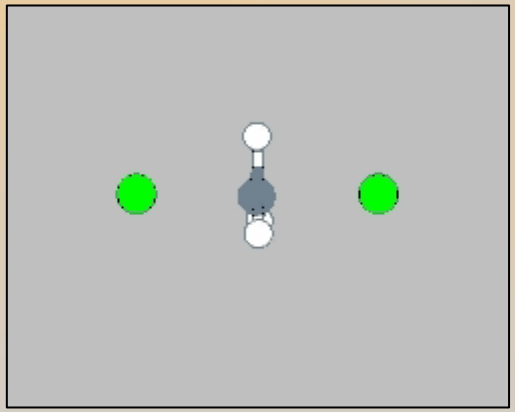
Modelowanie molekularne

metodami chemii kwantowej

Dr hab. Artur Michalak

Zakład Chemii Teoretycznej

Wydział Chemii UJ



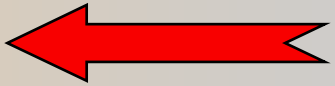
Wykład 6

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

• **Podstawowe idee i metody chemii kwantowej:**
Funkcja falowa, gęstość elektronowa; równanie Schrodingera; Teoria Funkcjonałów Gęstości (DFT); przyblienie Borna-Oppenheimera, zasada wariacyjna w mechanice kwantowej i w DFT, przyblienie 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 wiazami; analiza konformacyjna; problem minimum globalnego



• **Struktura elektronowa układów molekularnych:**
Orbitale molekularne, orbitale KS; wiazanie chemiczne; gęstość rónicowa; orbitale zlokalizowane; analiza populacyjna; analiza rzędów wiązań
• **Analiza wibracyjna; Wielkości termodynamiczne; Reaktywność chemiczna:**
Analiza wibracyjna; wielkosci 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; efety rozpuszczalnika; modelowanie w katalizie homo- i heterogenicznej; oddziaływania międzycząsteczkowe, i. in.

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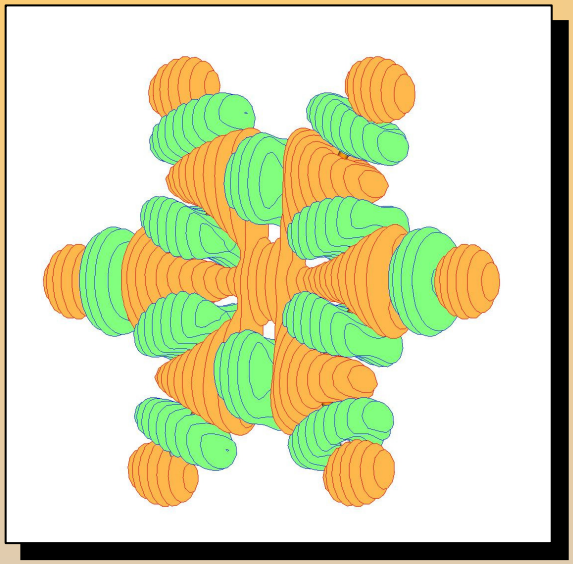

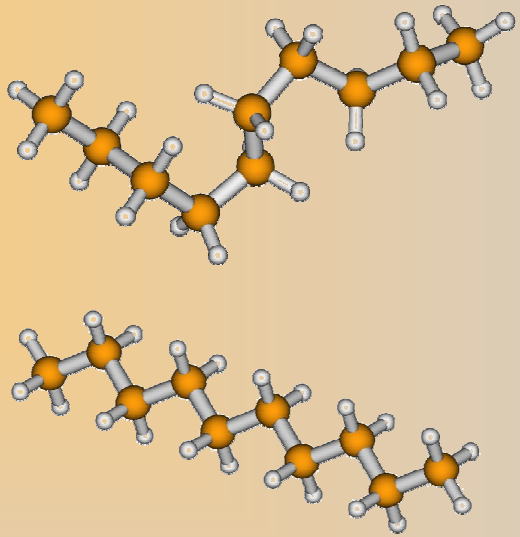

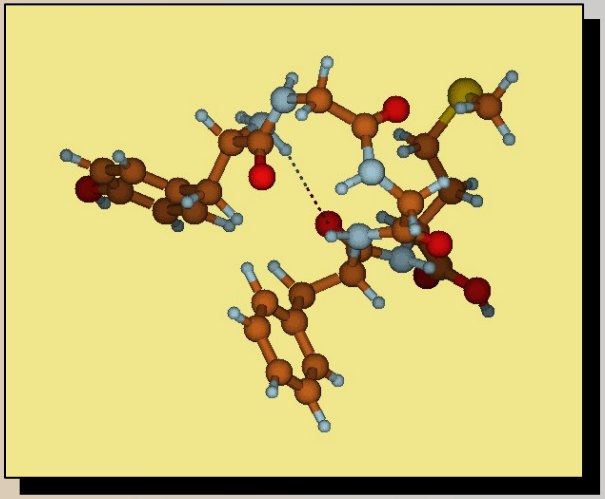

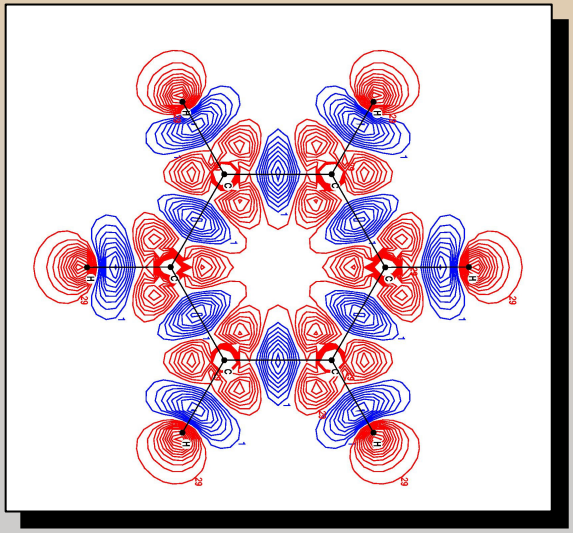

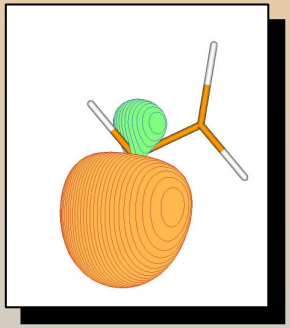

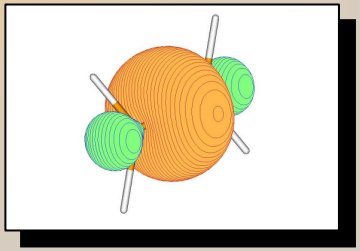

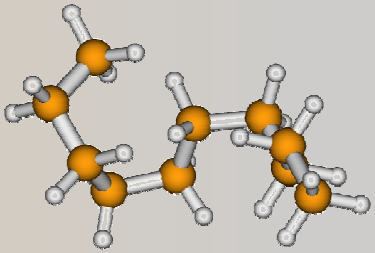

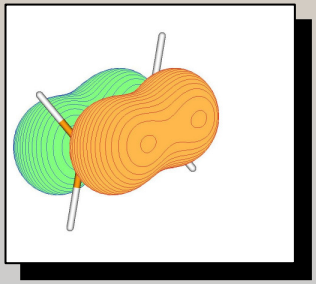

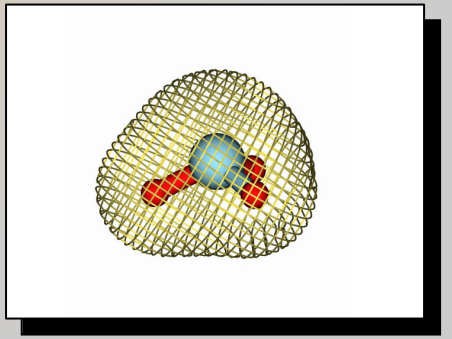

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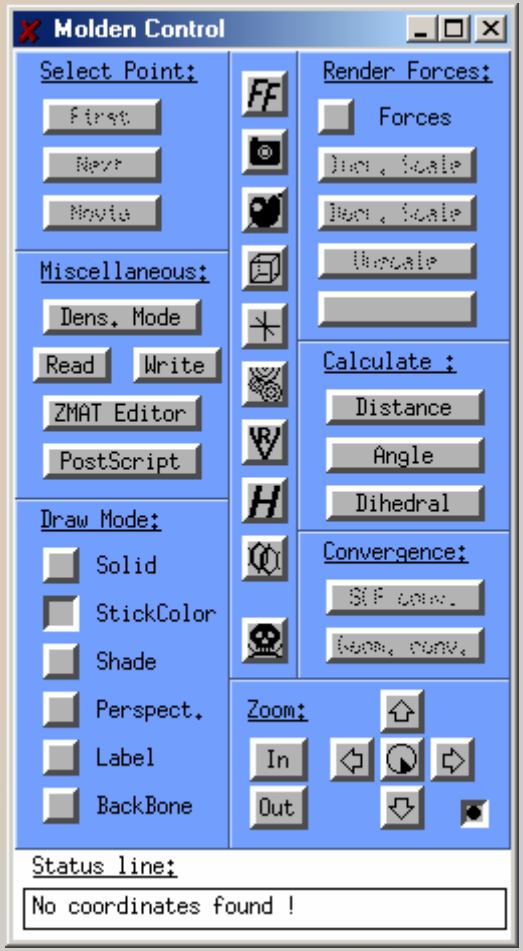

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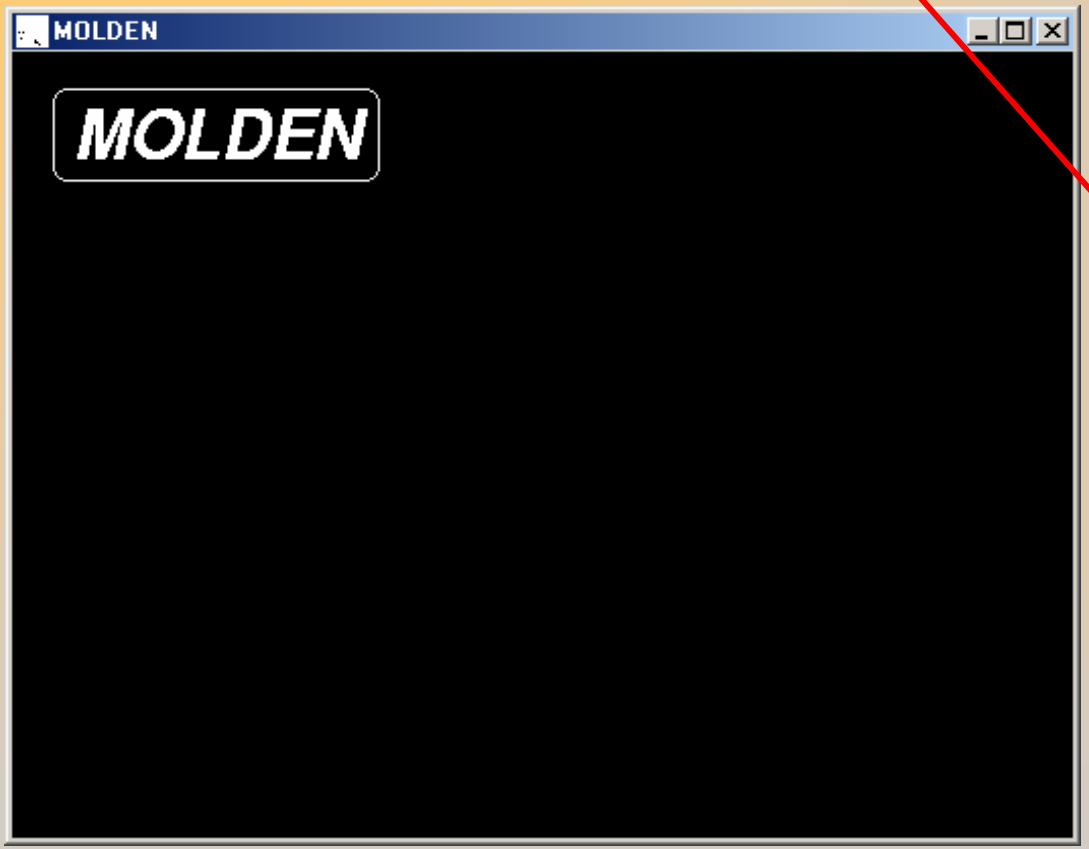

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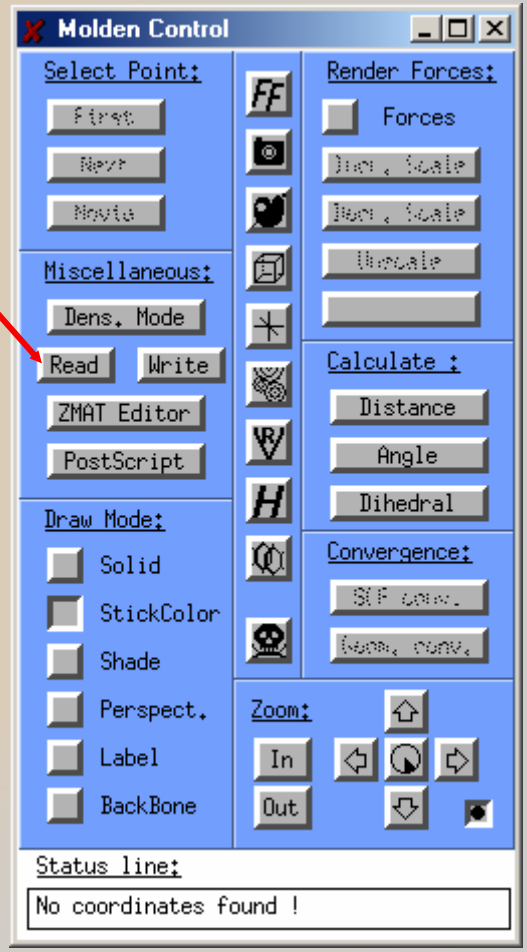

