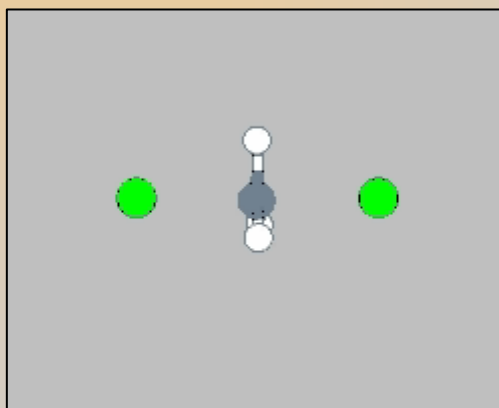


Modelowanie molekularne metodami chemii kwantowej

Dr hab. Artur Michalak
Zakład Chemii Teoretycznej
Wydział Chemii UJ



Wykład 6

<http://www.chemia.uj.edu.pl/~michalak/mmod2007/>

• Podstawowe idee i metody chemii kwantowej:

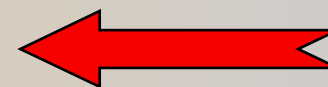
Funkcja falowa, gęstość elektronowa; równanie Schrodingera; Teoria Funkcjonałów Gęstości (DFT); przybliżenie Borna-Oppenheimera, zasada wariacyjna w mechanice kwantowej i w DFT, przybliżenie jednoelektronowe; metoda HF; korelacja elektronowa; metody korelacyjne oparte na funkcji falowej; metoda Kohna-Shama

• Dane do obliczeń kwantowo-chemicznych; GAMESS:

Geometria czasteczki; macierz Z; bazy funkcyjne w obliczeniach *ab initio* ; input/output programu GAMESS

• Struktura geometryczna układów molekularnych:

Optymalizacja geometrii; optymalizacja z wiązami; analiza konformacyjna; problem minimum globalnego



• Struktura elektronowa układów molekularnych:

Orbitale molekularne, orbitale KS; wiązanie chemiczne; gęstość różnicowa; orbitale zlokalizowane; analiza populacyjna; analiza rzędów wiązań

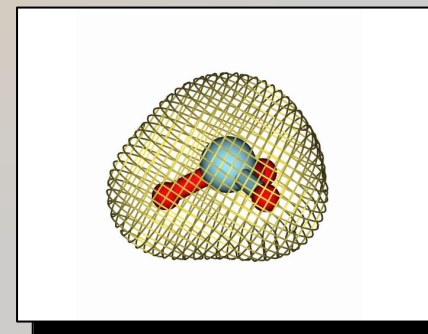
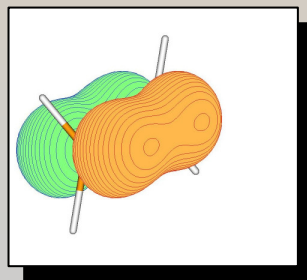
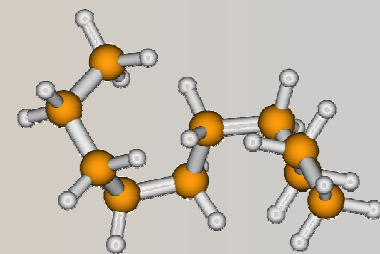
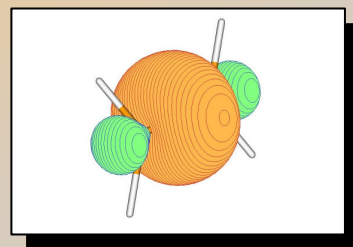
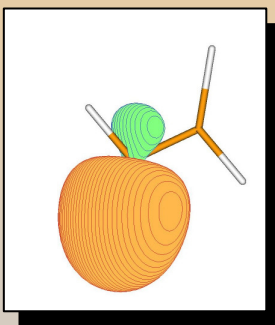
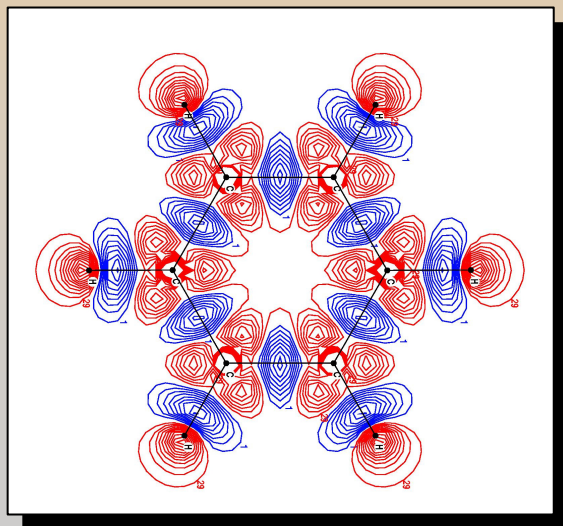
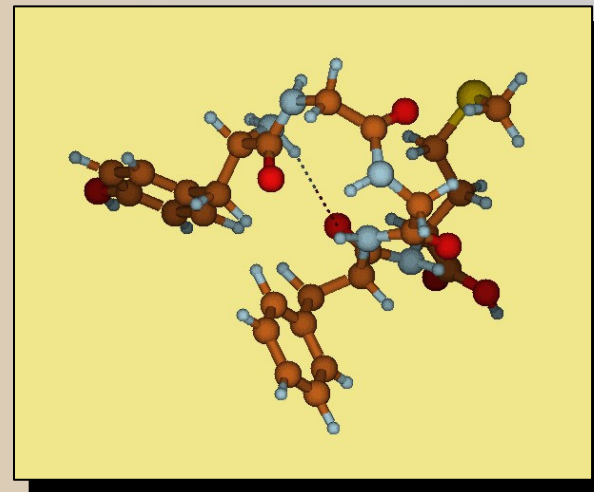
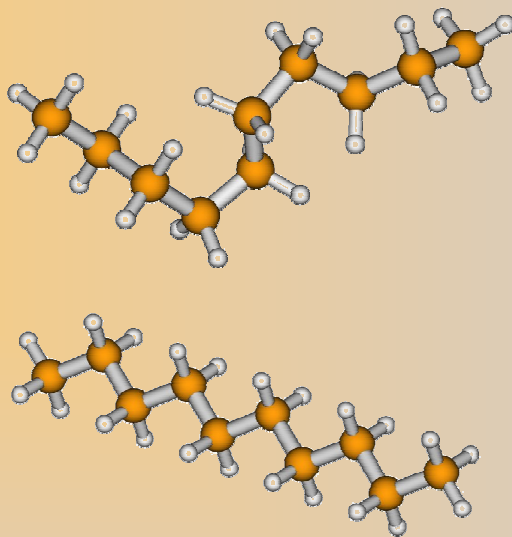
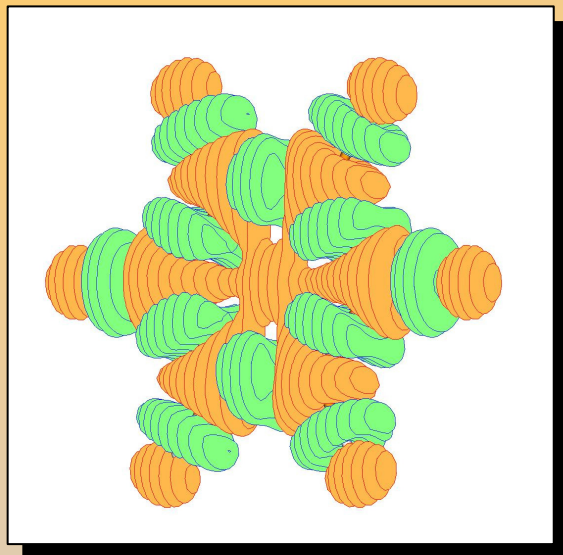
• Analiza wibracyjna; Wielkości termodynamiczne; Reaktywność chemiczna:

Analiza wibracyjna; wielkości termodynamiczne; modelowanie reakcji chemicznych; optymalizacja geometrii stanu przejściowego, IRC; indeksy reaktywności chemicznej, molekularny potencjał elektrostatyczny, funkcja Fukui'ego i teoria orbitali granicznych; jedno- i dwu-reagentowe indeksy reaktywności

• Inne zagadnienia:

Metody hybrydowe QM/MM; modelowanie wielkich układów; efekty rozpuszczalnika; modelowanie w katalizie homo- i heterogenicznej; oddziaływania międzycząsteczkowe, i. in.

MOLDEN



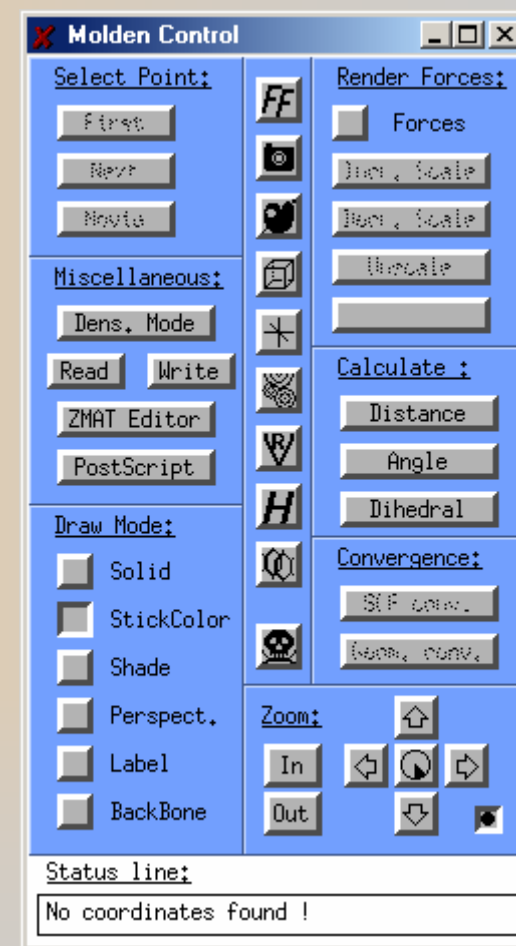
MOLDEN

Uruchomienie:

