) (kcal/mol)
Tautomer - CWW	0.0
Tautomer - DWW	14.9

1) Zero is the energy of the most stable tautomer

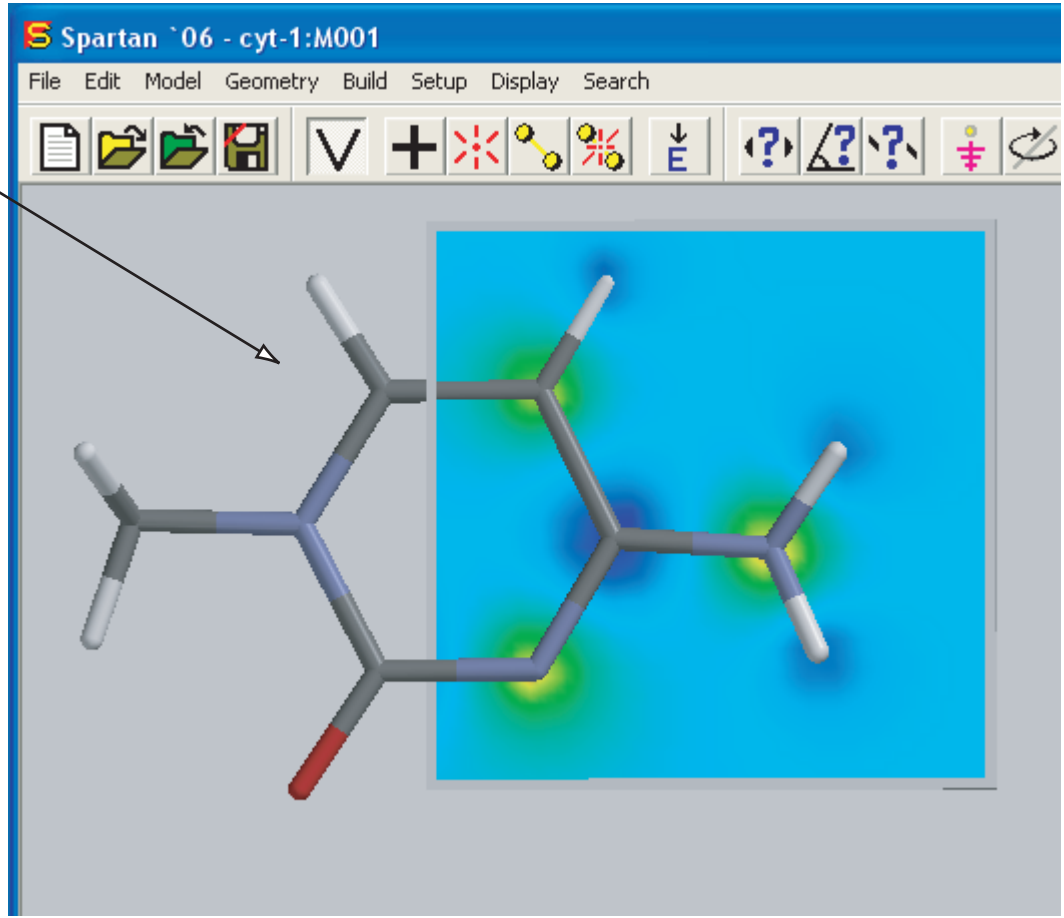
QM tautomerization - Cytosine

Energy of proton transfer in cytosine dimer and trimer



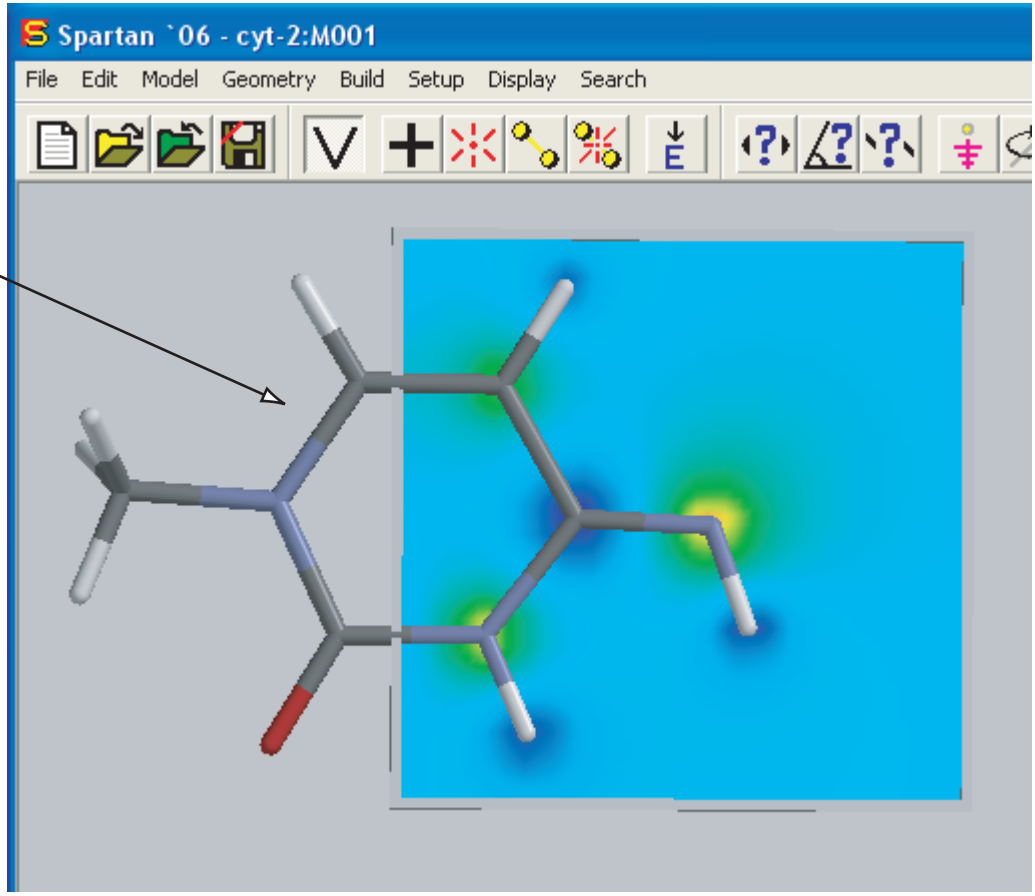
QM tautomerization - Cytosine

Electrostatic potential of cytosine tautomer - 1



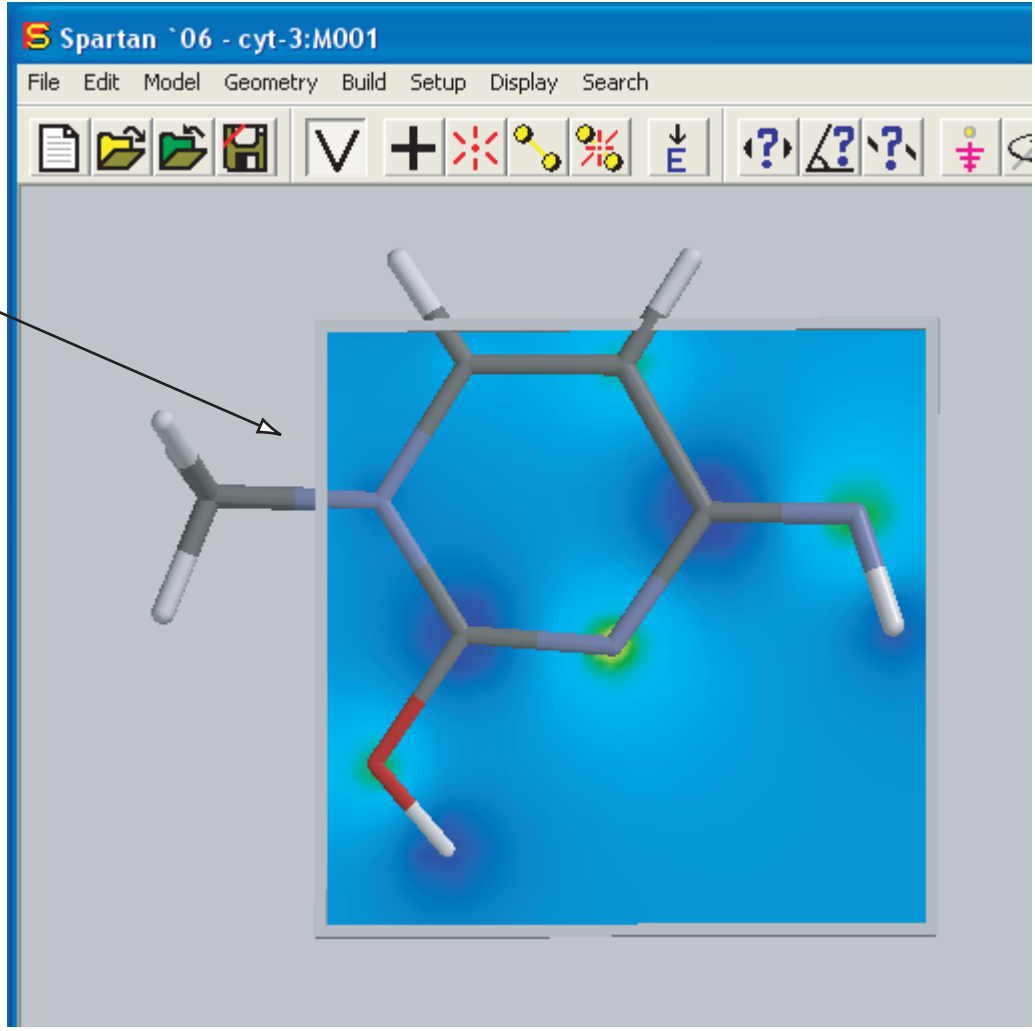
QM tautomerization - Cytosine

Electrostatic potential of cytosine tautomer - 2



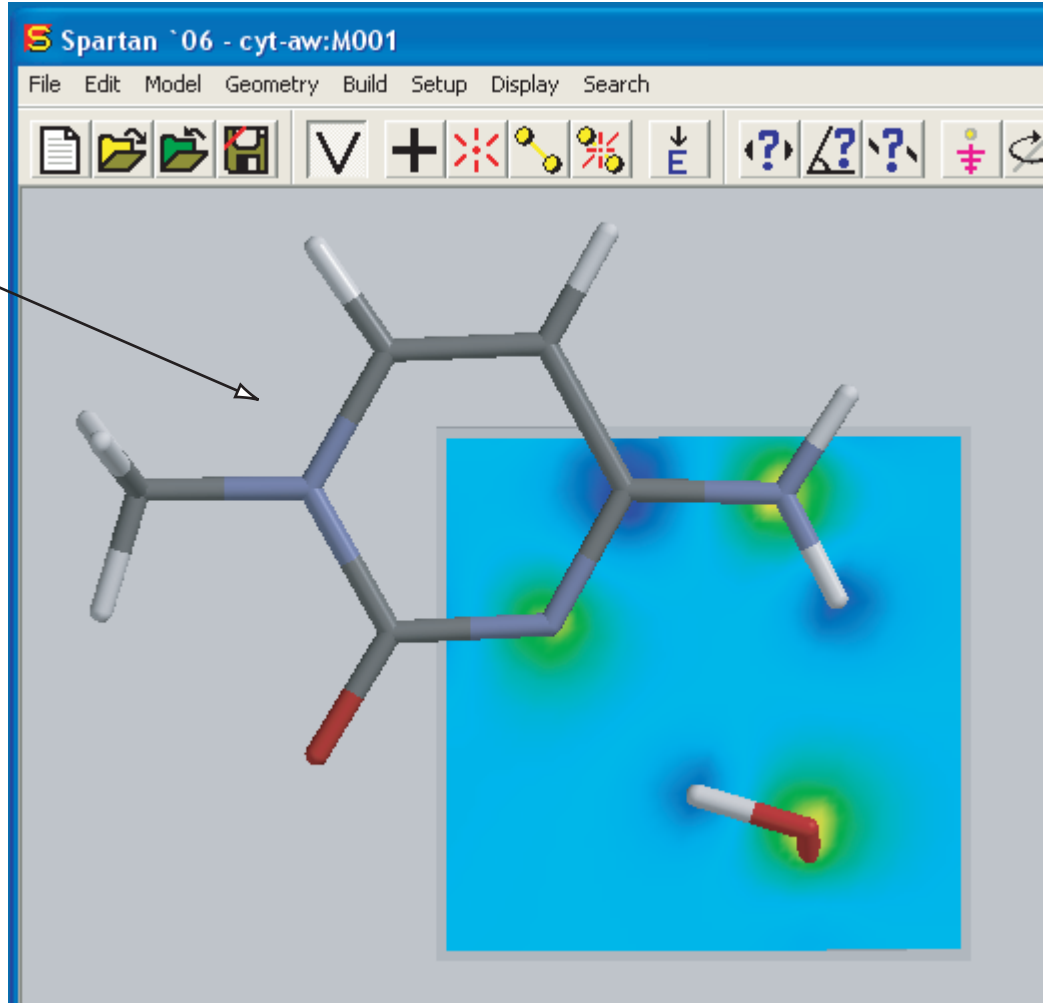
QM tautomerization - Cytosine

Electrostatic potential of cytosine tautomer - 3



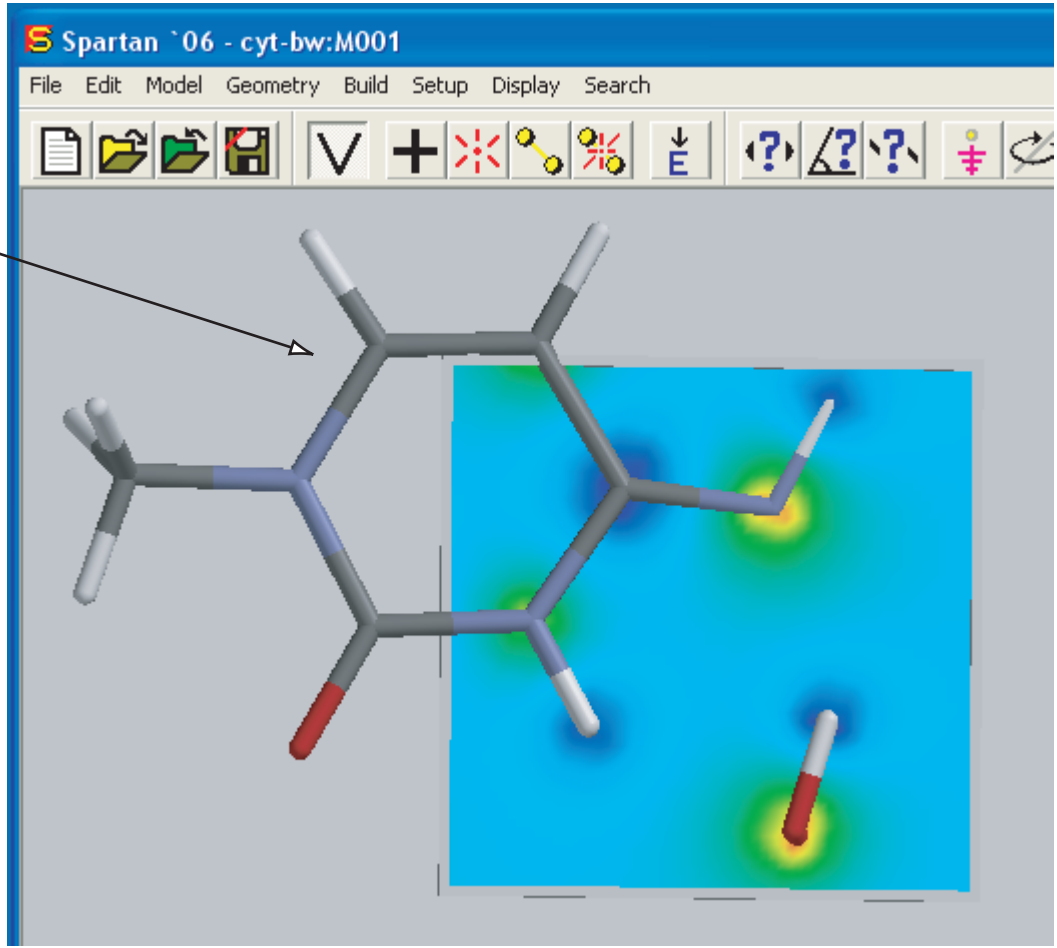
QM tautomerization - Cytosine

Electrostatic potential of cytosine water dimer (AW)



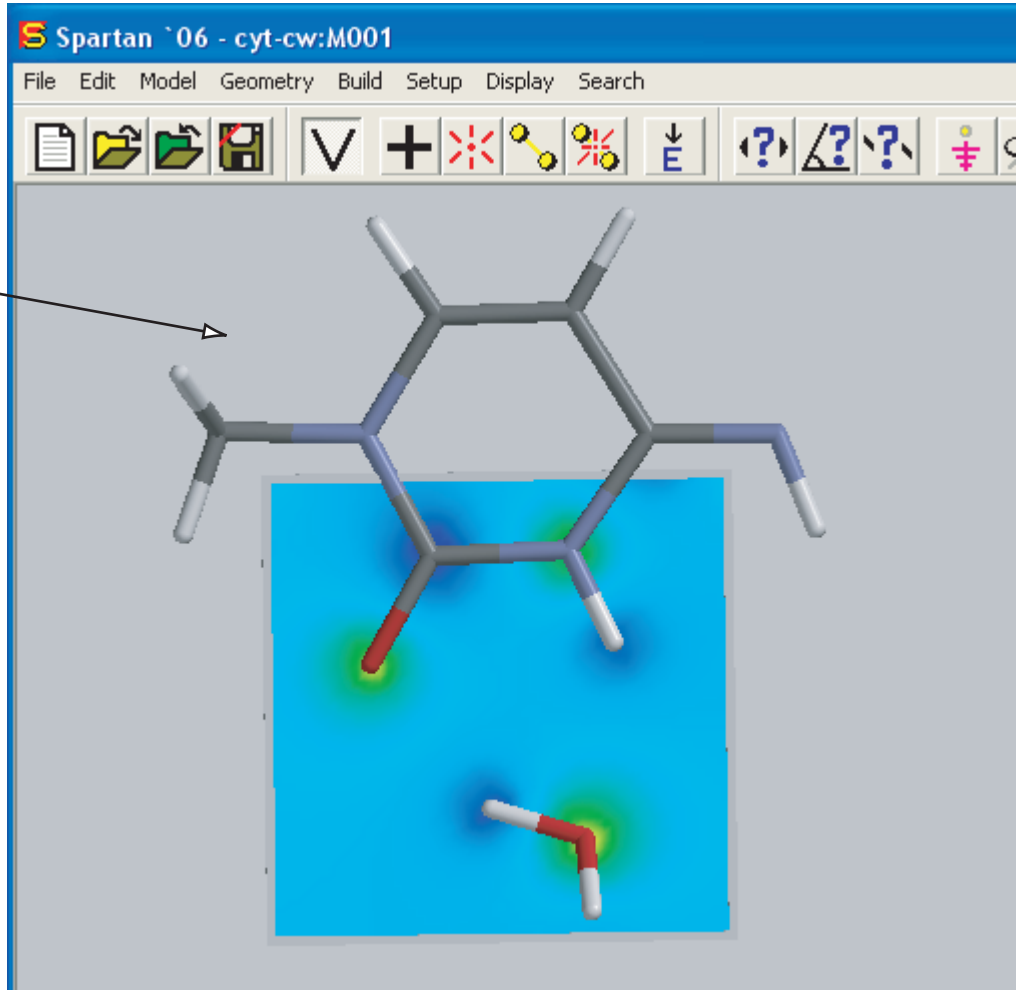
QM tautomerization - Cytosine

Electrostatic potential of cytosine water dimer (BW)



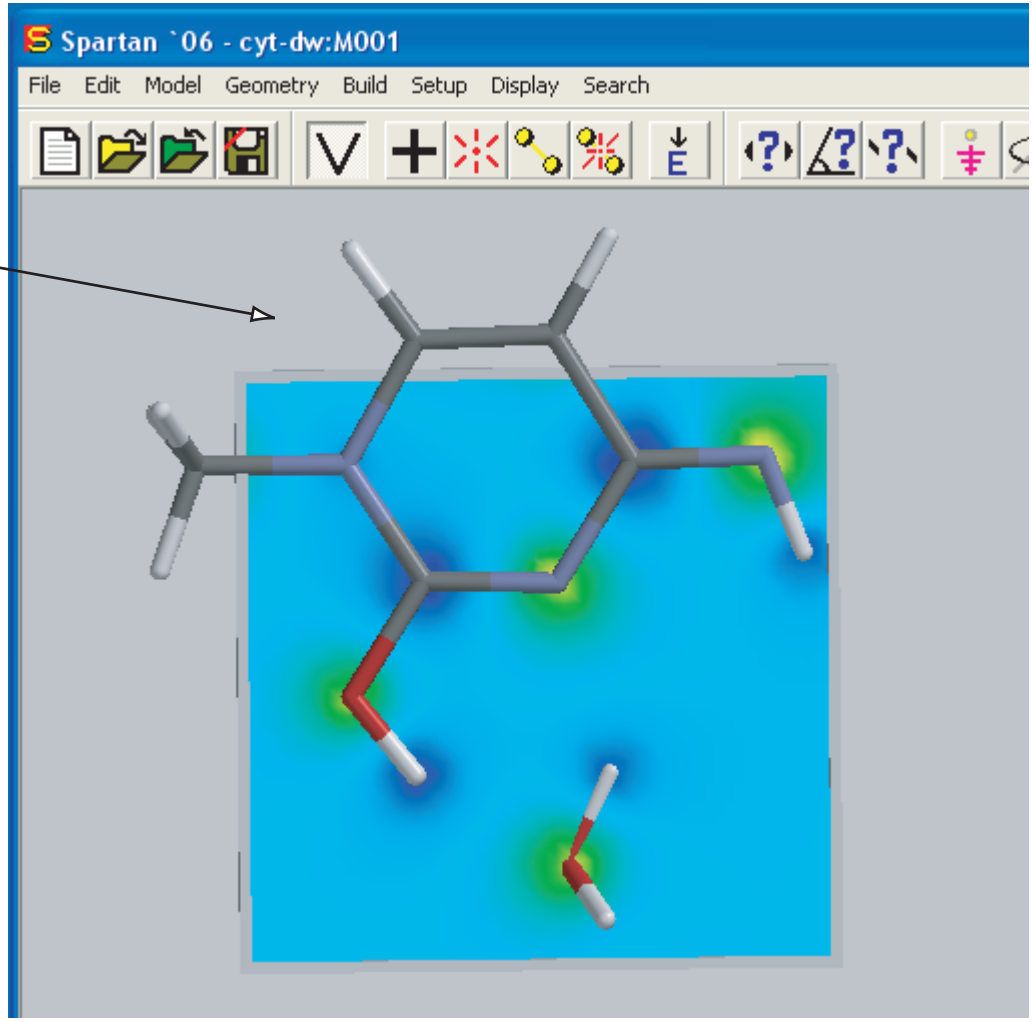
QM tautomerization - Cytosine

Electrostatic potential of cytosine water dimer (CW)