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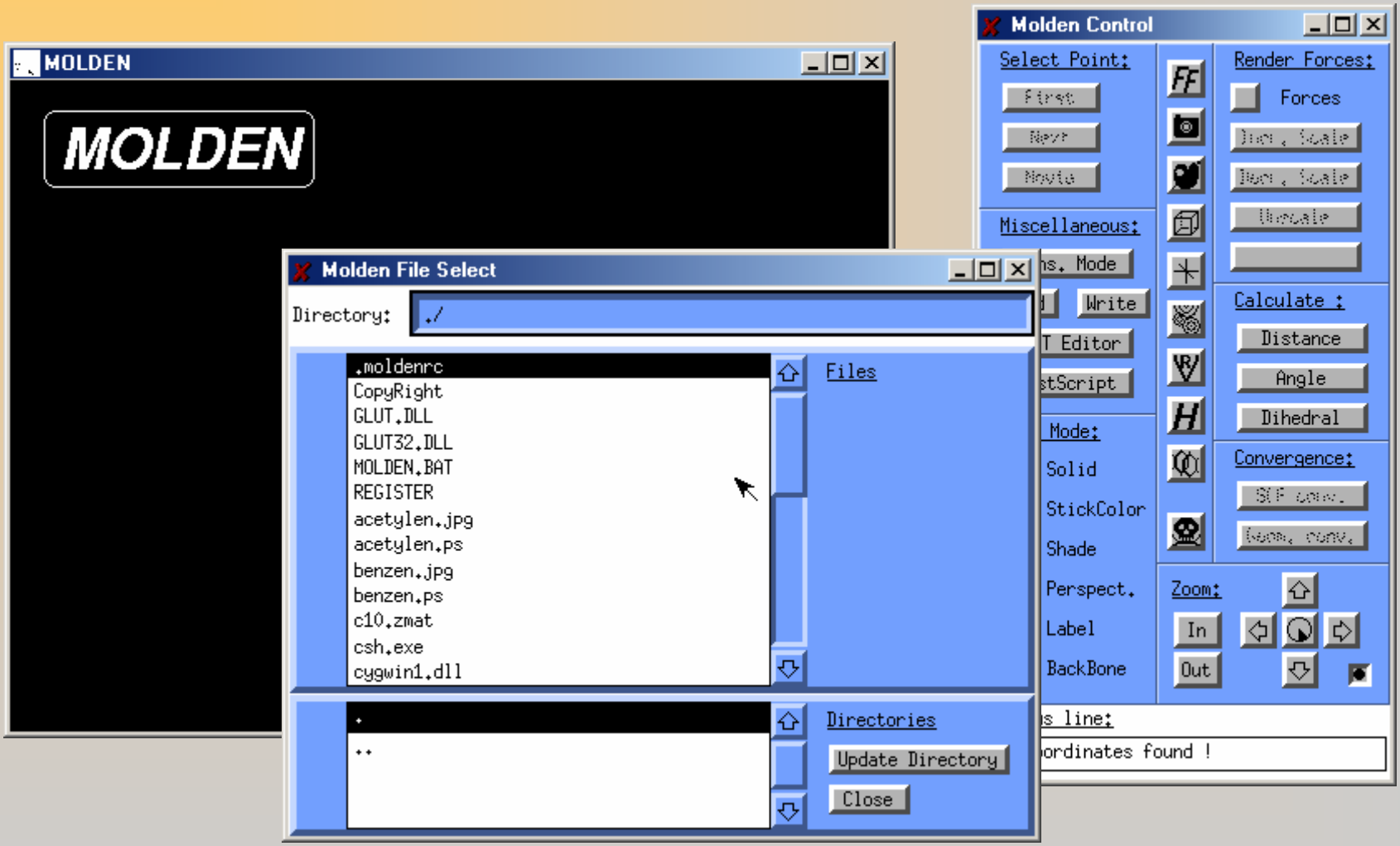
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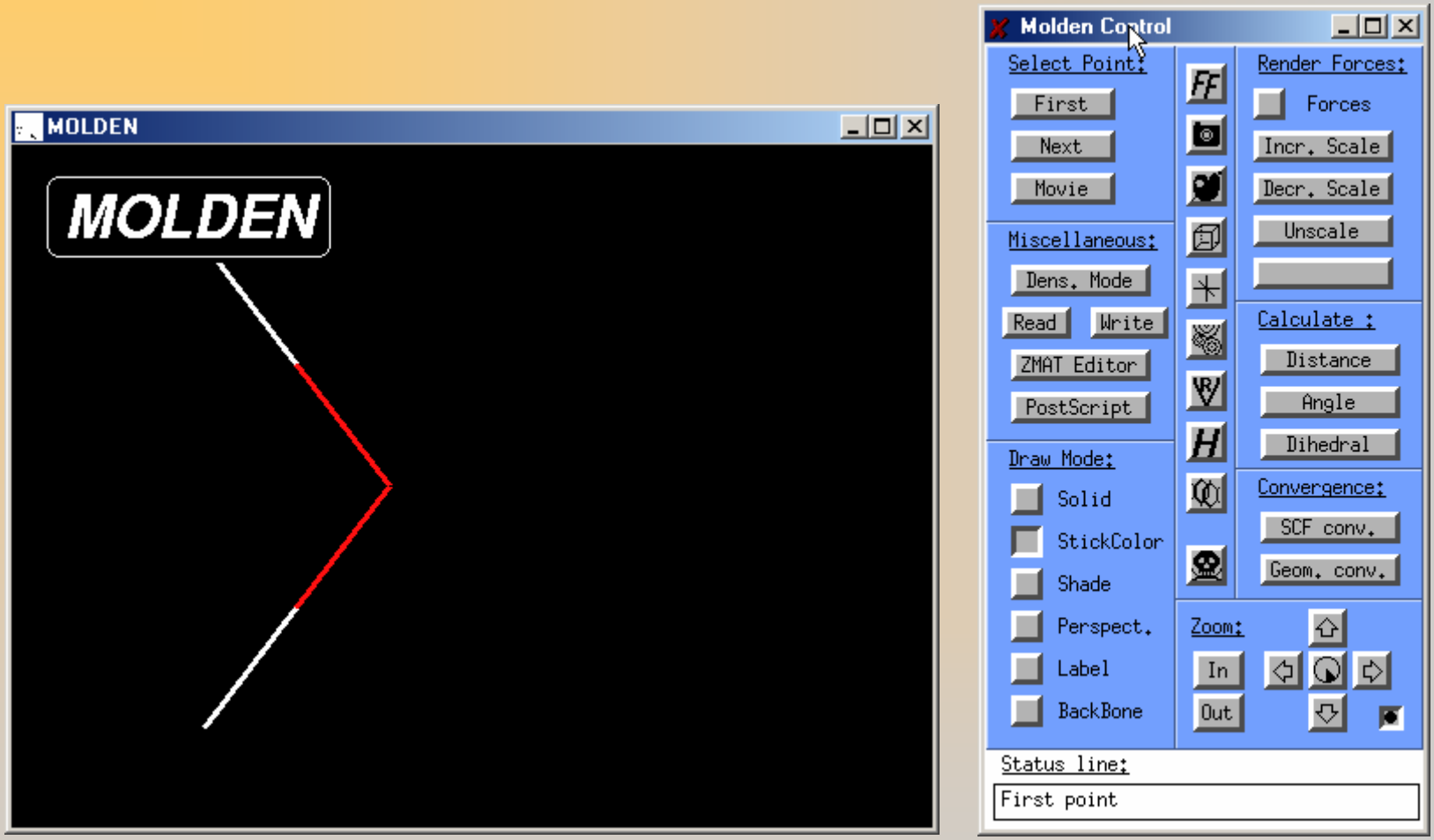
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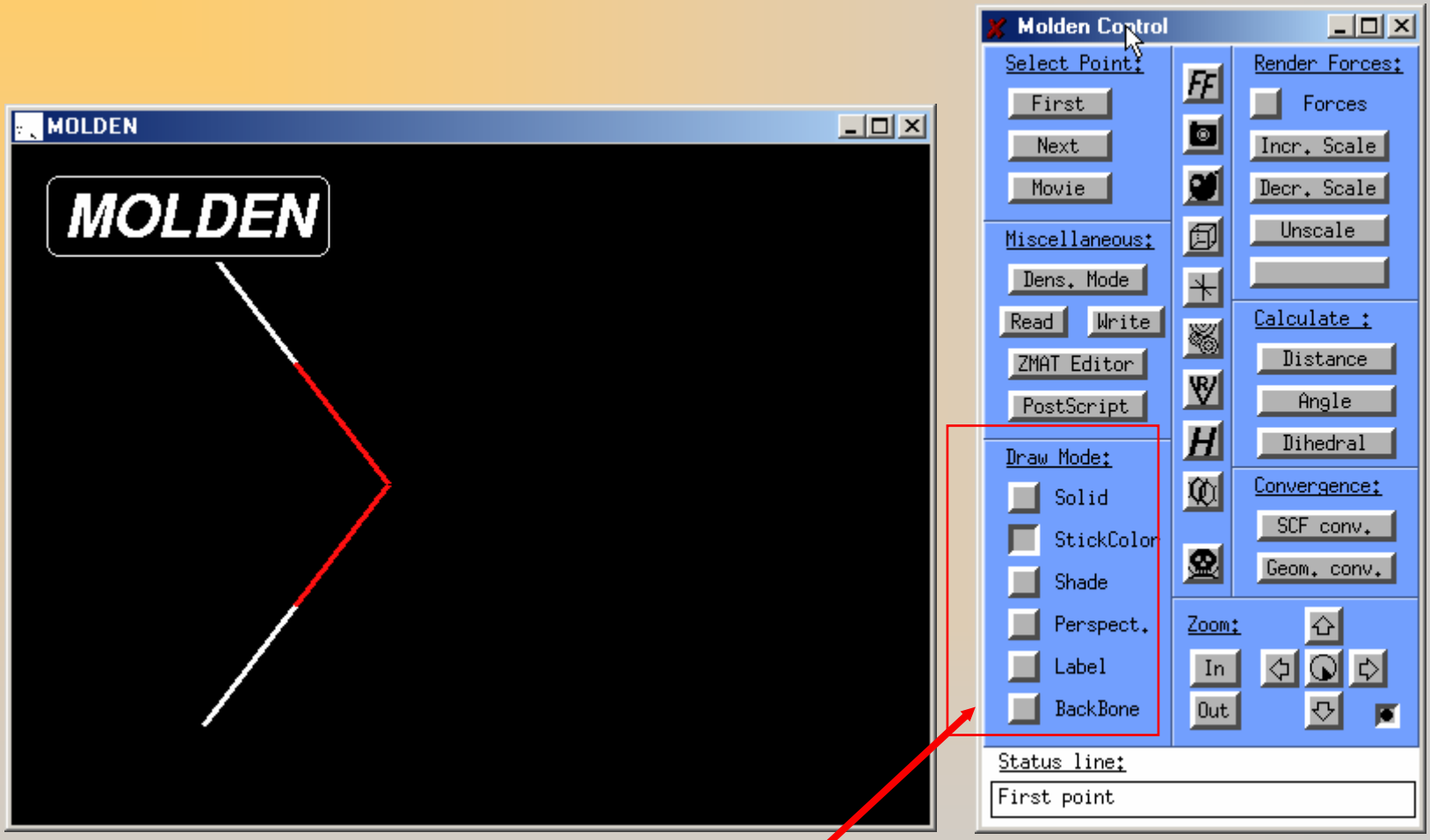

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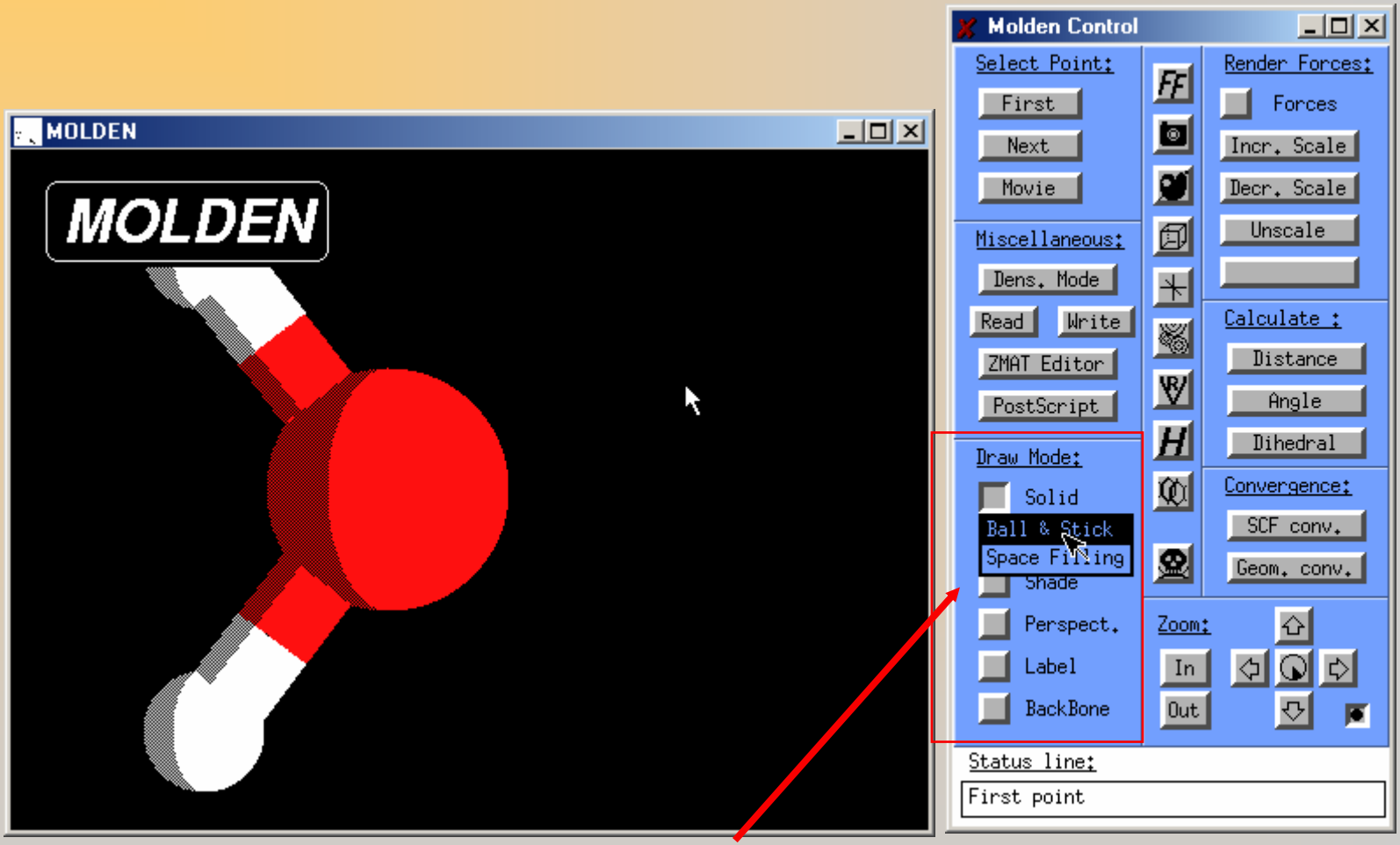