molden <Enter>

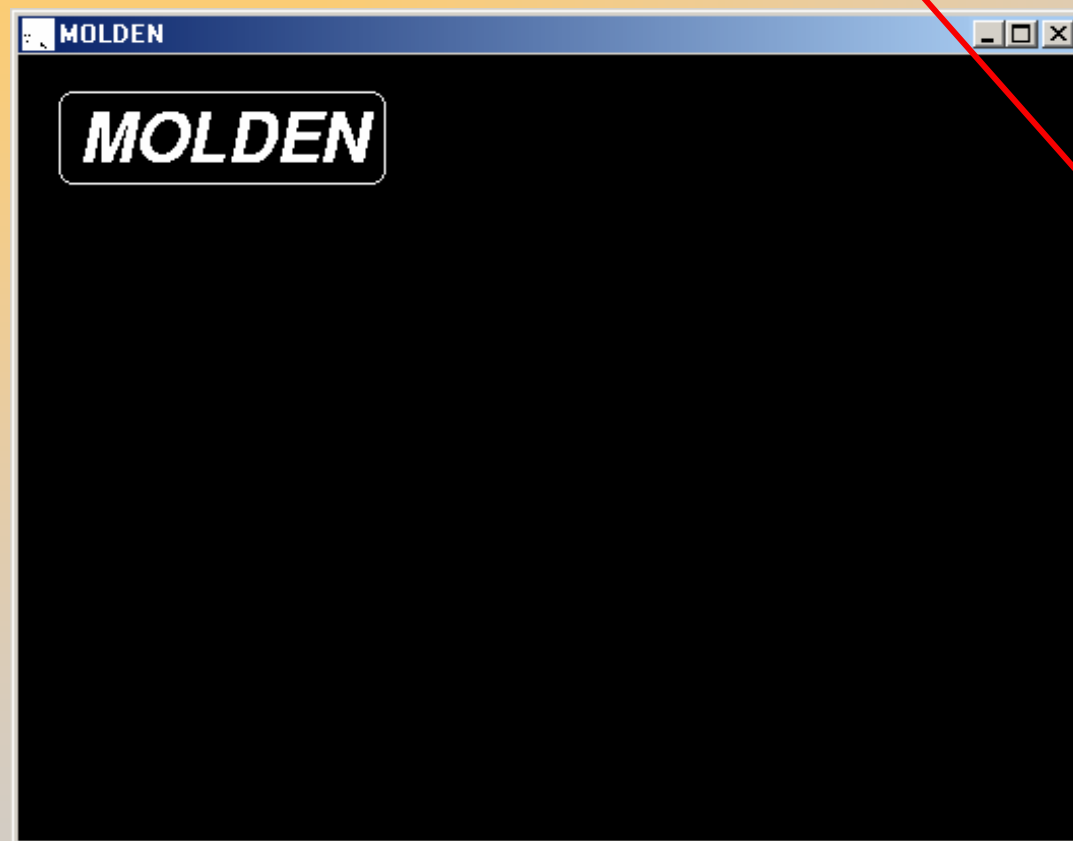


Okienko graficzne

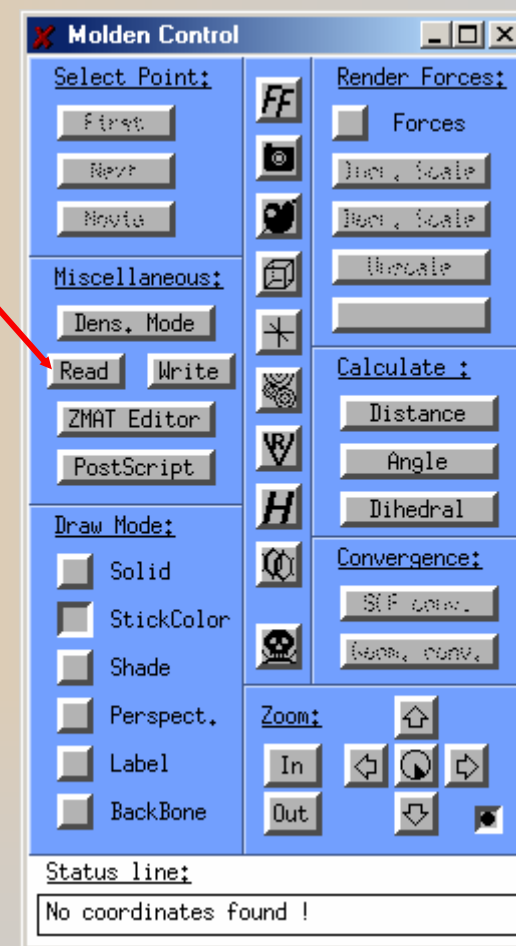


Okno kontrolne

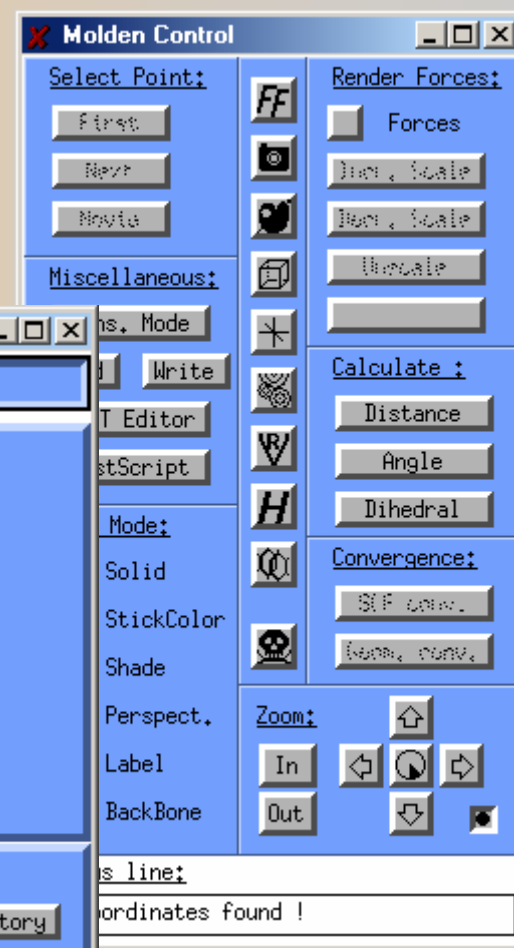
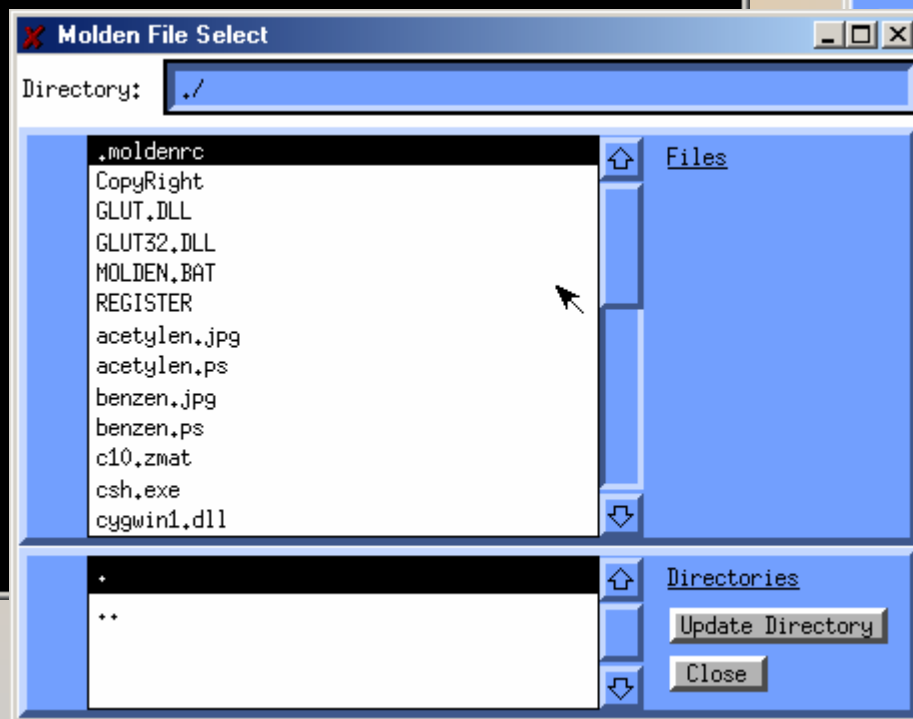
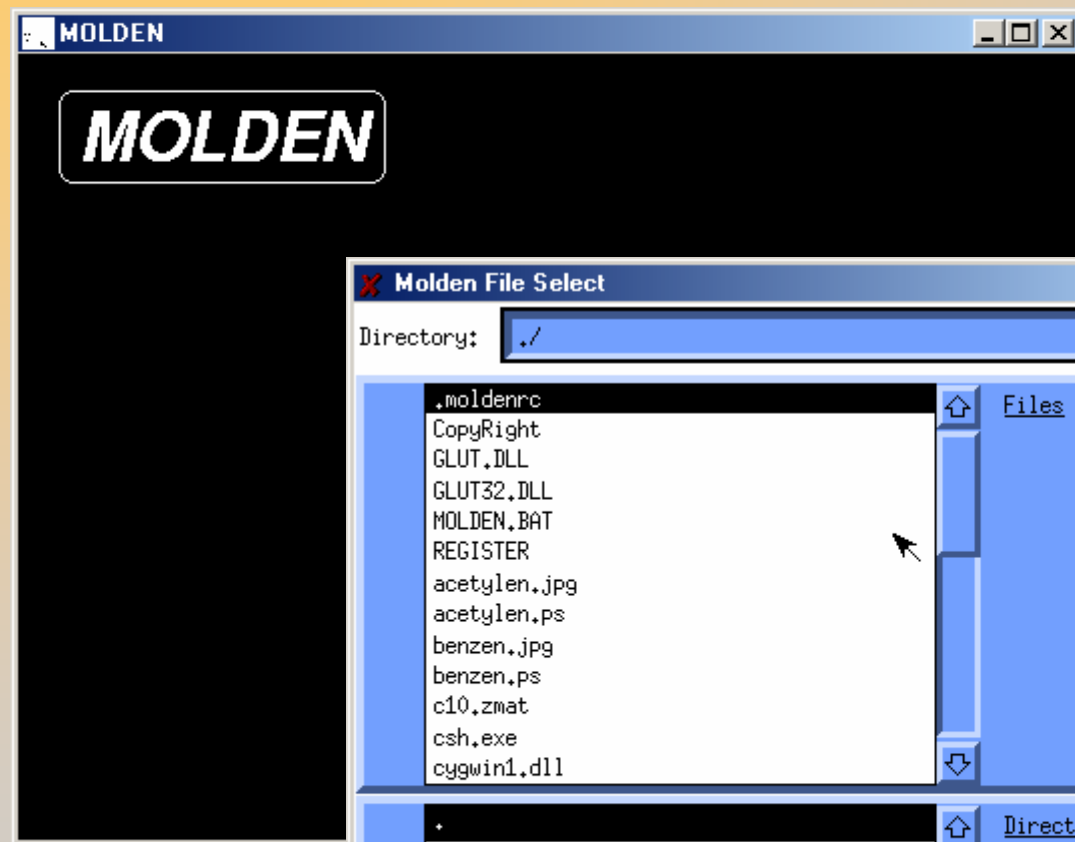
czytanie pliku

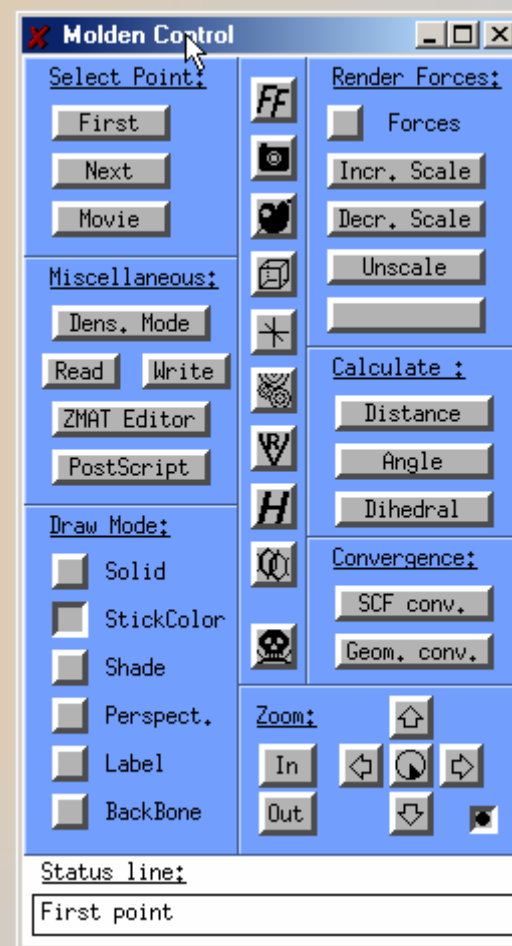
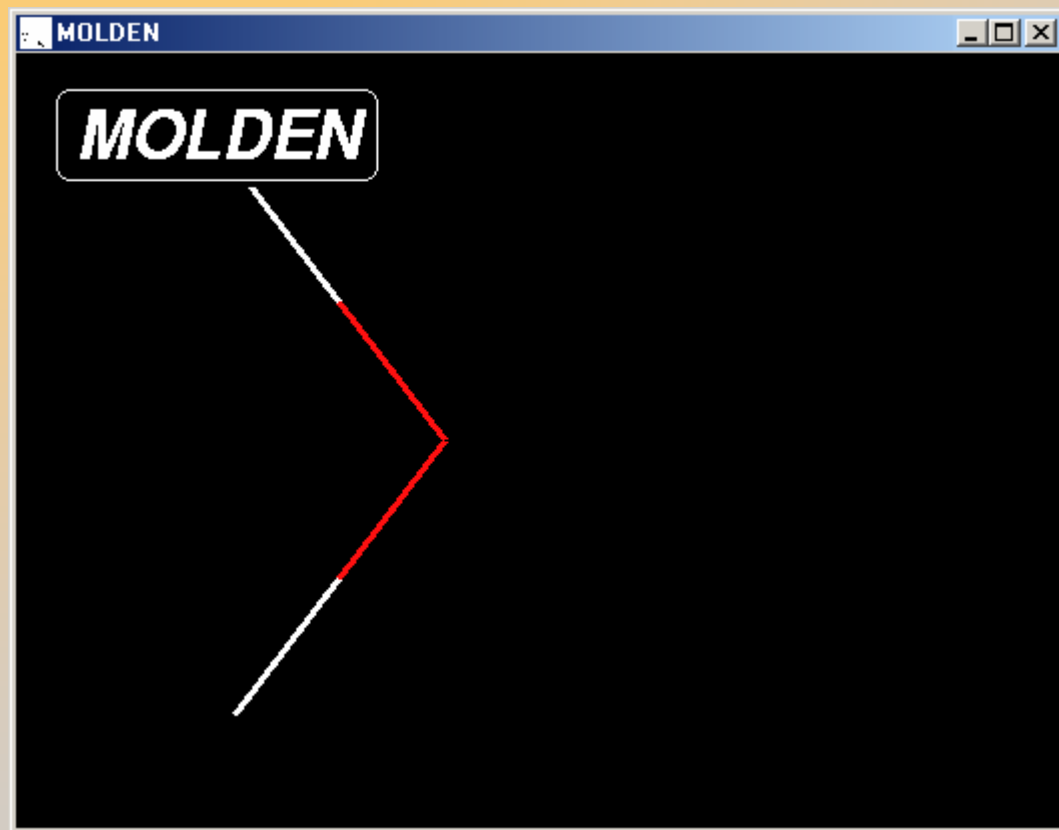


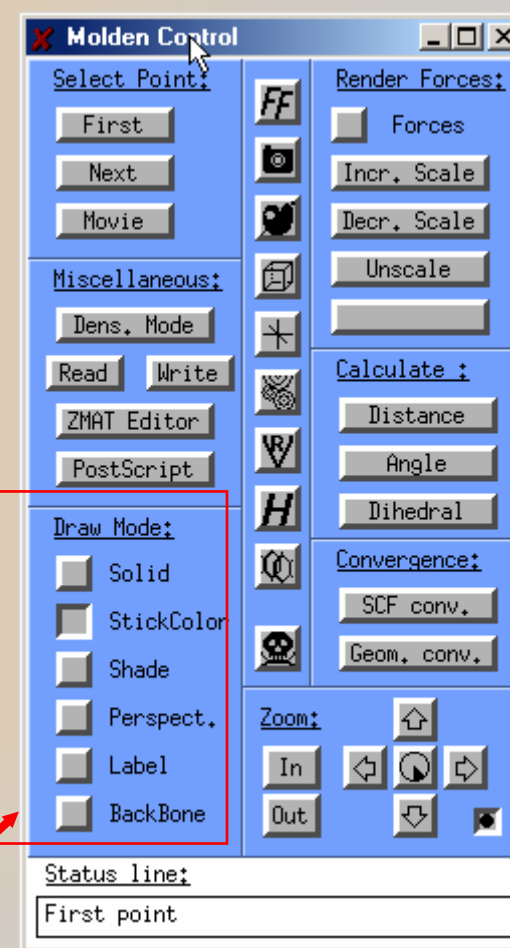
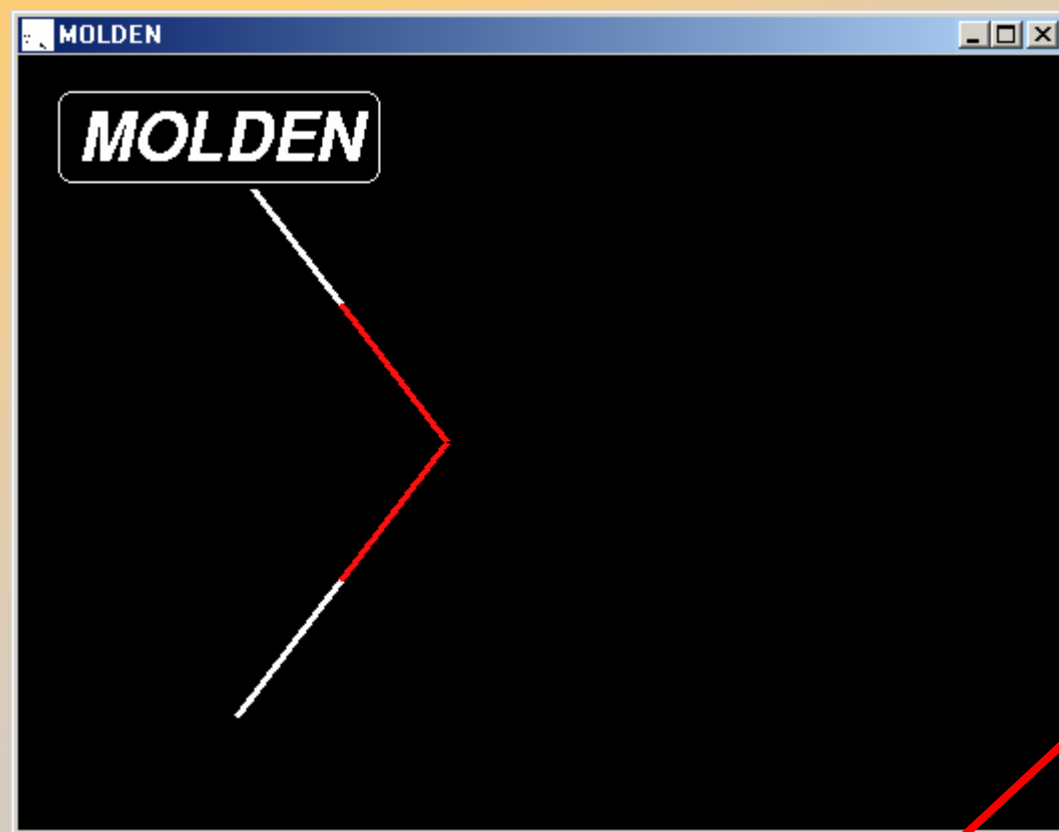
Okienko graficzne