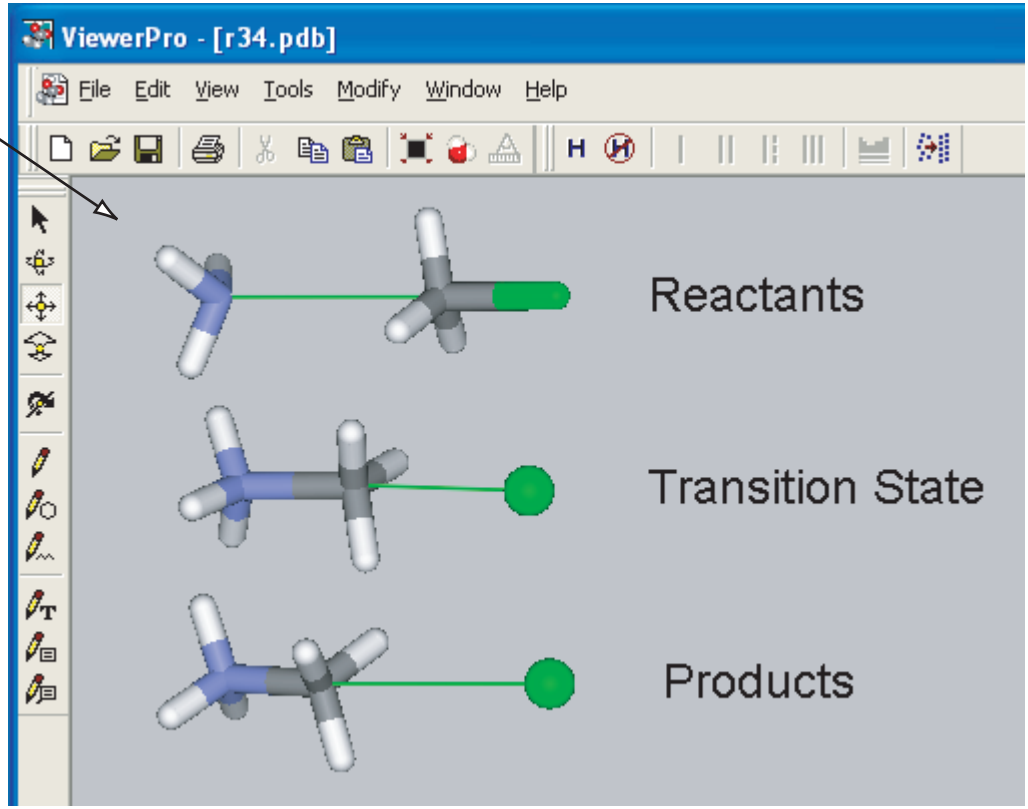
QM tautomerization - Cytosine

Electrostatic potential of cytosine water dimer (DW)

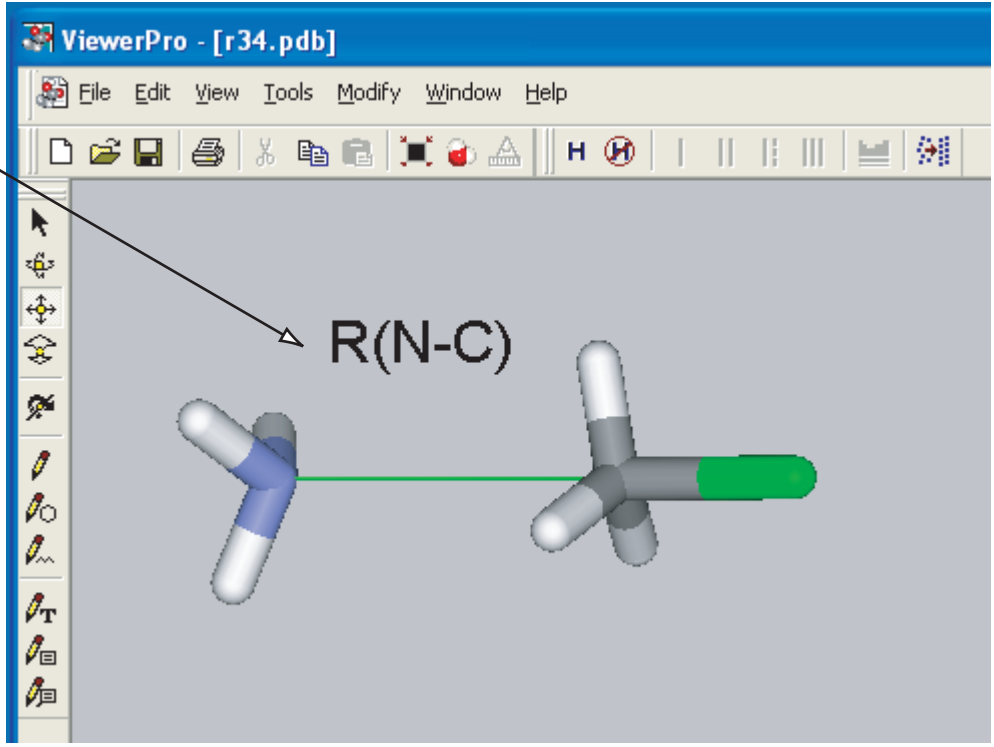


QM Reaction Profiles - Menshutkin reaction

Menshutkin reaction

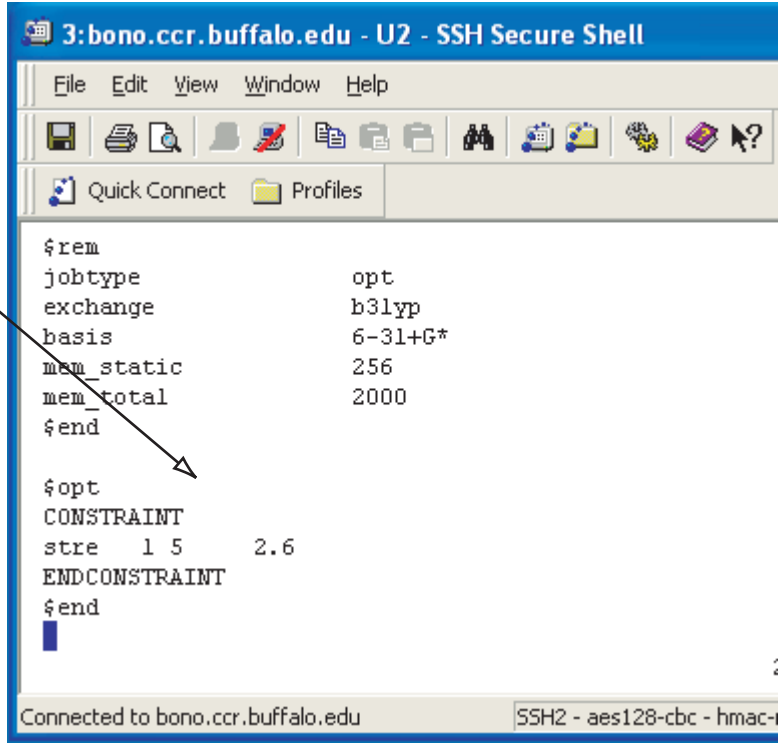


Reaction coordinate for reactants

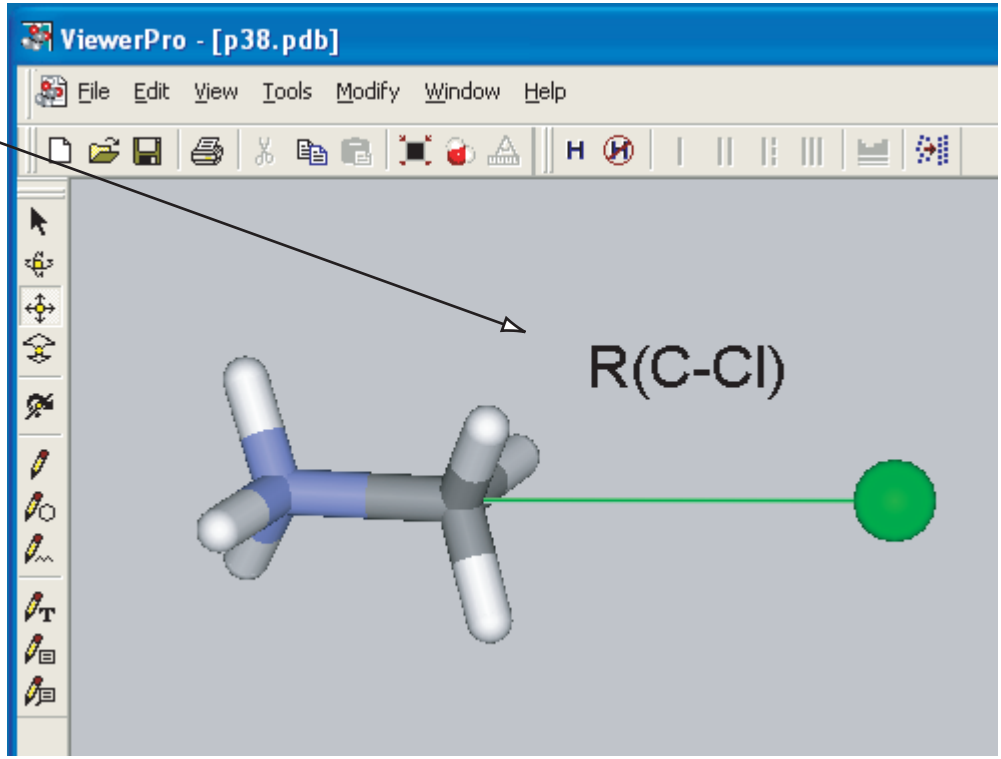


QM Reaction Profiles - Menshutkin reaction

Constrained geometry optimization

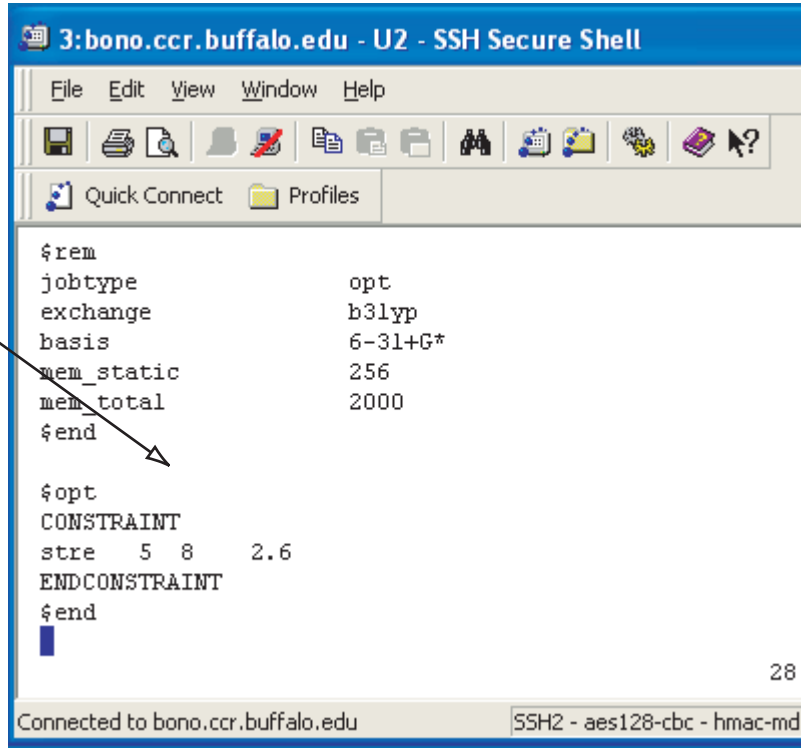


Reaction coordinate for products



QM Reaction Profiles - Menshutkin reaction

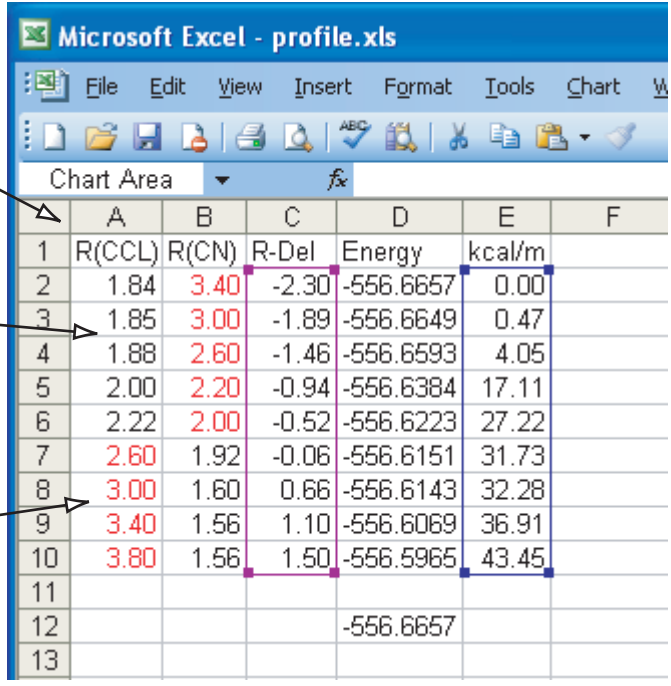
Constrained geometry optimization



Results of the calculations

Reactants

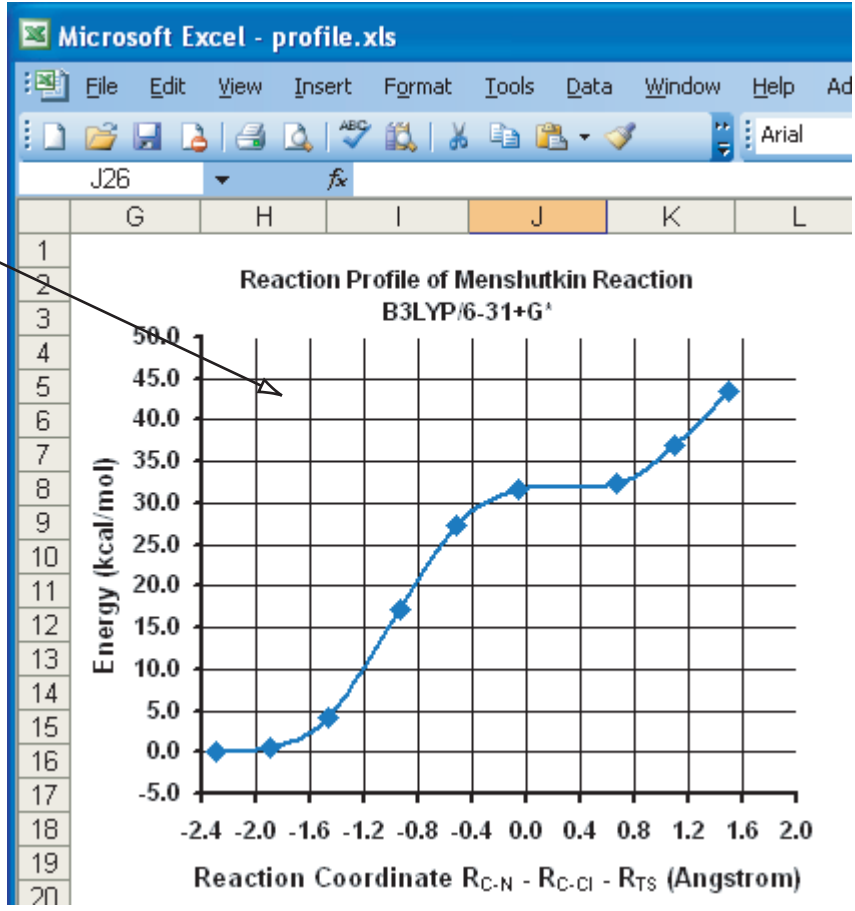
Products



	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						

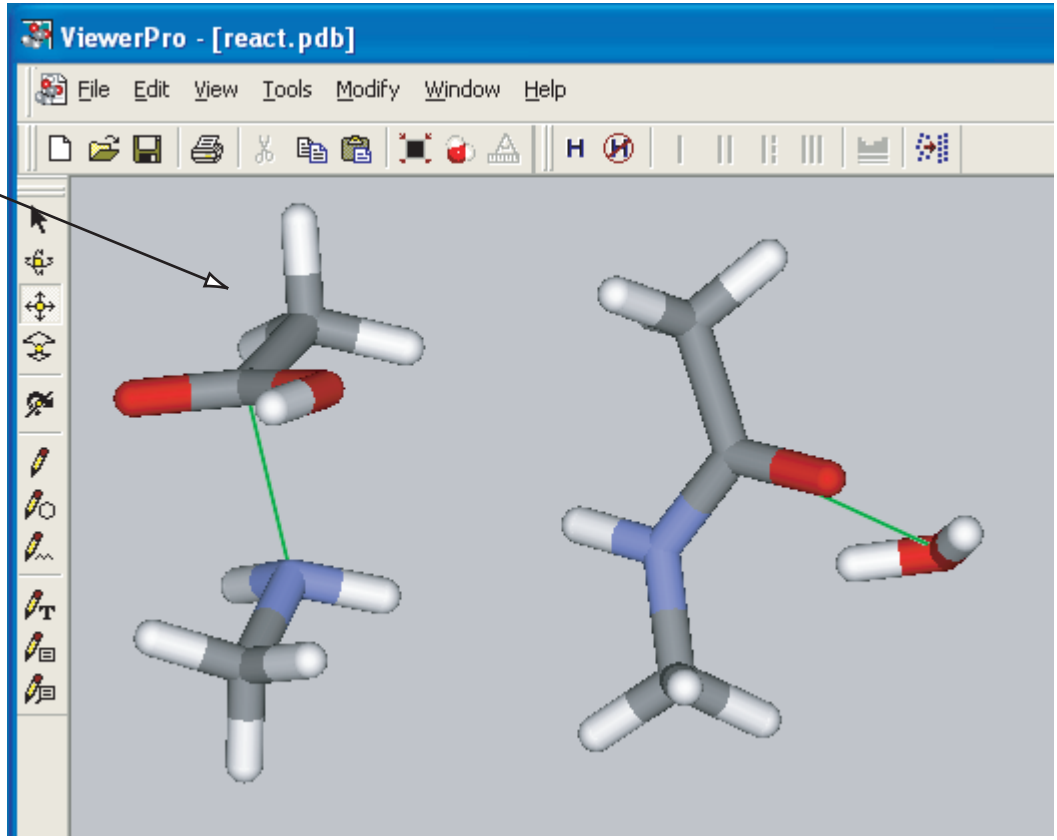
QM Reaction Profiles - Menshutkin reaction