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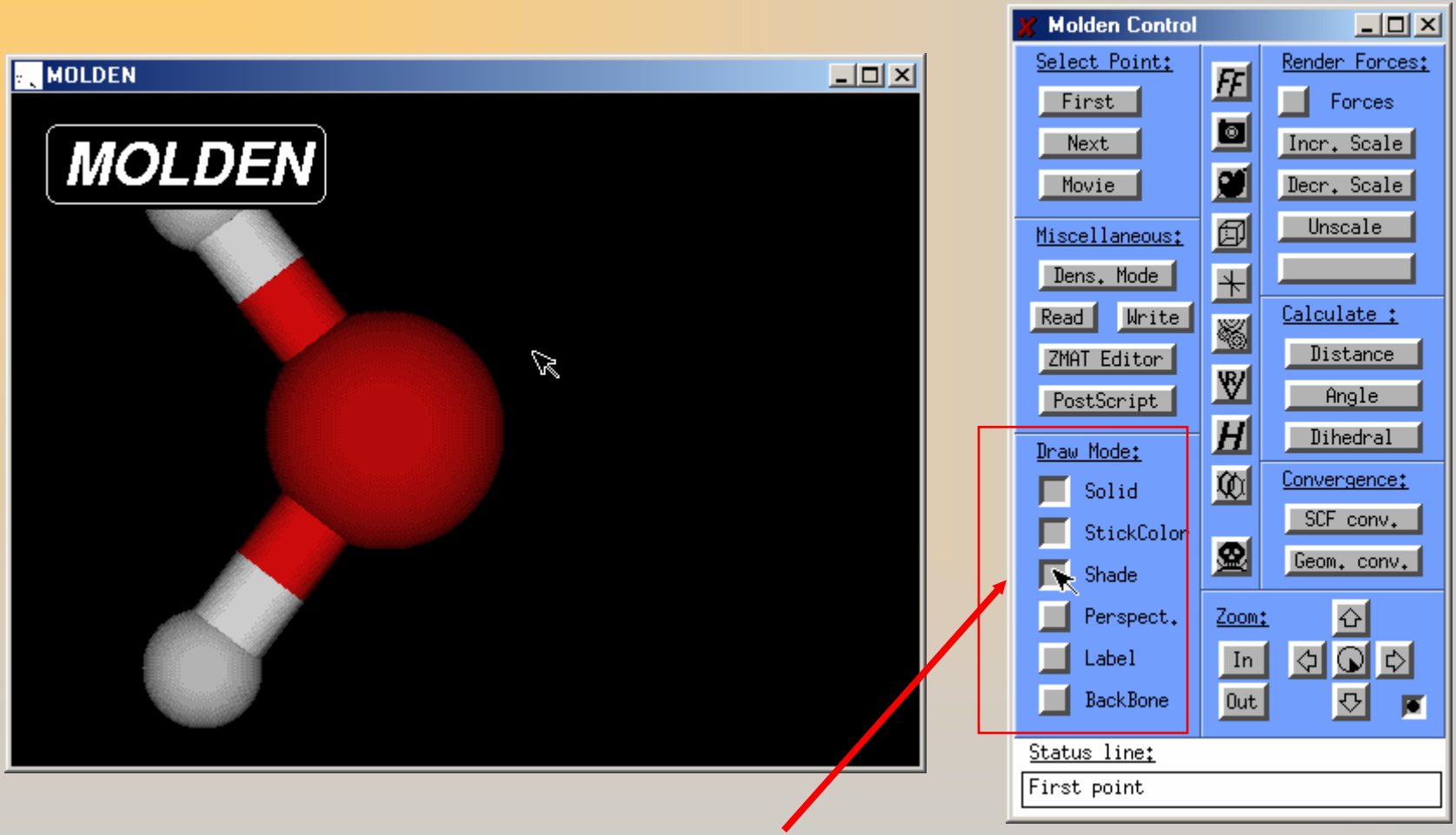

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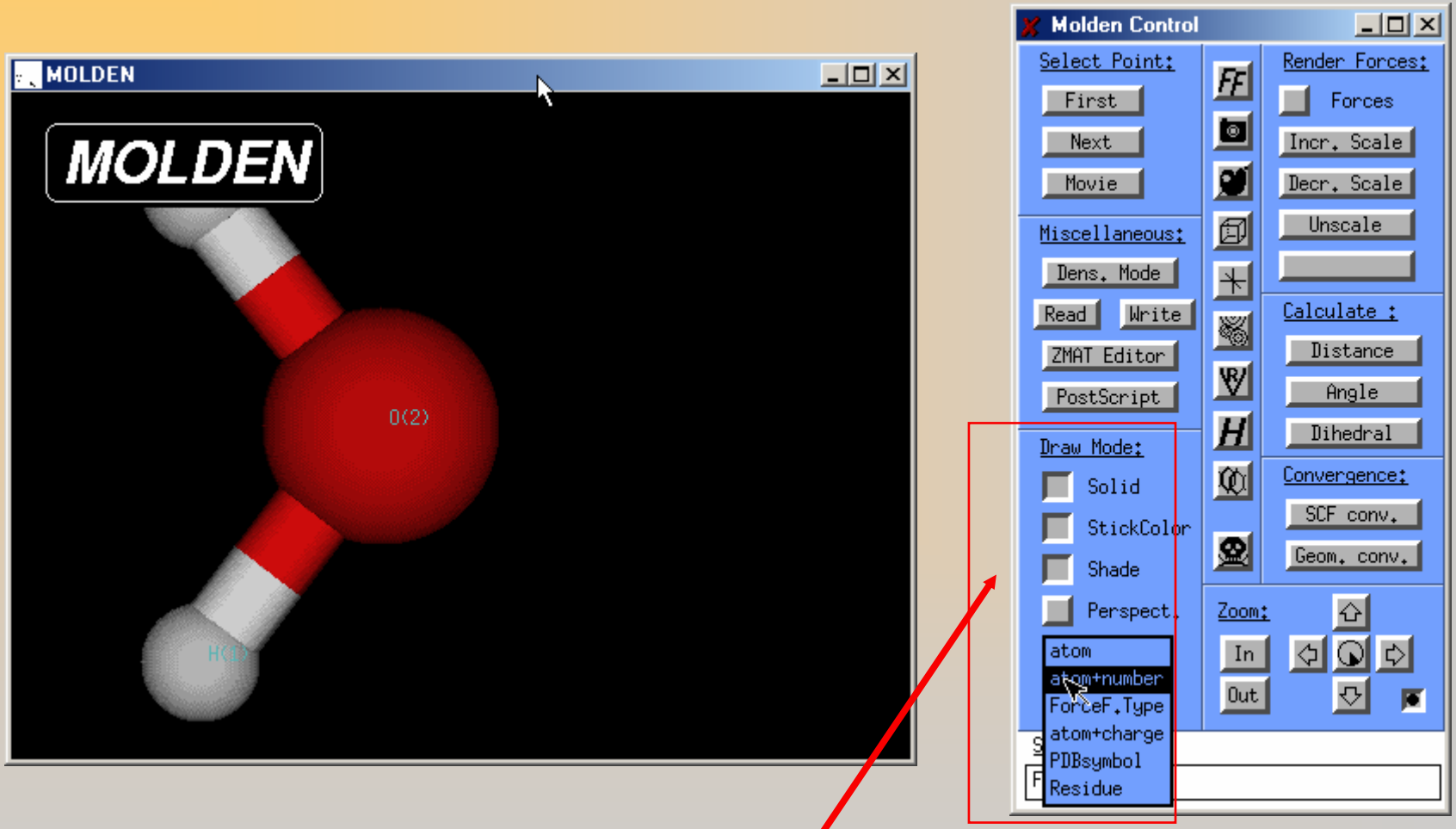

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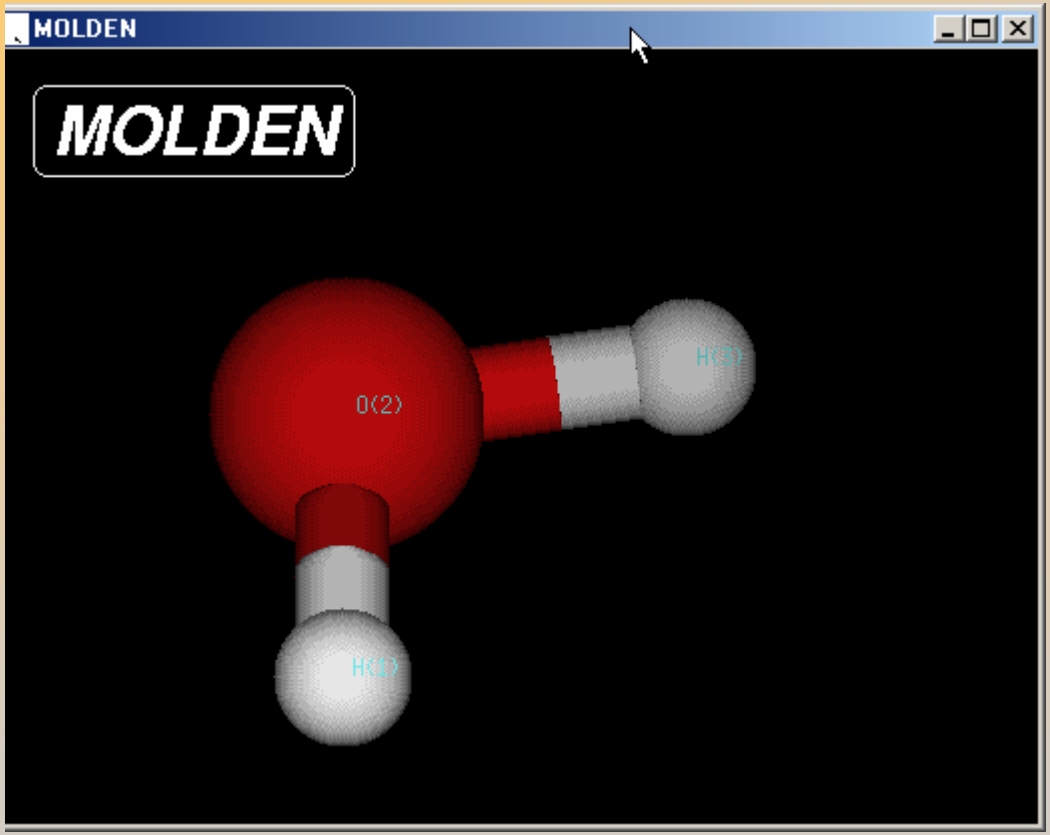

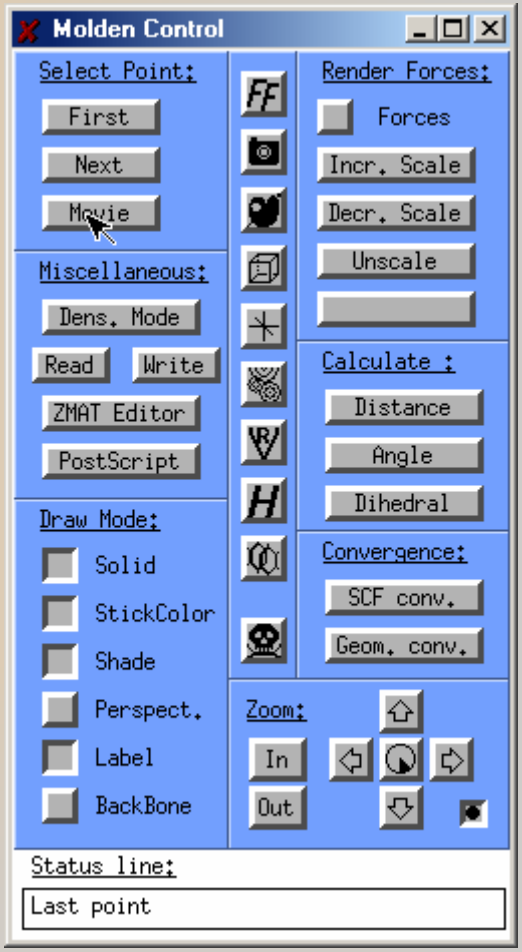

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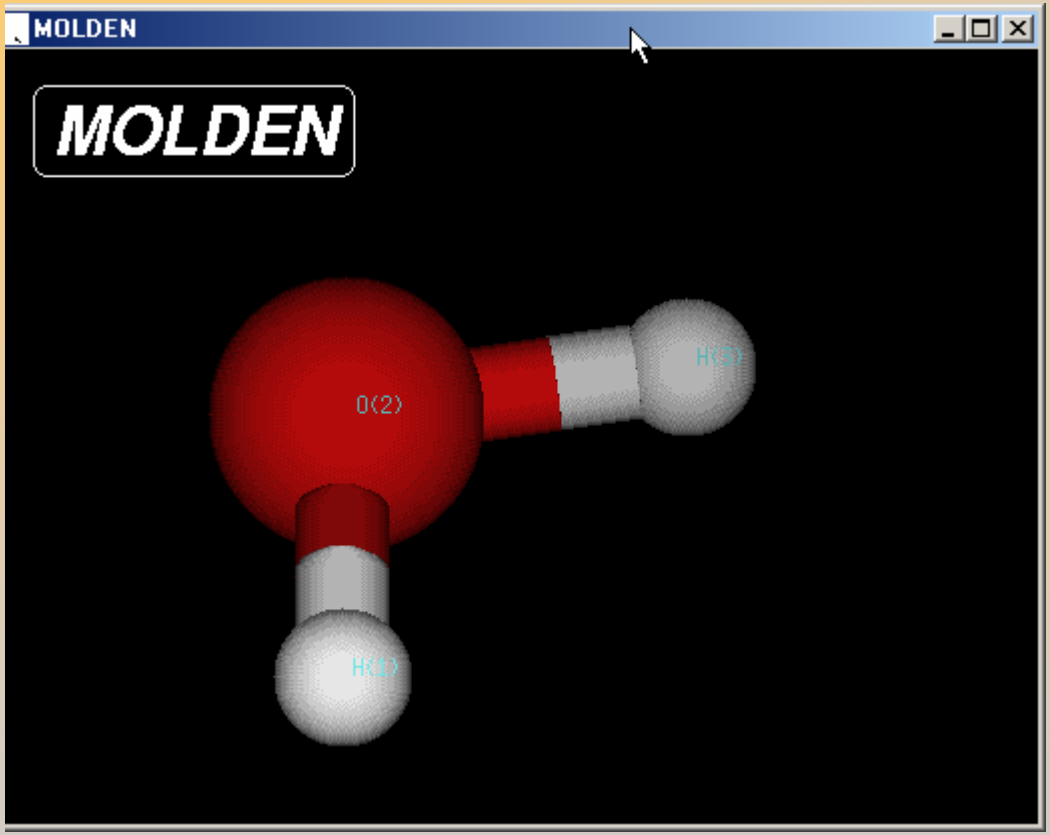
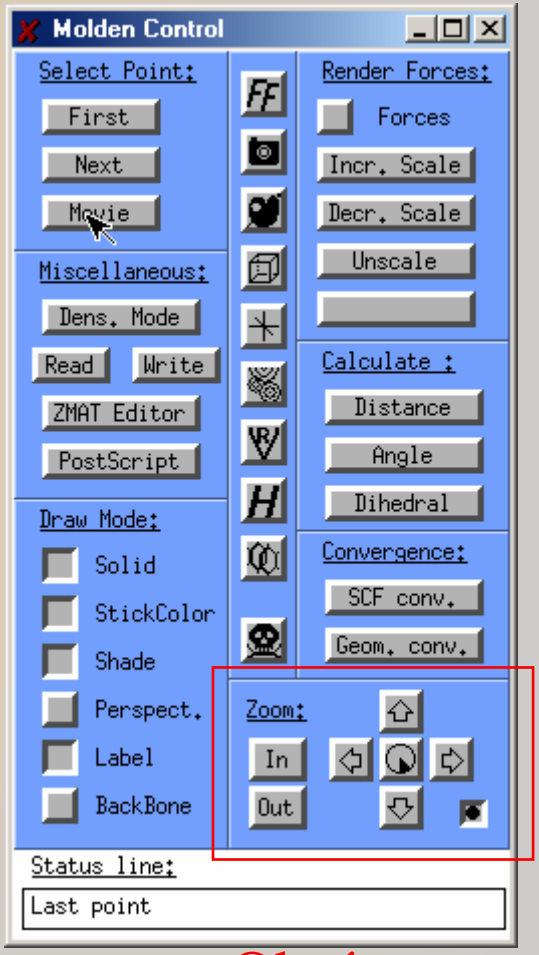
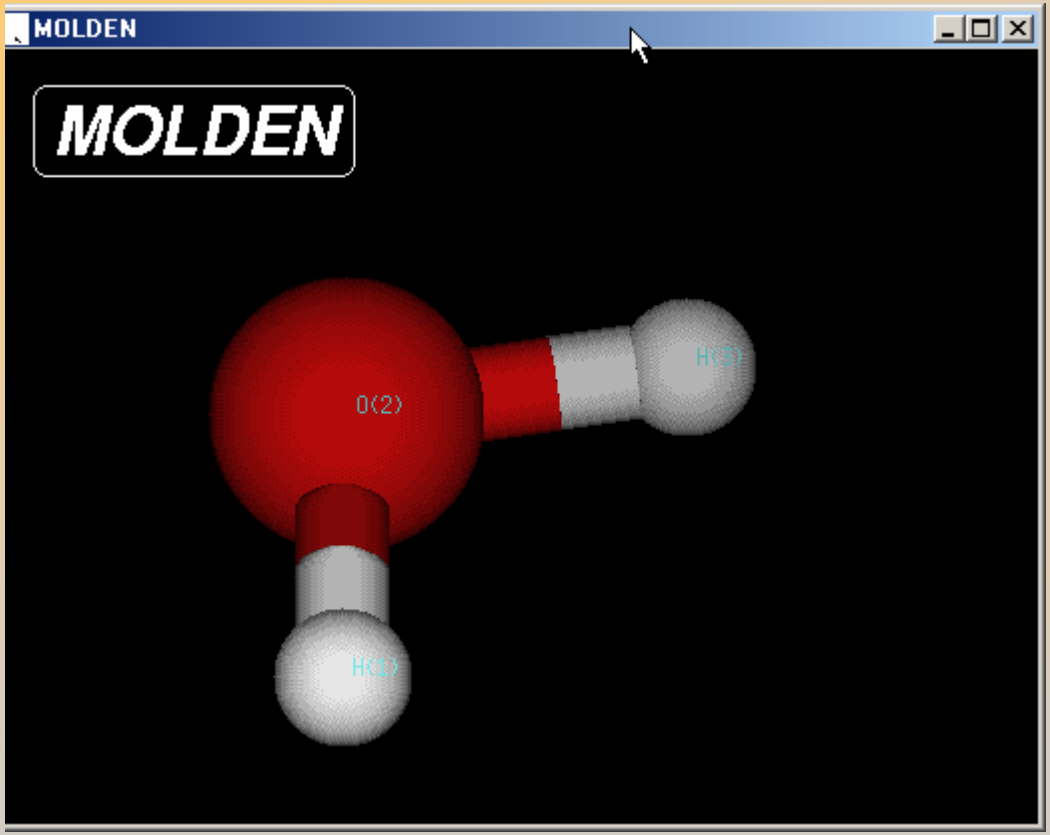