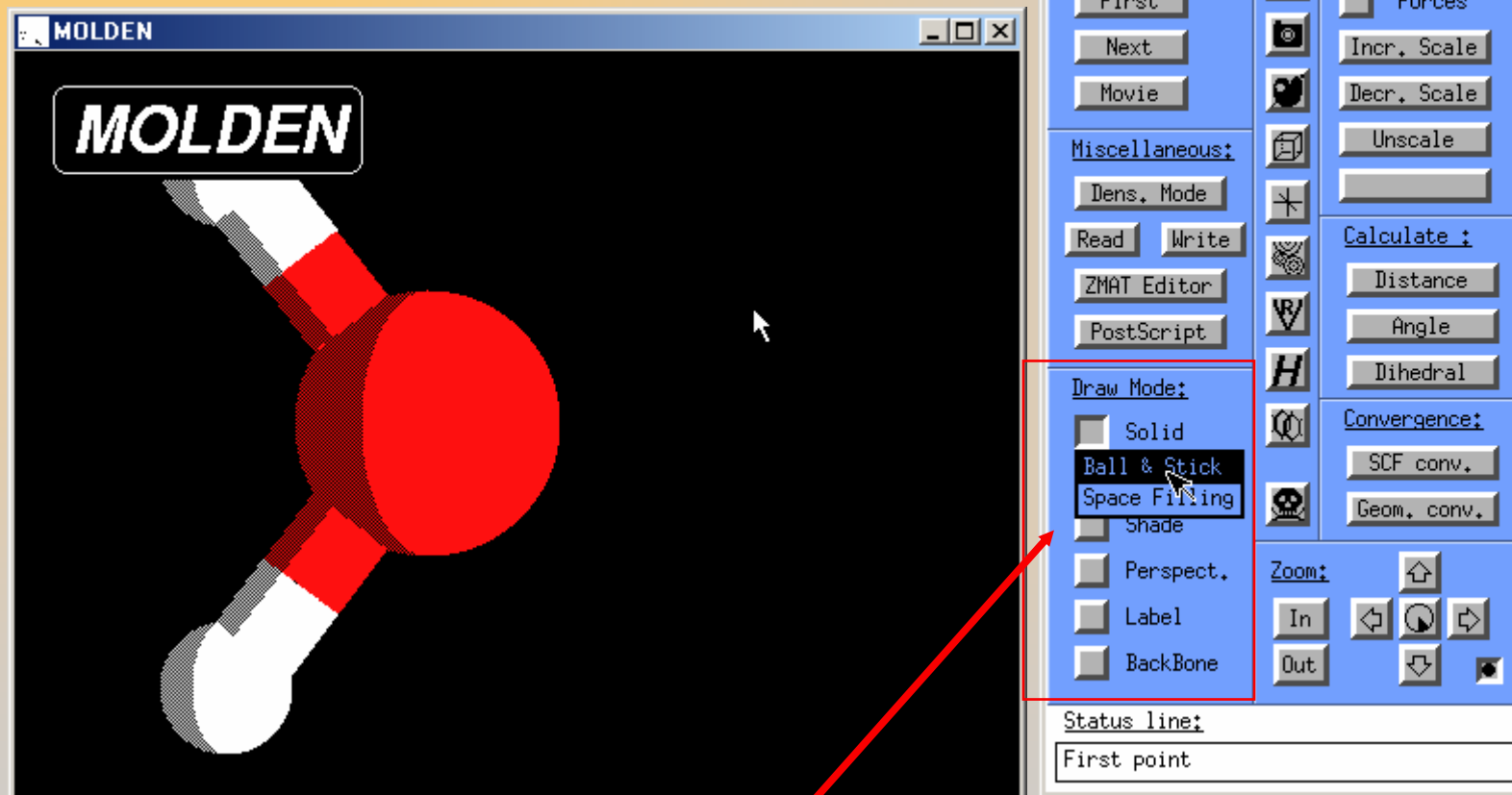
Okno kontrolne



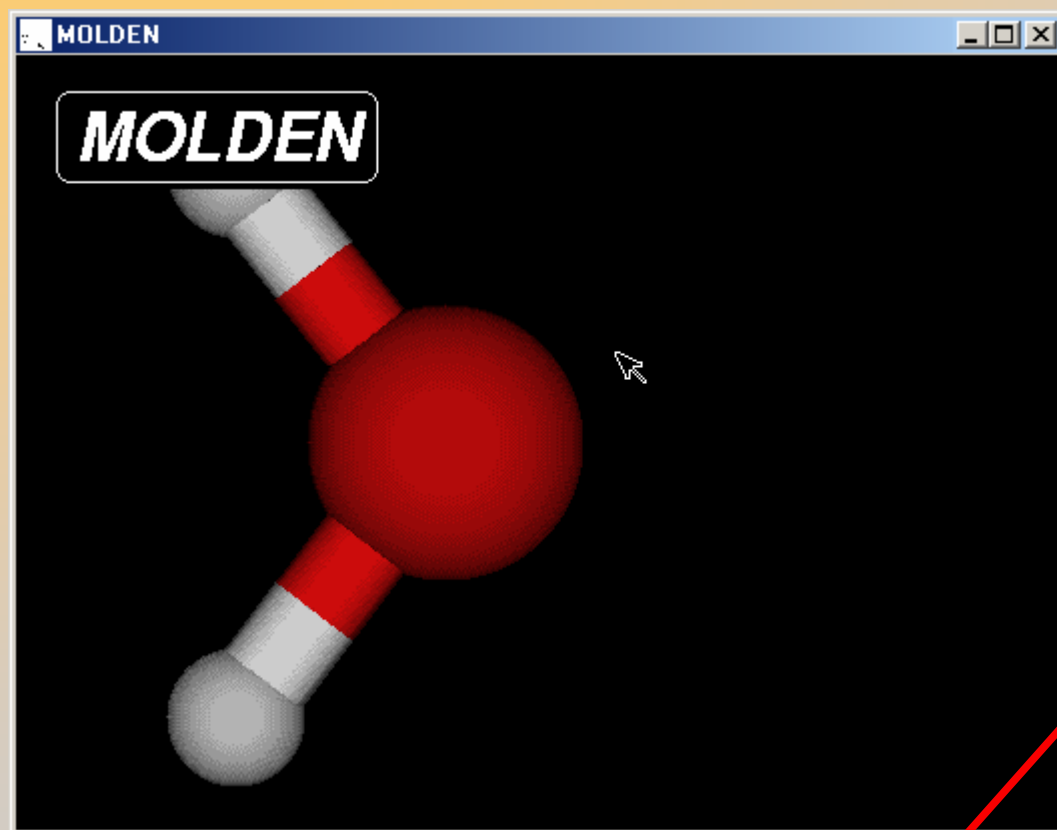




spóób wyświewtlania molekuly



sposób wyświetlania molekuły



Molden Control

Select Point:
First
Next
Movie

Miscellaneous:
Dens. Mode
Read Write
ZMAT Editor
PostScript

Draw Mode:
 Solid
 StickColor
 Shade
 Perspect.
 Label
 BackBone

Render Forces:
 Forces
Incr. Scale
Decr. Scale
Unscale

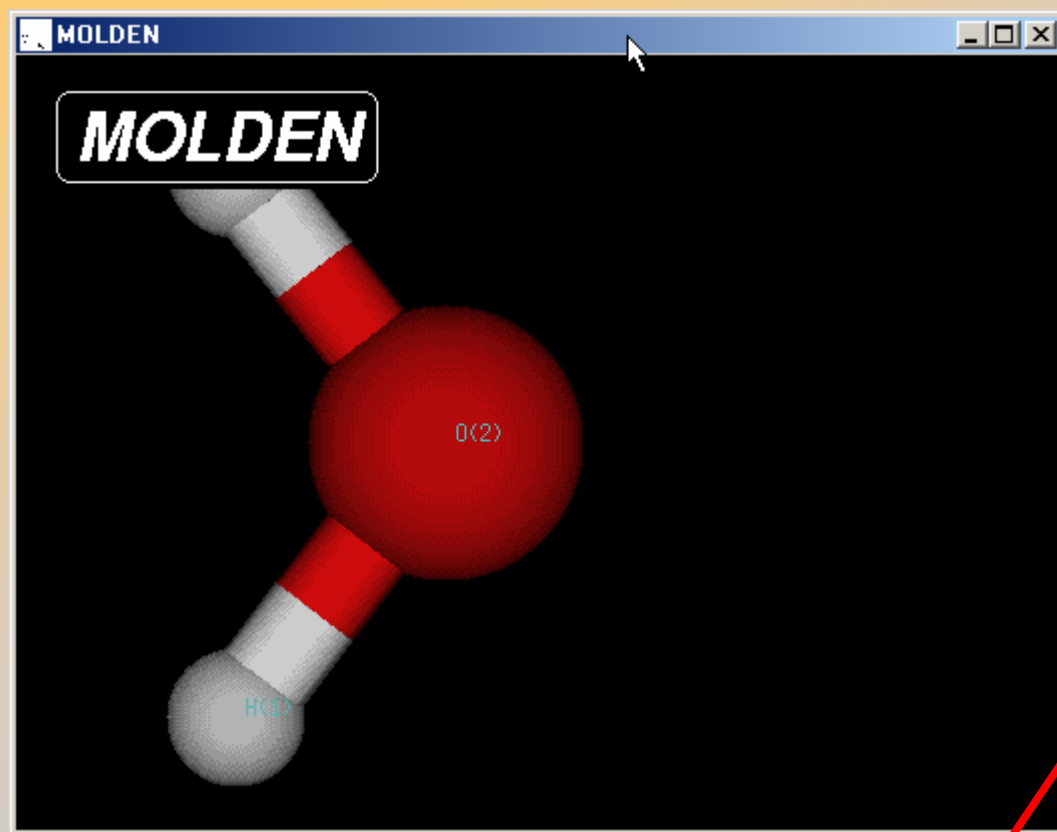
Calculate :
Distance
Angle
Dihedral

Convergence:
SCF conv.
Geom. conv.

Zoom:
In Out
Home

Status line:
First point

spóób wyświewtłania molekuly



Molden Control

Select Point:
First
Next
Movie

Miscellaneous:
Dens. Mode
Read Write
ZMAT Editor
PostScript

Draw Mode:
 Solid
 StickColor
 Shade
 Perspect.
atom
atom+number
ForceF.Type
atom+charge
PDBsymbol
Residue

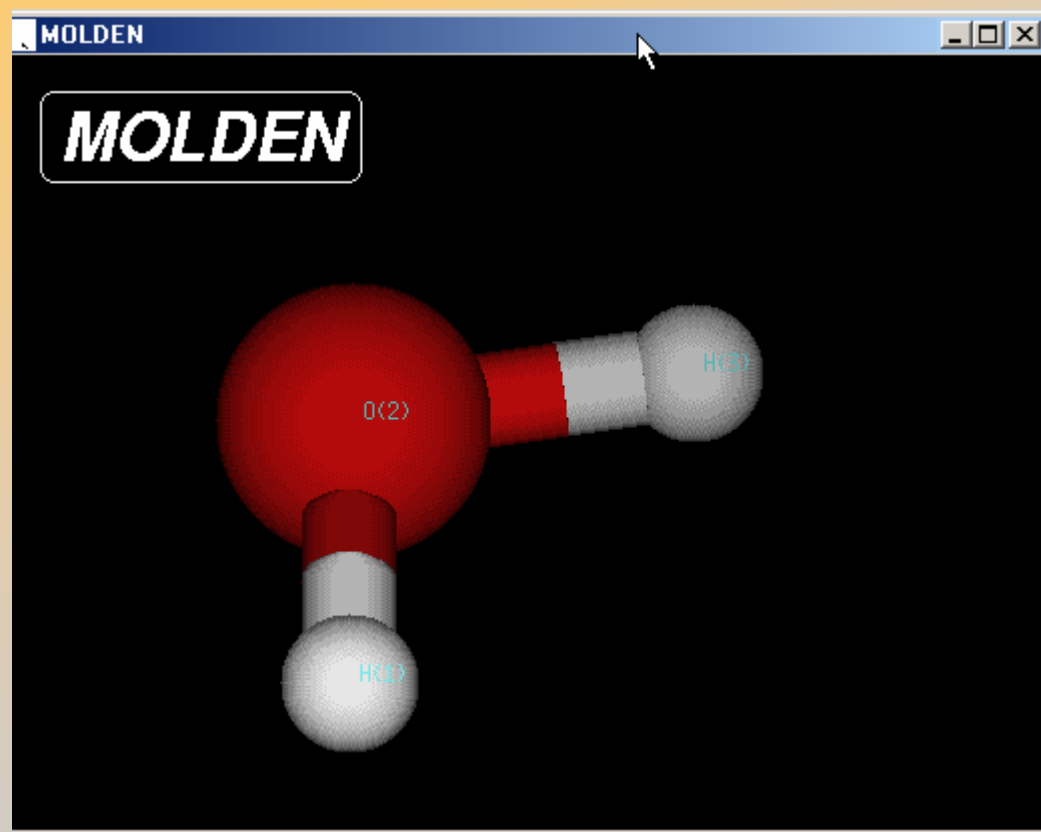
Render Forces:
 Forces
Incr. Scale
Decr. Scale
Unscale

Calculate :
Distance
Angle
Dihedral

Convergence:
SCF conv.
Geom. conv.

Zoom:
In Out

sposób wyświetlania molekuły

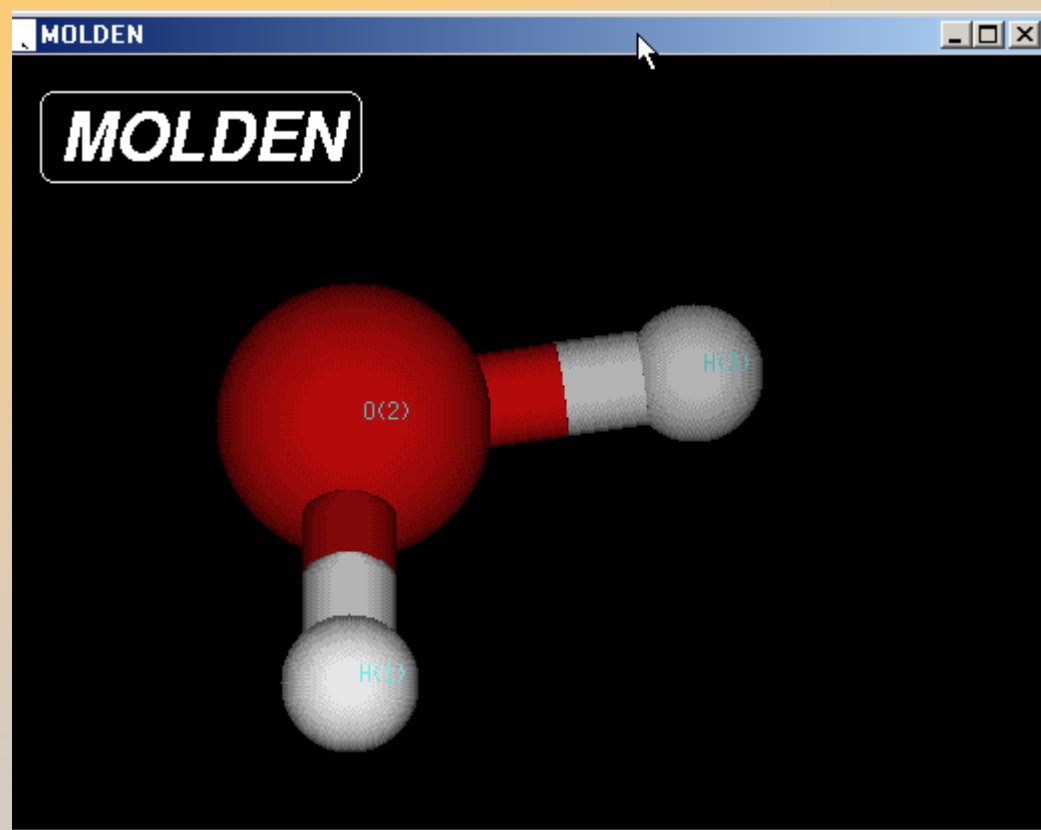


The Molden Control panel is a sidebar containing various controls for the MOLDEN application. It is organized into several sections:

- Select Point:** Buttons for First, Next, and Movie.
- Miscellaneous:** Buttons for Dens. Mode, Read, Write, ZMAT Editor, and PostScript.
- Draw Mode:** Checkboxes for Solid, StickColor, Shade, Perspect., Label, and BackBone.
- Render Forces:** A checkbox for Forces and buttons for Incr. Scale, Decr. Scale, and Unscale.
- Calculate:** Buttons for Distance, Angle, and Dihedral.
- Convergence:** Buttons for SCF conv. and Geom. conv.
- Zoom:** Buttons for In, Out, and a set of directional arrows.

At the bottom, there is a **Status line:** with the text "Last point".

obrót cząsteczki poprzez przeciągnięcie mysza



Molden Control

Select Point:
 First
 Next
 Movie

Miscellaneous:
 Dens. Mode
 Read Write
 ZMAT Editor
 PostScript

Draw Mode:
 Solid
 StickColor
 Shade
 Perspect.
 Label
 BackBone

Render Forces:
 Forces
 Incr. Scale
 Decr. Scale
 Unscale

Calculate :
 Distance
 Angle
 Dihedral

Convergence:
 SCF conv.
 Geom. conv.