Reaction profile



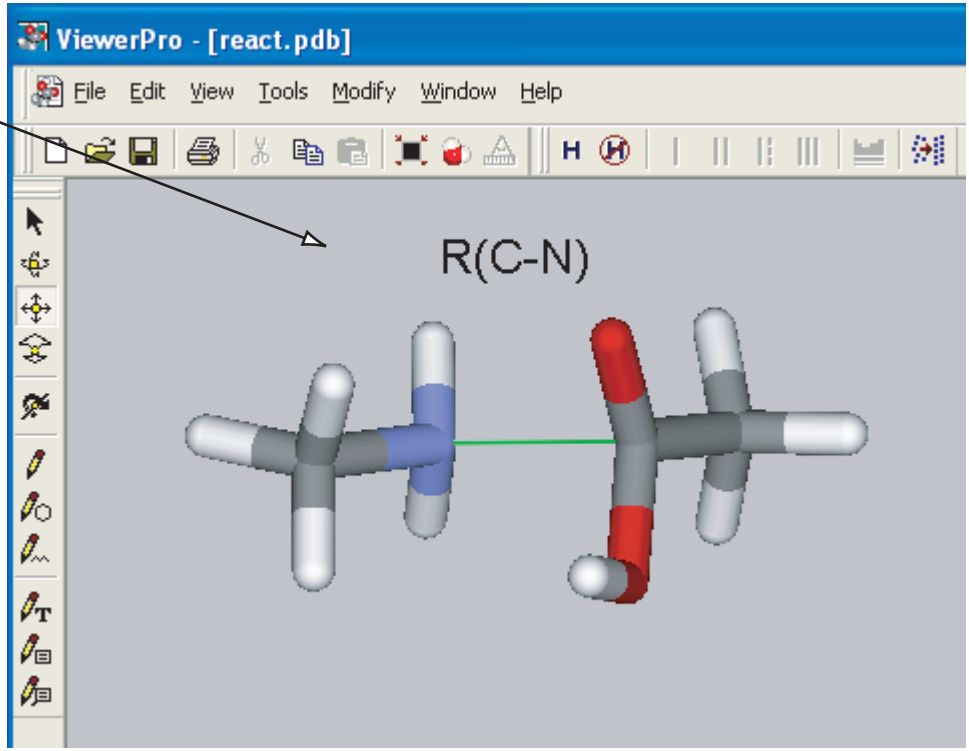
QM Reaction Profiles - Peptide Reaction

Creating a peptide bond

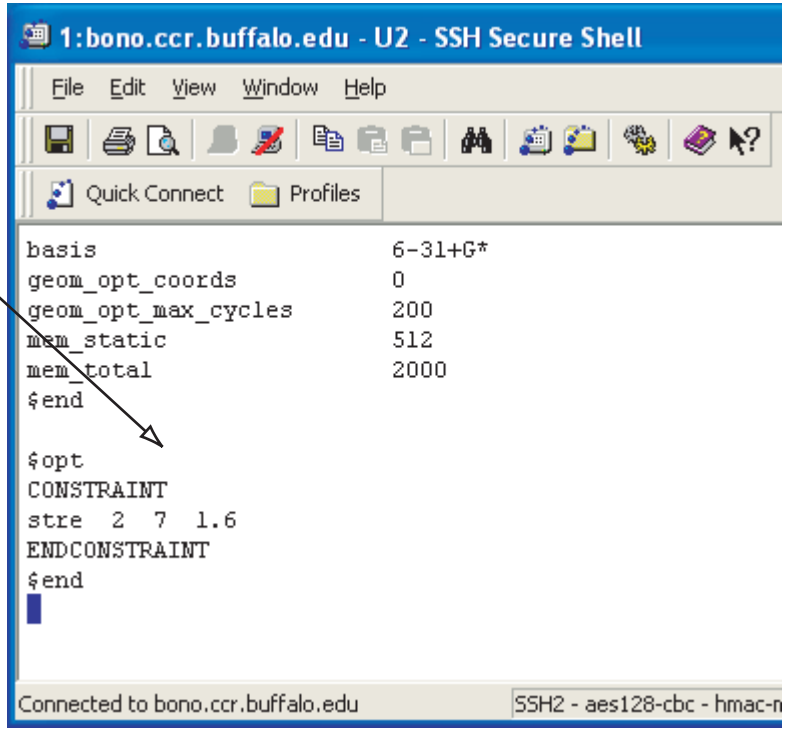


QM Reaction Profiles - Peptide Reaction

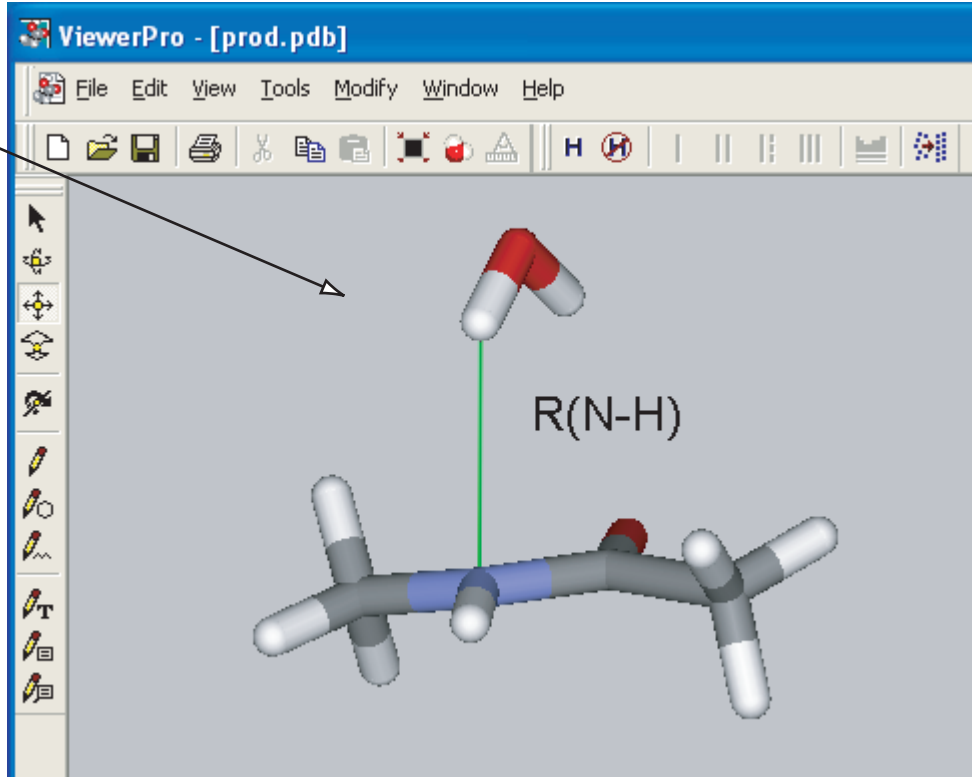
Reaction coordinate in reactants



Geometry optimization with a constrained distance

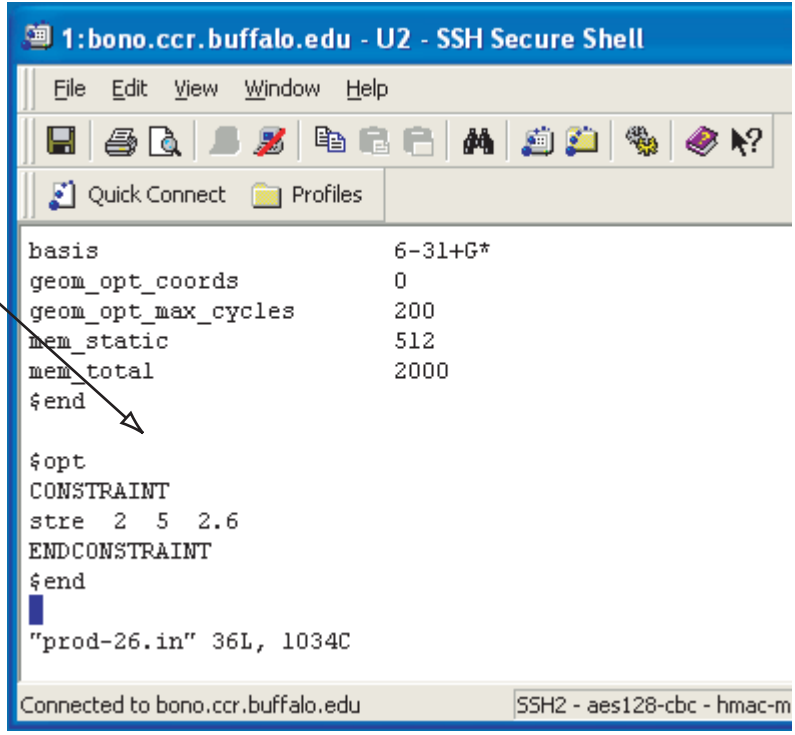


Reaction coordinate in products



QM Reaction Profiles - Peptide Reaction

Geometry optimization with a constrained distance

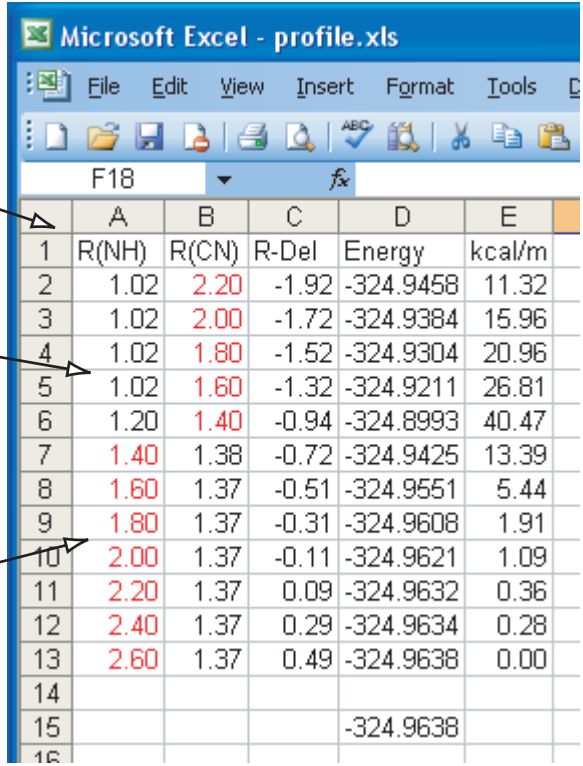


QM Reaction Profiles - Peptide Reaction

Results of the calculations

Reactants

Products



Microsoft Excel - profile.xls

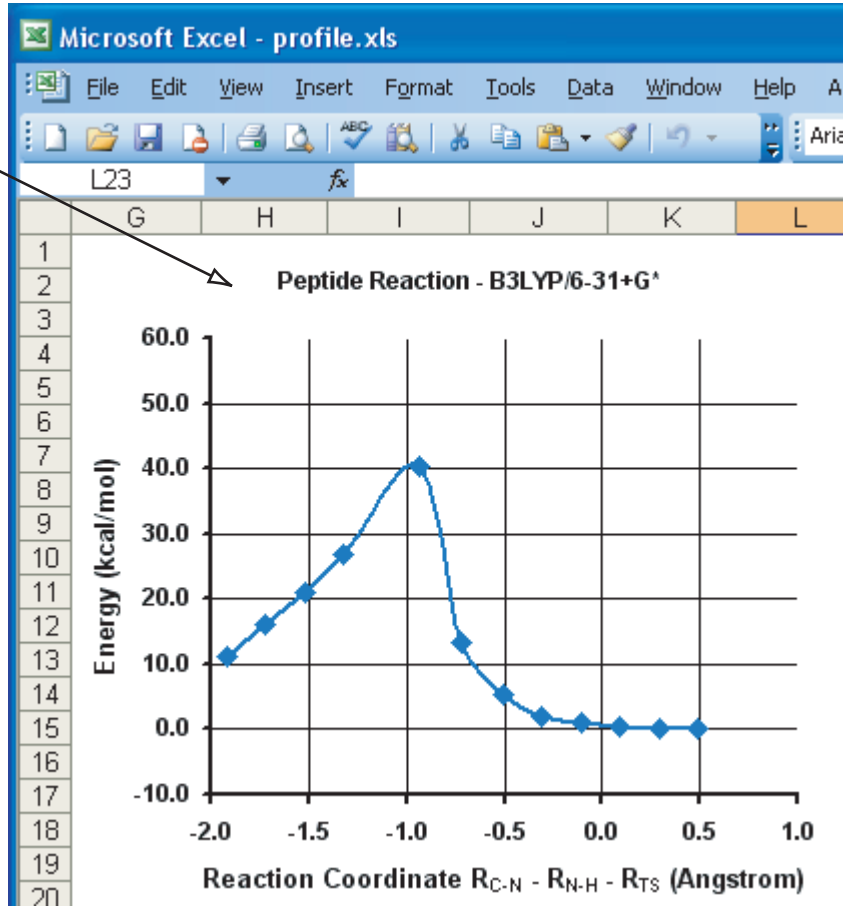
File Edit View Insert Format Tools

F18

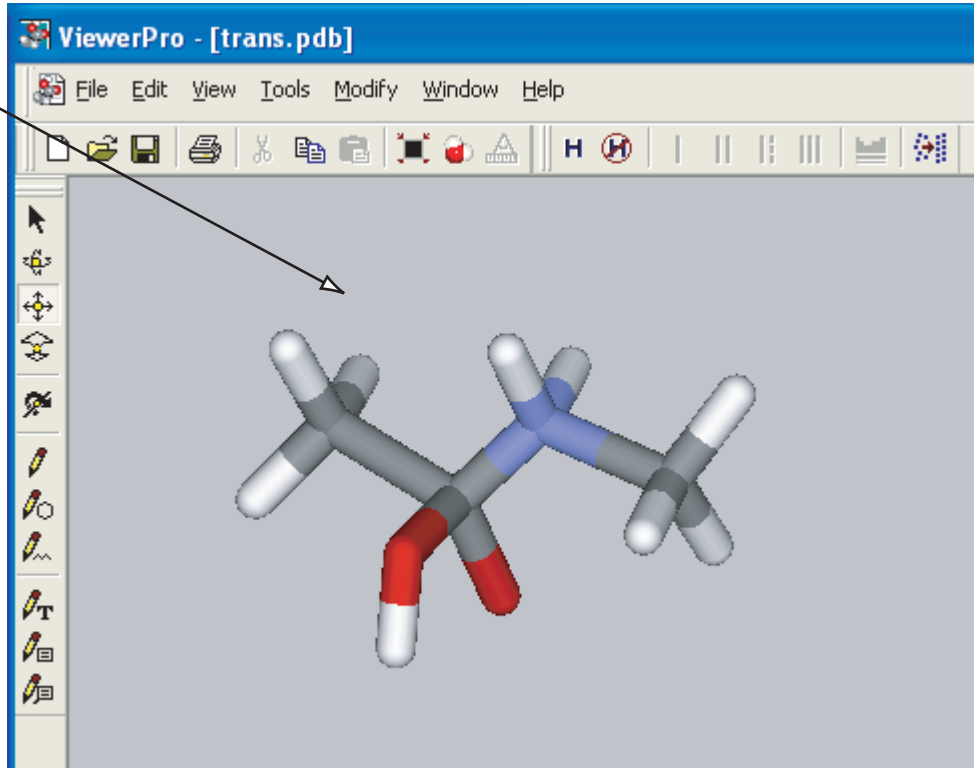
	A	B	C	D	E
1	R(NH)	R(CN)	R-Del	Energy	kcal/m
2	1.02	2.20	-1.92	-324.9458	11.32
3	1.02	2.00	-1.72	-324.9384	15.96
4	1.02	1.80	-1.52	-324.9304	20.96
5	1.02	1.60	-1.32	-324.9211	26.81
6	1.20	1.40	-0.94	-324.8993	40.47
7	1.40	1.38	-0.72	-324.9425	13.39
8	1.60	1.37	-0.51	-324.9551	5.44
9	1.80	1.37	-0.31	-324.9608	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	

QM Reaction Profiles - Peptide Reaction

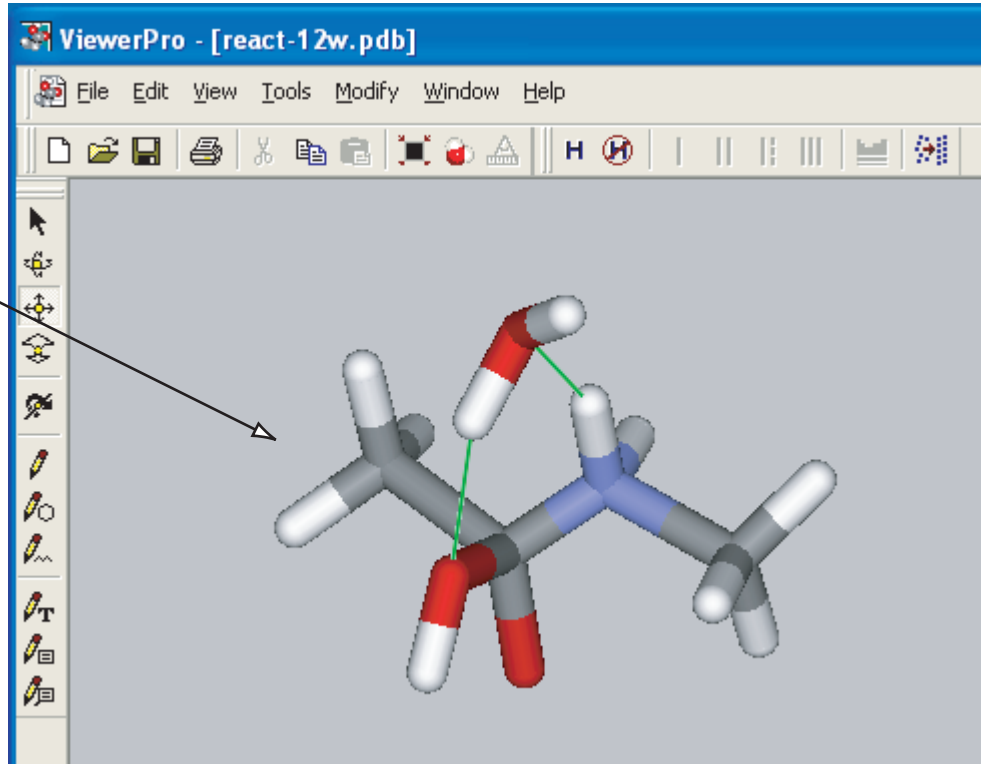
Reaction profile



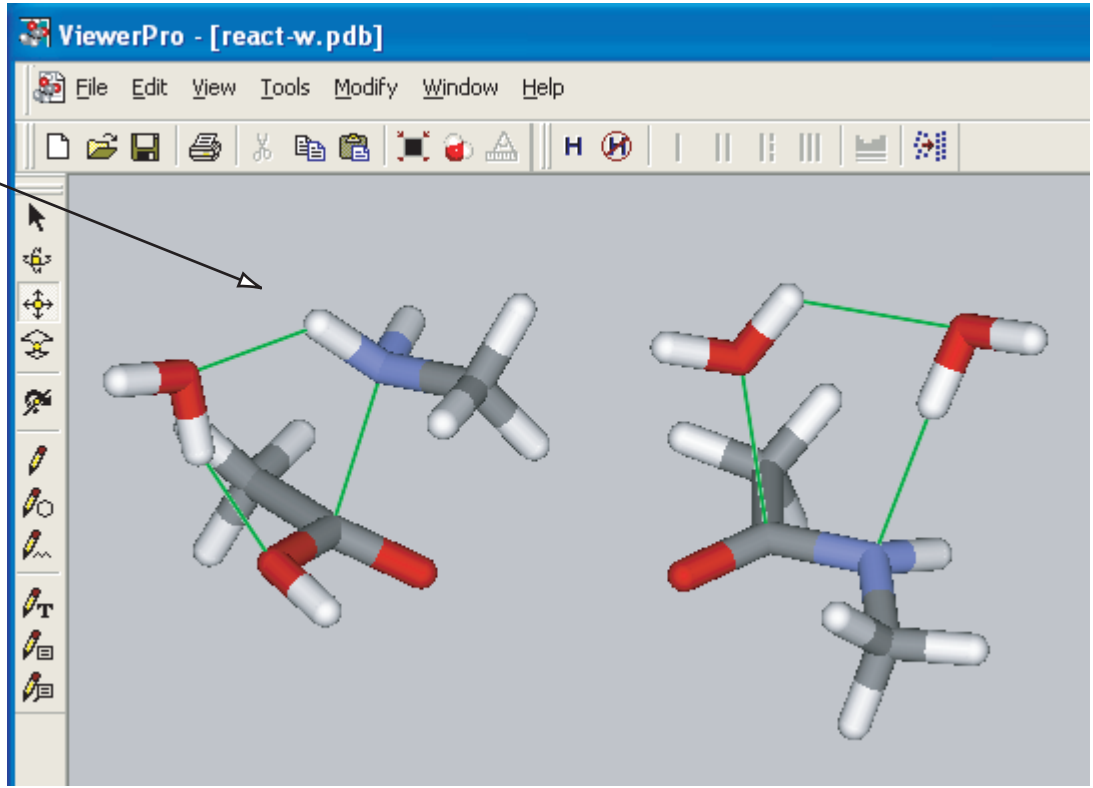
Transition state structure of the peptide reaction