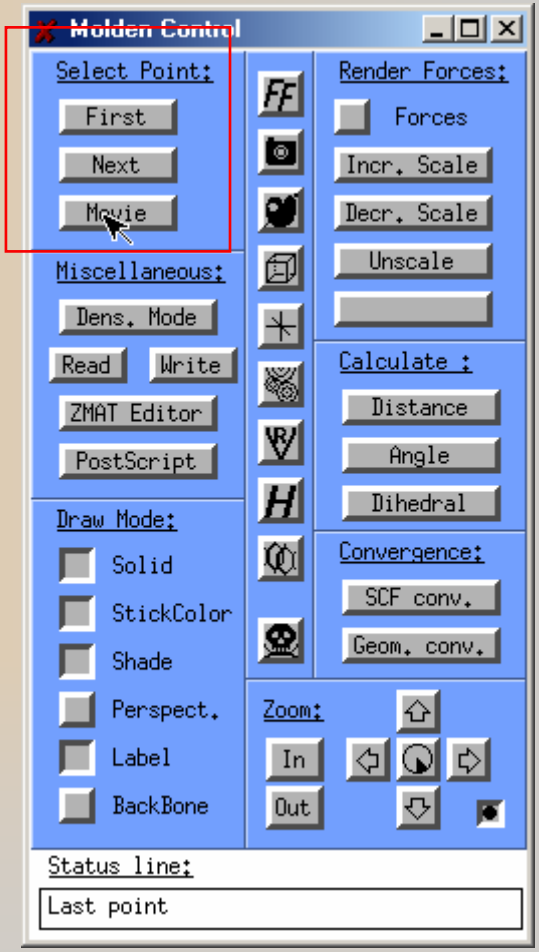


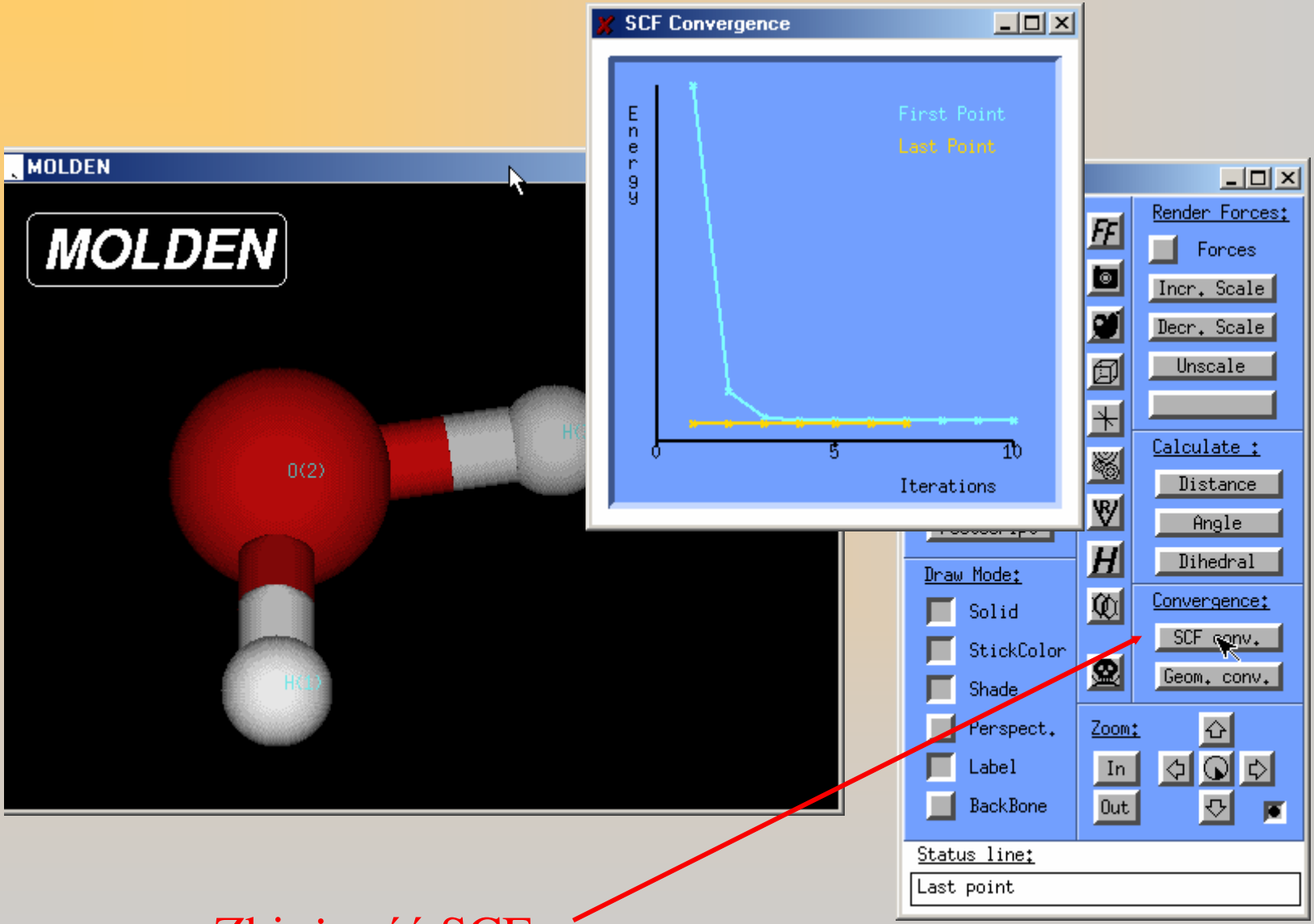
obrót cząsteczki poprzez przeciągniecie mysza

Obrót, przesunięcie, powiększenie

Wybór jednej z wielu geometrii







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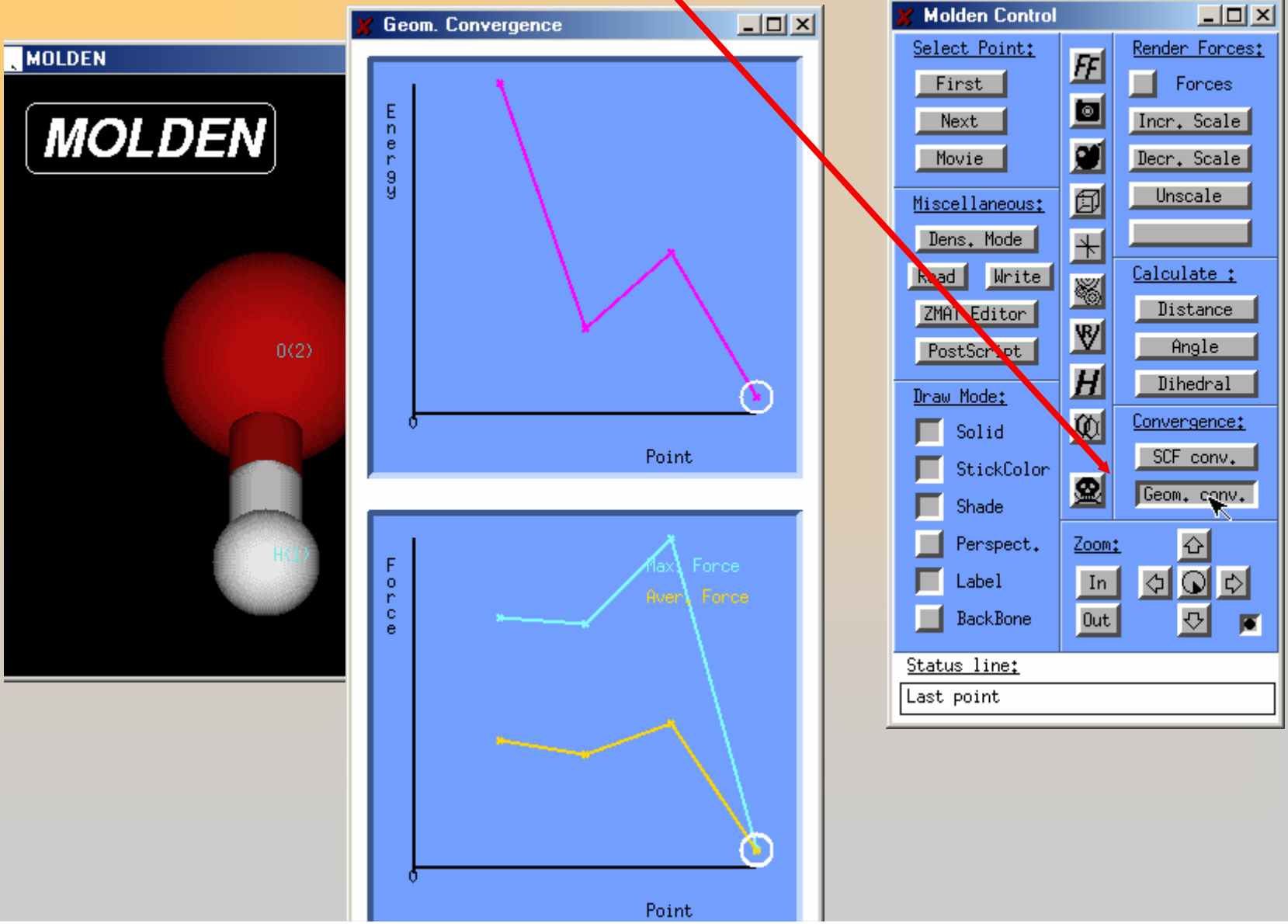
zbieżność geometrii



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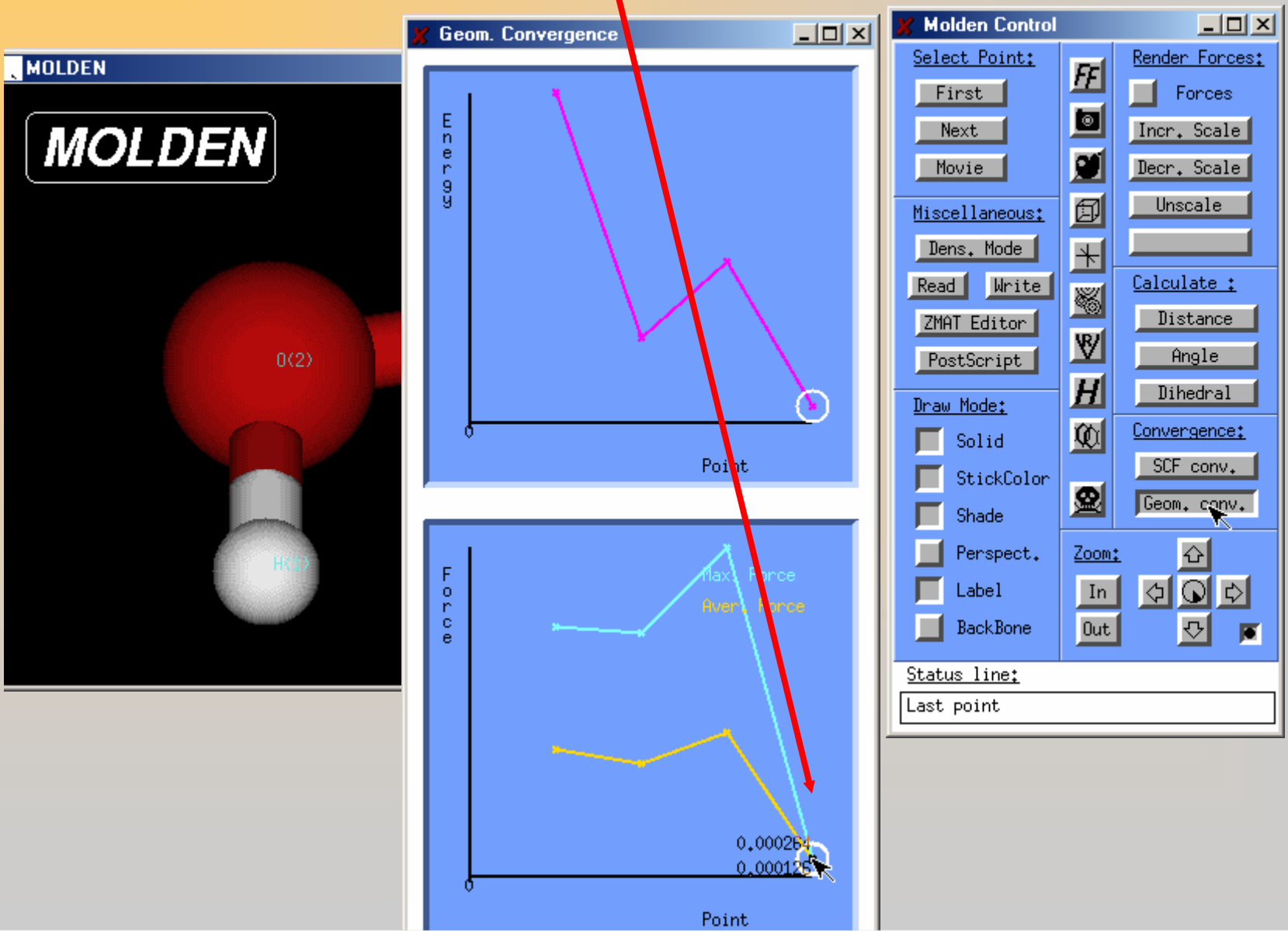