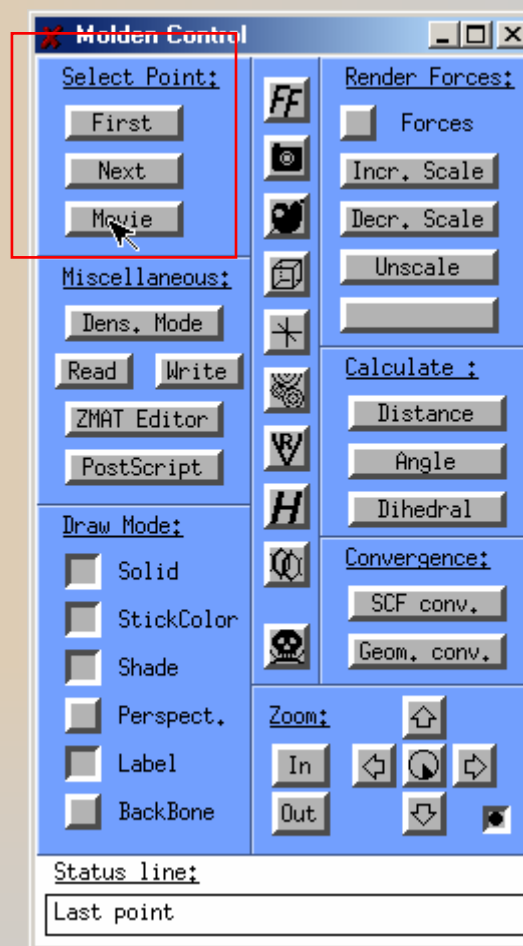
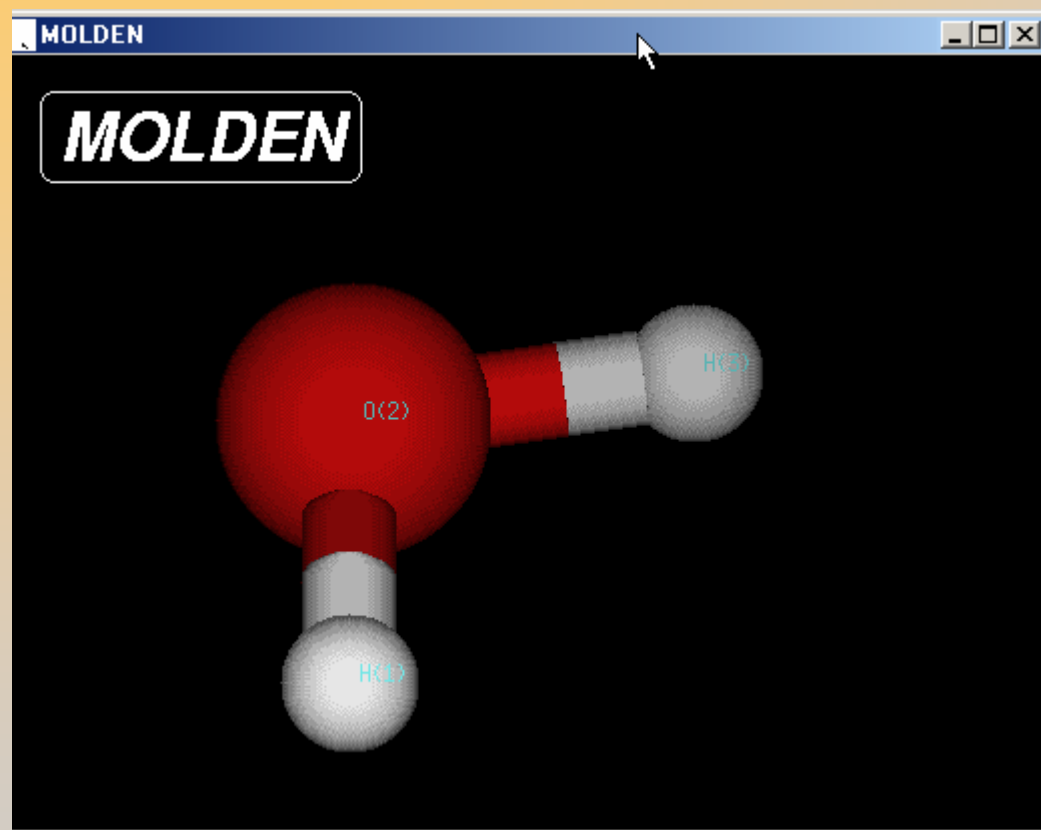
Zoom:
 In
 Out
 (directional arrows)

Status line:
 Last point

obrót cząsteczki poprzez przeciągnięcie mysza

Obrót,
 przesunięcie,
 powiększenie

Wybór jednej z wielu geometrii



Molden Control

Select Point:
First
Next
Movie

Render Forces:
Forces
Incr. Scale
Decr. Scale
Unscale

Miscellaneous:
Dens. Mode
Read Write
ZMAT Editor
PostScript

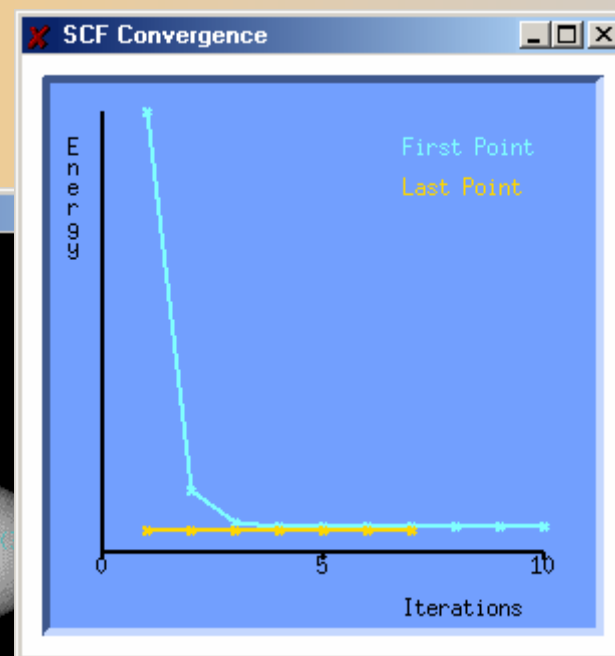
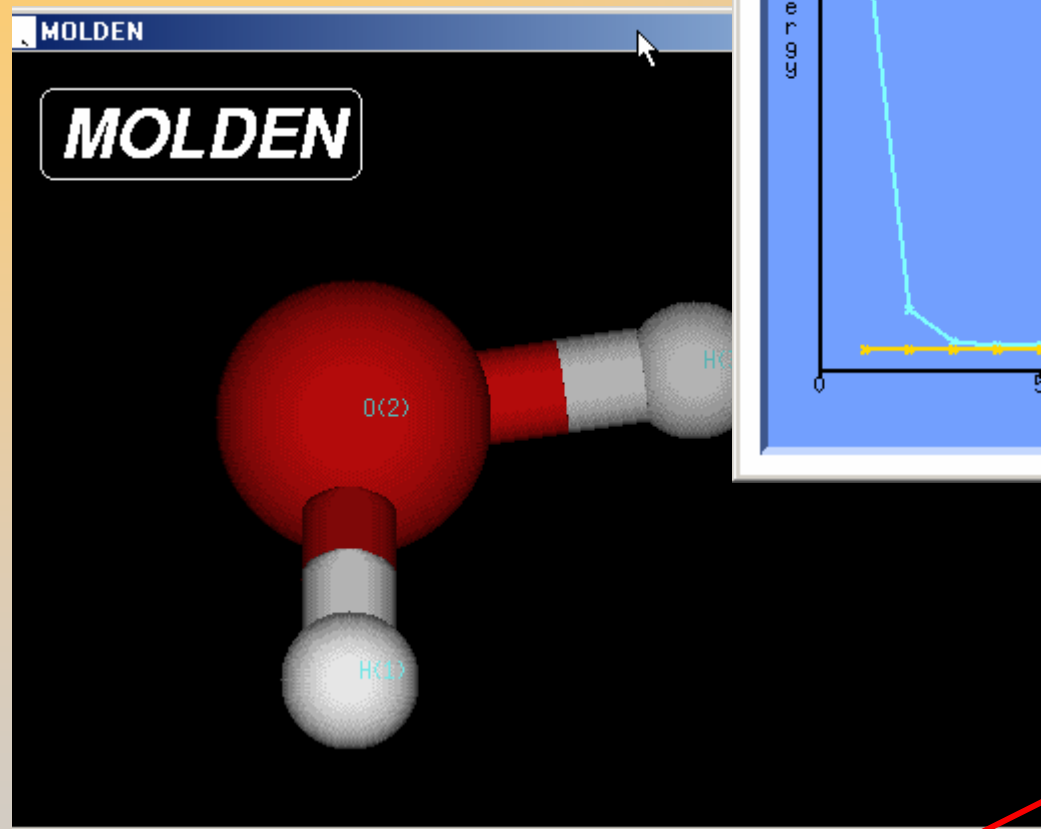
Calculate :
Distance
Angle
Dihedral

Convergence:
SCF conv.
Geom. conv.

Draw Mode:
Solid
StickColor
Shade
Perspect.
Label
BackBone

Zoom:
In
Out

Status line:
Last point



Render Forces:

Forces

Incr. Scale

Decr. Scale

Unscale

Calculate:

Distance

Angle

Dihedral

Convergence:

SCF conv.

Geom. conv.

Draw Mode:

Solid

StickColor

Shade

Perspect.

Label

BackBone

Zoom:

In

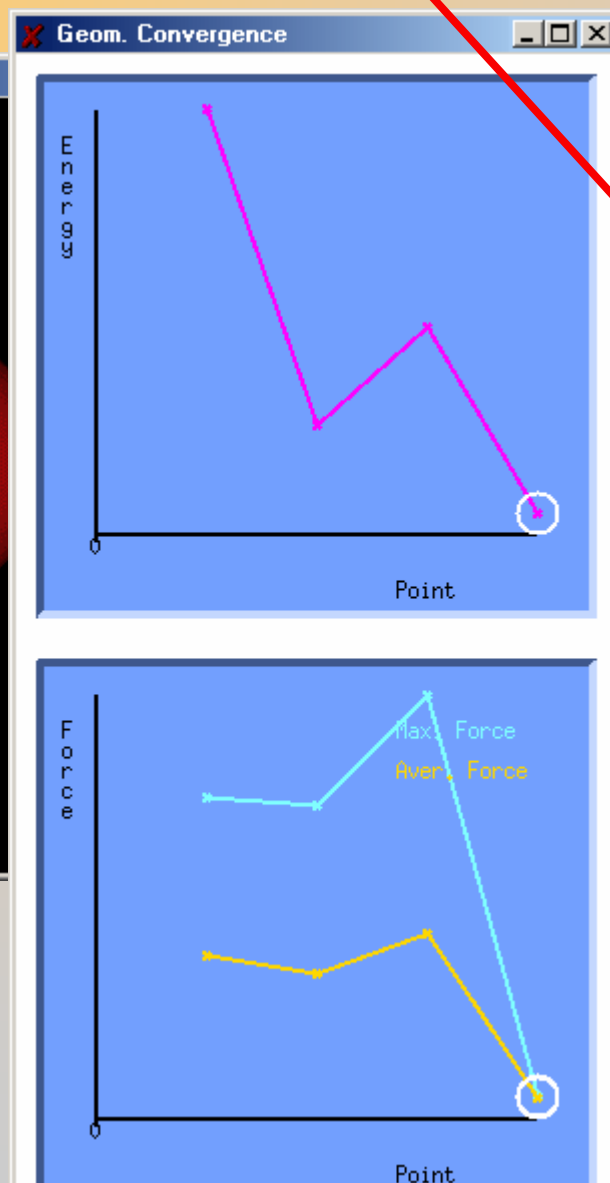
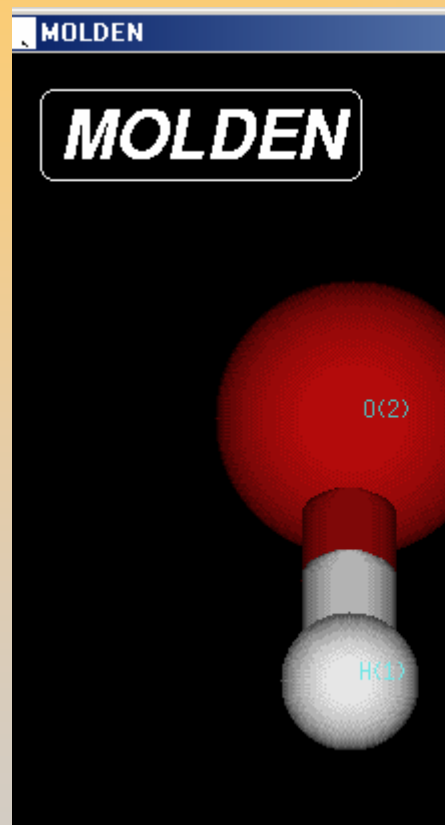
Out

Status line:

Last point

Zbieżność SCF

zbieżność geometrii



Molden Control

Select Point:

First

Next

Movie

Miscellaneous:

Dens. Mode

Read Write

ZMAT Editor

PostScript

Draw Mode:

Solid

StickColor

Shade

Perspect.

Label

BackBone

Render Forces:

Forces

Incr. Scale

Decr. Scale

Unscale

Calculate:

Distance

Angle

Dihedral

Convergence:

SCF conv.

Geom. conv.

Zoom:

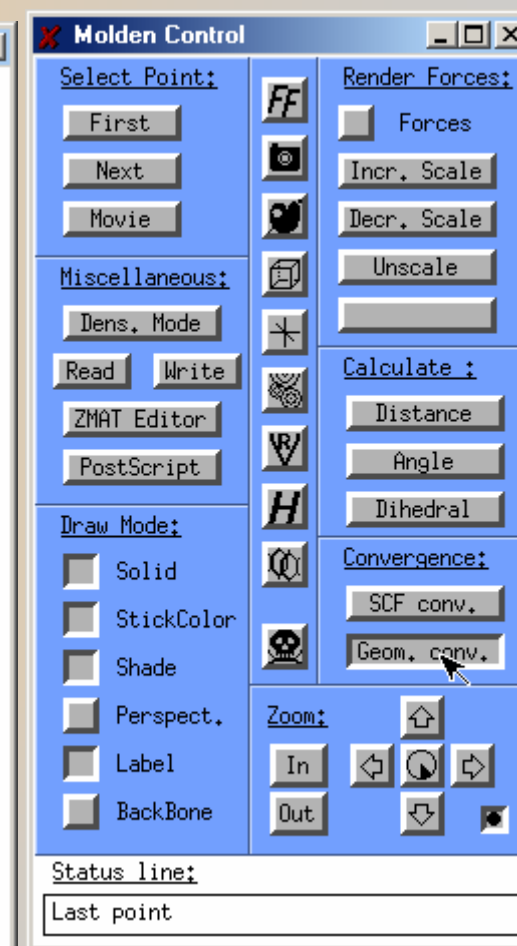
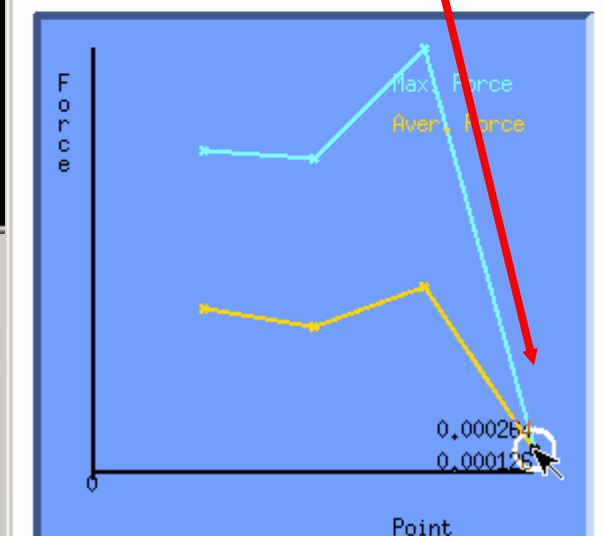
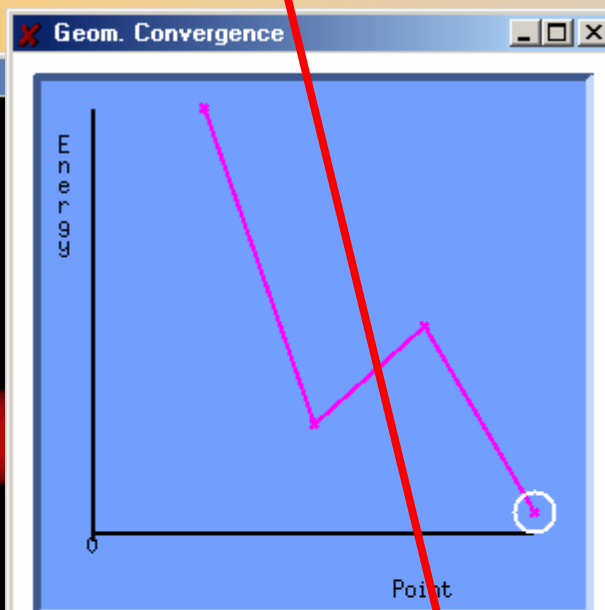
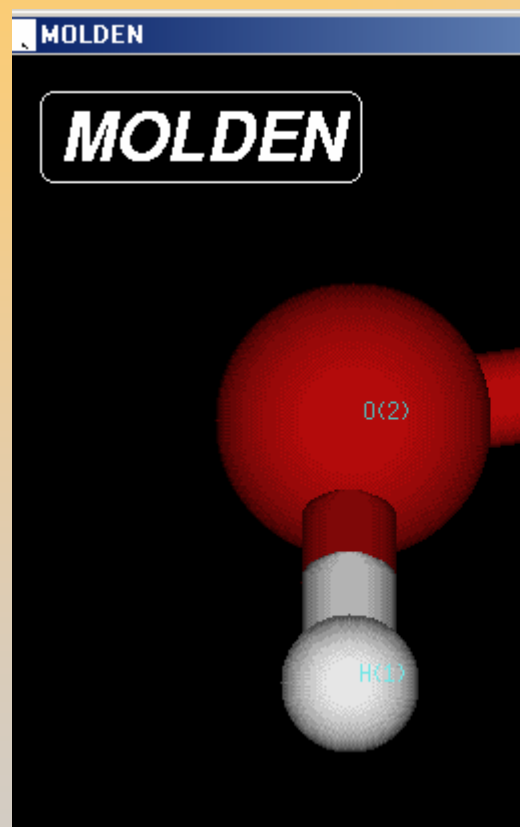
In

Out

Status line:

Last point

zbieżność geometrii:
wartości gradientów



Select Point:
First
Next
Movie

Miscellaneous:
Dens. Mode
Read Write
ZMAT Editor
PostScript

Draw Mode:
 Solid
 StickColor
 Shade
 Perspect.
 Label
 BackBone

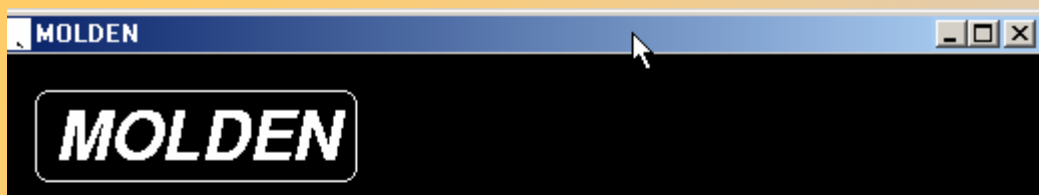
Render Forces:
 Forces
Incr. Scale
Decr. Scale
Unscale

Calculate :
Distance
Angle
Dihedral

Convergence:
SCF conv.
Geom. conv.