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

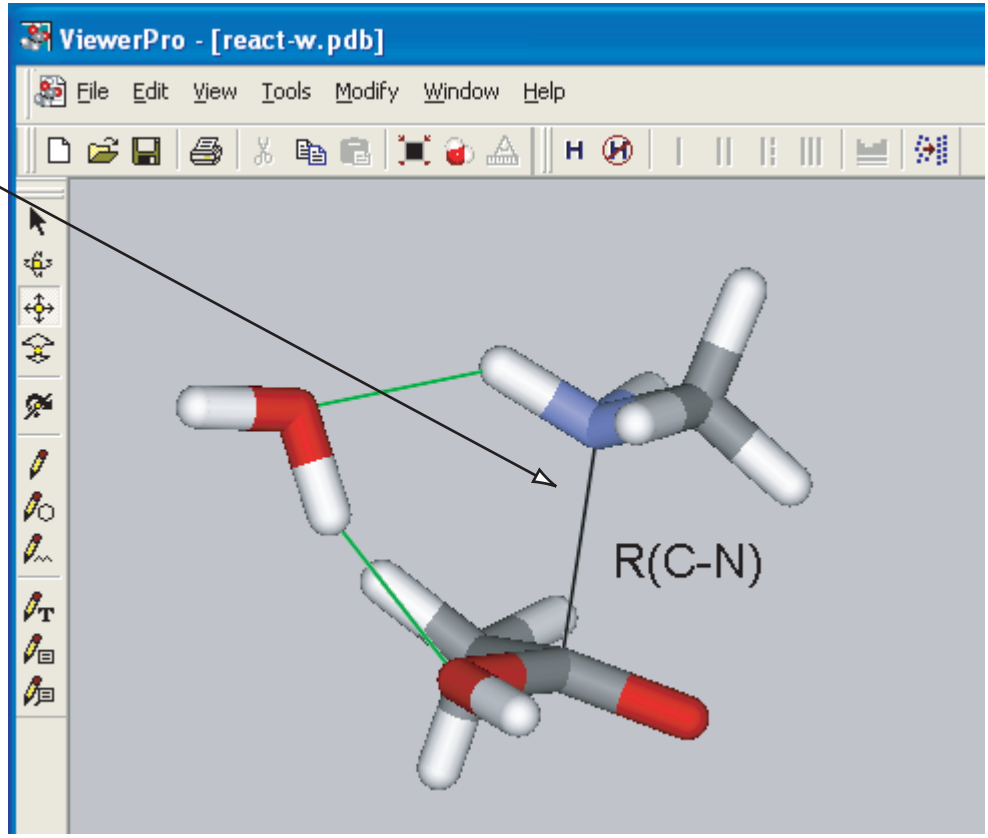


Reactants and products of the peptide reaction in a presence of a water molecule



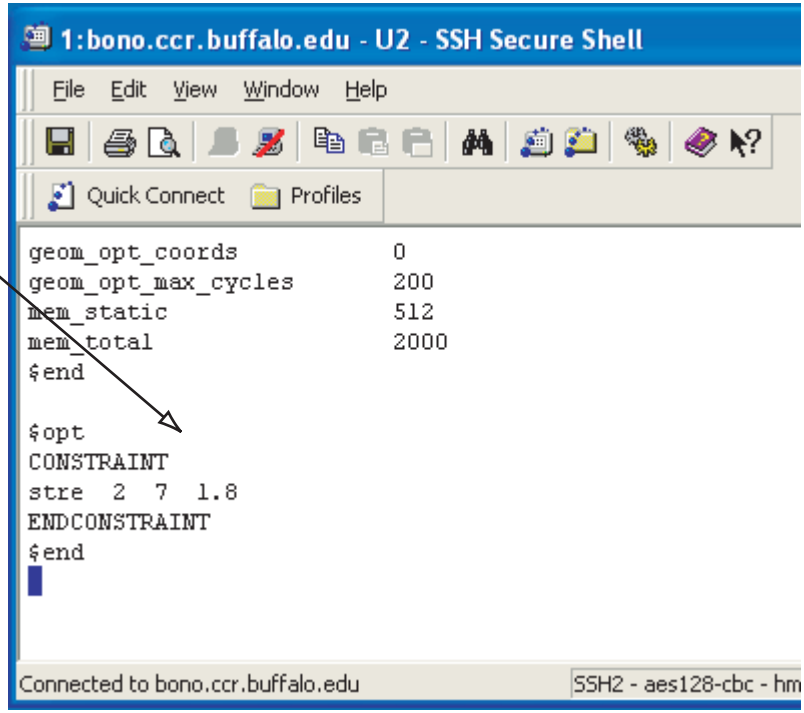
QM Reaction Profiles - Peptide Reaction

Reaction coordinate for reactants



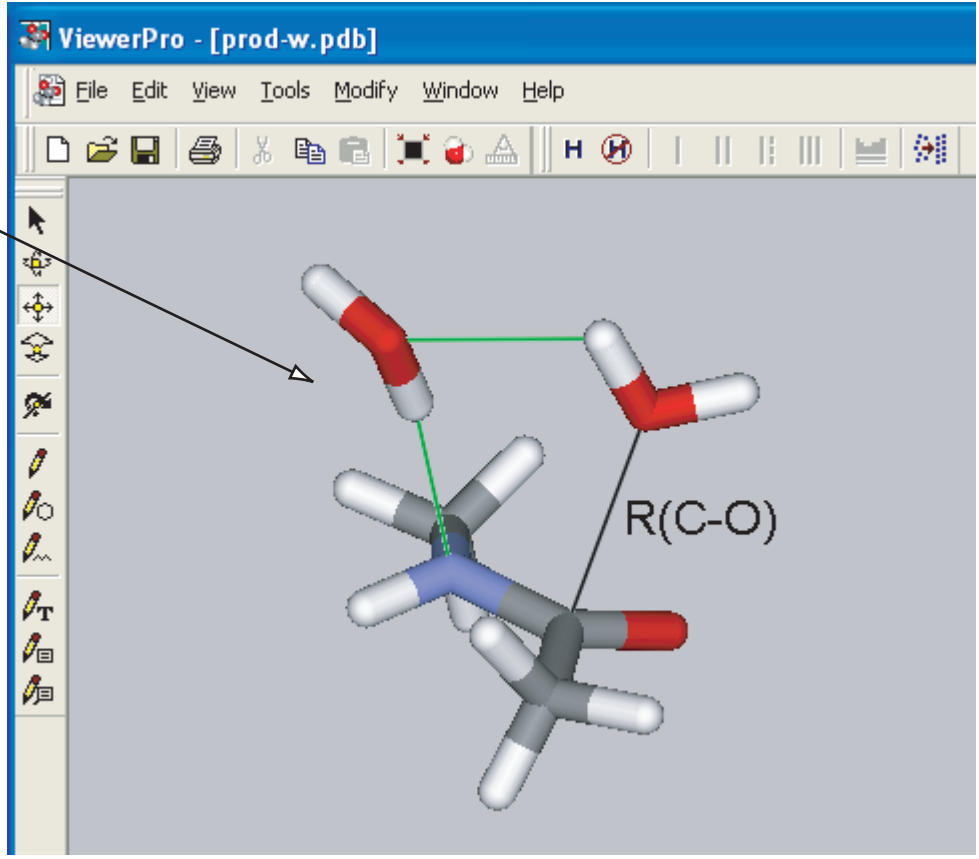
QM Reaction Profiles - Peptide Reaction

Geometry optimization with a constrained distance

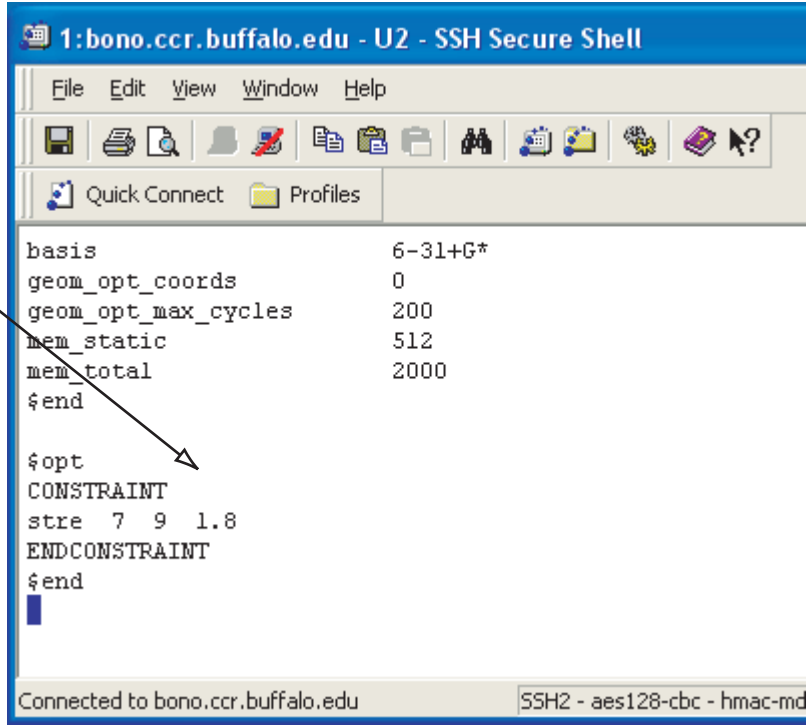


QM Reaction Profiles - Peptide Reaction

Reaction coordinate for products



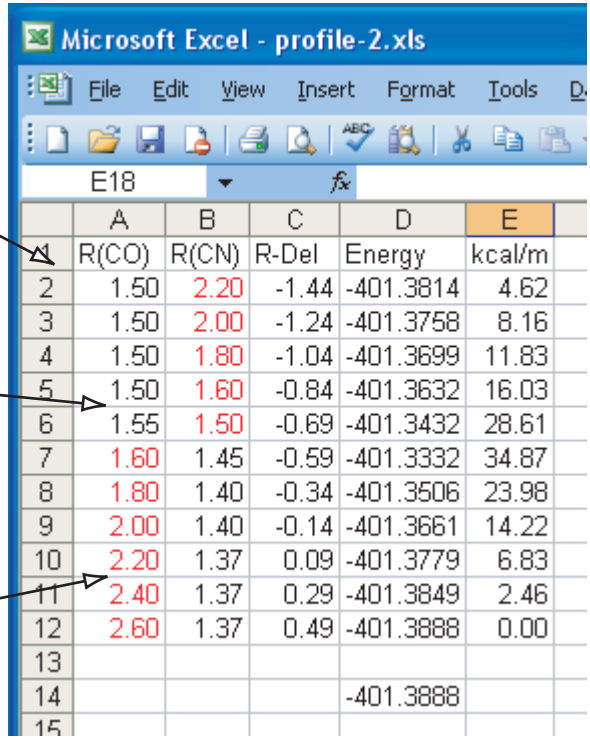
Geometry optimization with a constrained distance



Final results

Reactants

Products



Microsoft Excel - profile-2.xls

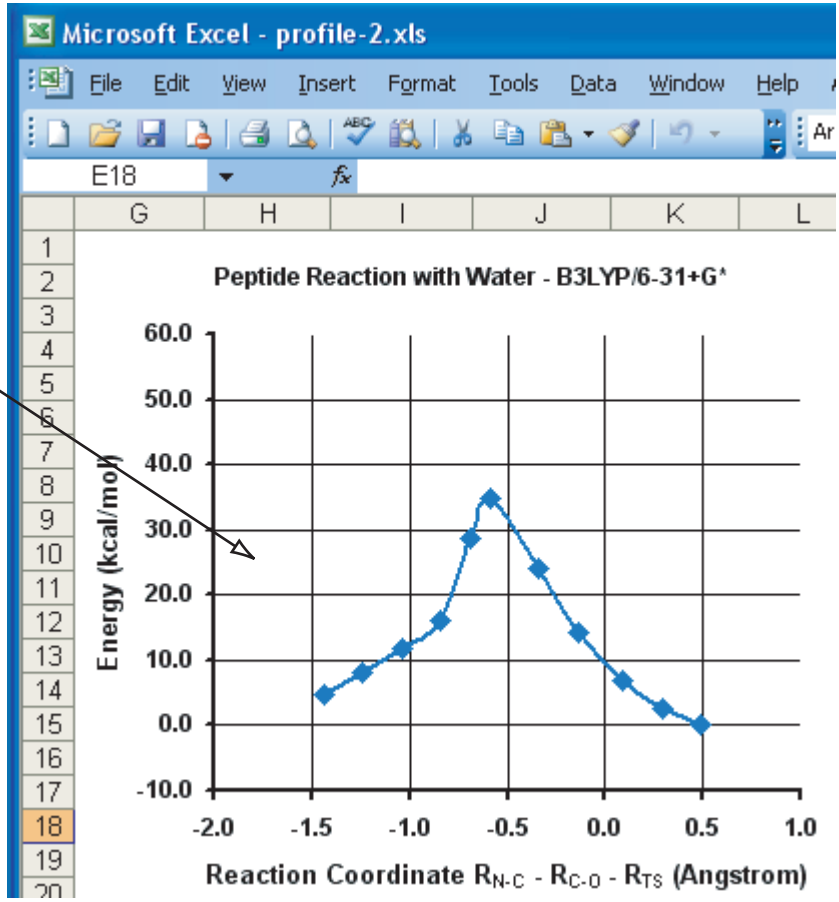
File Edit View Insert Format Tools D

E18

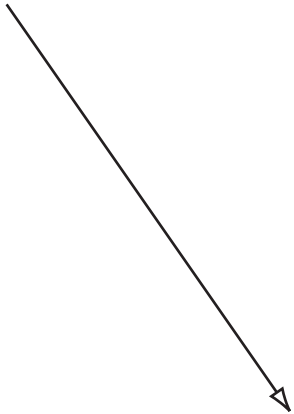
	A	B	C	D	E
1	R(CO)	R(CN)	R-Del	Energy	kcal/m
2	1.50	2.20	-1.44	-401.3814	4.62
3	1.50	2.00	-1.24	-401.3758	8.16
4	1.50	1.80	-1.04	-401.3699	11.83
5	1.50	1.60	-0.84	-401.3632	16.03
6	1.55	1.50	-0.69	-401.3432	28.61
7	1.60	1.45	-0.59	-401.3332	34.87
8	1.80	1.40	-0.34	-401.3506	23.98
9	2.00	1.40	-0.14	-401.3661	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



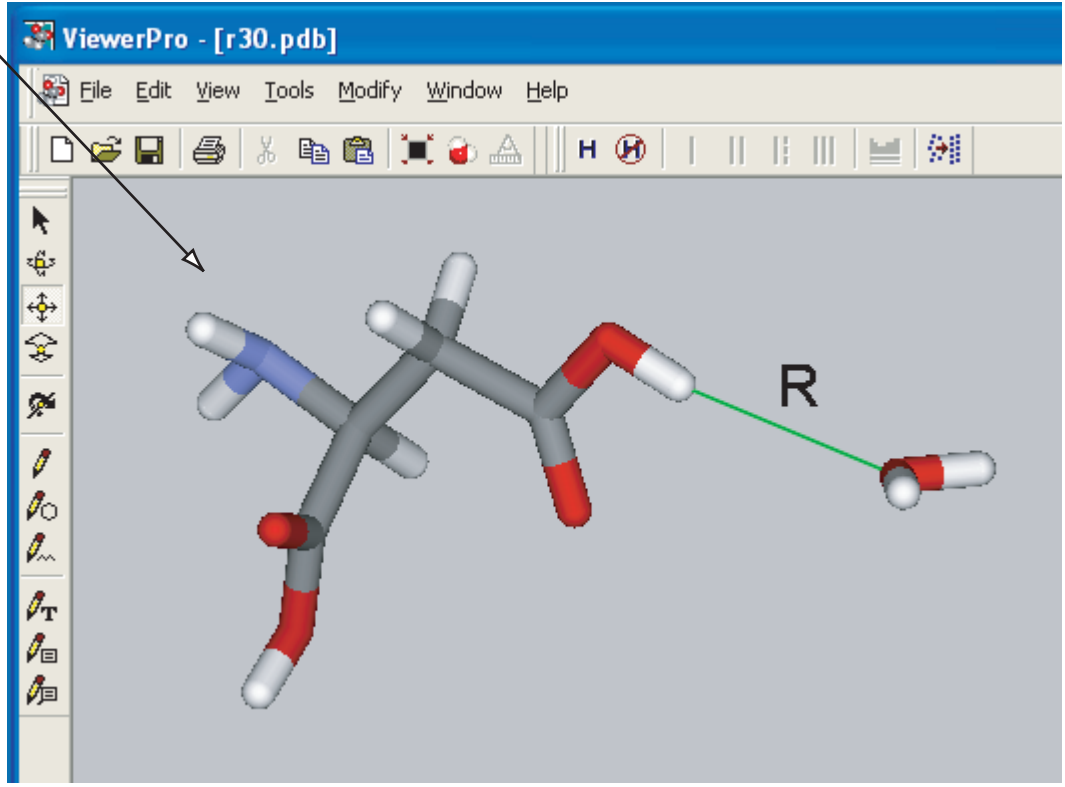
$$HA + H_2O \rightarrow H_3O^+ + A^-$$

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

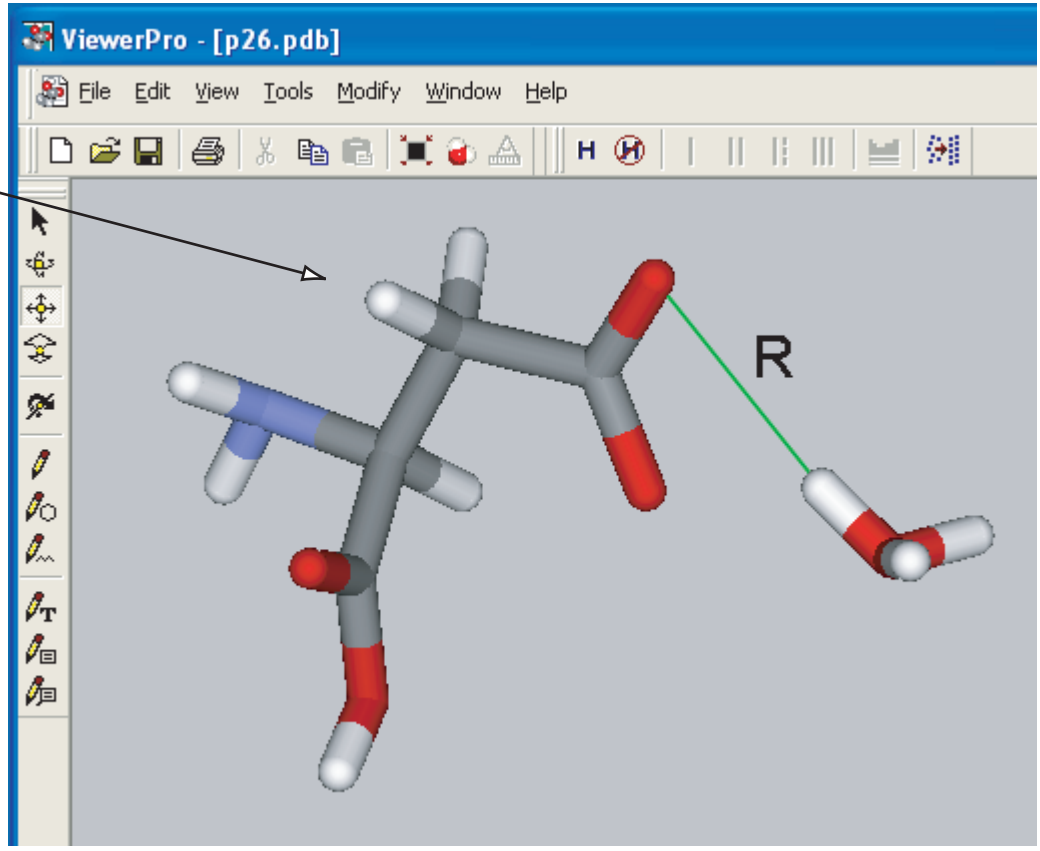
$$K_a = e^{-\frac{\Delta G}{RT}}$$

$$pK_a = -Log_{10} K_a$$

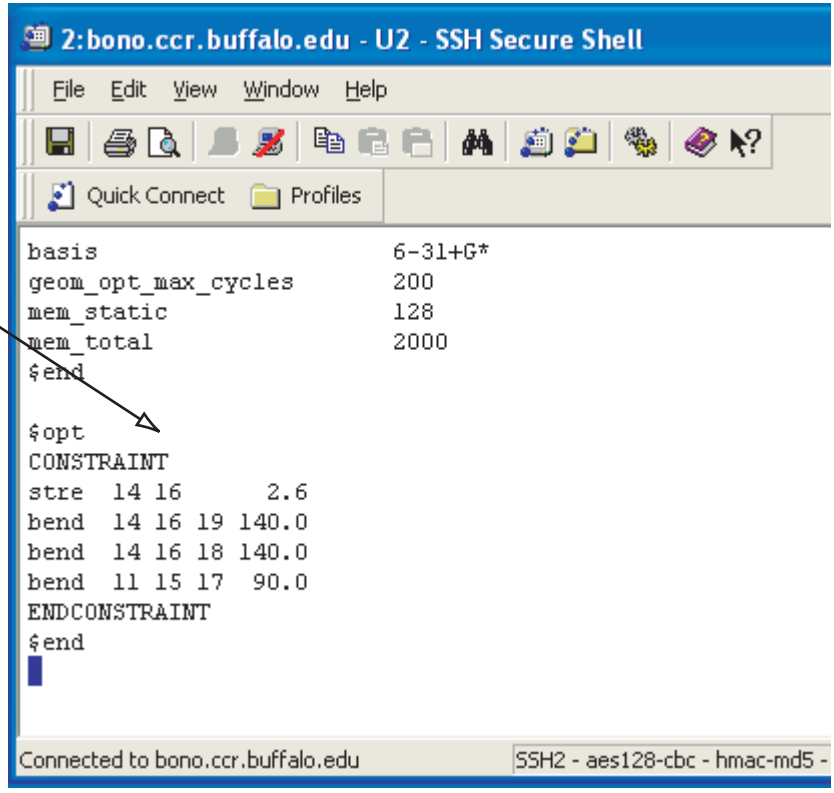
Reactants in the deprotonation reaction of aspartic acid with water



Products in the deprotonation reaction of aspartic acid with water



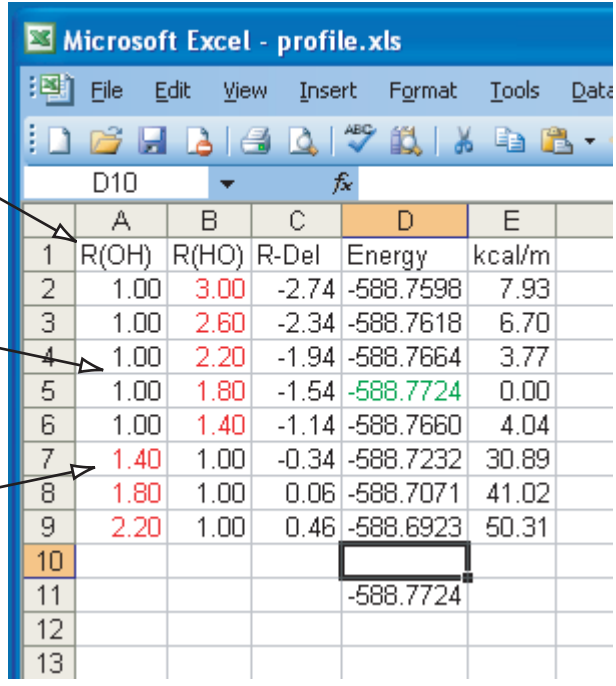
Geometry optimization with constrained distances and angles



Final results

Reactants

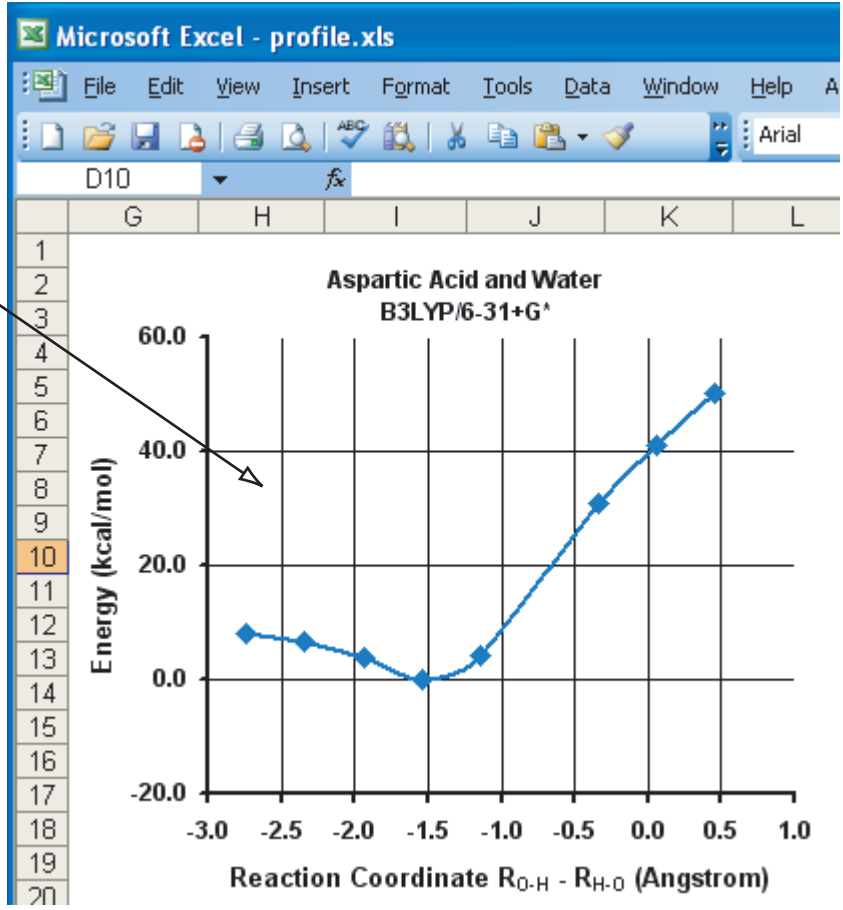
Products



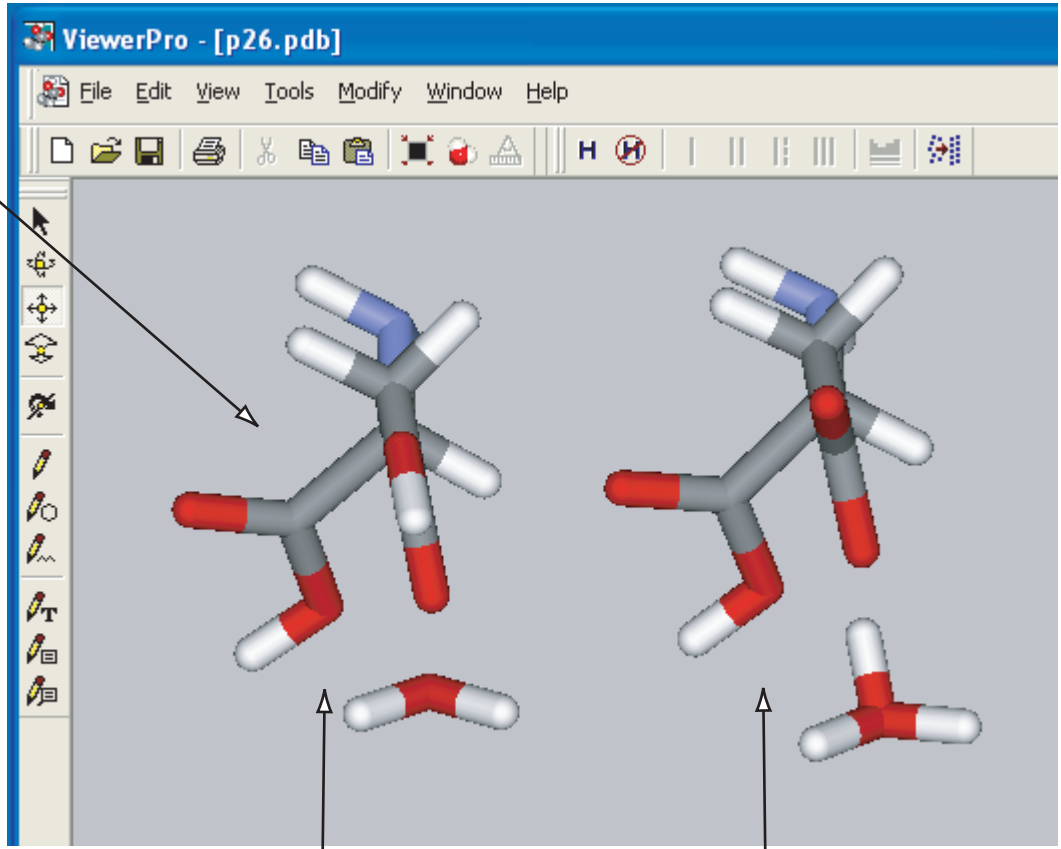
	A	B	C	D	E
1	R(OH)	R(HO)	R-Del	Energy	kcal/m
2	1.00	3.00	-2.74	-588.7598	7.93
3	1.00	2.60	-2.34	-588.7618	6.70
4	1.00	2.20	-1.94	-588.7664	3.77
5	1.00	1.80	-1.54	-588.7724	0.00
6	1.00	1.40	-1.14	-588.7660	4.04
7	1.40	1.00	-0.34	-588.7232	30.89
8	1.80	1.00	0.06	-588.7071	41.02
9	2.20	1.00	0.46	-588.6923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