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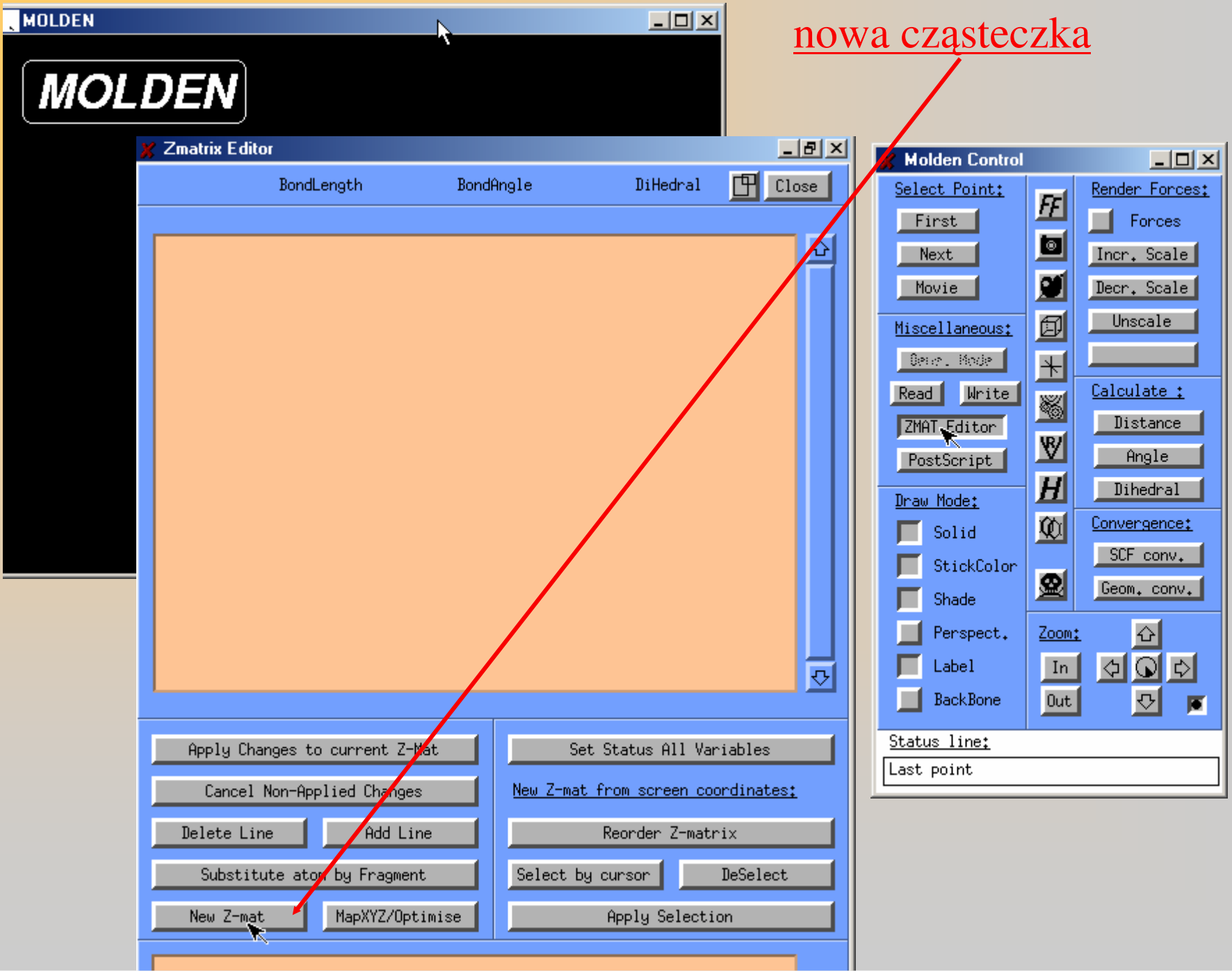
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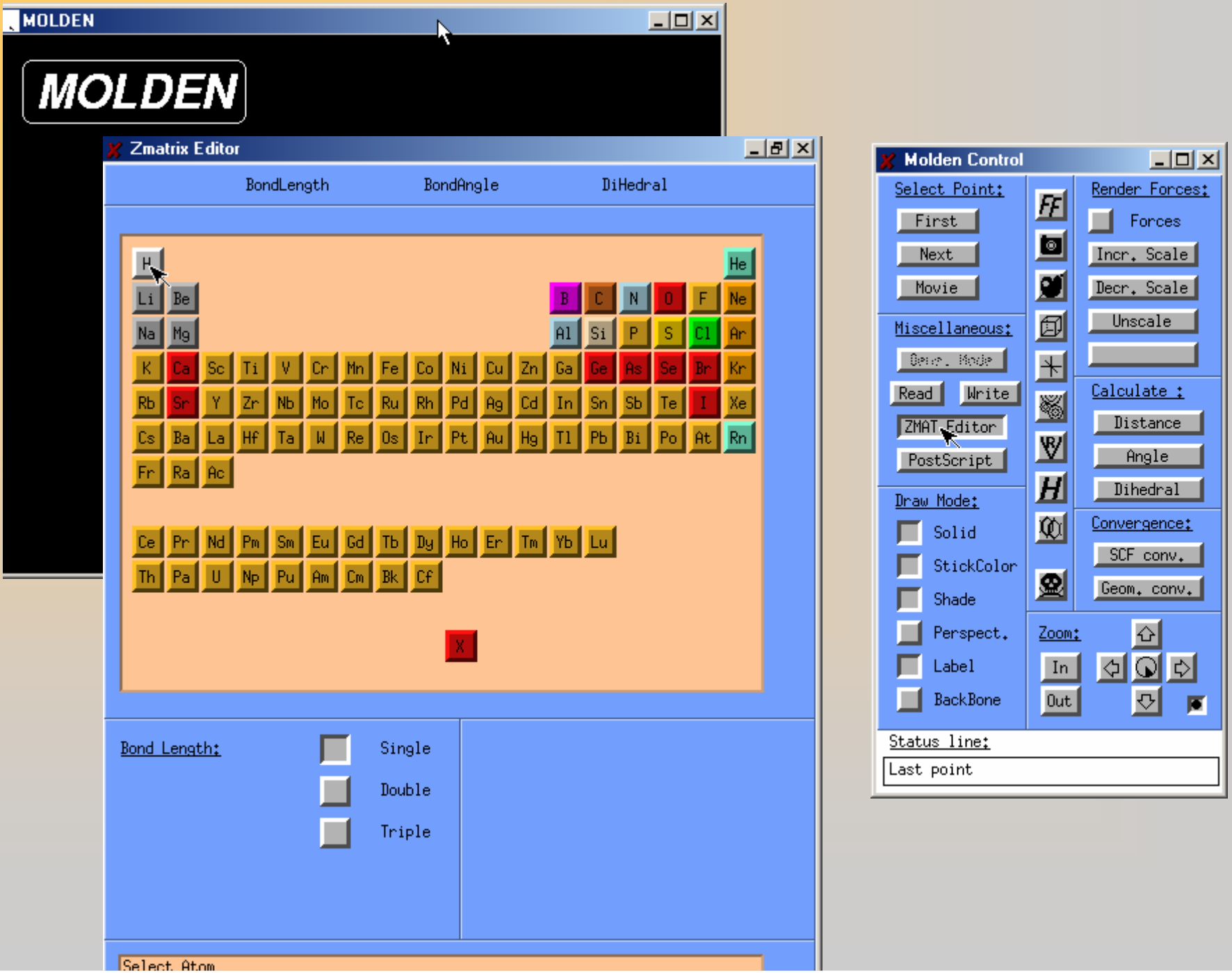
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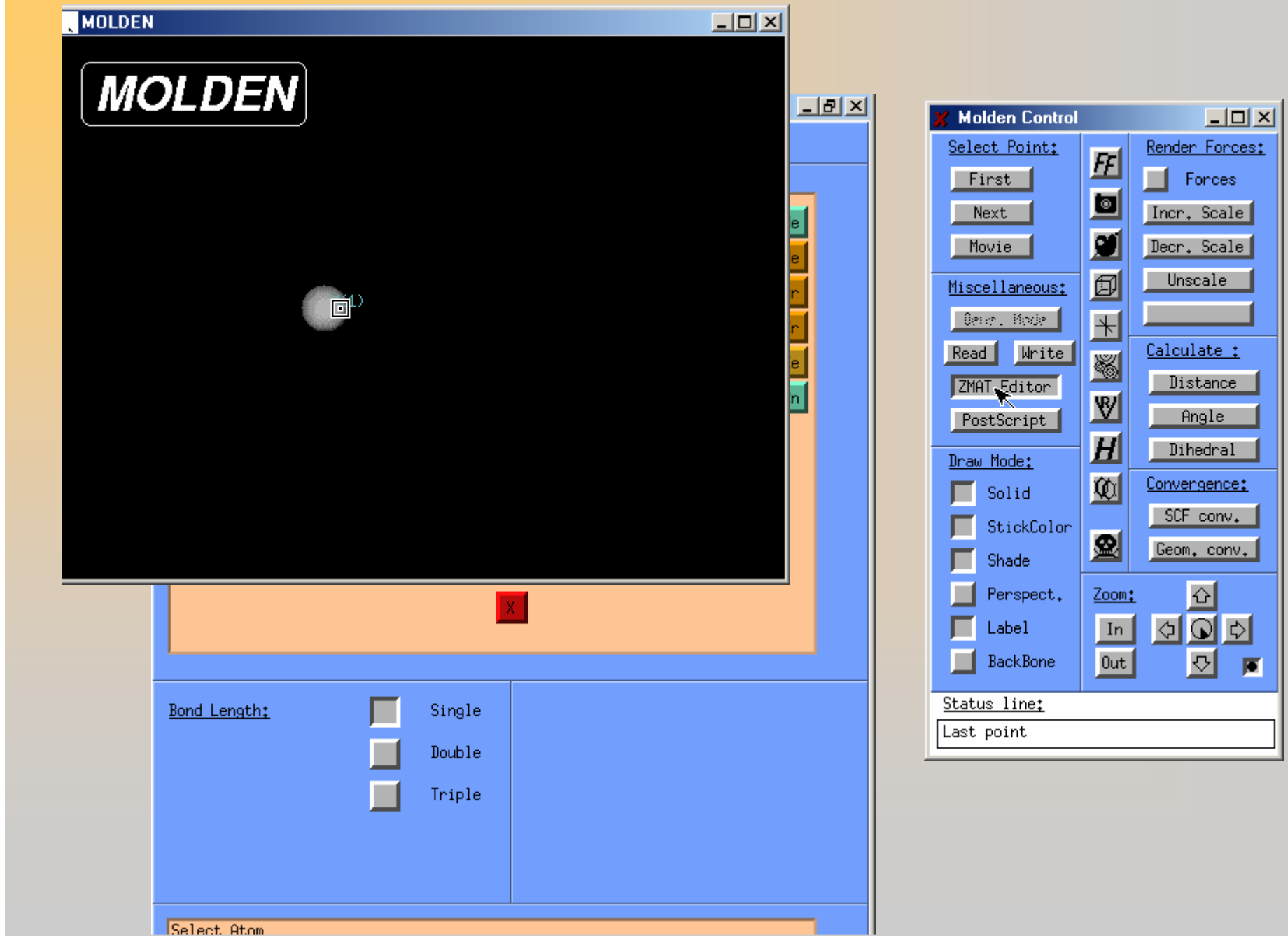
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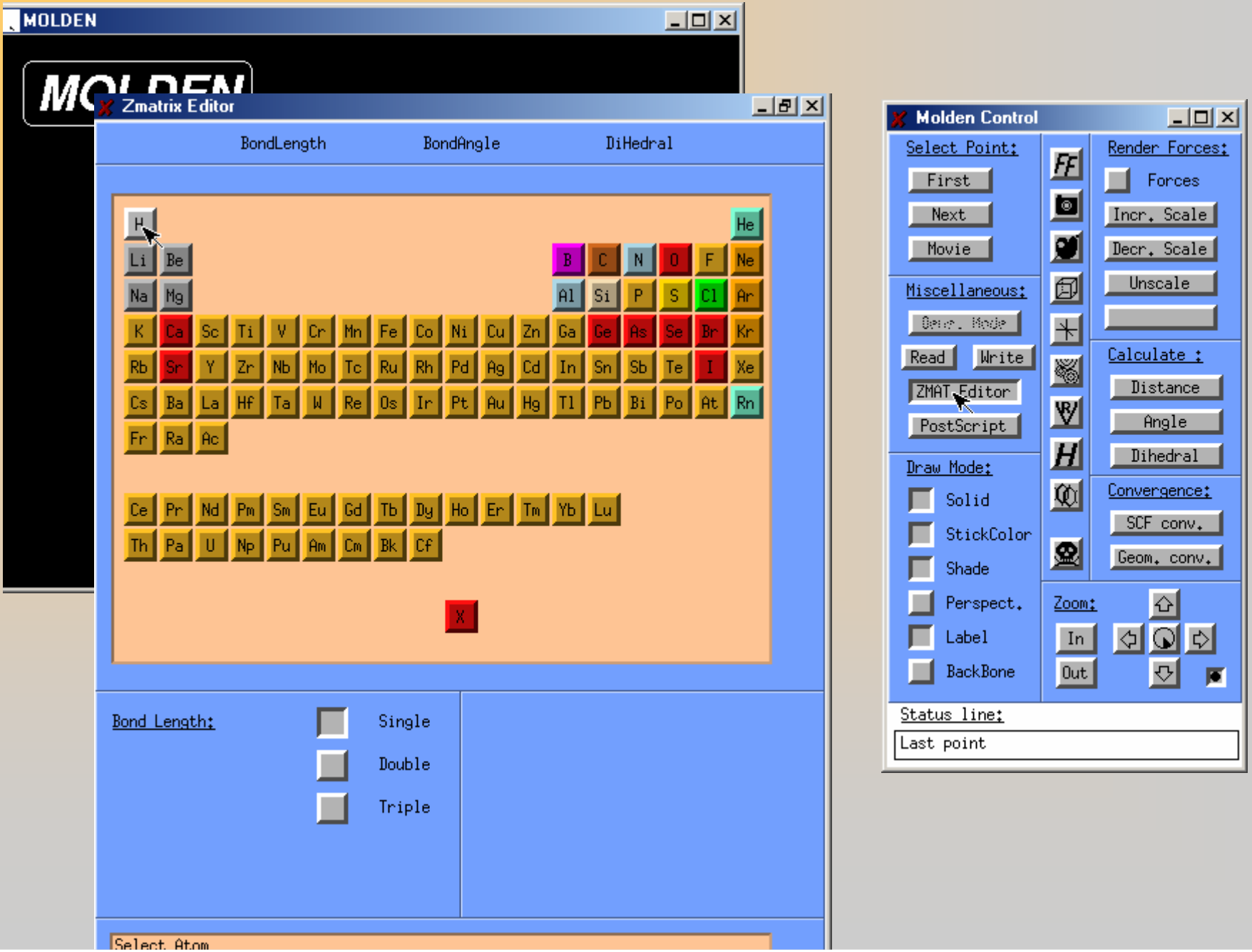
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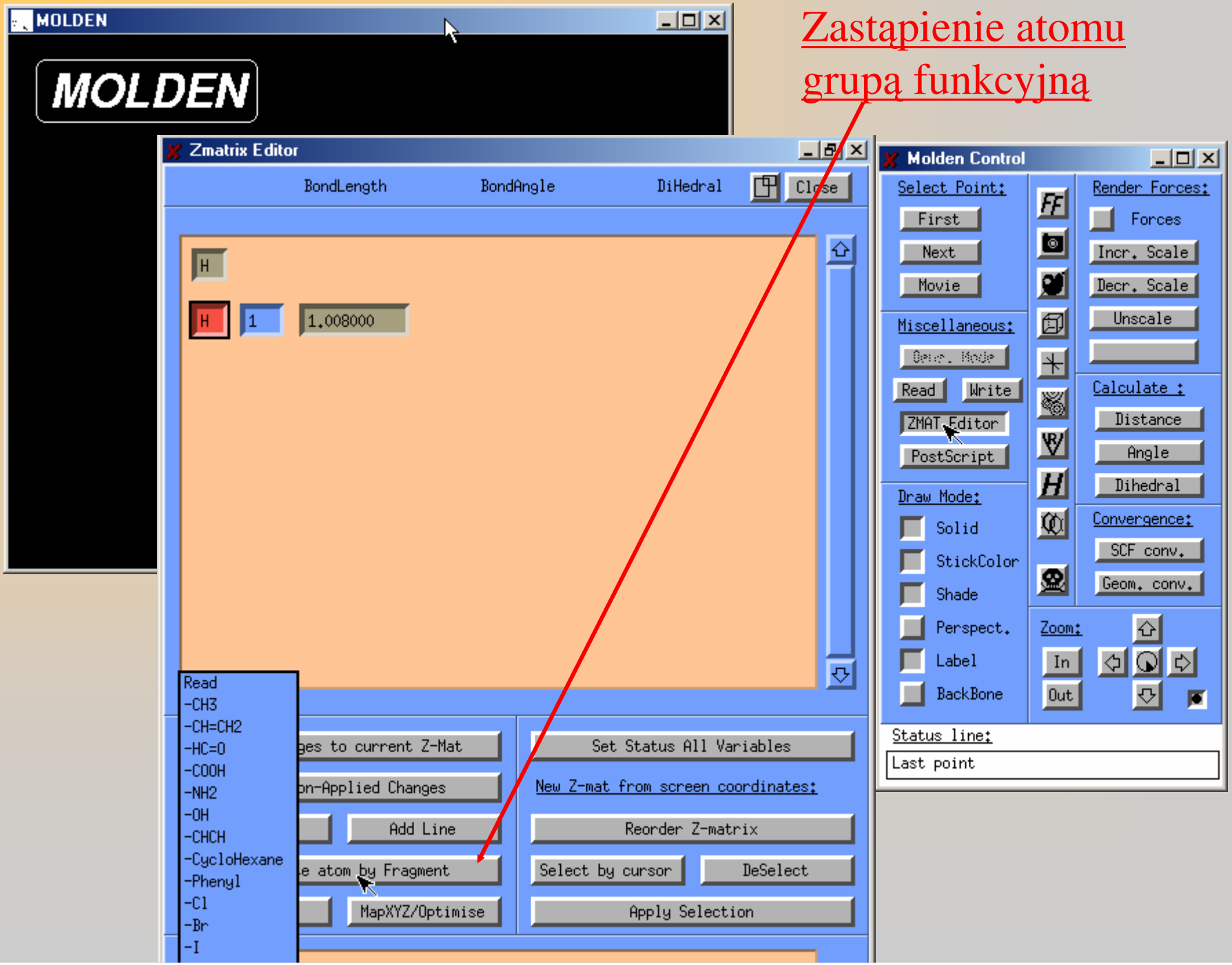