Zoom:
In Out
Directional arrows

Status line:
Last point



edytor macierzy Z

Zmatrix Editor

BondLength BondAngle Dihedral [Close]

H				
O	1	0.989577		
H	2	0.989577	1	100.018240

Apply Changes to current Z-Mat Set Status All Variables

Cancel Non-Applied Changes New Z-mat from screen coordinates:

Delete Line Add Line Reorder Z-matrix

Substitute atom by Fragment Select by cursor DeSelect

New Z-mat MapXYZ/Optimise Apply Selection

Molden Control

Select Point: First Next Movie

Miscellaneous: Gen. Mode Read Write ZMAT Editor PostScript

Draw Mode: Solid StickColor Shade Perspect. Label BackBone

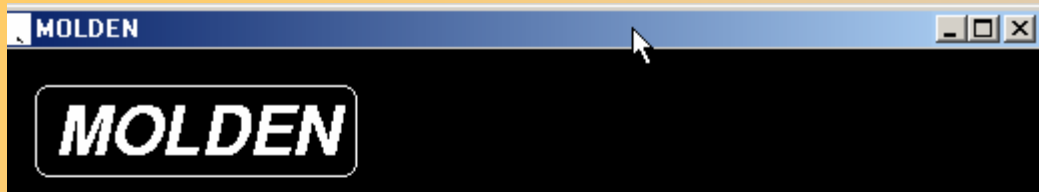
Render Forces: Forces Incr. Scale Decr. Scale Unscale

Calculate: Distance Angle Dihedral

Convergence: SCF conv. Geom. conv.

Zoom: In Out

Status line: Last point



nowa cząsteczka

Zmatrix Editor

BondLength BondAngle DiHedral [Close]

[Apply Changes to current Z-Mat] [Set Status All Variables]

[Cancel Non-Applied Changes]

[Delete Line] [Add Line] [New Z-mat from screen coordinates]

[Substitute atom by Fragment] [Reorder Z-matrix]

[New Z-mat] [MapXYZ/Optimise] [Select by cursor] [DeSelect]

[Apply Selection]

Molden Control

Select Point: [First] [Next] [Movie]

Miscellaneous: [Geom. Mode] [Read] [Write] [ZMAT Editor] [PostScript]

Draw Mode: [Solid] [StickColor] [Shade] [Perspect.] [Label] [BackBone]

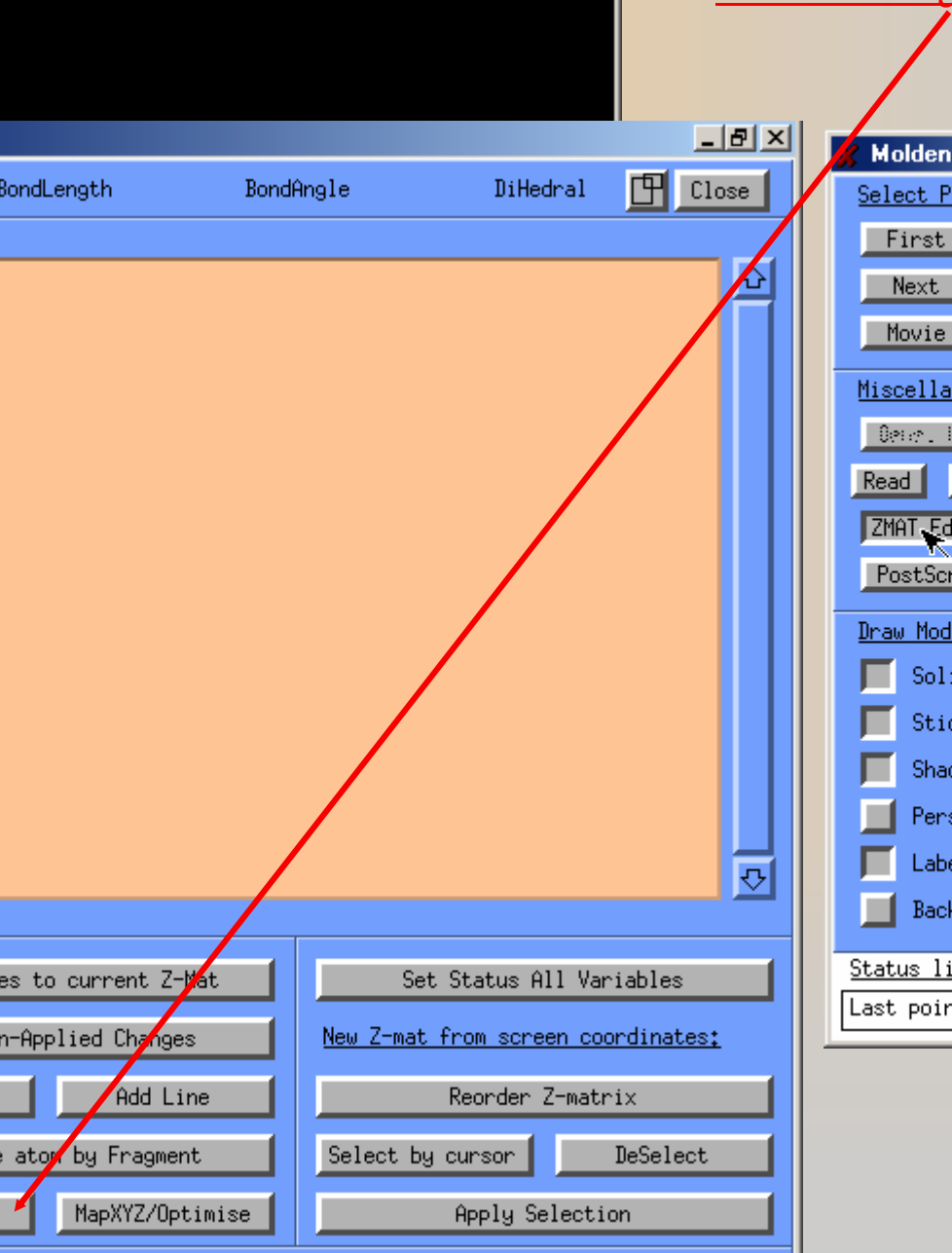
Render Forces: [FF] [Forces] [Incr. Scale] [Decr. Scale] [Unscale]

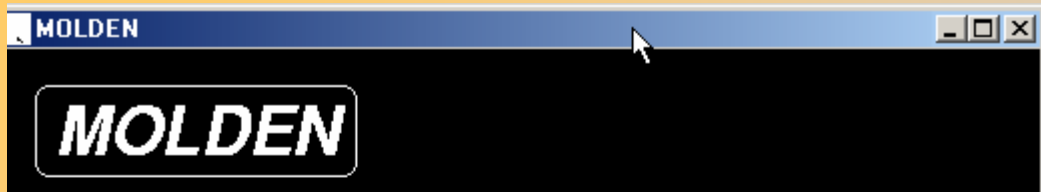
Calculate: [Distance] [Angle] [Dihedral]

Convergence: [SCF conv.] [Geom. conv.]

Zoom: [In] [Out] [Home] [Left] [Right] [Up] [Down]

Status line: [Last point]





Zmatrix Editor

BondLength BondAngle DiHedral

H																							He
Li	Be									B	C	N	O	F									Ne
Na	Mg									Al	Si	P	S	Cl									Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br							Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I							Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At							Rn
Fr	Ra	Ac																					
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu										
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf															

Single
 Double
 Triple

Select Atom

Molden Control

Select Point:

Miscellaneous:

Draw Mode:
 Solid
 StickColor
 Shade
 Perspect.
 Label
 BackBone

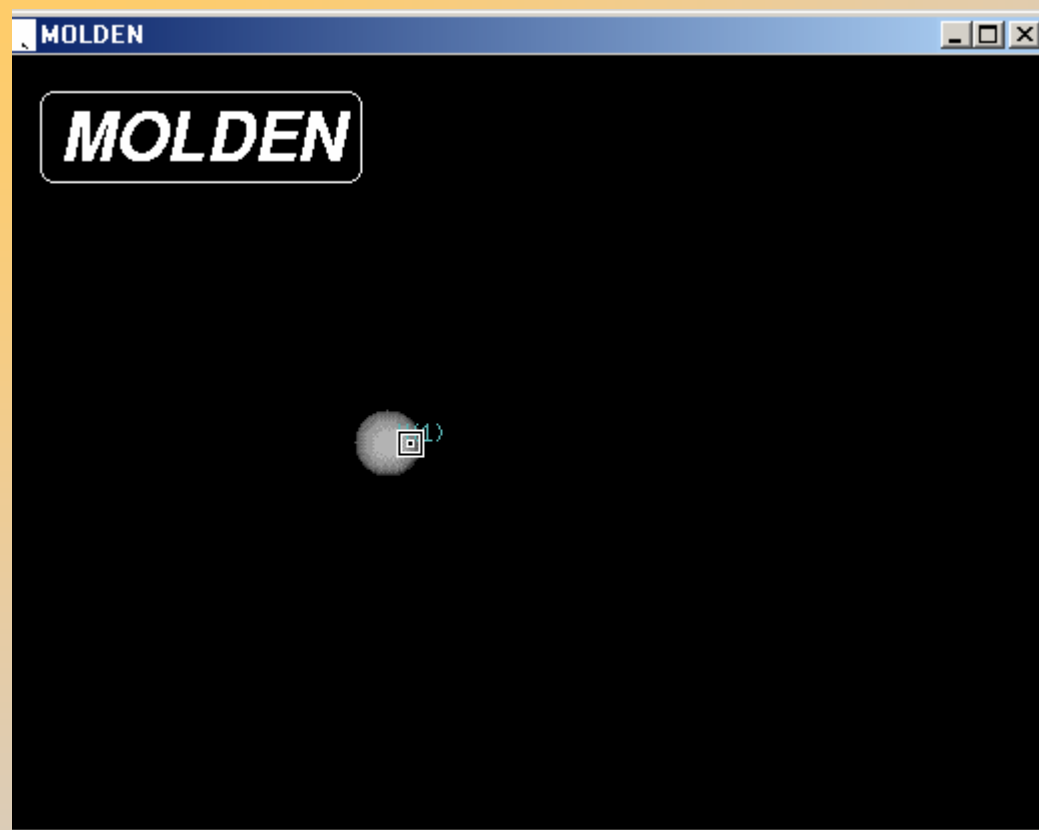
Render Forces:
 Forces

Calculate :

Convergence:

Zoom:

Status line:
Last point



Bond Length:

- Single
- Double
- Triple

Select Atom

The "Molden Control" panel is a blue window with a close button in the top left. It is organized into several sections:

- Select Point:** Buttons for "First", "Next", and "Movie".
- Miscellaneous:** Buttons for "Geom. Mode", "Read", "Write", "ZMAT Editor", and "PostScript".
- Draw Mode:** Checkboxes for "Solid", "StickColor", "Shade", "Perspect.", "Label", and "BackBone".
- Render Forces:** A checkbox for "Forces" and buttons for "Incr. Scale", "Decr. Scale", and "Unscale".
- Calculate:** Buttons for "Distance", "Angle", and "Dihedral".
- Convergence:** Buttons for "SCF conv." and "Geom. conv.".
- Zoom:** Buttons for "In", "Out", and a set of directional arrows.
- Status line:** A text box at the bottom containing "Last point".

MOLDEN

MOLDEN
Zmatrix Editor

BondLength

BondAngle

DiHedral

A periodic table of elements displayed in a grid. The elements are color-coded: H (grey), He (green), Li (grey), Be (grey), B (purple), C (orange), N (blue), O (red), F (yellow), Ne (orange), Na (grey), Mg (grey), Al (grey), Si (grey), P (yellow), S (yellow), Cl (green), Ar (orange), K (yellow), Ca (red), Sc (yellow), Ti (yellow), V (yellow), Cr (yellow), Mn (yellow), Fe (yellow), Co (yellow), Ni (yellow), Cu (yellow), Zn (yellow), Ga (yellow), Ge (red), As (red), Se (red), Br (red), Kr (orange), Rb (yellow), Sr (red), Y (yellow), Zr (yellow), Nb (yellow), Mo (yellow), Tc (yellow), Ru (yellow), Rh (yellow), Pd (yellow), Ag (yellow), Cd (yellow), In (yellow), Sn (yellow), Sb (yellow), Te (red), I (red), Xe (orange), Cs (yellow), Ba (yellow), La (yellow), Hf (yellow), Ta (yellow), W (yellow), Re (yellow), Os (yellow), Ir (yellow), Pt (yellow), Au (yellow), Hg (yellow), Tl (yellow), Pb (yellow), Bi (yellow), Po (yellow), At (red), Rn (orange), Fr (yellow), Ra (yellow), Ac (yellow). A mouse cursor is pointing to the Hydrogen (H) atom.

X

Bond Length:

- Single
- Double
- Triple

Select Atom

Molden Control

Select Point:

- First
- Next
- Movie

Miscellaneous:

- Geom. Mode
- Read
- Write
- ZMAT Editor
- PostScript

Draw Mode:

- Solid
- StickColor
- Shade
- Perspect.
- Label
- BackBone

FF

☉

♥

☐

✳

☉

∇

H

☉

☉

☉

☉

In

Out

Render Forces:

- Forces
- Incr. Scale
- Decr. Scale
- Unscale

Calculate :

- Distance
- Angle
- Dihedral

Convergence:

- SCF conv.
- Geom. conv.