QM calculations of pKa in amino acids and base pairs

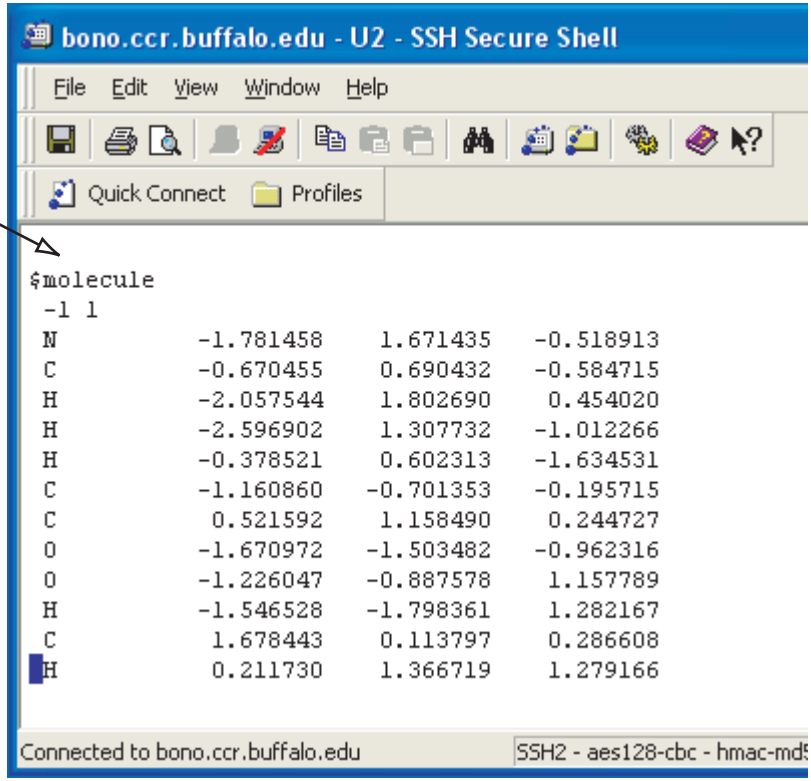
Potential energy surface of the deprotonation reaction



Separate calculations for all molecules used in the reaction



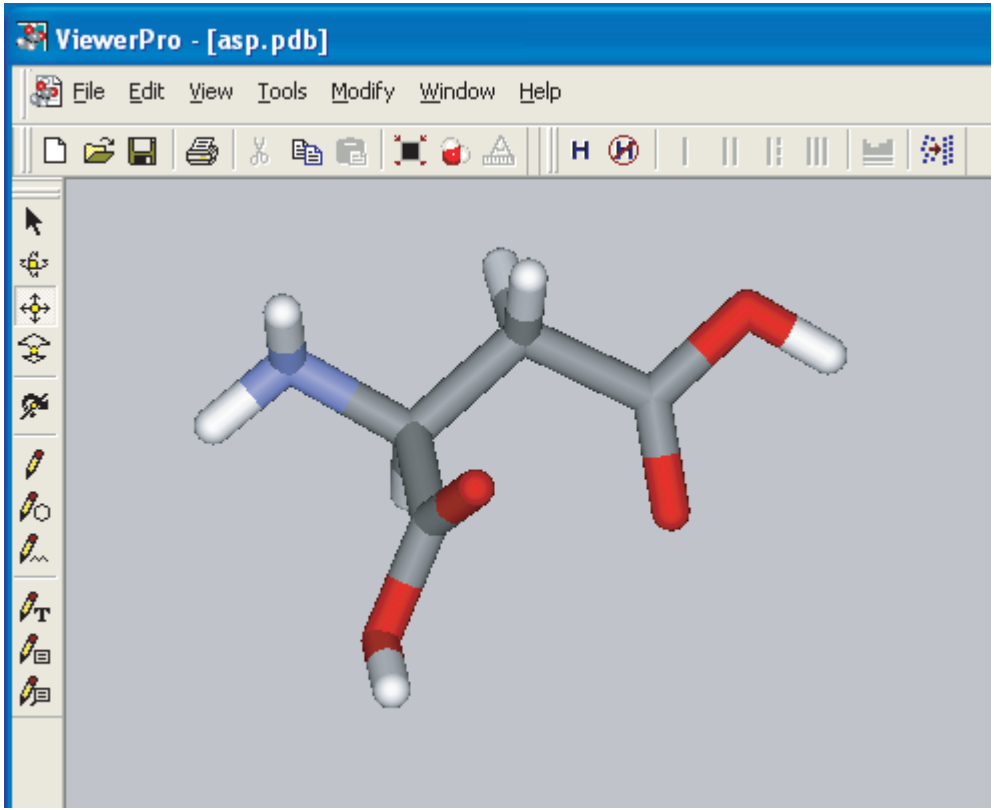
Calculations of the anion in the singlet electronic state



Aspartic Acid

Deprotonation energy:

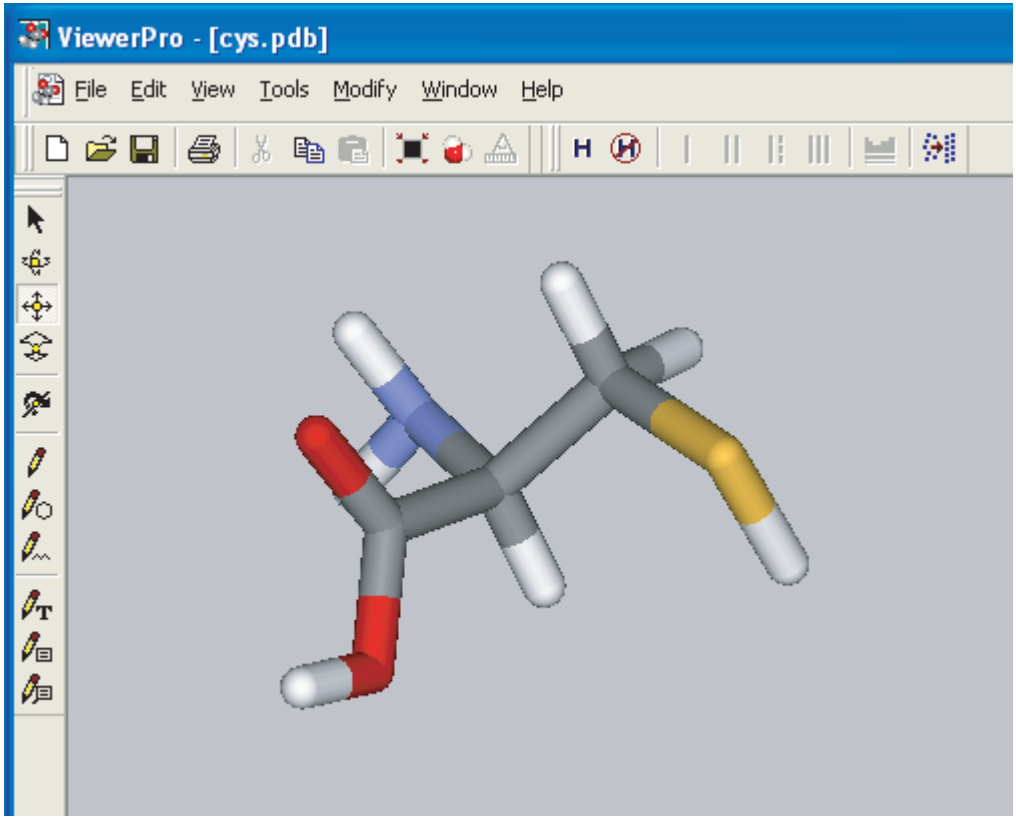
E = 173 kcal/mol



Cysteine

Deprotonation energy:

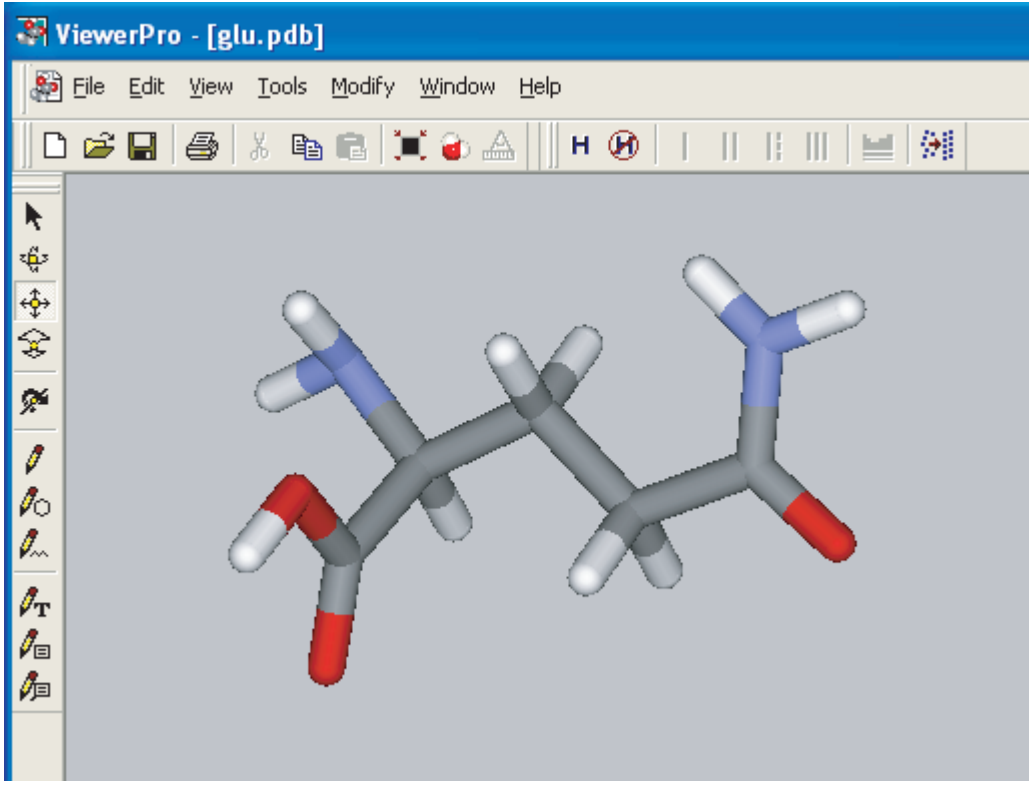
E = 181 kcal/mol



Glutamic Acid

Deprotonation energy:

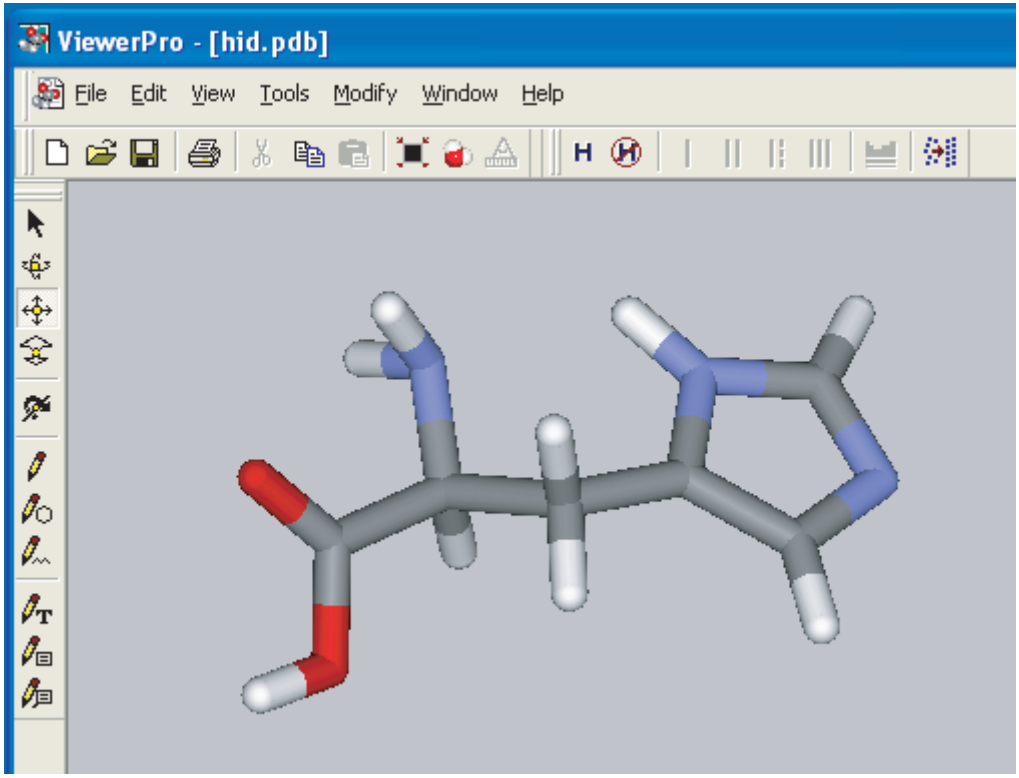
E = 199 kcal/mol



Histidine (δ)

Deprotonation energy:

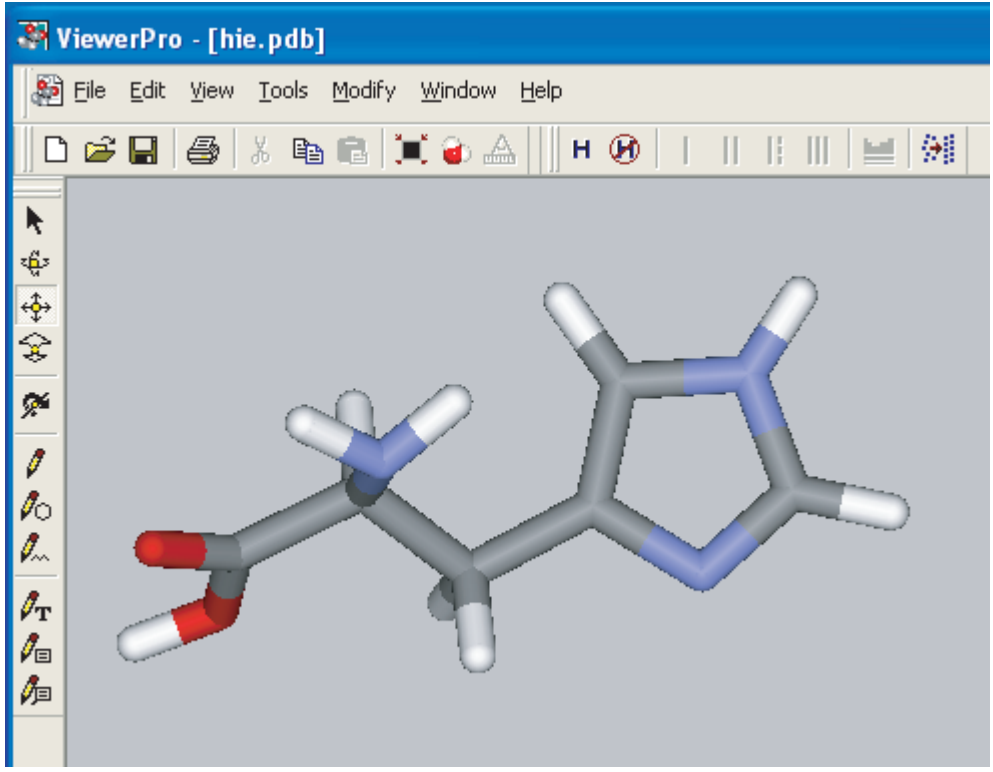
E = 181 kcal/mol



Histidine (ε)

Deprotonation energy:

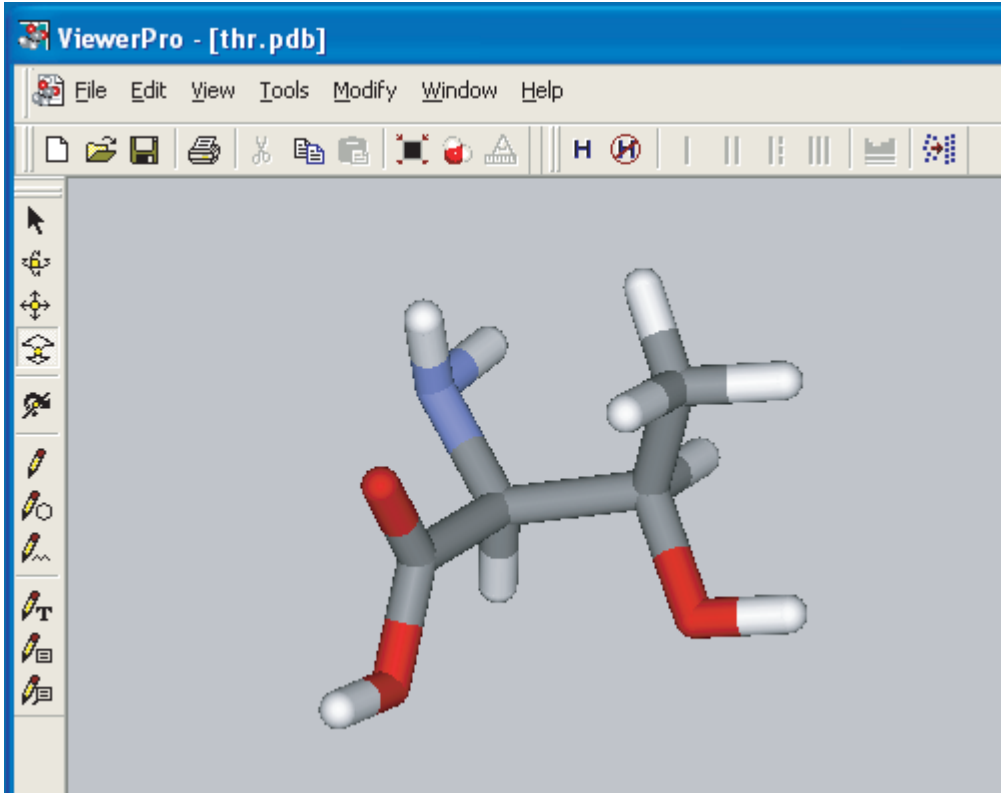
E = 175 kcal/mol



Threonine

Deprotonation energy:

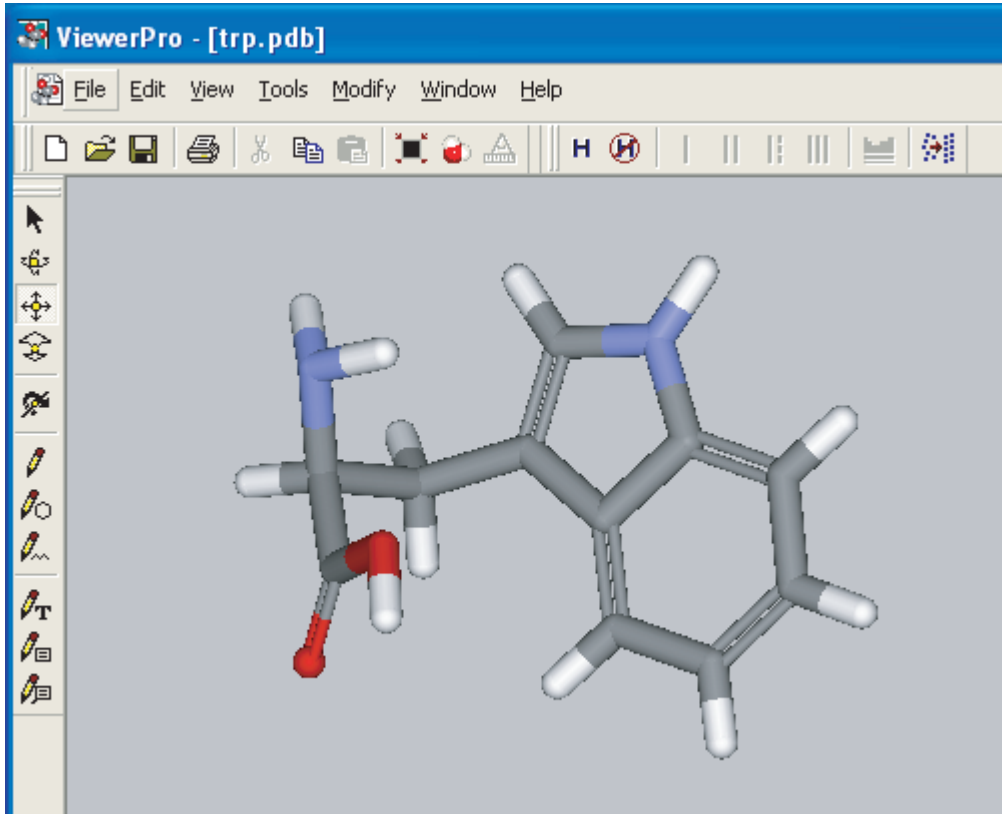
E = 196 kcal/mol



Triptophan

Deprotonation energy:

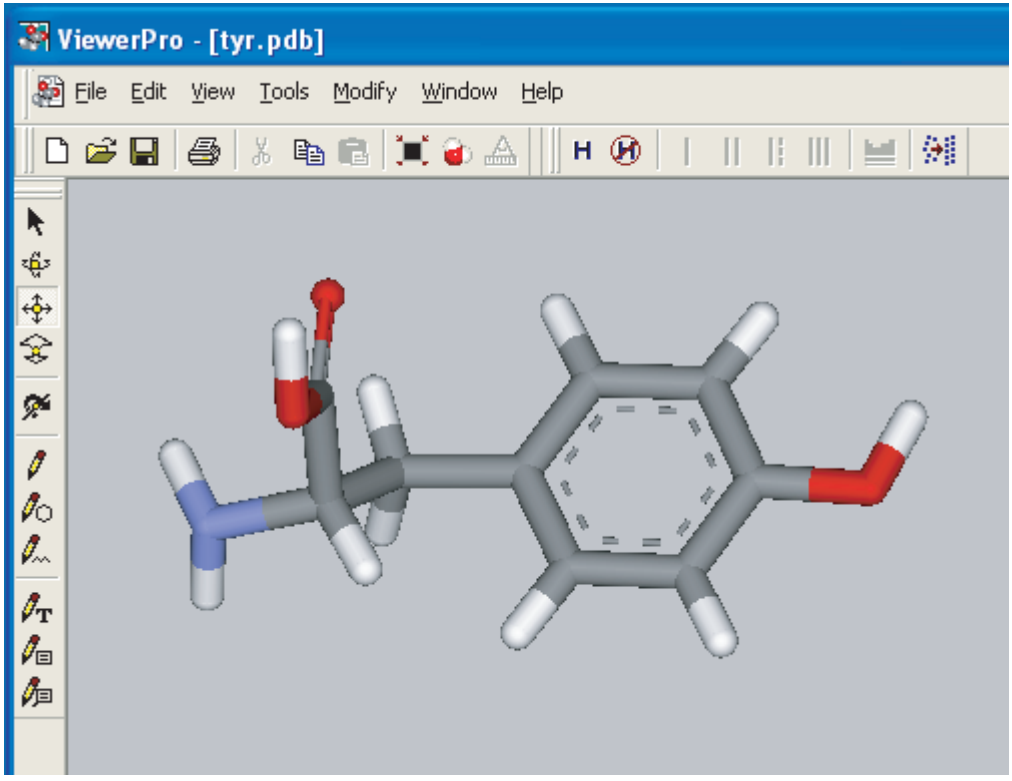
E = 180 kcal/mol



Tyrosine

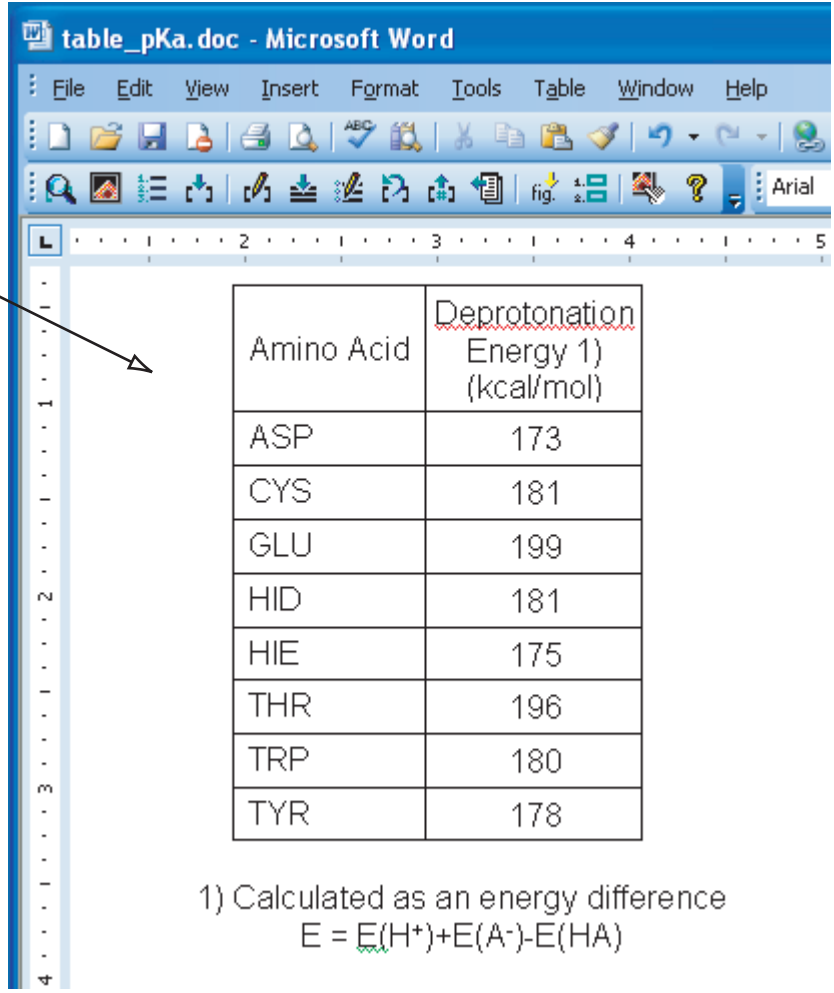
Deprotonation energy:

E = 178 kcal/mol



QM calculations of pKa in amino acids and base pairs

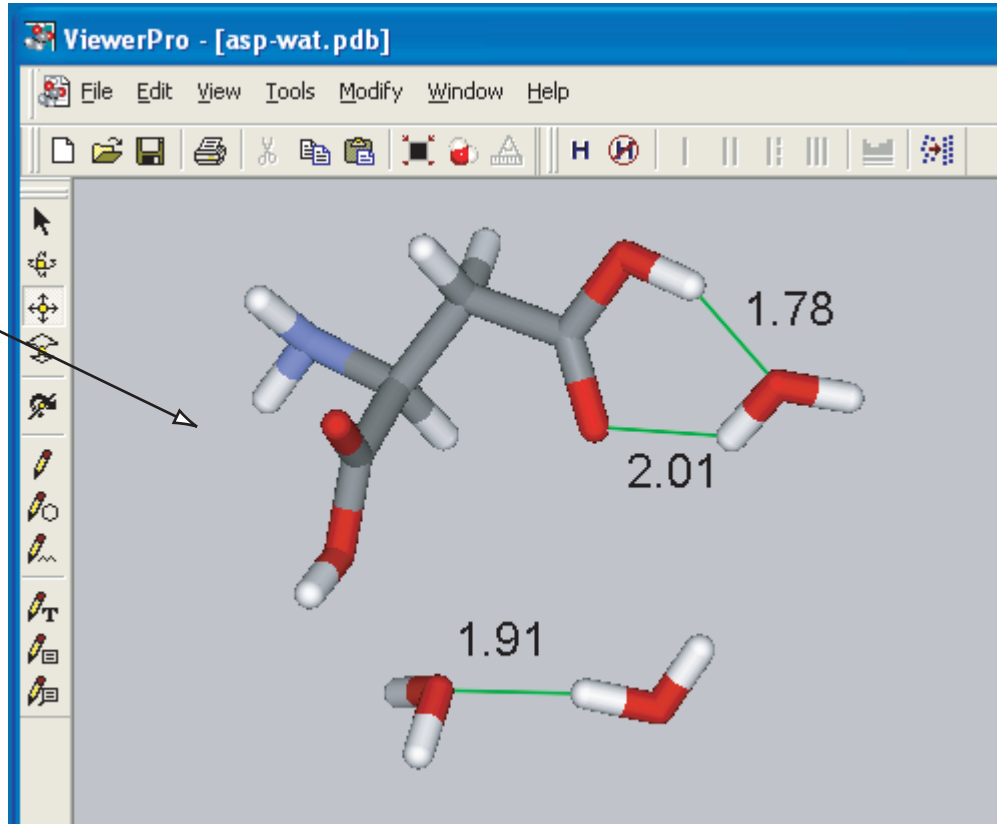
Final results



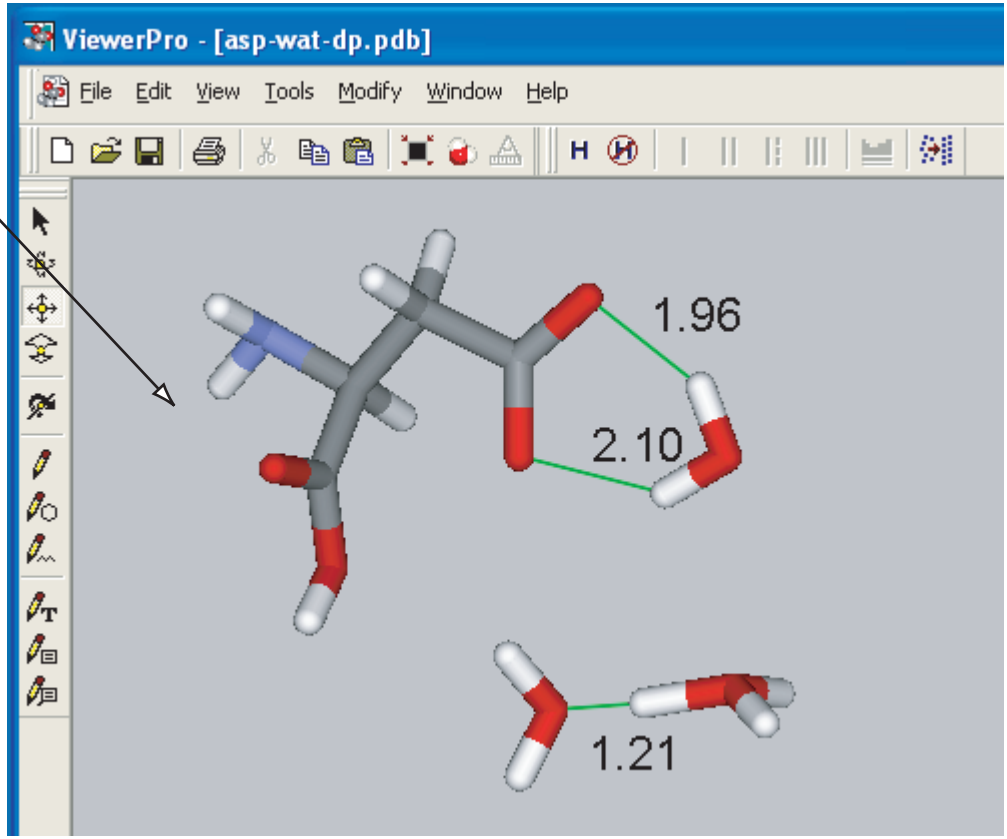
Amino Acid	Deprotonation Energy 1) (kcal/mol)
ASP	173
CYS	181
GLU	199
HID	181
HIE	175
THR	196
TRP	180
TYR	178

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

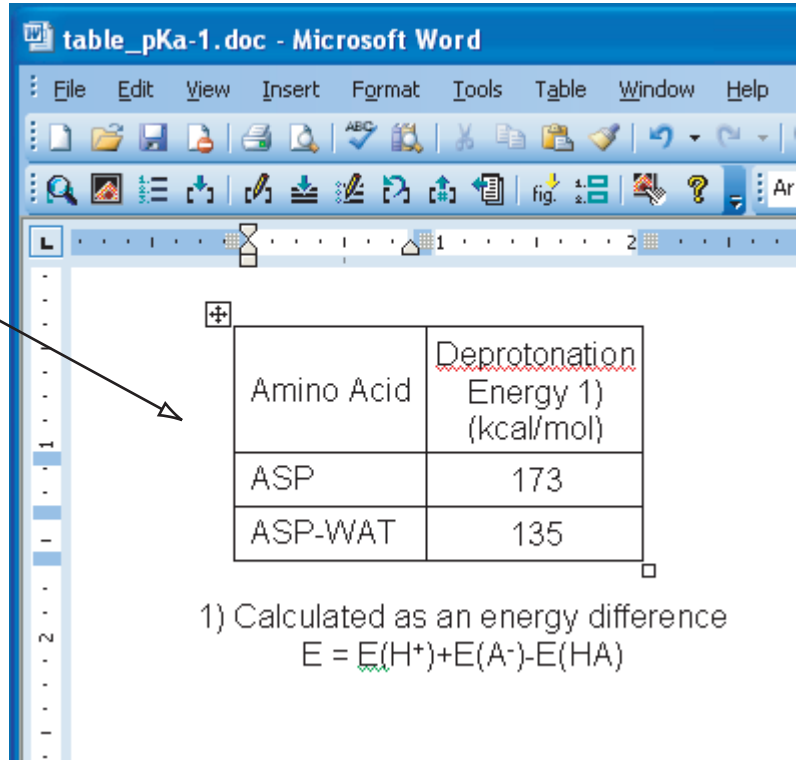
Stabilization of neutral aspartic acid and water by two water molecules