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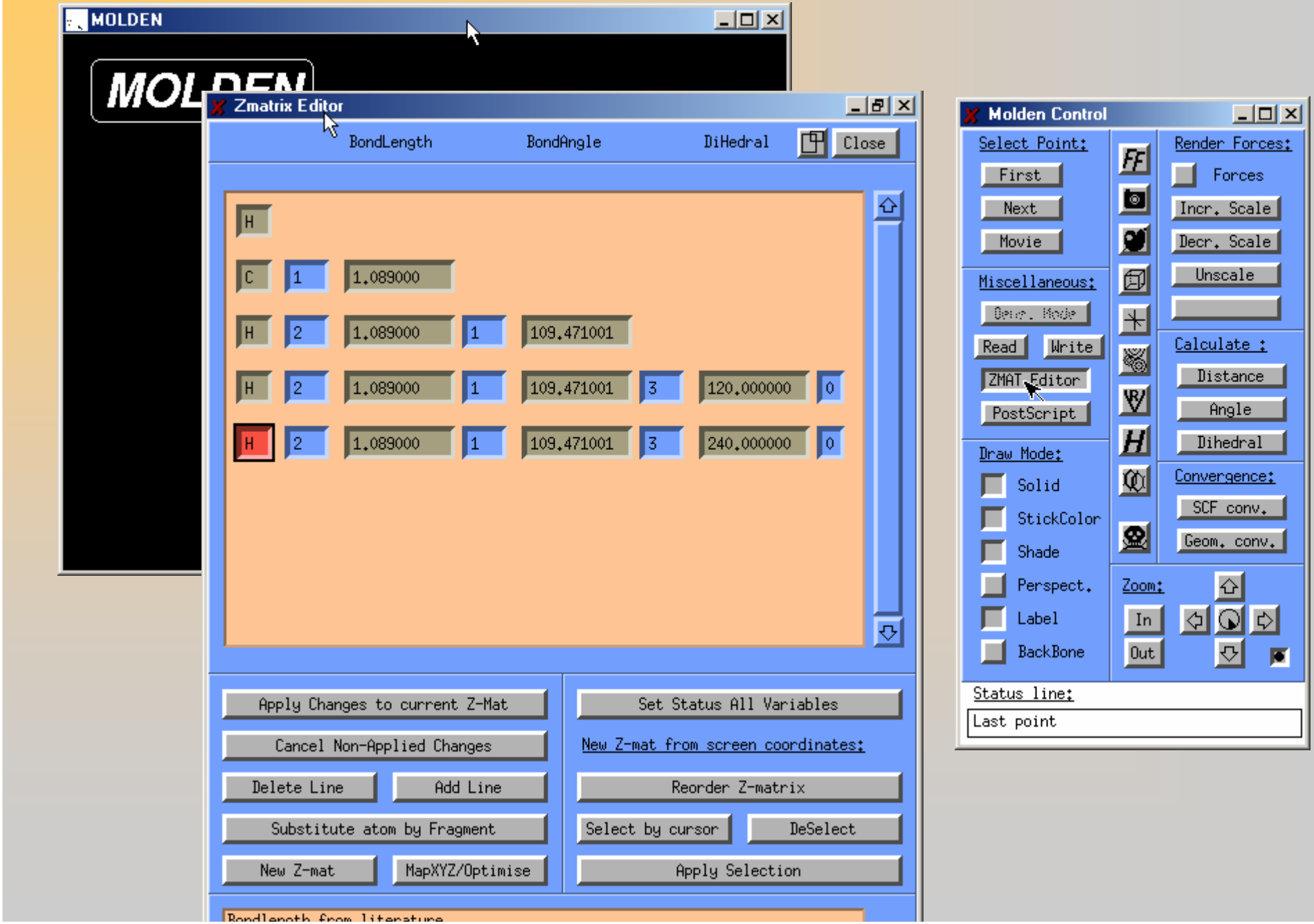
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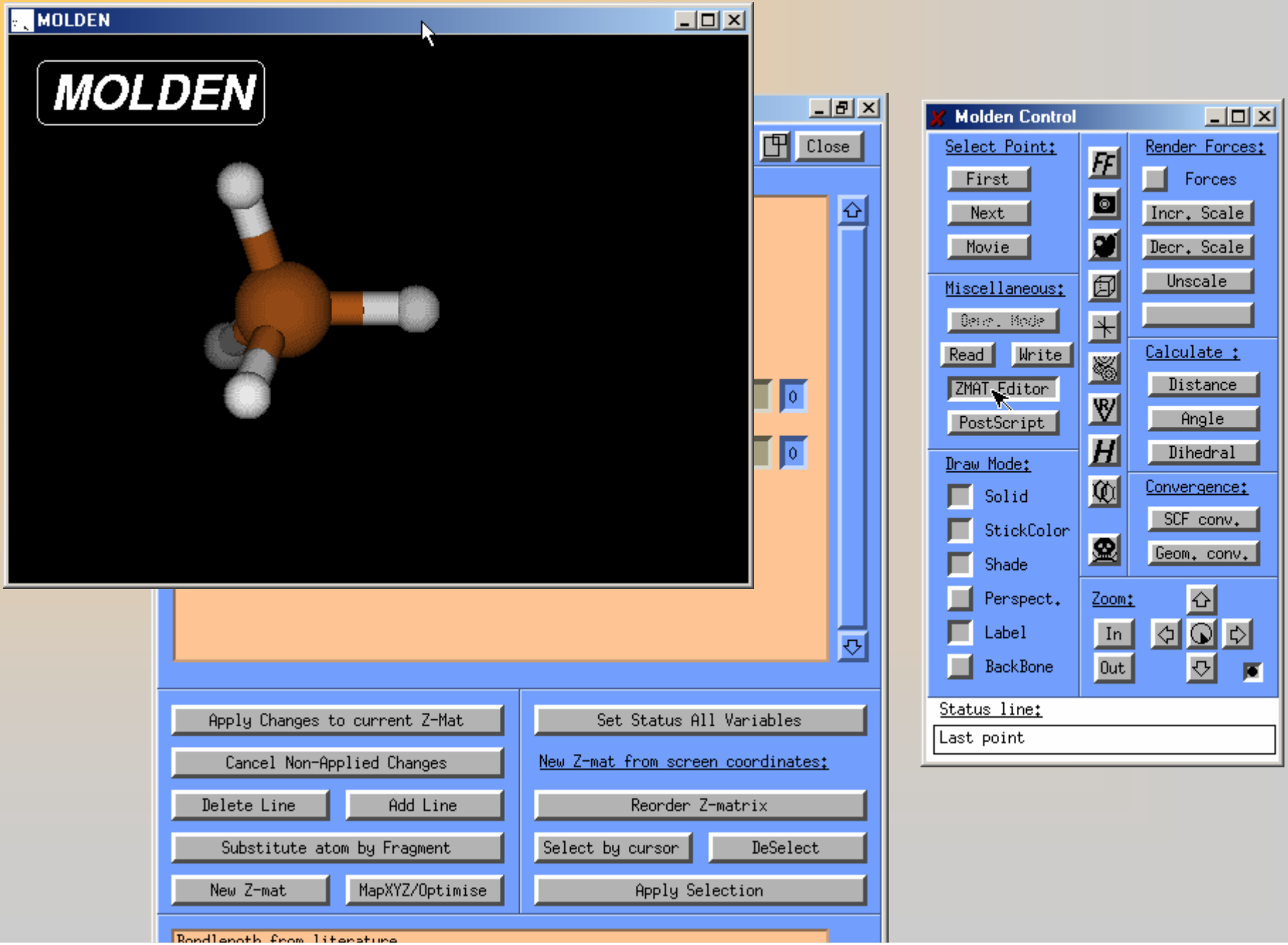