Zoom:

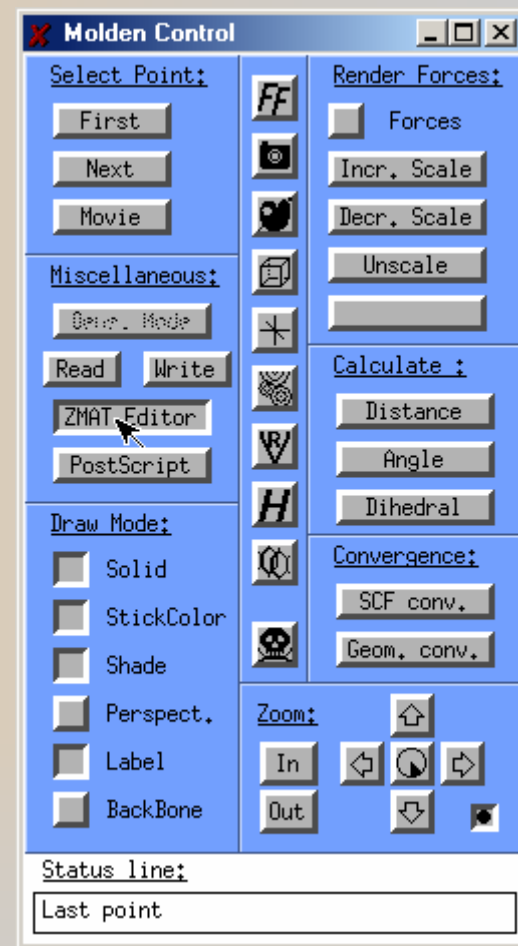
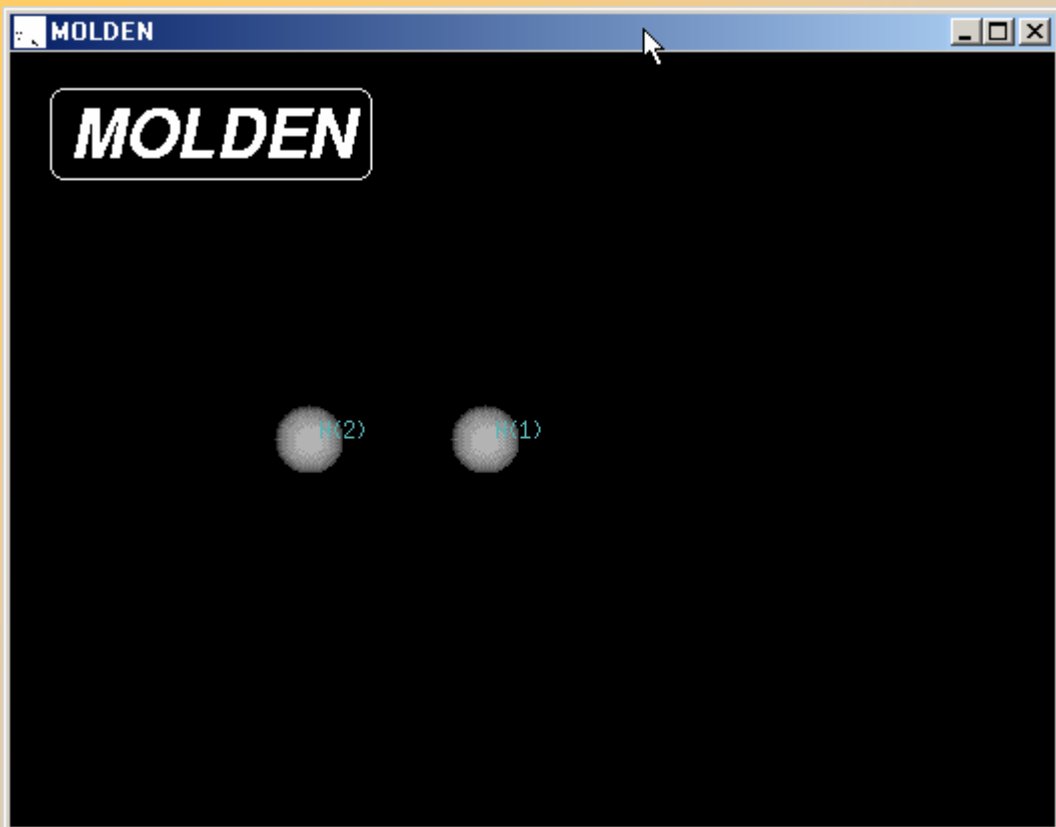
In

Out

- ⬆
- ⬅
- ↻
- ➡
- ⬇
- ☑

Status line:

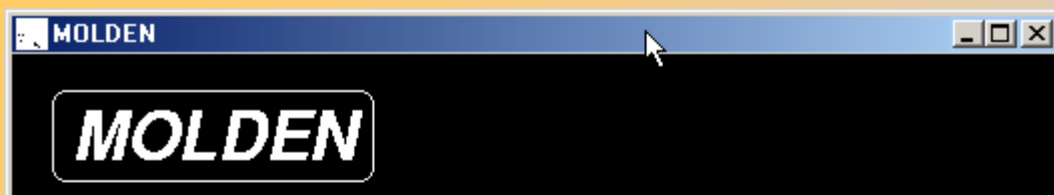
Last point



Bond Length:

- Single
- Double
- Triple

Select Atom



Zastąpienie atomu
grupą funkcyjjną

Zmatrix Editor

BondLength BondAngle DiHedral Close

H

H 1 1.008000

Read

- CH3
- CH=CH2
- HC=O
- COOH
- NH2
- OH
- CHCH
- CycloHexane
- Phenyl
- Cl
- Br
- I

Changes to current Z-Mat

Non-Applied Changes

Add Line

Replace atom by Fragment

MapXYZ/Optimise

Set Status All Variables

New Z-mat from screen coordinates:

Reorder Z-matrix

Select by cursor DeSelect

Apply Selection

Molden Control

Select Point:

First Next Movie

Miscellaneous:

Geom. Mode

Read Write

ZMAT Editor

PostScript

Draw Mode:

Solid

StickColor

Shade

Perspect.

Label

BackBone

Render Forces:

Forces

Incr. Scale

Decr. Scale

Unscale

Calculate:

Distance

Angle

Dihedral

Convergence:

SCF conv.

Geom. conv.

Zoom:

In Out

Status line:

Last point



Zmatrix Editor

BondLength BondAngle DiHedral Close

Atom	Order	BondLength	BondAngle	DiHedral
H	1	1.089000		
C	2	1.089000	109.471001	
H	3	1.089000	109.471001	120.000000
H	4	1.089000	109.471001	240.000000

Buttons: Apply Changes to current Z-Mat, Cancel Non-Applied Changes, Delete Line, Add Line, Substitute atom by Fragment, New Z-mat, MapXYZ/Optimise, Set Status All Variables, New Z-mat from screen coordinates, Reorder Z-matrix, Select by cursor, DeSelect, Apply Selection

Molden Control

Select Point: First, Next, Movie

Render Forces: Forces, Incr. Scale, Decr. Scale, Unscale

Miscellaneous: Gen. Mode, Read, Write, ZMAT Editor, PostScript

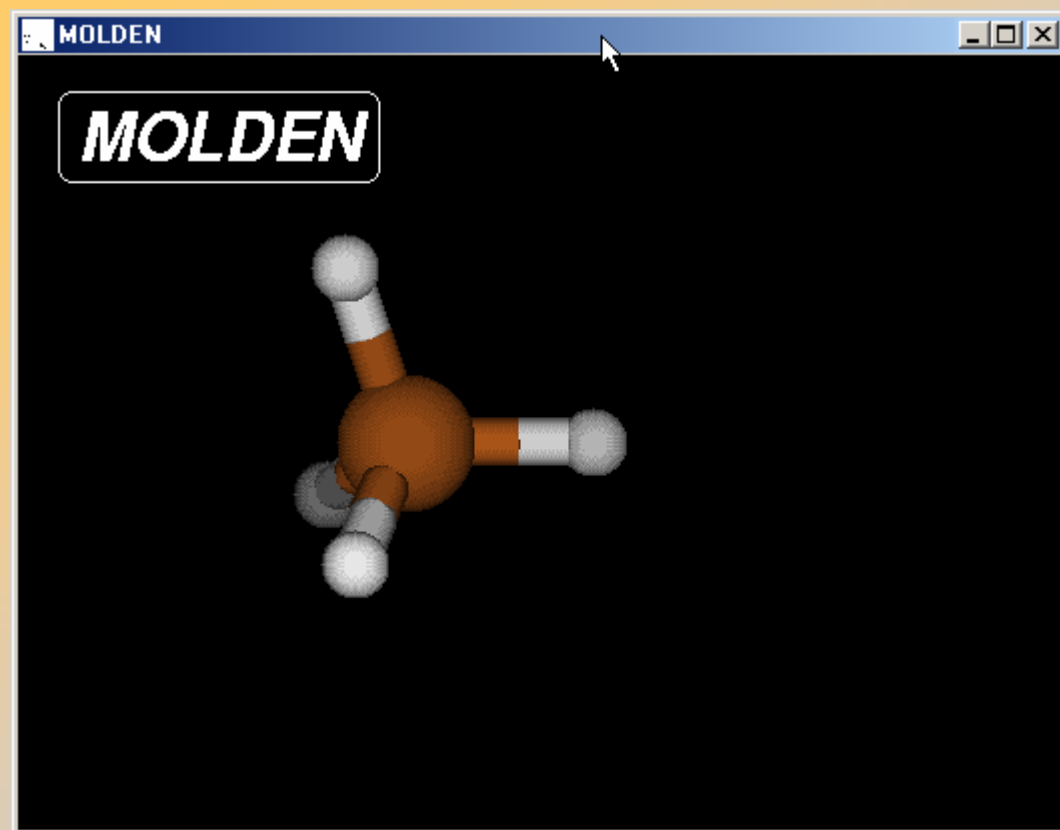
Draw Mode: Solid, StickColor, Shade, Perspect., Label, BackBone

Calculate: Distance, Angle, Dihedral

Convergence: SCF conv., Geom. conv.

Zoom: In, Out

Status line: Last point



Close

0

0

Apply Changes to current Z-Mat

Cancel Non-Applied Changes

Delete Line

Add Line

Substitute atom by Fragment

New Z-mat

MapXYZ/Optimise

Set Status All Variables

New Z-mat from screen coordinates:

Reorder Z-matrix

Select by cursor

DeSelect

Apply Selection

Molden Control

Select Point:

First

Next

Movie

Miscellaneous:

Gen. Mode

Read

Write

ZMAT Editor

PostScript

Draw Mode:

Solid

StickColor

Shade

Perspect.

Label

BackBone

Render Forces:

Forces

Incr. Scale

Decr. Scale

Unscale

Calculate :

Distance

Angle

Dihedral

Convergence:

SCF conv.

Geom. conv.

Zoom:

In

Out

Status line:

Last point



Zmatrix Editor

BondLength BondAngle DiHedral Close

H							
C	1	1.089000					
H	2	1.089000	1	109.471001			
H	2	1.089000	1	109.471001	3	120.000000	0
H	2	1.089000	1	109.471001	3	240.000000	0

- Read
- CH3
- CH=CH2
- HC=O
- COOH
- NH2
- OH
- CHCH
- CycloHexane
- Phenyl
- Cl
- Br
- I

Changes to current Z-Mat

Non-Applied Changes

Add Line

MapXYZ/Optimise

Set Status All Variables

New Z-mat from screen coordinates:

Reorder Z-matrix

Select by cursor DeSelect

Apply Selection

Control

Point:

Render Forces:

Forces

Incr. Scale

Decr. Scale

Unscale

Calculate :

Distance

Angle

Dihedral

Convergence:

SCF conv.

Geom. conv.

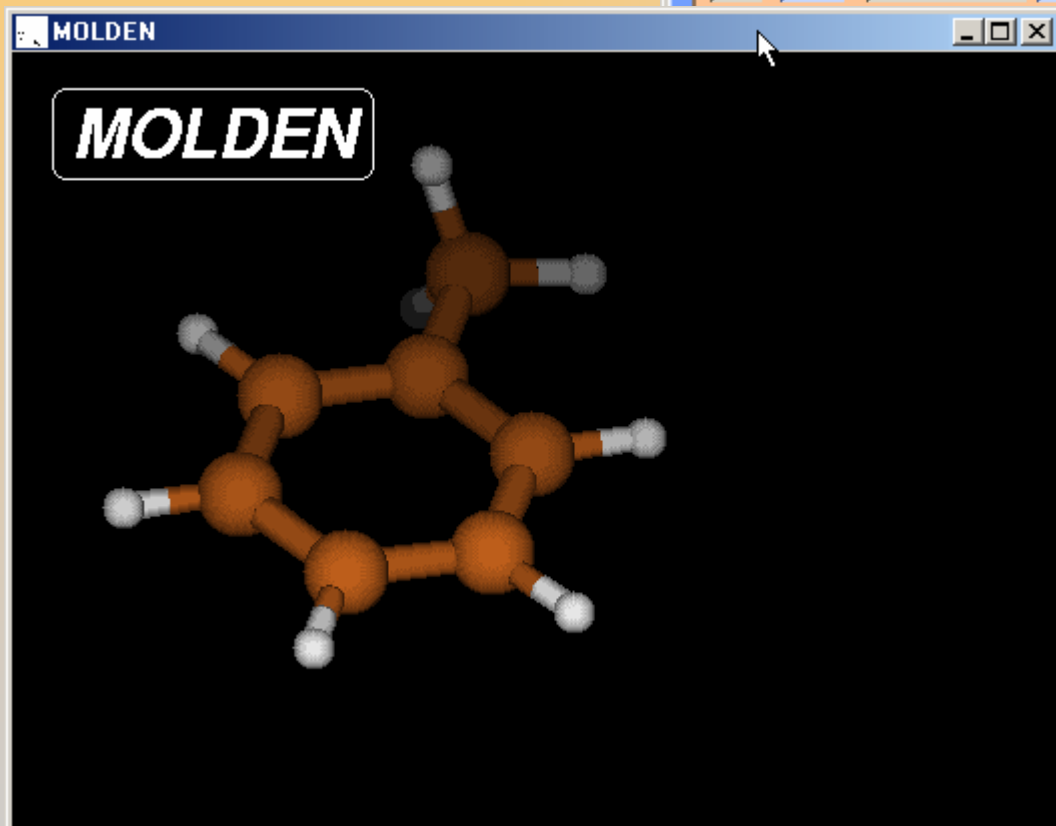
Zoom:

In

Out

line:

int



Zmatrix Editor

BondLength BondAngle DiHedral Close

Atom 1	Atom 2	BondLength	Atom 1	Atom 2	BondAngle	Atom 1	Atom 2	Atom 3	DiHedral
C	7	1.400000	6	7	120.000000	5	6	7	0.000000
C	8	1.400000	7	8	120.000000	6	7	8	0.000000
					120.000000	7			0.000000
					120.000000	7			180.000000
					120.000000	8			180.000000
					120.000000	9			180.000000
					120.000000	7			180.000000
					120.000000	8			180.000000

Mat Set Status All Variables

vs New Z-mat from screen coordinates;

ne Reorder Z-matrix

nt Select by cursor DeSelect

Apply Selection

new z-mat mapatz7optimise

er Forces:

Forces

. Scale

. Scale

scale

ulate :

stance

Angle

hedral

ergence:

F conv.

n. conv.

MOLDEN

- Read
- CH3
- CH=CH2
- HC=O
- COOH
- NH2
- OH
- CHCH
- CycloHexane
- Phenyl
- Cl
- Br
- I
- OCH3
- SH
- NO2
- CH4
- Period. Chain
- Amino Acid
- Sequence
- Cancel

Build Sequence Window

Residues:

GLY	ALA	SER	CYS	THR	ILE	VAL	MET	ASP	ASN
LEU	LYS	GLU	GLN	PRO	ARG	HIS	PHE	TYR	TRP

Conformation: Alpha-Helix PHI -58.000 PSI -47.000

Build Undo Read Close

Molden Control

Under Forces:

Forces

cr. Scale

cr. Scale

Unscale

Calculate :

Distance

Angle

Dihedral

convergence:

SCF conv.

Geom. conv.

Zoom:

In

Out

Status line:

Last point

budowanie sekwencji aminokwasów

The screenshot displays the MOLDEN software interface with three main windows:

- Zmatrix Editor:** A table for editing dihedral angles (Phi, Psi, Chi1, Chi2, Chi3, Chi4) for residues GLY, ALA, CYS, and MET. The current sequence is G G A C M.
- Build Sequence Window:** A window for building a sequence of residues. The current sequence is GLY-GLY-ALA-CYS-MET. The conformation is set to Alpha-Helix, with PHI at -58,000 and PSI at -47,000.
- Molder Control:** A control panel for rendering forces and navigation.