Stabilization of ionic aspartic acid and water by two water molecules



Deprotonation energy of acetic acid stabilized by a water molecule

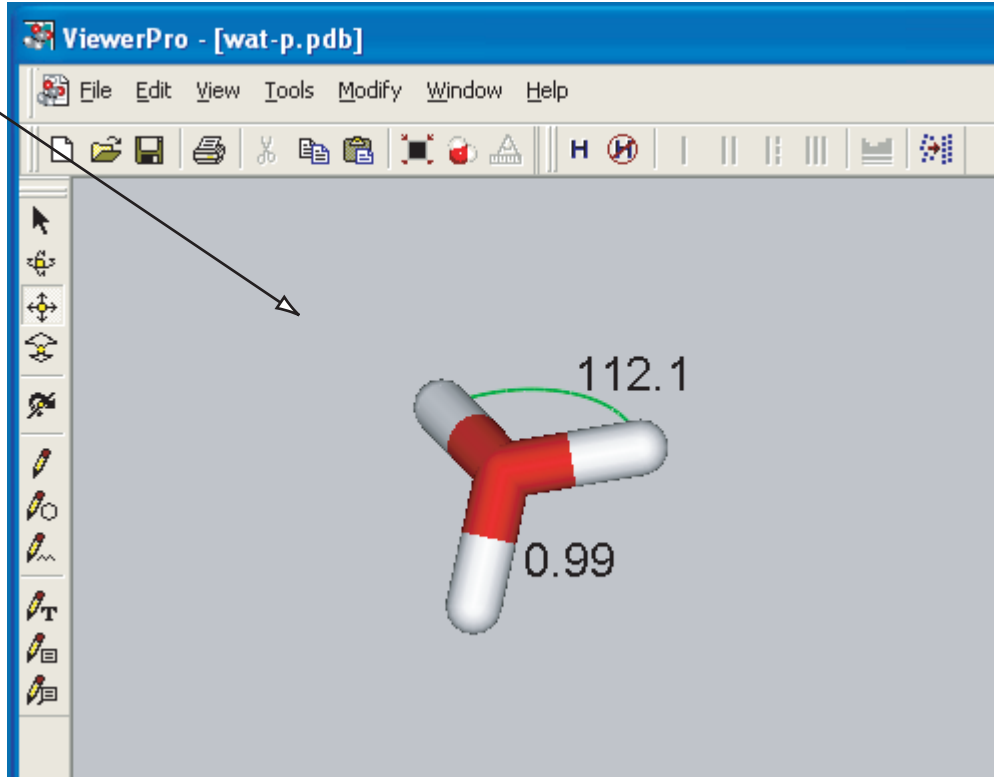


Amino Acid	Deprotonation Energy 1) (kcal/mol)
ASP	173
ASP-WAT	135

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

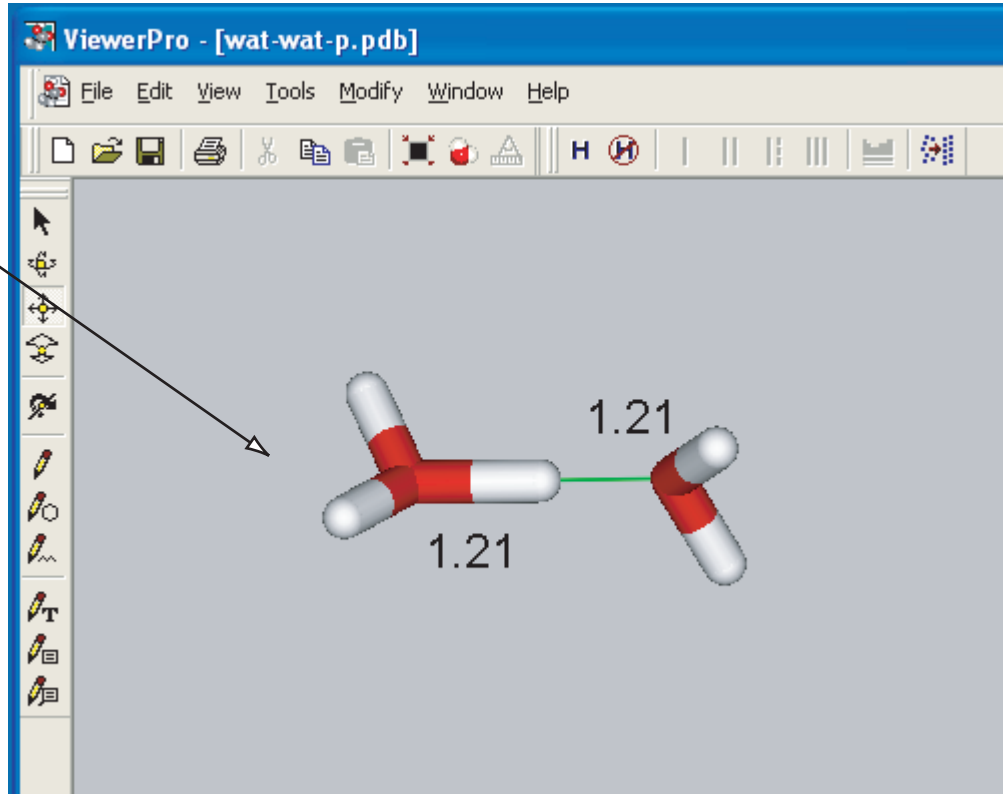
QM calculations of hydronium ion

Optimal geometry of hydronium ion



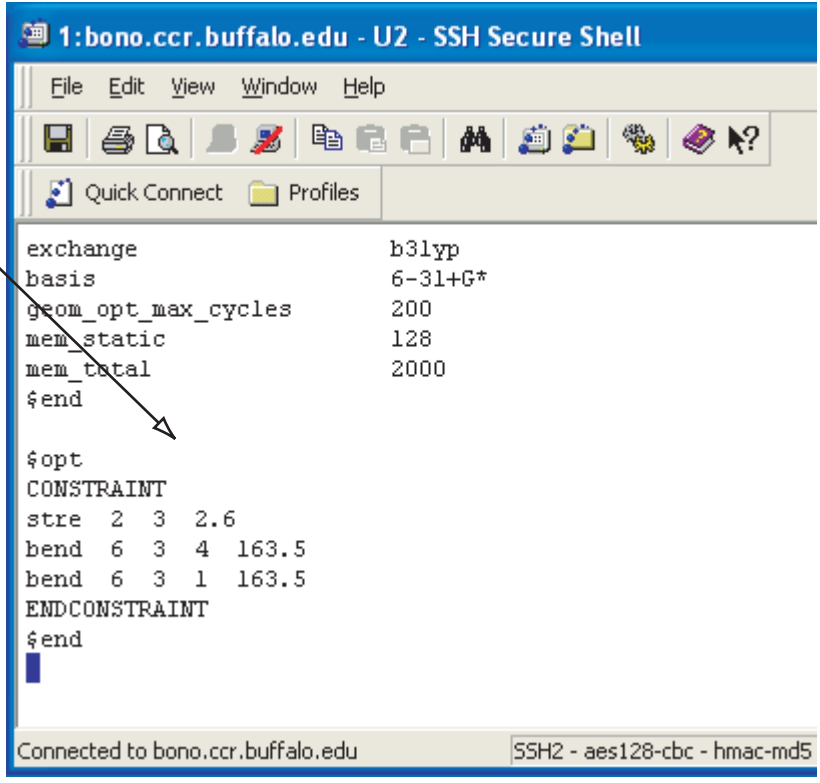
QM calculations of hydronium ion

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

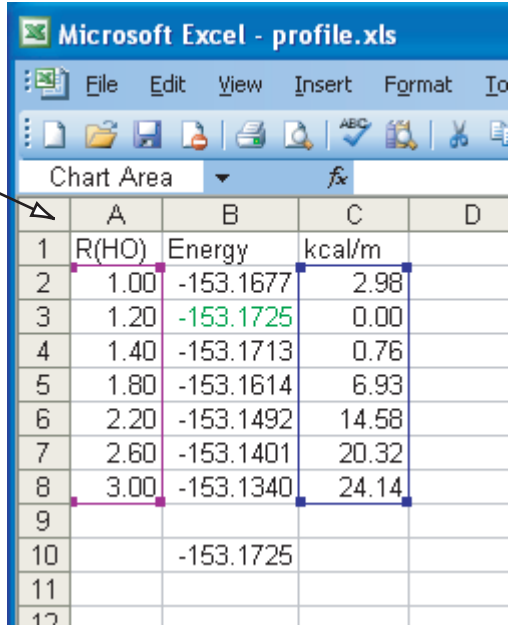


QM calculations of hydronium ion

Geometry optimization with a constrained distance and angles



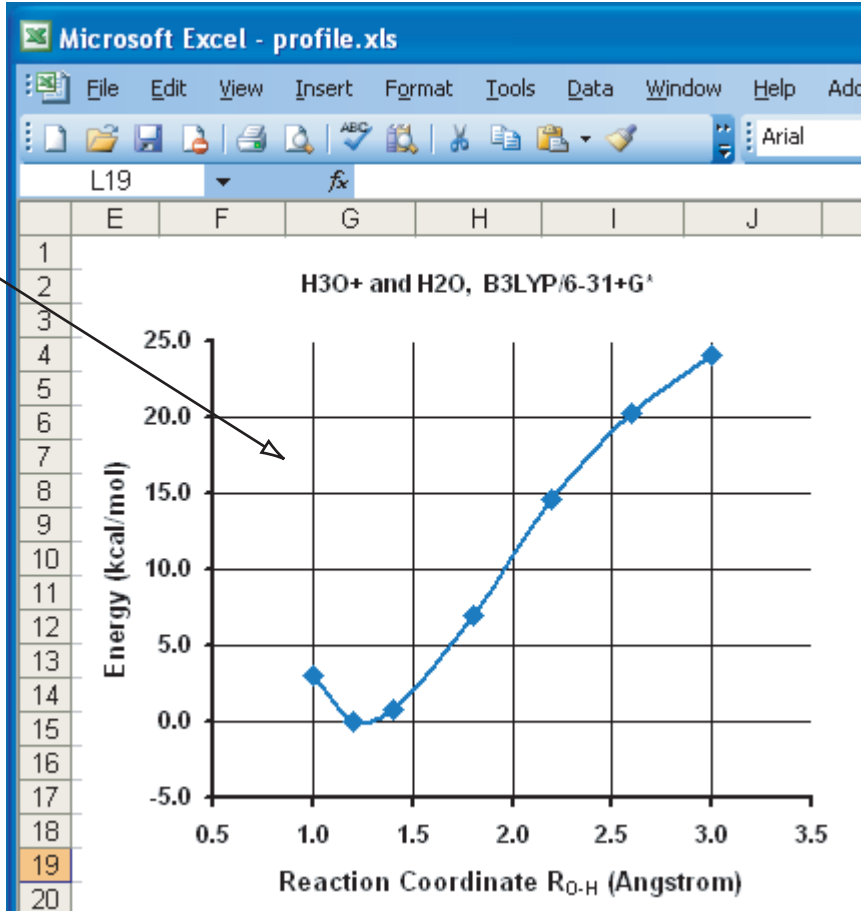
Results of the calculation



	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				

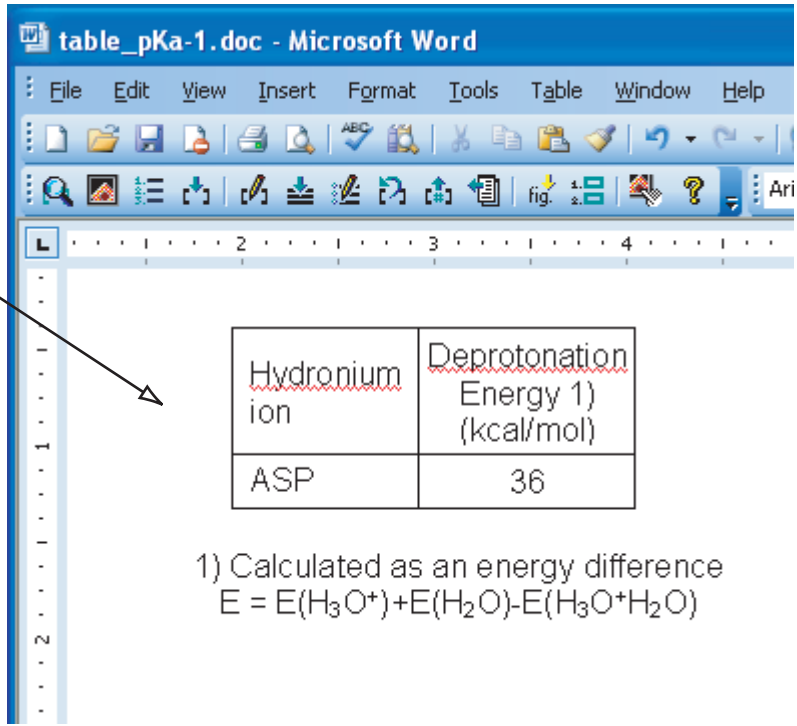
QM calculations of hydronium ion

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



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

1) Calculated as an energy difference
$E = E(H_3O^+)+E(H_2O)-E(H_3O^+H_2O)$

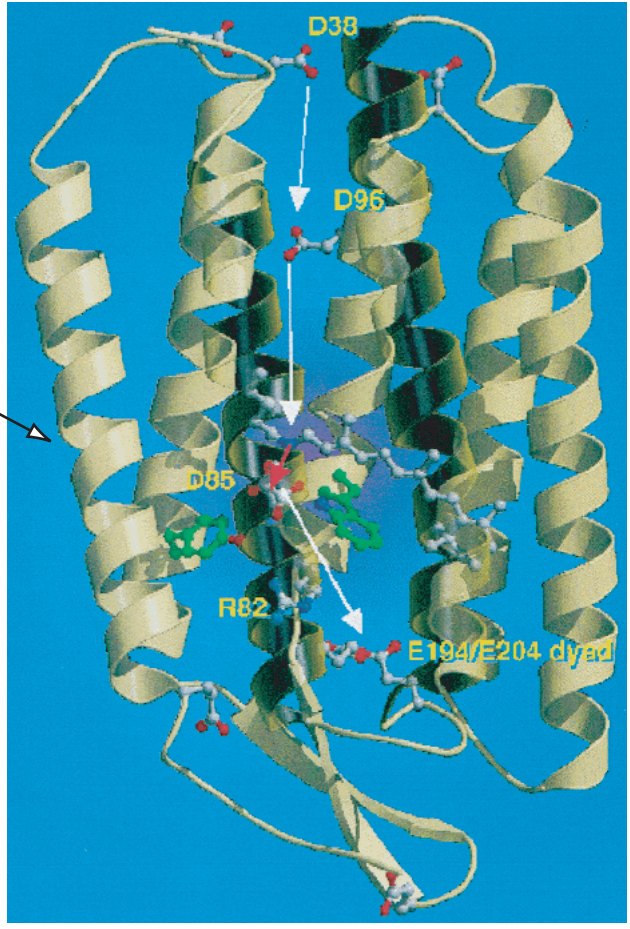
Schrodinger equation

$$H\Psi = E\Psi$$

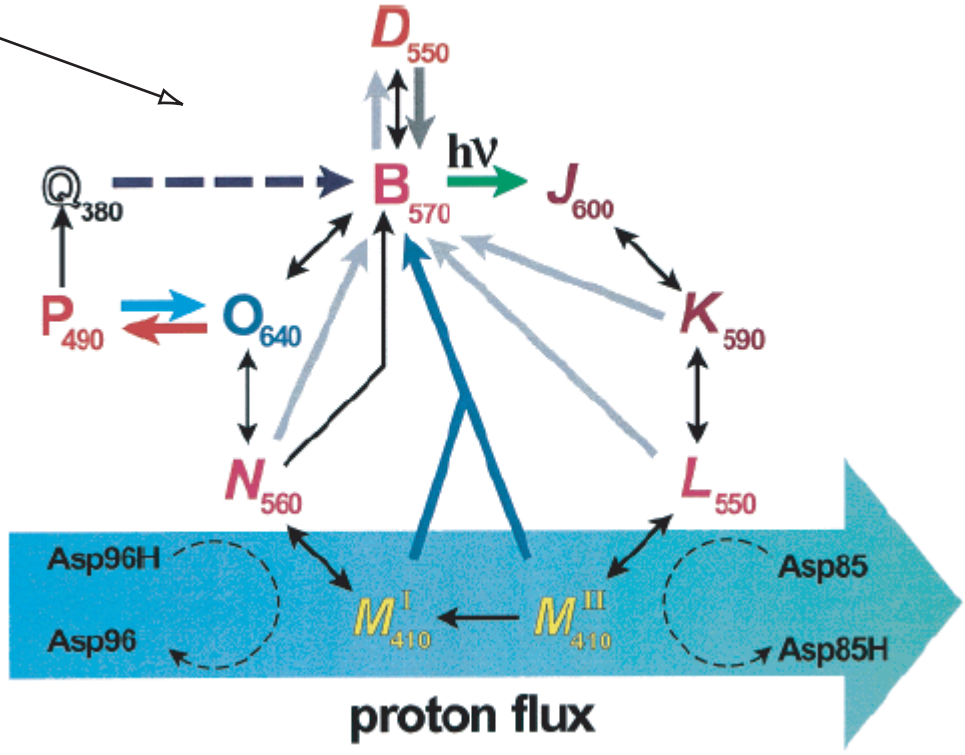
Ground electronic state $\longrightarrow$ $\Psi_g \quad E_g$

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

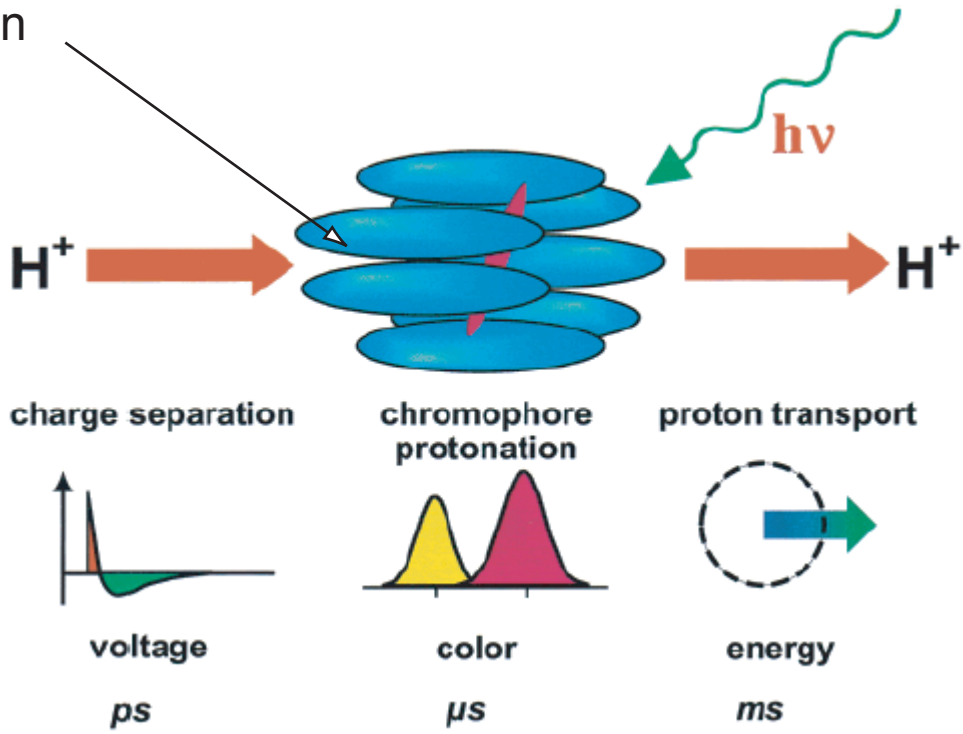
Bacteriorhodopsin



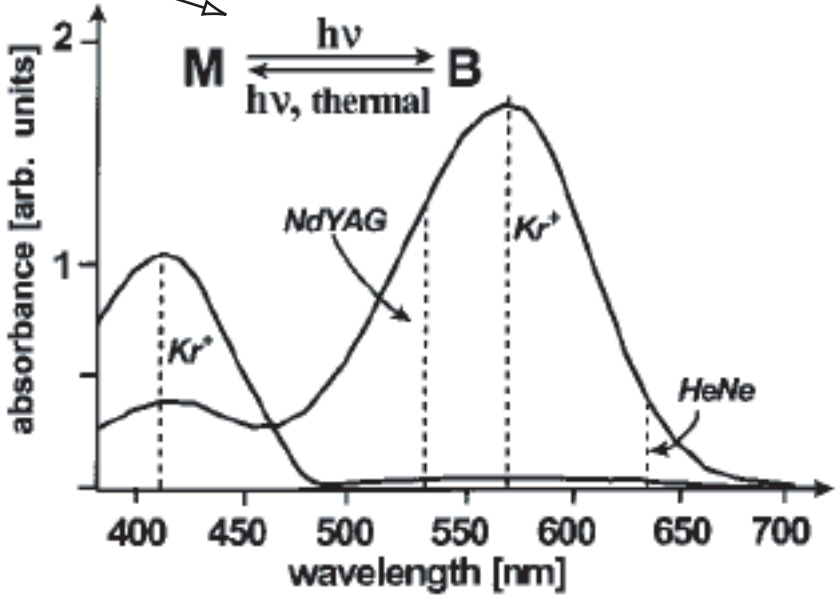
The reaction cycle of bacteriorhodopsin



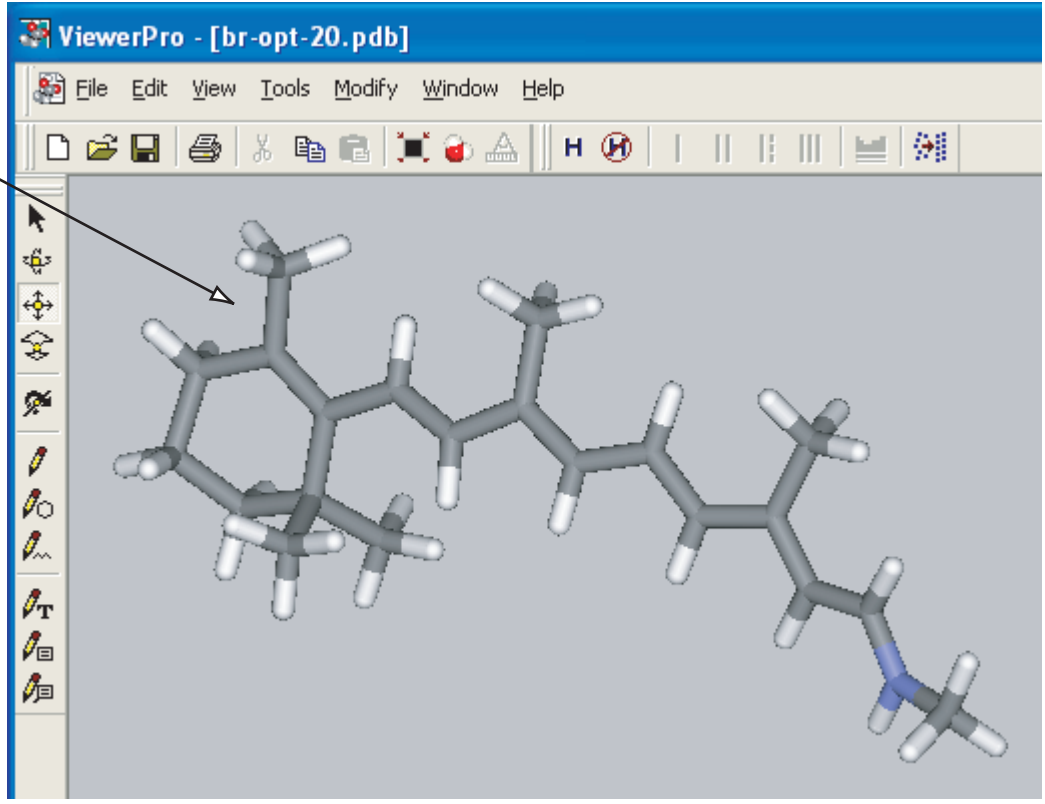
Molecular function of bacteriorhodopsin



Experimental UV spectrum of bR



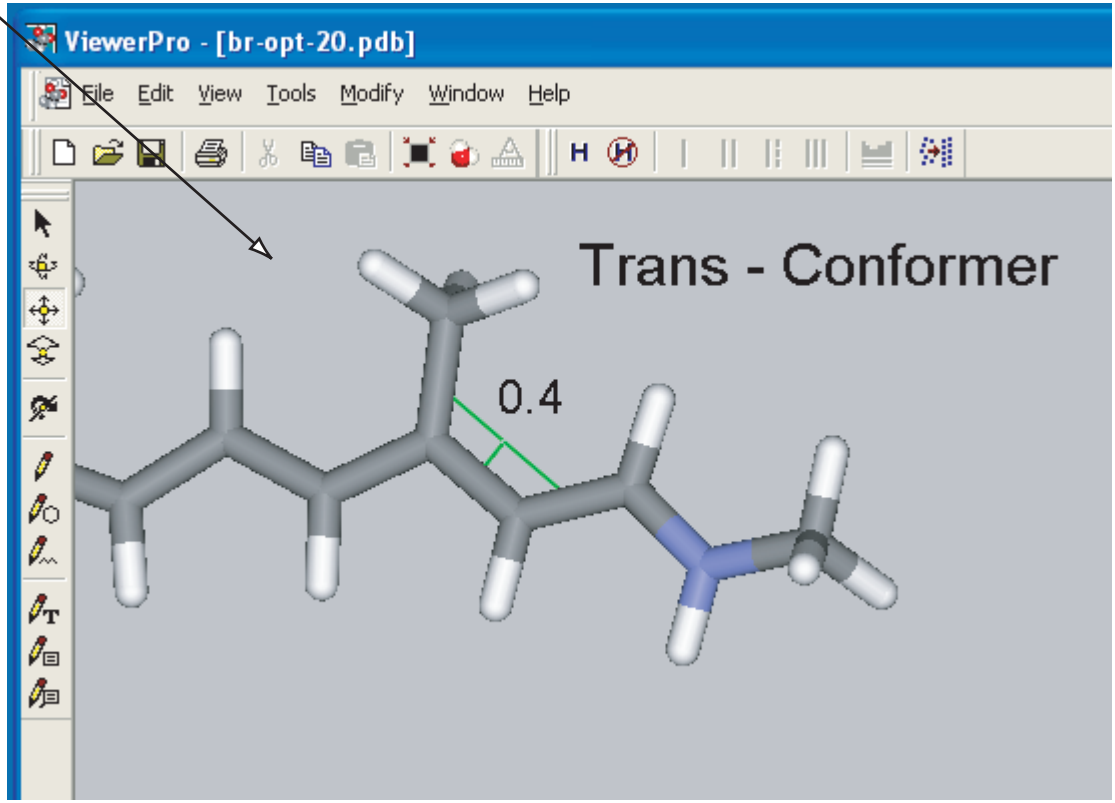
The active site of bacteriorhodopsin



QM calculations of excited electronic states

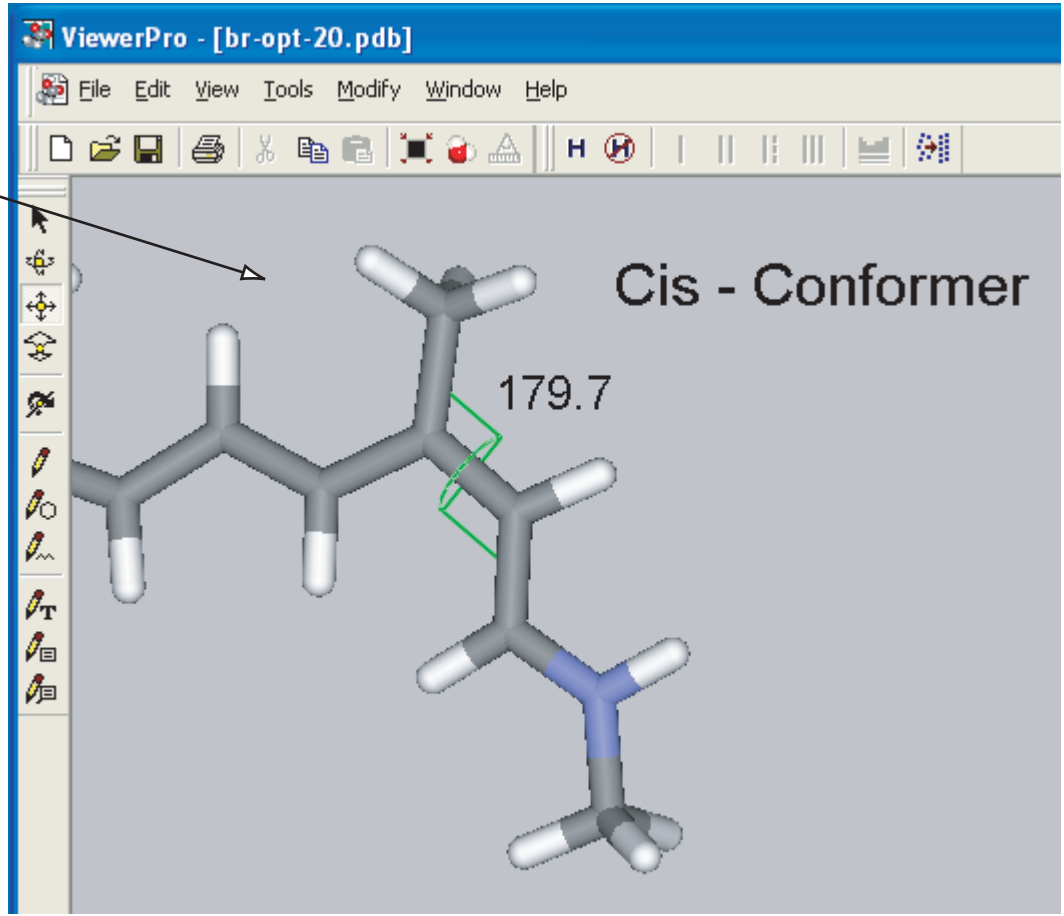
The trans conformer
of retinal

E = 570 nm
(17500 cm-1)

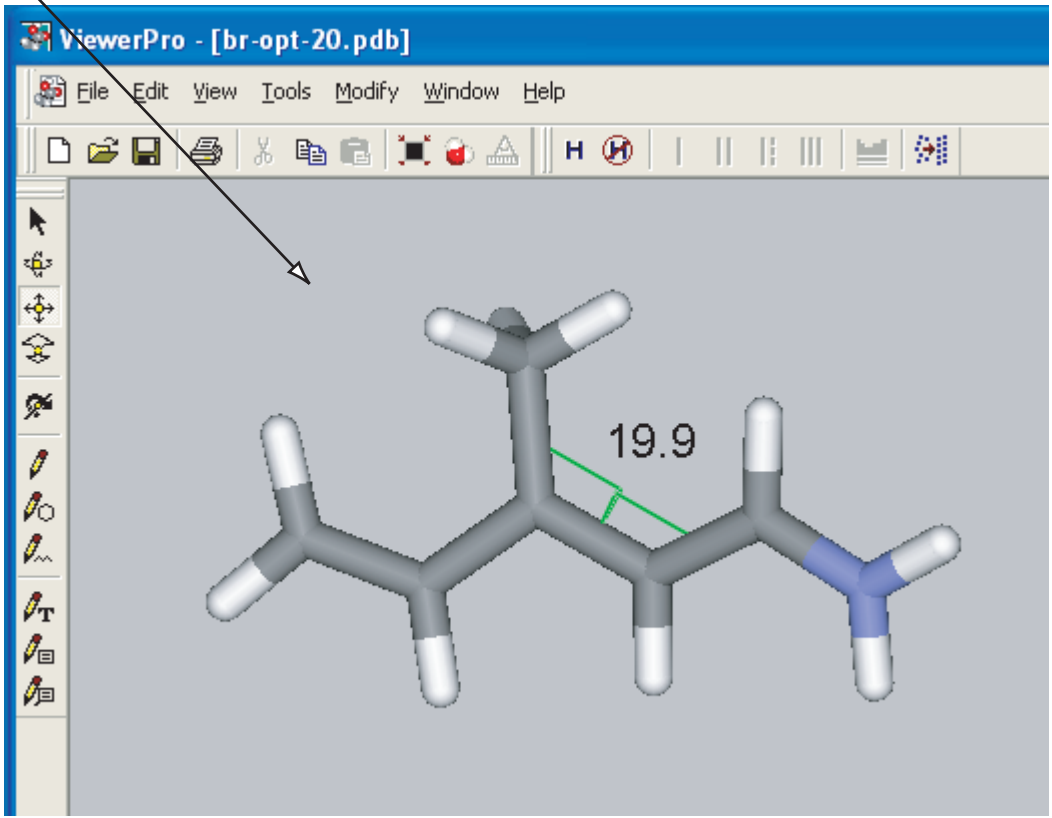


The cis conformer of retinal

E = 410 nm (24400 cm-1)

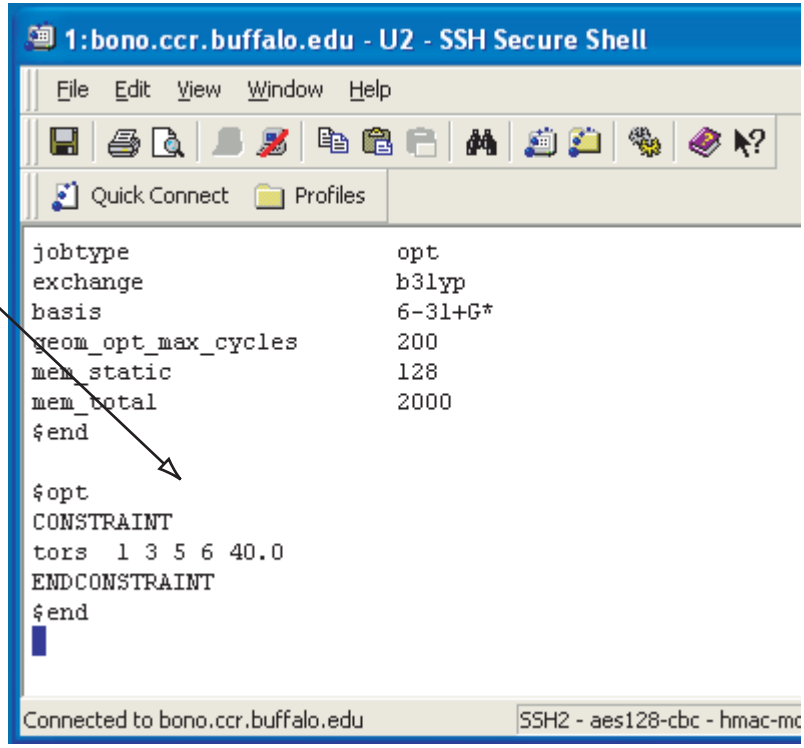


A small computational model of retinal



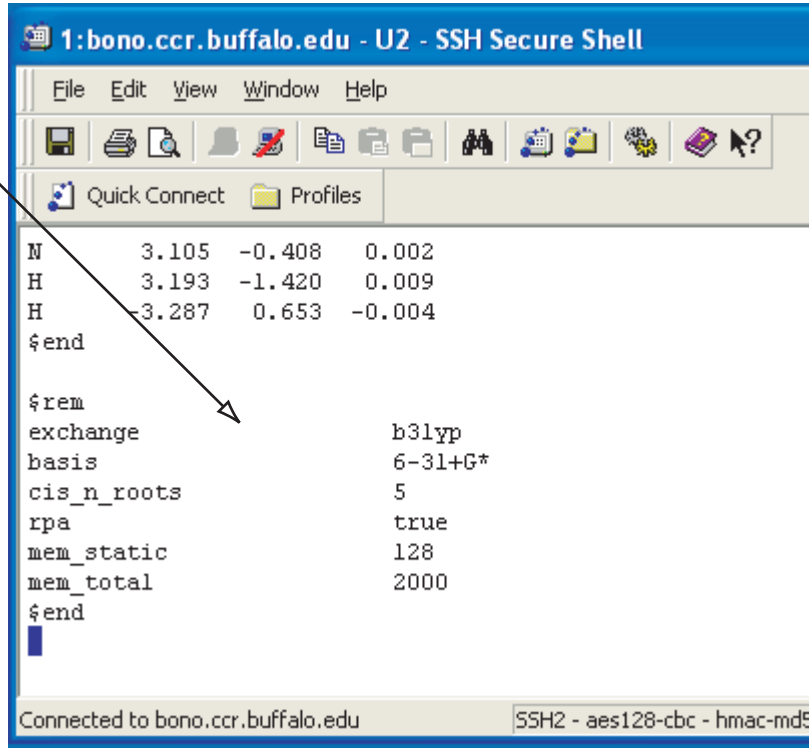
QM calculations of excited electronic states