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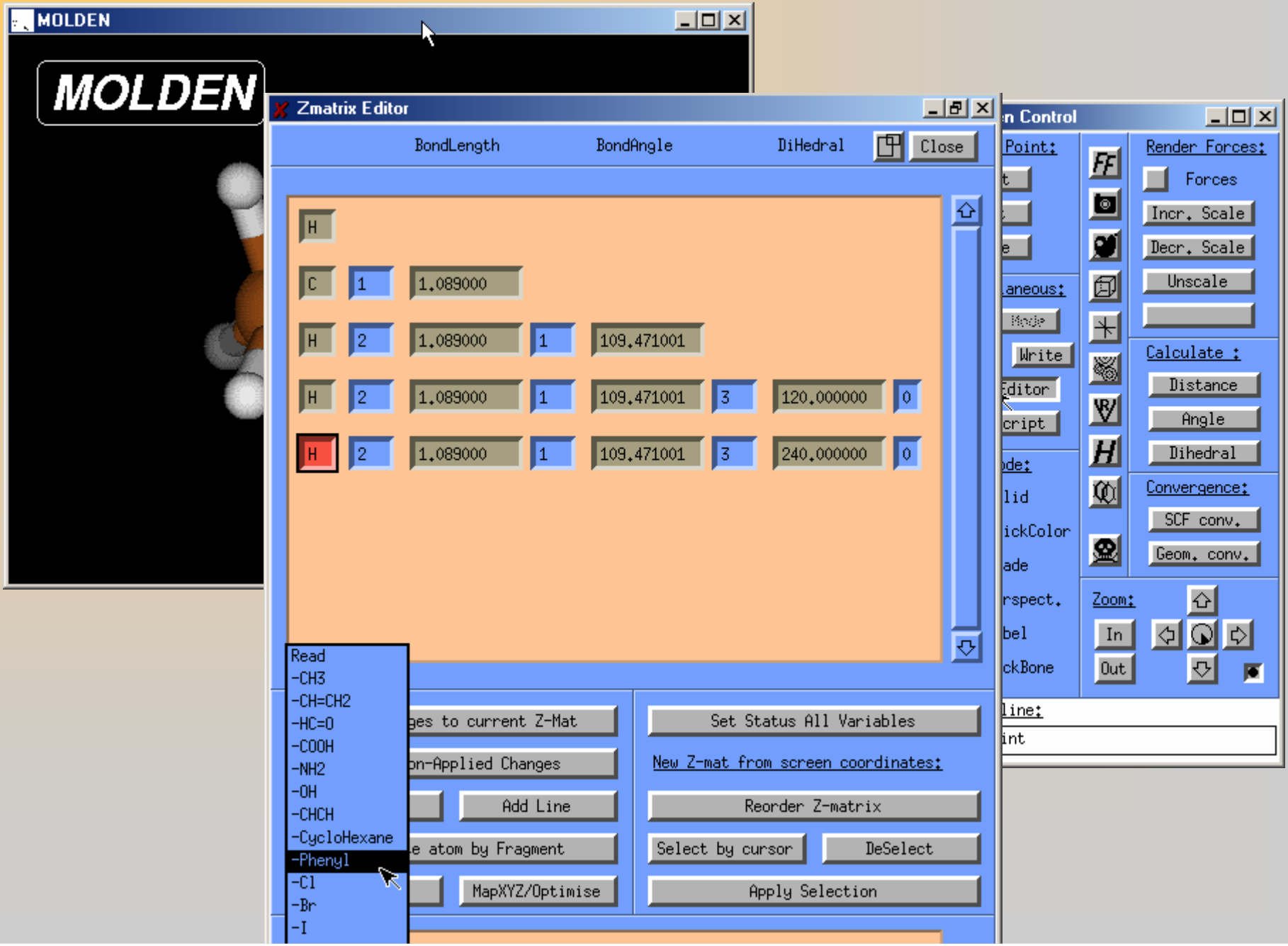
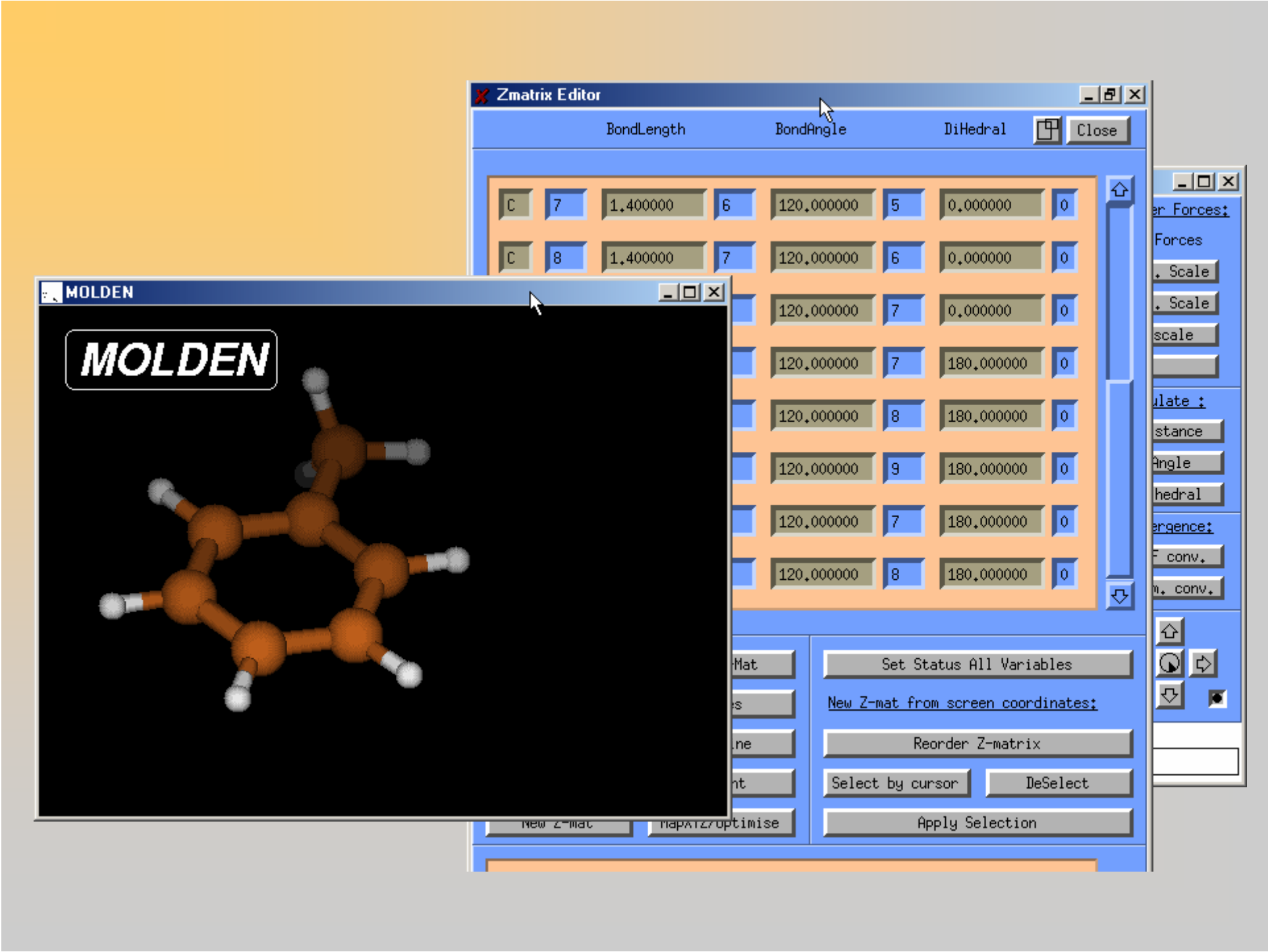
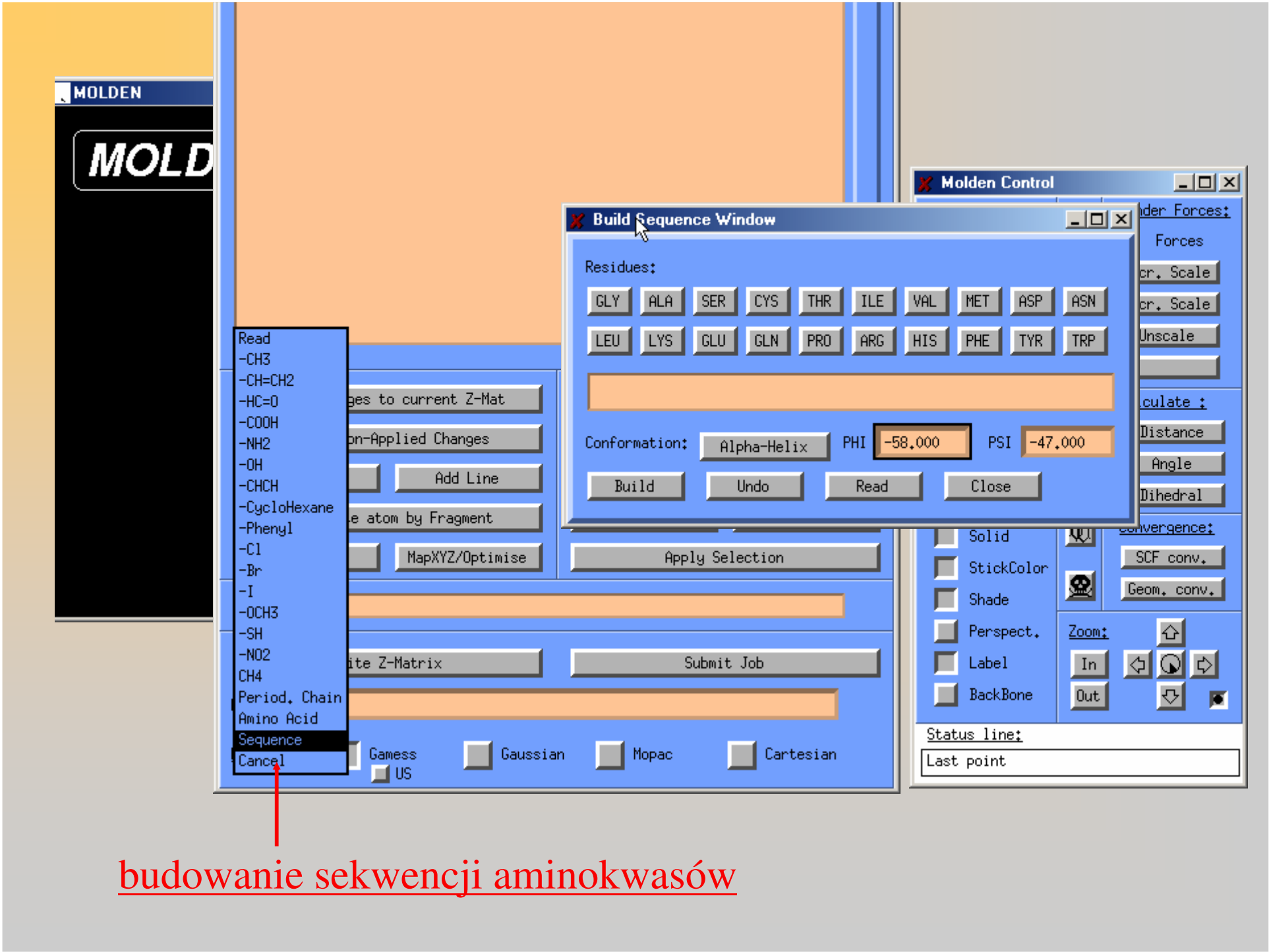
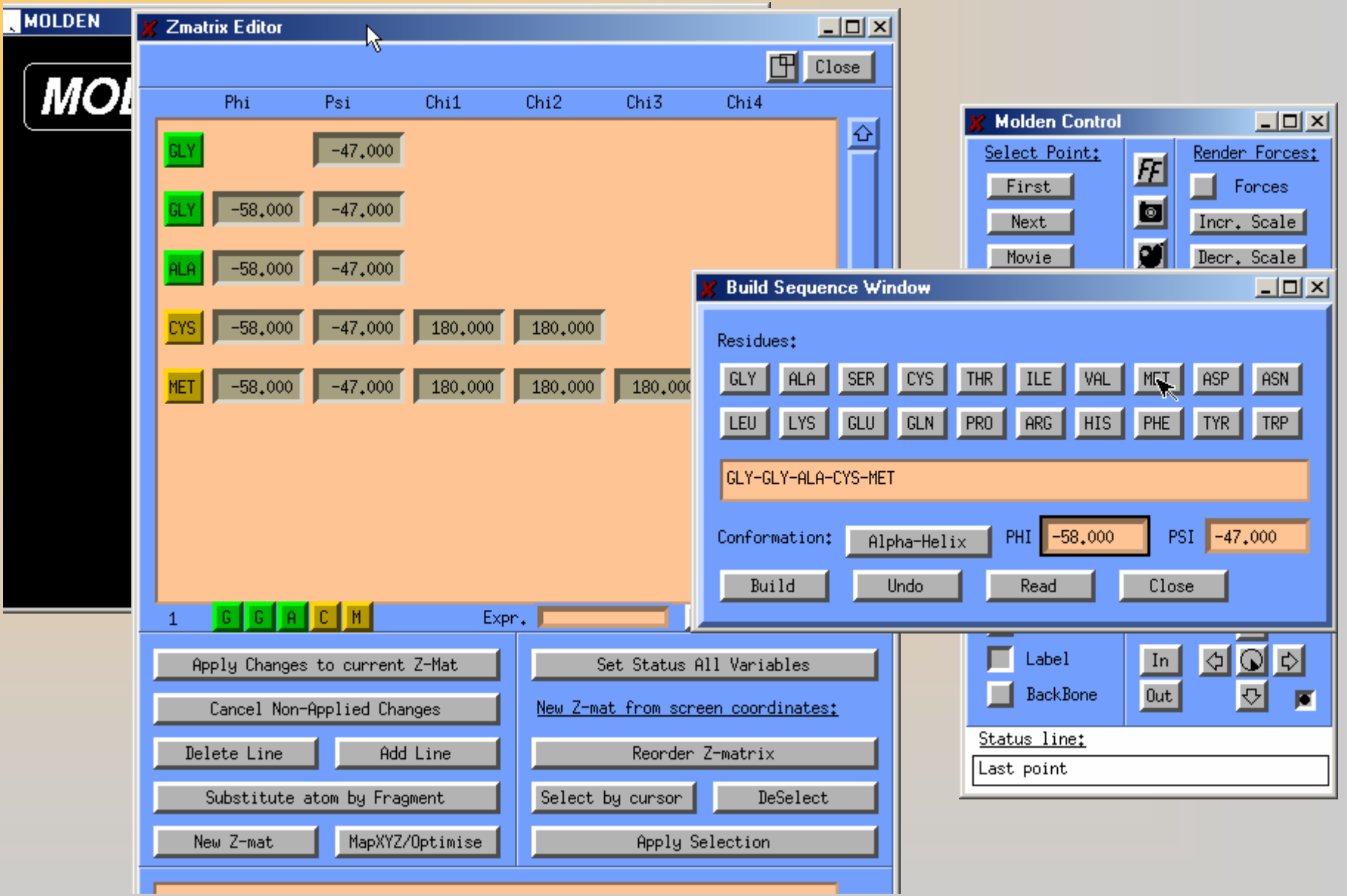