Zmatrix Editor Data:

Residue	Phi	Psi	Chi1	Chi2	Chi3	Chi4
GLY		-47,000				
GLY	-58,000	-47,000				
ALA	-58,000	-47,000				
CYS	-58,000	-47,000	180,000	180,000		
MET	-58,000	-47,000	180,000	180,000	180,000	

Build Sequence Window Data:

Residues: GLY ALA SER CYS THR ILE VAL MET ASP ASN
 LEU LYS GLU GLN PRO ARG HIS PHE TYR TRP

Sequence: GLY-GLY-ALA-CYS-MET

Conformation: Alpha-Helix PHI: -58,000 PSI: -47,000

Molder Control Data:

Render Forces: Forces
 Incr. Scale
 Decr. Scale

Zmatrix Editor Controls:

- Apply Changes to current Z-Mat
- Cancel Non-Applied Changes
- Delete Line
- Add Line
- Substitute atom by Fragment
- New Z-mat
- MapXYZ/Optimise
- Set Status All Variables
- New Z-mat from screen coordinates:
- Reorder Z-matrix
- Select by cursor
- DeSelect
- Apply Selection

Molder Control Navigation:

Label In Out BackBone

Status line: Last point

budowanie sekwencji aminokwasów

Zmatrix Editor

	Phi	Psi	Chi1	Chi2	Chi3	Chi4
GLY		-47,000				
GLY	-58,000	-47,000				
ALA	-58,000	-47,000				
CYS	-58,000	-47,000	180,000	180,000		
MET	-58,000	-47,000	180,000	180,000	180,000	

1 G G A C M Expr. Full Z-Mat

Molden Control

Select Point: First Next Movie

Render Forces: Forces Incr. Scale Decr. Scale

THR ILE VAL MET ASP ASN
PRO ARG HIS PHE TYR TRP

PHI -58,000 PSI -47,000

Read Close

Label In Out
BackBone

Status line:
Last point

budowanie sekwencji aminokwasów – pełna macierz Z

MOLDEN

Zmatrix Editor

BondLength BondAngle DiHedral Close

N							
C	1	1.460000					
C	2	1.510000	1	111.600000			
N	3	1.340000	2	112.700000	1	-47.000000	0
O	3	1.220000	2	122.500000	4	180.000000	0
H	1	1.020000	2	121.000000	3	61.000000	0
H	2	1.110000	3	107.900000	1	120.342000	0
H	2	1.110000	3	107.900000	1	-120.342000	0

Full Z-Mat

Apply Changes to current Z-Mat Set Status All Variables

Cancel Non-Applied Changes New Z-mat from screen coordinates:

Delete Line Add Line Reorder Z-matrix

Substitute atom by Fragment Select by cursor DeSelect

New Z-mat MapXYZ/Optimise Apply Selection

Molden Control

Select Point: Render Forces:

First FF Forces

Next [Target Icon] Incr. Scale

Movie [Heart Icon] Decr. Scale

THR ILE VAL MET ASP ASN

PRO ARG HIS PHE TYR TRP

PHI -58,000 PSI -47,000

Read Close

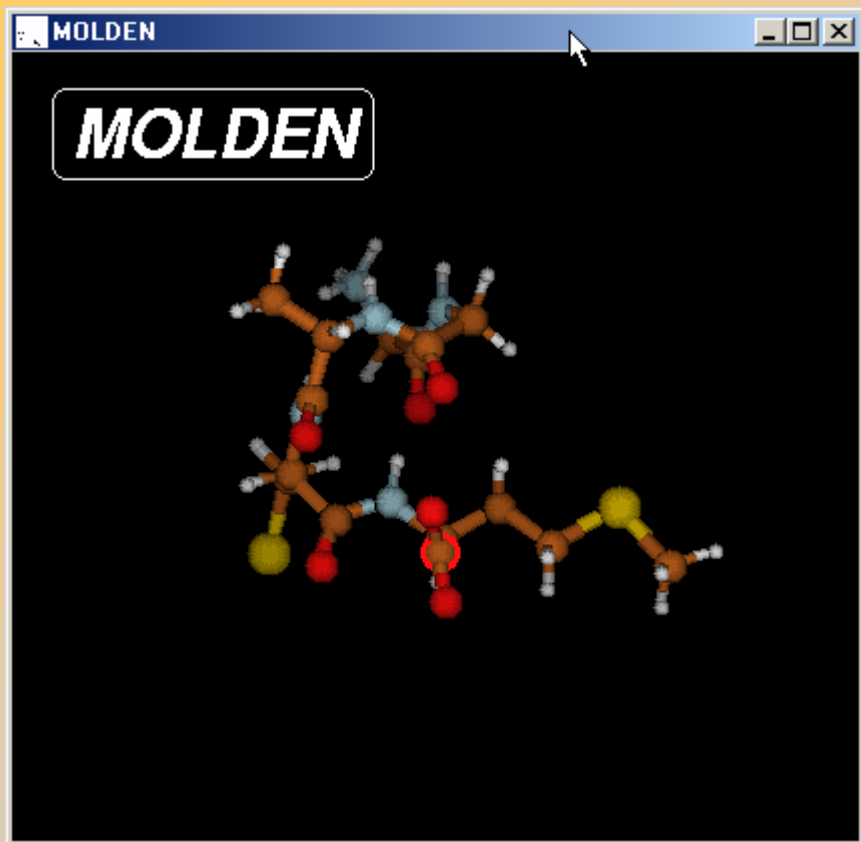
Label In [Left Arrow] [Refresh] [Right Arrow]

BackBone Out [Down Arrow] [Target Icon]

Status line:

Last point

budowanie sekwencji aminokwasów – pełna macierz Z



DiHedral Close

000			
000	1	-47,000000	0
000	4	180,000000	0
000	3	61,000000	0
000	1	120,342000	0
000	1	-120,342000	0

Full Z-Mat

Molden Control

Select Point: First Next Movie

Render Forces: Forces Incr. Scale Decr. Scale

THR ILE VAL MET ASP ASN
PRO ARG HIS PHE TYR TRP

PHI -58,000 PSI -47,000

Read Close

Apply Changes to current Z-Mat

Cancel Non-Applied Changes

Delete Line Add Line

Substitute atom by Fragment

New Z-mat MapXYZ/Optimise

Set Status All Variables

New Z-mat from screen coordinates:

Reorder Z-matrix

Select by cursor DeSelect

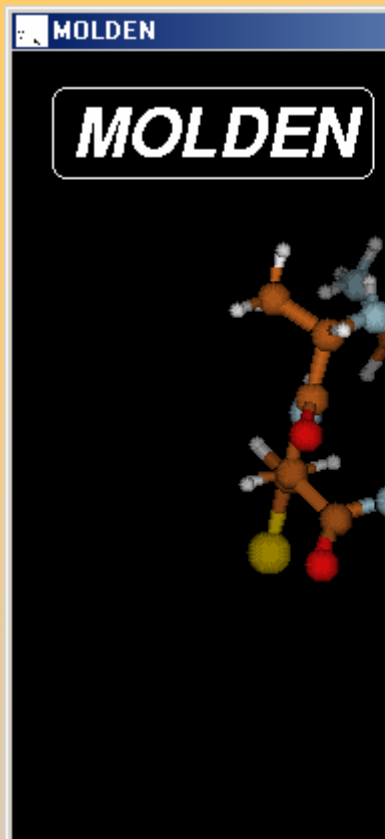
Apply Selection

Label In Out

BackBone

Status line:

Last point



C	2	1,510000	1	111,600000			
N	3	1,340000	2	112,700000	1	-47,000000	0
O	3	1,220000	2	122,500000	4	180,000000	0
H	1	1,020000	2	121,000000	3	61,000000	0
H	2	1,110000	3	107,900000	1	120,342000	0
H	2	1,110000	3	107,900000	1	-120,342000	0

Full Z-Mat

Apply Changes to current Z-Mat Set Status All Variables

Cancel Non-Applied Changes New Z-mat from screen coordinates:

Delete Line Add Line Reorder Z-matrix

Substitute atom by Fragment Select by cursor DeSelect

New Z-mat MapXYZ/Optimise Apply Selection

Write Z-Matrix Submit Job

File name ? nazwapliku

Format: Gamess Gaussian Mopac Cartesian
 US

Render Control

Render Point: FF Render Forces: Forces

Dist Incr. Scale

Ext Decr. Scale

Vie Unscale

Planeous:

Write Calculate: Distance

Editor Angle

Script Dihedral

Mode: H Convergence: SCF conv.

Solid Geom. conv.

StickColor

Shade Zoom:

Perspect. In

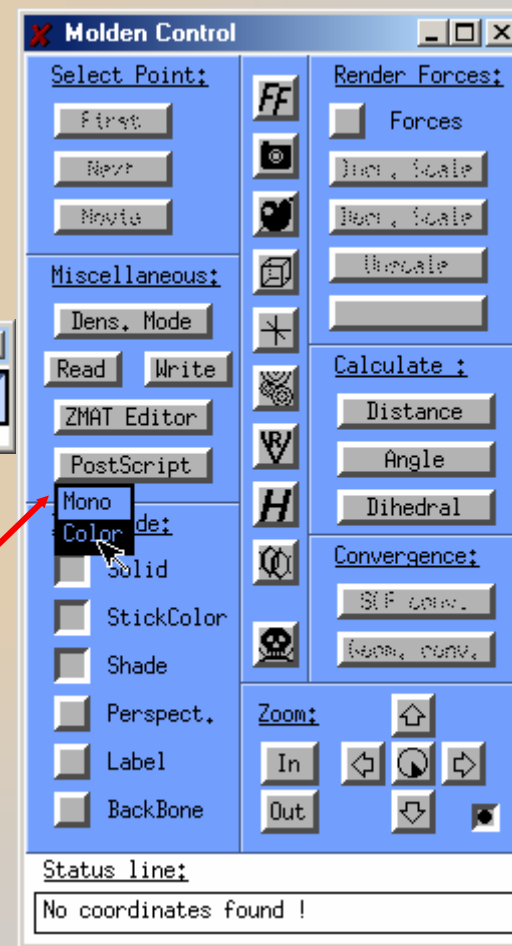
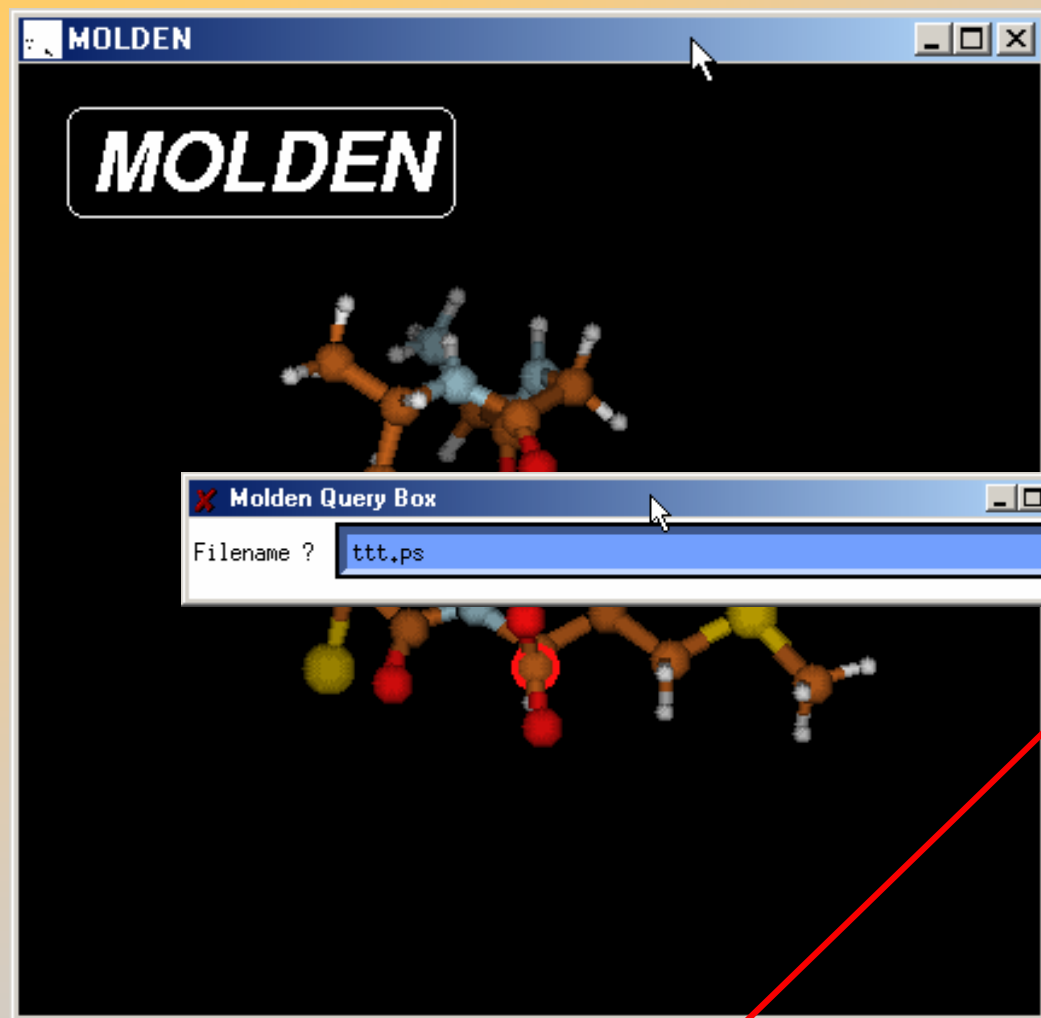
Label Out

BackBone

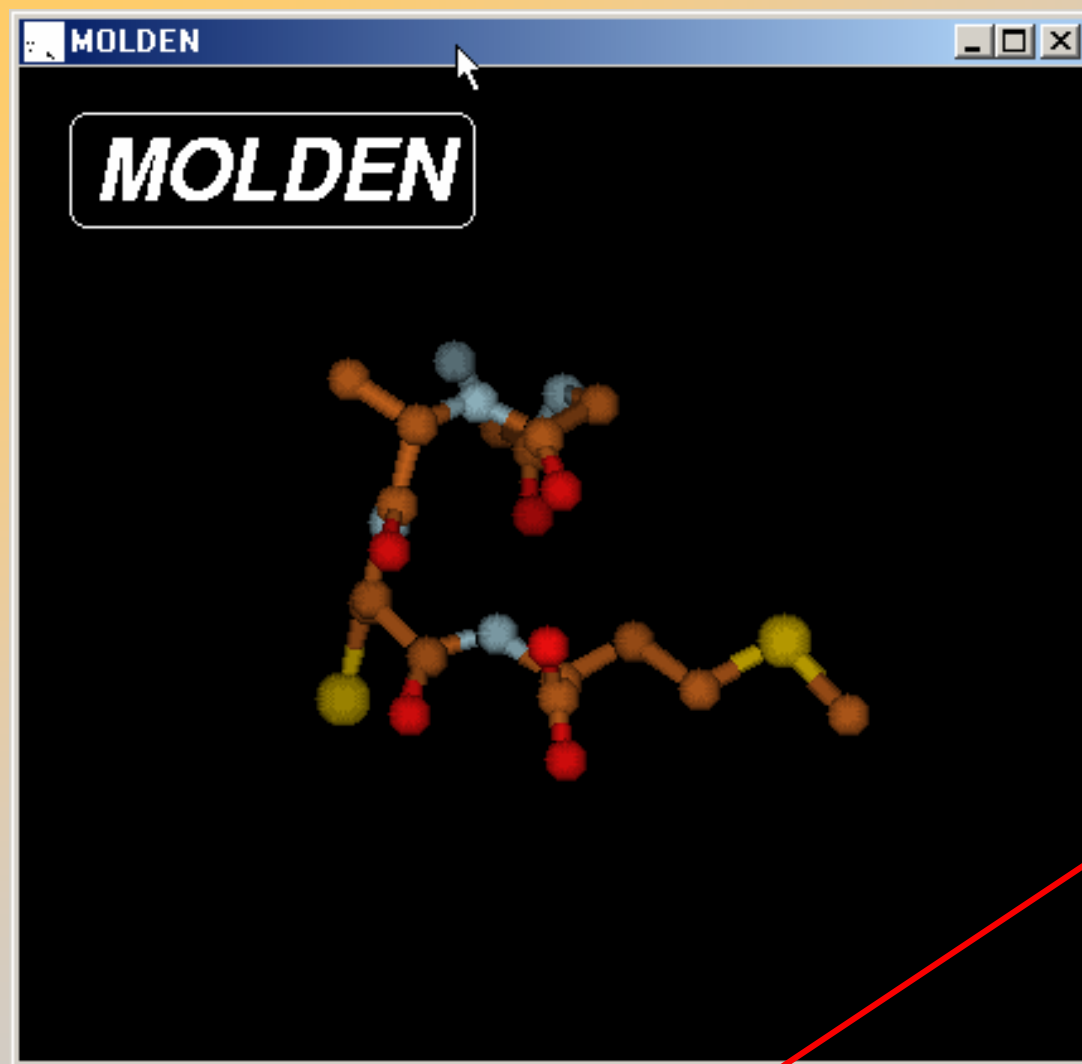
line: _____

point _____

Zapis macierzy Z w pliku (format MOPACa)



Zapis rysunku w pliku (postscript)



Molden Control

Select Point:
First
Next
None

Miscellaneous:
Dens. Mode
Read Write
ZMAT Editor
PostScript

Draw Mode:
 Solid
 StickColor
 Shade
 Perspect.
 Label
 BackBone

Add to Backbone:
Res. Conn.
Rings
Hets/AAs
 SulfurBond
 H-bonds

Calculate :
Distance
Angle
Dihedral

Convergence:
SIF conv.
Geom. conv.