Geometry optimization of retinal with a constrined dihedral angle

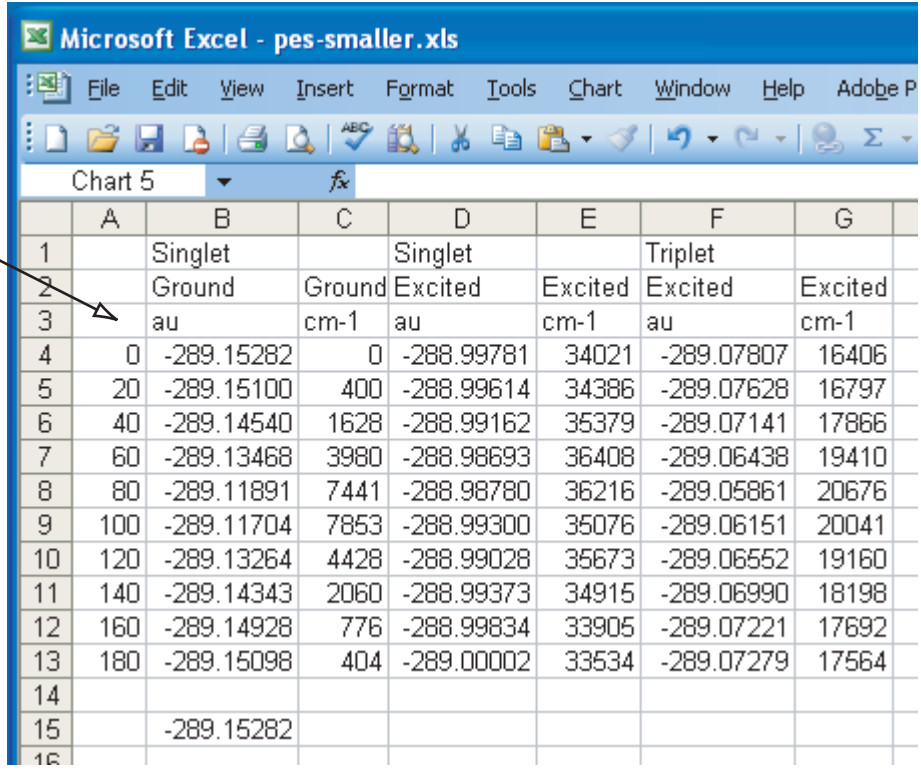


QM calculations of excited electronic states

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



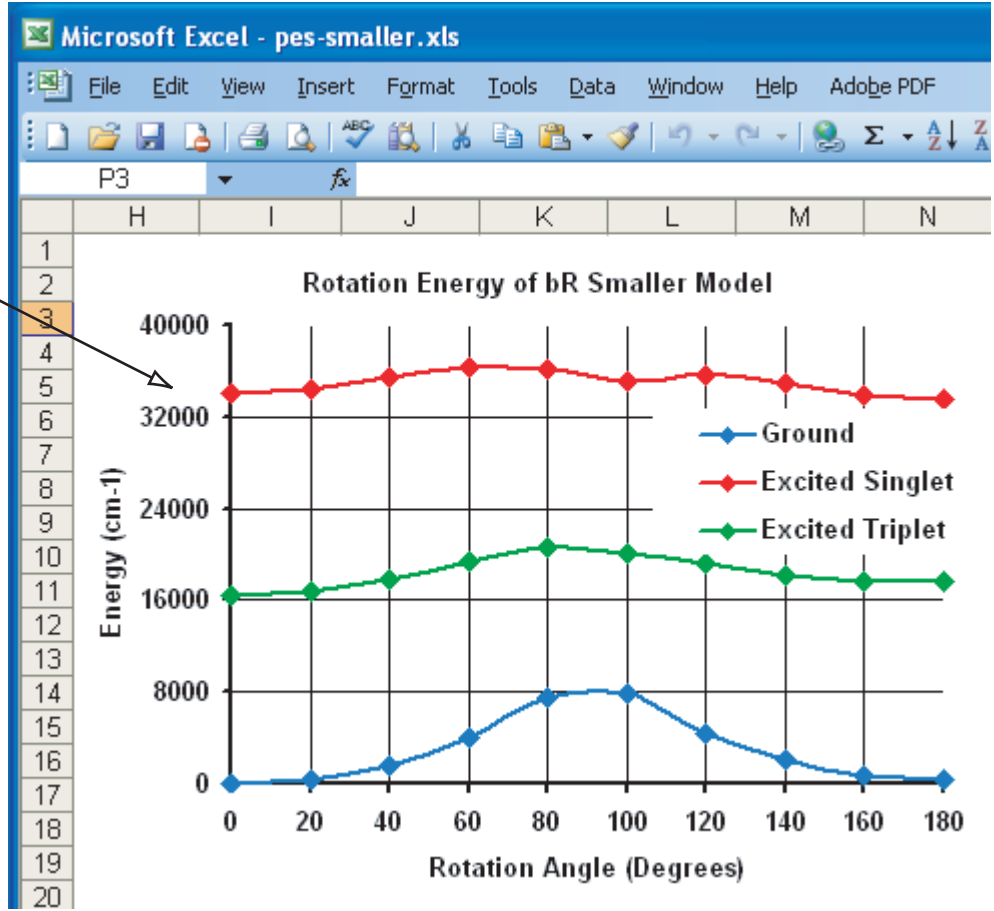
Results of the calculations for the ground electronic state, the excited singlet and triplet



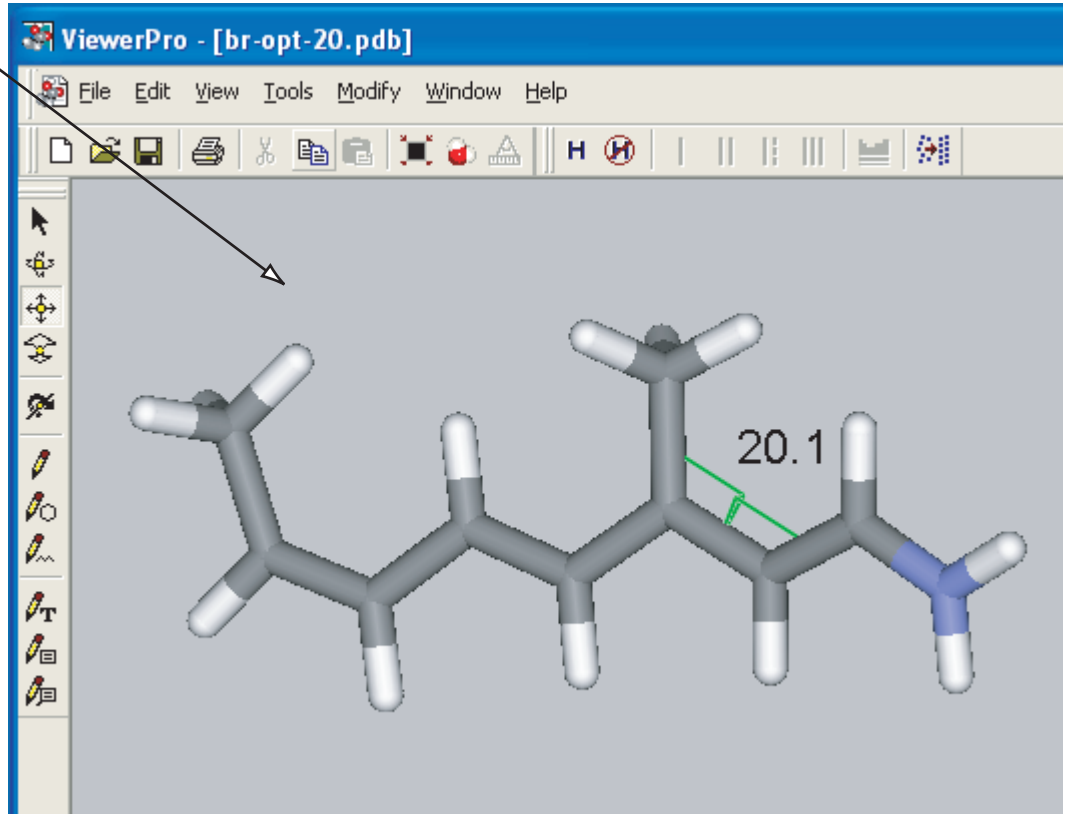
	A	B	C	D	E	F	G
1		Singlet		Singlet		Triplet	
2		Ground	Ground	Excited	Excited	Excited	Excited
3		au	cm-1	au	cm-1	au	cm-1
4	0	-289.15282	0	-288.99781	34021	-289.07807	16406
5	20	-289.15100	400	-288.99614	34386	-289.07628	16797
6	40	-289.14540	1628	-288.99162	35379	-289.07141	17866
7	60	-289.13468	3980	-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					

QM calculations of excited electronic states

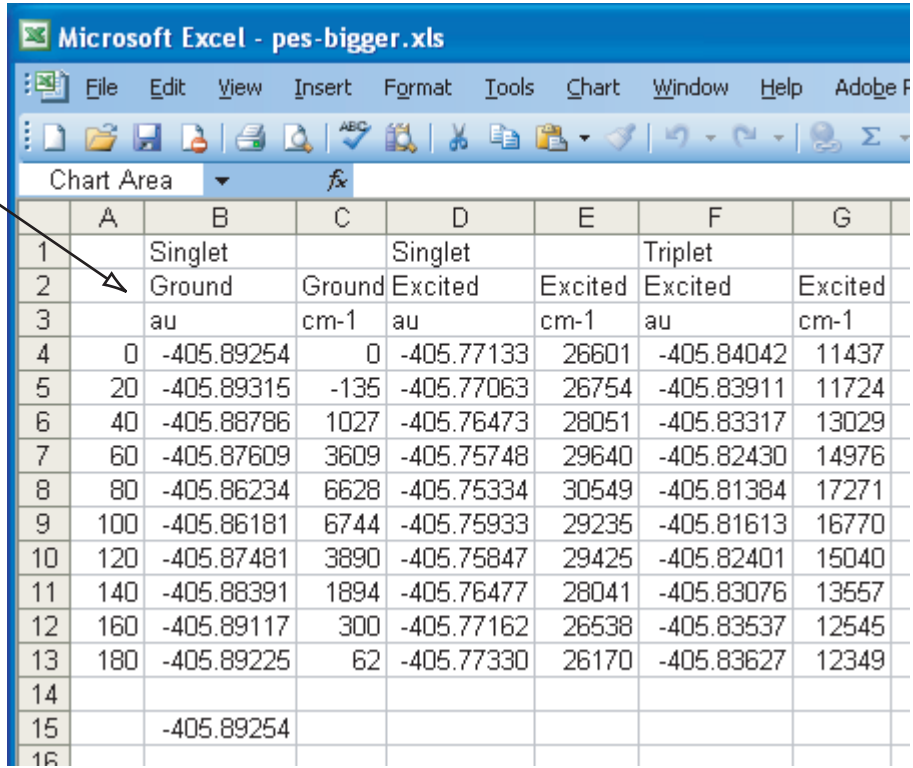
Results of the calculations for the ground electronic state, the excited singlet and triplet



The bigger model of retinal



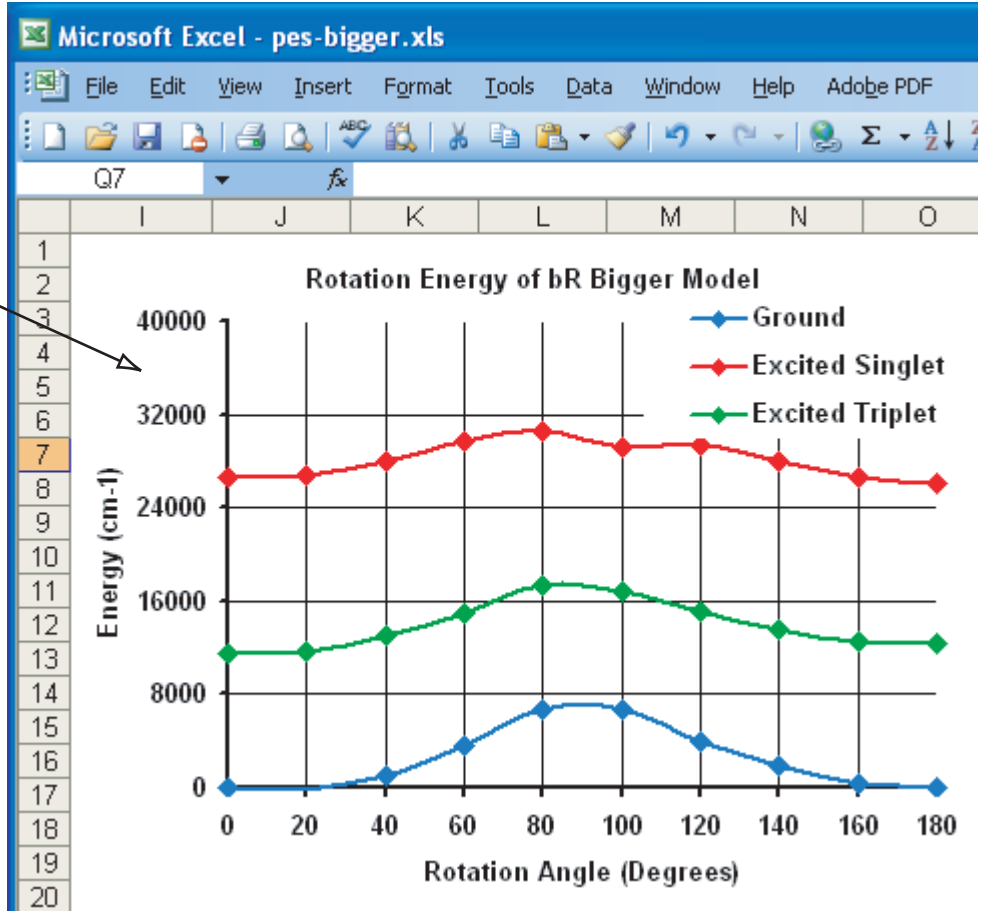
Results of the calculations for the ground electronic state, the excited singlet and triplet



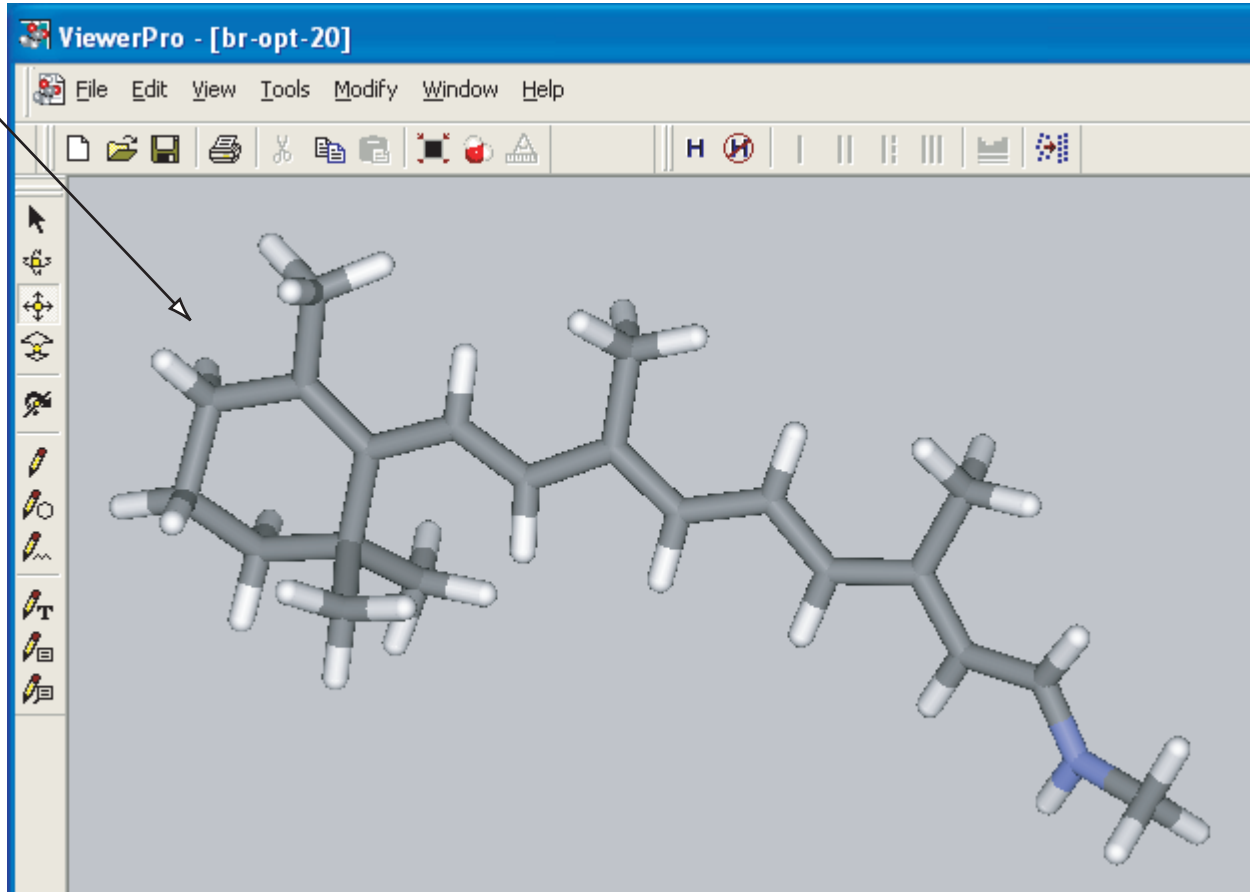
	A	B	C	D	E	F	G
1		Singlet		Singlet		Triplet	
2		Ground	Ground	Excited	Excited	Excited	Excited
3		au	cm-1	au	cm-1	au	cm-1
4	0	-405.89254	0	-405.77133	26601	-405.84042	11437
5	20	-405.89315	-135	-405.77063	26754	-405.83911	11724
6	40	-405.88786	1027	-405.76473	28051	-405.83317	13029
7	60	-405.87609	3609	-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					

QM calculations of excited electronic states

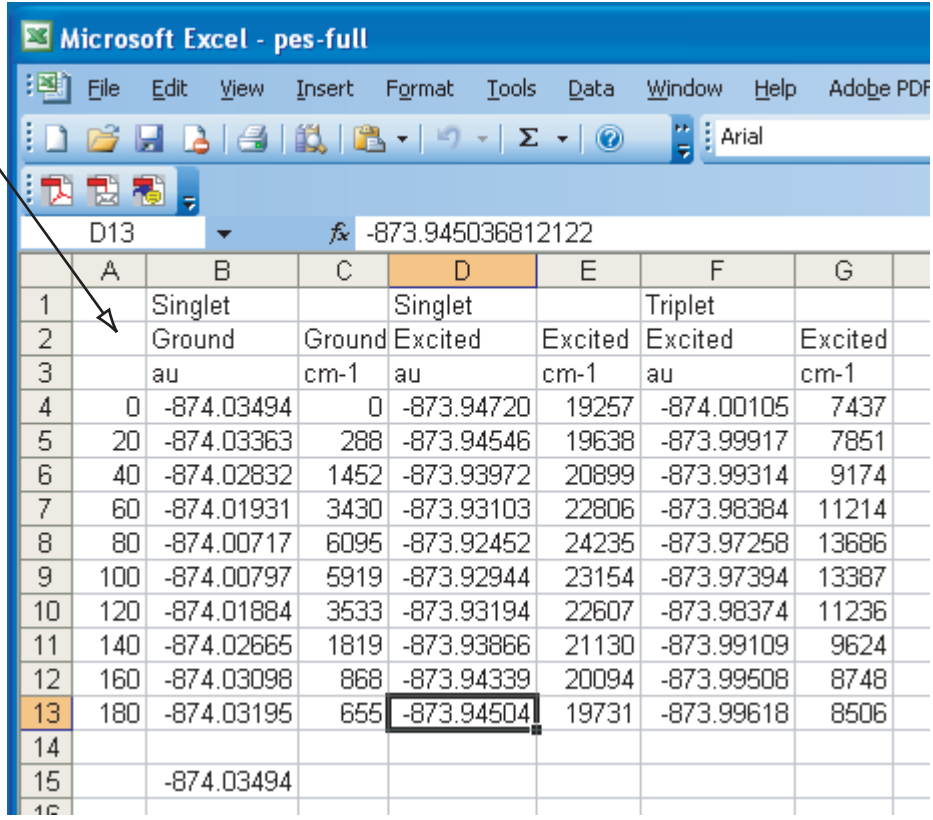
Results of the calculations for the ground electronic state, the excited singlet and triplet



The full model of retinal



The results of the calculations



Microsoft Excel - pes-full

File Edit View Insert Format Tools Data Window Help Adobe PDF

Arial

D13 -873.945036812122

	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	-874.03494	0	-873.94720	19257	-874.00105	7437
5	20	-874.03363	288	-873.94546	19638	-873.99917	7851
6	40	-874.02832	1452	-873.93972	20899	-873.99314	9174
7	60	-874.01931	3430	-873.93103	22806	-873.98384	11214
8	80	-874.00717	6095	-873.92452	24235	-873.97258	13686
9	100	-874.00797	5919	-873.92944	23154	-873.97394	13387
10	120	-874.01884	3533	-873.93194	22607	-873.98374	11236
11	140	-874.02665	1819	-873.93866	21130	-873.99109	9624
12	160	-874.03098	868	-873.94339	20094	-873.99508	8748
13	180	-874.03195	655	-873.94504	19731	-873.99618	8506
14							
15		-874.03494					

QM calculations of excited electronic states

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