Zoom:
In Out

Status line:
No Electrostatic Potential !

Atomy wodoru nie wyświetlane

The image shows the MOLDEN software interface. On the left is a 3D ball-and-stick model of a benzene ring. On the right is the 'Molden Control' panel. The 'Calculate' section is highlighted with a red box and contains buttons for 'Distance', 'Angle', and 'Dihedral'. A red arrow points from this section to the text below.

MOLDEN

Molden Control

Select Point:
First
Next
Next

Miscellaneous:
Dens. Mode
Read Write
ZMAT Editor
PostScript

Draw Mode:
 Solid
 StickColor
 Shade
 Perspect.
 Label
 BackBone

Render Forces:
 Forces
Dist. Scale
Dist. Scale
UnScale

Calculate :
Distance
Angle
Dihedral

Convergence:
Self conv.
Geom. conv.

Zoom:
In Out
← → ↻ ↺ ↻ ↺

Status line:
Click on two atoms !

Pomiar odległości, kątów i kątów torsyjnych

The image shows the MOLDEN software interface. On the left, a window titled 'MOLDEN' displays a ball-and-stick model of a benzene ring. On the right, the 'Molden Control' panel is visible. The 'Calculate' section is highlighted with a red box and contains three buttons: 'Distance', 'Angle', and 'Dihedral'. A red arrow points from the 'Distance' button to the molecular model. The 'Status line' at the bottom of the control panel reads 'Click on two atoms !'.

Pomiar odległości, kątów i kątów torsyjnych

Po wybraniu odpowiedniego przycisku należy wskazać odpowiednio dwa, trzy lub cztery atomy (klikając)

The image shows the Molden software interface. On the left, three 'Molden Calculate' windows are open, each displaying a different measurement: Distance (1.08900 Angstrom, 2.05791 a.u.), Covalent Angle (120.000 Degrees), and Dihedral (0.000 Degrees). On the right, the 'Molden Control' panel is visible, featuring various controls for the visualization. A red box highlights the 'Calculate' section, which includes buttons for 'Distance', 'Angle', and 'Dihedral'. Blue arrows point from the text below to the three 'Molden Calculate' windows, and a red arrow points from the 'Calculate' section to the text below.

Pomiar odległości, kątów i kątów torsyjnych

Po wybraniu odpowiedniego przycisku należy wskazać odpowiednio dwa, trzy lub cztery atomy (klikając).

Pojawi się jedno z trzech okienek widocznych powyżej

MOLDEN

Zmatrix Editor

	BondLength	BondAngle	DiHedral				
H	4	1.089000	3	120.000000	5	180.000000	0
H	5	1.089000	4	120.000000	6	180.000000	0
H	6	1.089000	5	120.000000	4	180.000000	0
H	7	1.089000	6	120.000000	5	180.000000	0
C	1	1.400000	2	120.000000	3	180.000000	0
C	13	1.400000	1	120.000000	2	180.000000	0
C	14	1.400000	13	120.000000	1	0.000000	0
C	15	1.400000	14	120.000000	13	0.000000	0

Buttons: Apply Changes to current Z-Mat, Cancel Non-Applied Changes, Delete Line, Add Line, Substitute atom by Fragment, New Z-mat, MapXYZ/Optimise, Set Status All Variables, New Z-mat from screen coordinates, Reorder Z-matrix, Select by cursor, DeSelect, Apply Selection, Variable, Write Z-Matrix, Submit Job, File name ?

Zaznaczenie kąta w edytorze macierzy Z powoduje zaznaczenie atomów definiujących kąt

The image shows the MOLDEN software interface. On the left, a ball-and-stick model of a benzene ring is displayed with several atoms highlighted by colored circles (cyan, green, yellow, red). On the right, the Zmatrix Editor dialog box is open, showing a table of bond lengths, bond angles, and dihedrals for the molecule. A context menu is open over the table, highlighting the 'animate' option.

	BondLength	BondAngle	DiHedral		
H 4	1,089000	3	120,000000	5	180,000000
H 5	1,089000	4	120,000000	6	180,000000
H 6	1,089000	5	120,000000	4	180,000000
H 7	1,089000	6	120,000000	5	180,000000
C 1	1,400000	2	120,000000	3	176,000000
C 13	1,400000	1	120,000000	2	180,000000
C 14	1,400000	13	120,000000	1	180,000000
C 15	1,400000	14	120,000000	13	180,000000

The context menu options are: constant, variable, mark, unmark, **animate**, link, -link.

Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

The screenshot displays the MOLDEN software interface. The main window shows a ball-and-stick model of a benzene ring with orange carbon atoms and white hydrogen atoms. The 'MOLDEN' logo is visible in the top left corner of the main window. To the right, a control panel is open, showing a table of bond angles and dihedral angles. The table has columns for 'BondAngle' and 'DiHedral'. The values for bond angles are consistently 120.000000, and for dihedral angles, they are 180.000000 for most entries, with some being 0.000000. Below the table, there are several buttons for controlling the model, including 'Z-Mat', 'Set Status All Variables', 'New Z-mat from screen coordinates:', 'Reorder Z-matrix', 'Select by cursor', 'DeSelect', 'Apply Selection', and 'Submit Job'. A 'File name ?' field is visible at the bottom of the control panel.

	BondAngle	DiHedral	
3	120,000000	5	180,000000 0
4	120,000000	6	180,000000 0
5	120,000000	4	180,000000 0
6	120,000000	5	180,000000 0
2	120,000000	3	180,000000 0
1	120,000000	2	180,000000 0
13	120,000000	1	0,000000 0
14	120,000000	13	0,000000 0

Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

The screenshot displays the MOLDEN software interface. The main window shows a ball-and-stick model of a benzene ring with carbon atoms in orange and hydrogen atoms in white. The 'MOLDEN' logo is visible in the top left corner of the window. To the right, a control panel is open, titled 'BondAngle' and 'DiHedral'. It contains a table of bond and dihedral angles, with the value '180,000000' highlighted in the cell for bond 3 and dihedral 3. Below the table are several buttons for manipulating the model, including 'Z-Mat', 'Set Status All Variables', 'New Z-mat from screen coordinates', 'Reorder Z-matrix', 'Select by cursor', 'DeSelect', 'Apply Selection', and 'Submit Job'. A 'File name ?' input field is located at the bottom of the control panel.

	BondAngle	DiHedral	
3	120,000000	5	180,000000 0
4	120,000000	6	180,000000 0
5	120,000000	4	180,000000 0
6	120,000000	5	180,000000 0
2	120,000000	3	180,000000 0
1	120,000000	2	180,000000 0
13	120,000000	1	0,000000 0
14	120,000000	13	0,000000 0

Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

The screenshot shows the MOLDEN software interface. The main window displays a ball-and-stick model of a benzene ring. The control panel on the right is titled 'BondAngle' and 'DiHedral' and contains a table of parameters. The table has columns for atom indices and values for bond angles and dihedral angles. The value '180,000000' is highlighted in the table.

	BondAngle	DiHedral	
3	120,000000	5	180,000000 0
4	120,000000	6	180,000000 0
5	120,000000	4	180,000000 0
6	120,000000	5	180,000000 0
2	120,000000	3	180,000000 0
1	120,000000	2	180,000000 0
13	120,000000	1	0,000000 0
14	120,000000	13	0,000000 0

Below the table are buttons for 'Z-Mat', 'Set Status All Variables', 'New Z-mat from screen coordinates', 'Reorder Z-matrix', 'Select by cursor', 'DeSelect', and 'Apply Selection'. At the bottom, there is a 'Submit Job' button and a 'File name ?' input field.

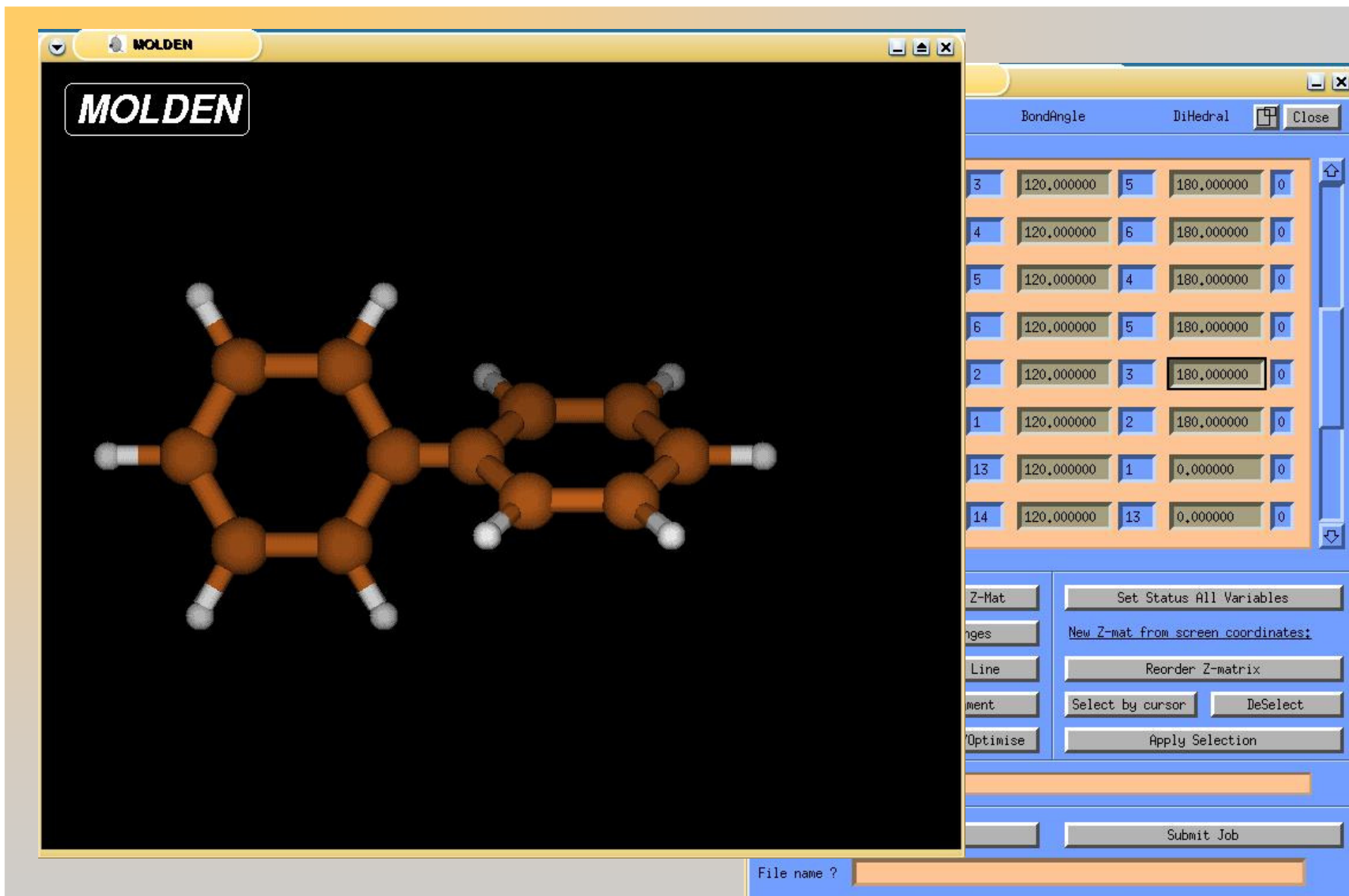
Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

The screenshot shows the MOLDEN software interface. The main window displays a ball-and-stick model of a molecule. To the right, there is a control panel with a table of bond and dihedral angles. The table has columns for BondAngle and DiHedral, with values in degrees. The value 180.000000 is highlighted in the DiHedral column for the second row.

	BondAngle	DiHedral		
3	120.000000	5	180.000000	0
4	120.000000	6	180.000000	0
5	120.000000	4	180.000000	0
6	120.000000	5	180.000000	0
2	120.000000	3	180.000000	0
1	120.000000	2	180.000000	0
13	120.000000	1	0.000000	0
14	120.000000	13	0.000000	0

Below the table, there are buttons for Z-Mat, Set Status All Variables, New Z-mat from screen coordinates, Reorder Z-matrix, Select by cursor, DeSelect, Apply Selection, and Submit Job. A File name ? field is visible at the bottom.

Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.



Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

The screenshot displays the MOLDEN software interface. The main window shows a ball-and-stick model of a molecule with orange carbon atoms and white hydrogen atoms. The 'MOLDEN' logo is visible in the top left corner of the window. To the right, a control panel is open, showing a table of bond angles and dihedral angles. The table has columns for 'BondAngle' and 'DiHedral'. The values are as follows:

	BondAngle	DiHedral	
3	120,000000	5	180,000000
4	120,000000	6	180,000000
5	120,000000	4	180,000000
6	120,000000	5	180,000000
2	120,000000	3	180,000000
1	120,000000	2	180,000000
13	120,000000	1	0,000000
14	120,000000	13	0,000000

Below the table, there are several buttons: 'Z-Mat', 'Set Status All Variables', 'New Z-mat from screen coordinates:', 'Reorder Z-matrix', 'Select by cursor', 'DeSelect', 'Apply Selection', and 'Submit Job'. A 'File name ?' input field is visible at the bottom of the control panel.

Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

The screenshot displays the MOLDEN software interface. The main window shows a ball-and-stick model of a molecule, likely a substituted benzene ring. The control panel on the right is titled 'BondAngle' and 'DiHedral' and contains a table of parameters. The table has columns for bond angle and dihedral angle values, and a 'Close' button. Below the table are buttons for 'Z-Mat', 'Set Status All Variables', 'New Z-mat from screen coordinates', 'Reorder Z-matrix', 'Select by cursor', 'DeSelect', 'Apply Selection', and 'Submit Job'. A 'File name ?' input field is visible at the bottom.

	BondAngle	DiHedral	
3	120,000000	5	180,000000 0
4	120,000000	6	180,000000 0
5	120,000000	4	180,000000 0
6	120,000000	5	180,000000 0
2	120,000000	3	180,000000 0
1	120,000000	2	180,000000 0
13	120,000000	1	0,000000 0
14	120,000000	13	0,000000 0

Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

The screenshot displays the MOLDEN software interface. On the left, a ball-and-stick model of a molecule is shown against a black background. The molecule consists of a benzene ring (six carbon atoms in a hexagonal ring) attached to a chain of three carbon atoms, with hydrogen atoms (white) and oxygen atoms (red) also present. The MOLDEN logo is visible in the top left corner of the window.

On the right side, there is a control panel with a table for defining bond angles and dihedral angles. The table has columns for BondAngle and DiHedral, and a Close button. The table contains the following data:

	BondAngle	DiHedral	
3	120,000000	5	180,000000 0
4	120,000000	6	180,000000 0
5	120,000000	4	180,000000 0
6	120,000000	5	180,000000 0
2	120,000000	3	180,000000 0
1	120,000000	2	180,000000 0
13	120,000000	1	0,000000 0
14	120,000000	13	0,000000 0

Below the table, there are several buttons: Z-Mat, Set Status All Variables, New Z-mat from screen coordinates, Line, Reorder Z-matrix, Select by cursor, DeSelect, Apply Selection, and Submit Job. A File name ? field is visible at the bottom of the interface.

Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.

cdn