MOLDEN
MOLDEN
Zmatrix Editor
BondLength
BondAngle
DiHedral
Close
H
C 1 1.089000
H 2 1.089000 1 109.471001
H 2 1.089000 1 109.471001 3 120.000000 0
H 2 1.089000 1 109.471001 3 240.000000 0
Read
-CH3
-CH=CH2
-HC=O
-COOH
-NH2
-OH
-CHCH
-CycloHexane
-Phenyl
-Cl
-Br
-I
Add Line
MapXYZ/Optimise
Set Status All Variables
New Z-mat from screen coordinates:
Reorder Z-matrix
Select by cursor
DeSelect
Apply Selection
Render Forces:
Forces
Incr. Scale
Decr. Scale
Unscale
Calculate :
Distance
Angle
Dihedral
Convergence:
SCF conv.
Geom. conv.
Zoom:
In
Out
Write

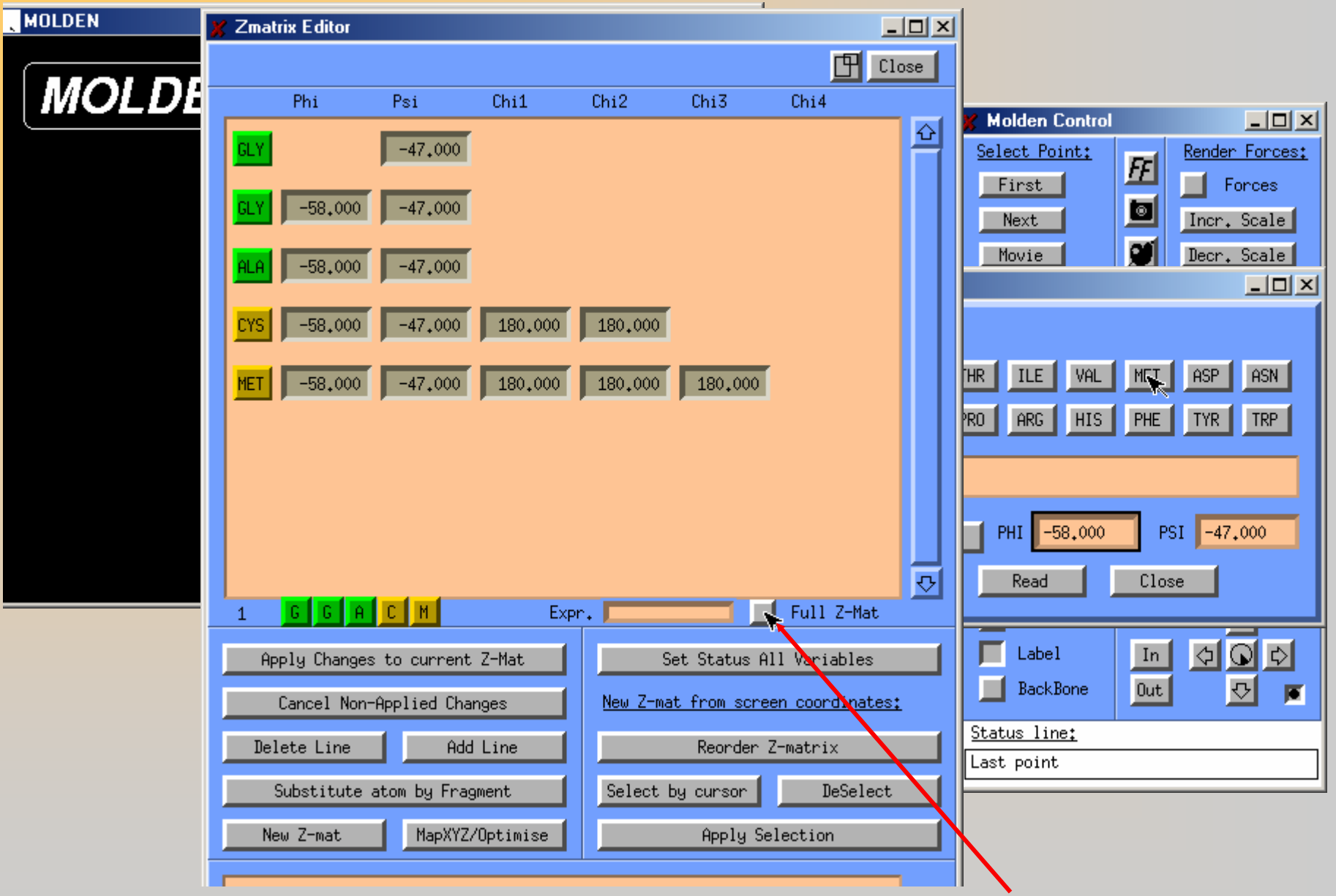

Zmatrix Editor
BondLength
BondAngle
DiHedral
Close
C 7 1.400000 6 120.000000 5 0.000000 0
C 8 1.400000 7 120.000000 6 0.000000 0
120.000000 7 0.000000 0
120.000000 7 180.000000 0
120.000000 8 180.000000 0
120.000000 9 180.000000 0
120.000000 7 180.000000 0
120.000000 8 180.000000 0
Set Status All Variables
New Z-mat from screen coordinates:
Reorder Z-matrix
Select by cursor
DeSelect
Apply Selection
MOLDEN
MOLDEN



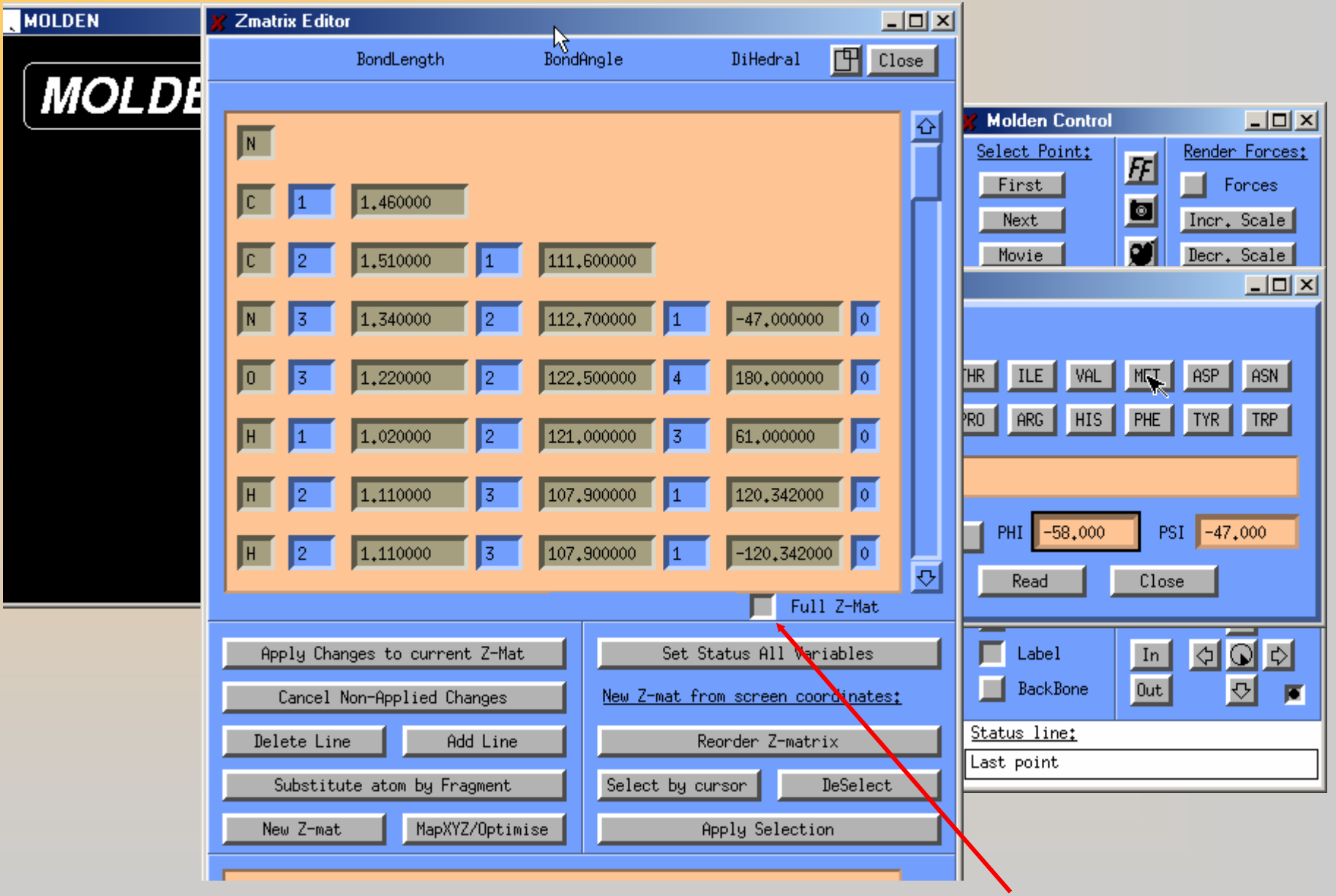
budowanie sekwencji aminokwasów



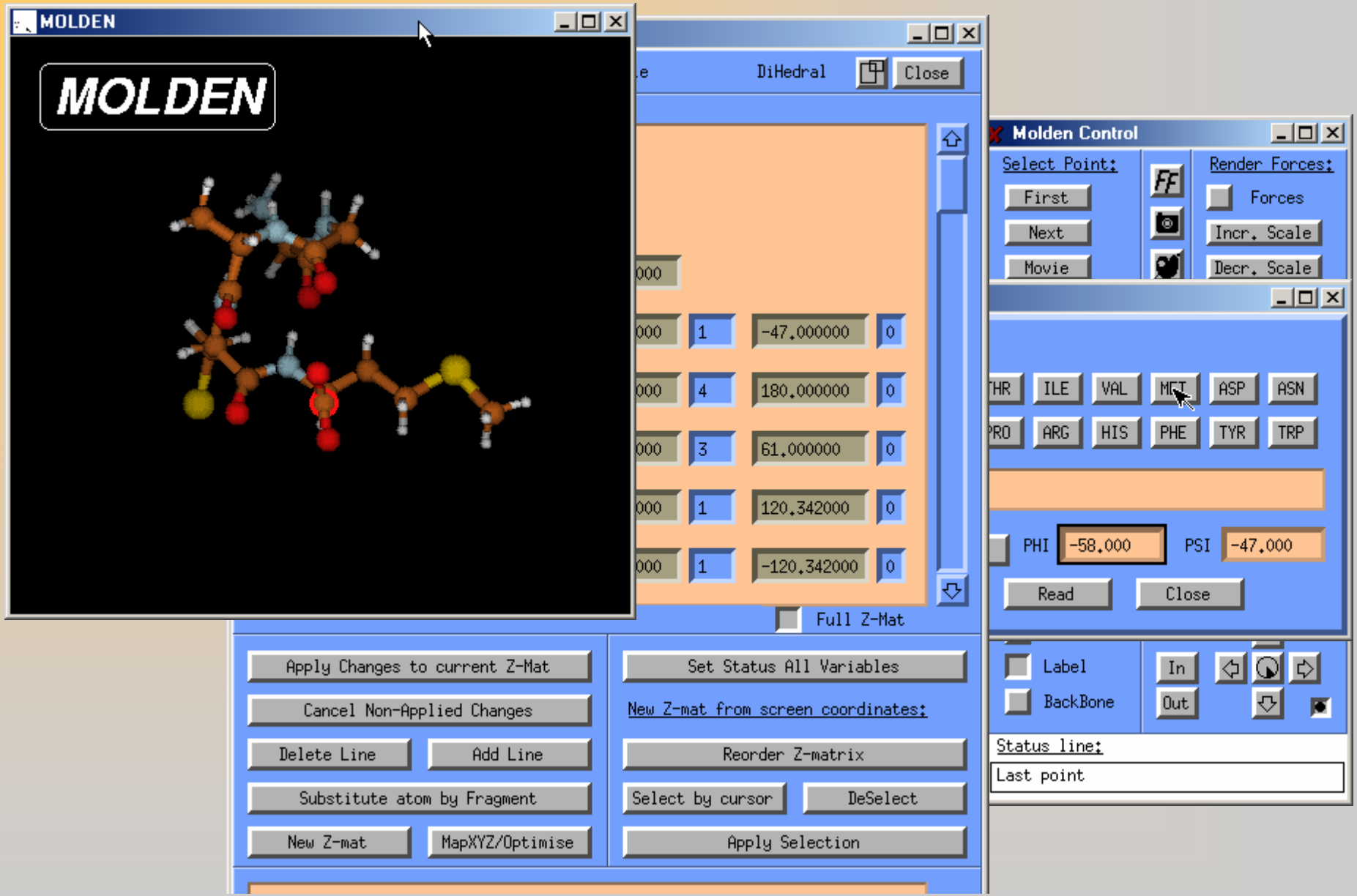
budowanie sekwencji aminokwasów

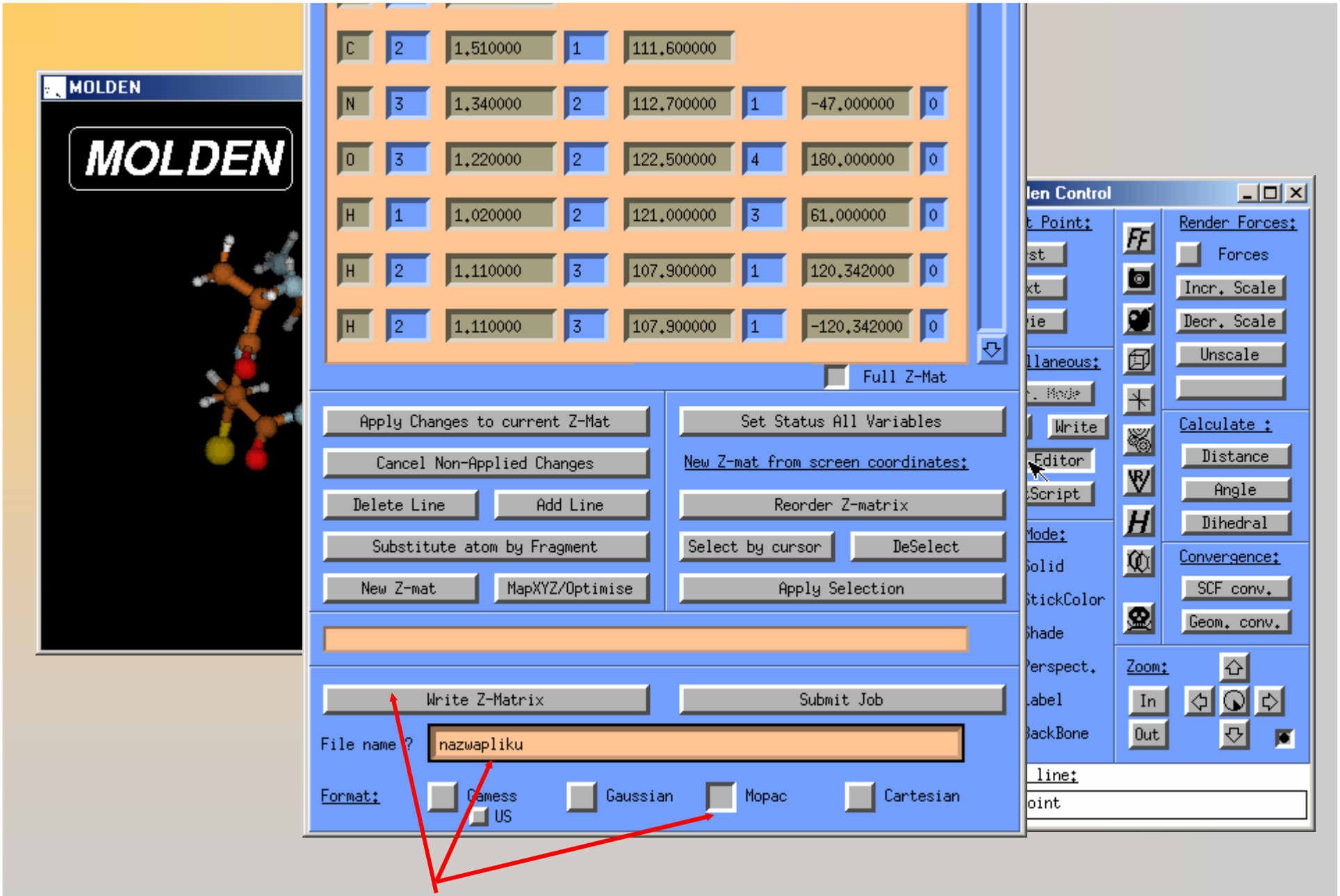


budowanie sekwencji aminokwasów – pełna macierz Z

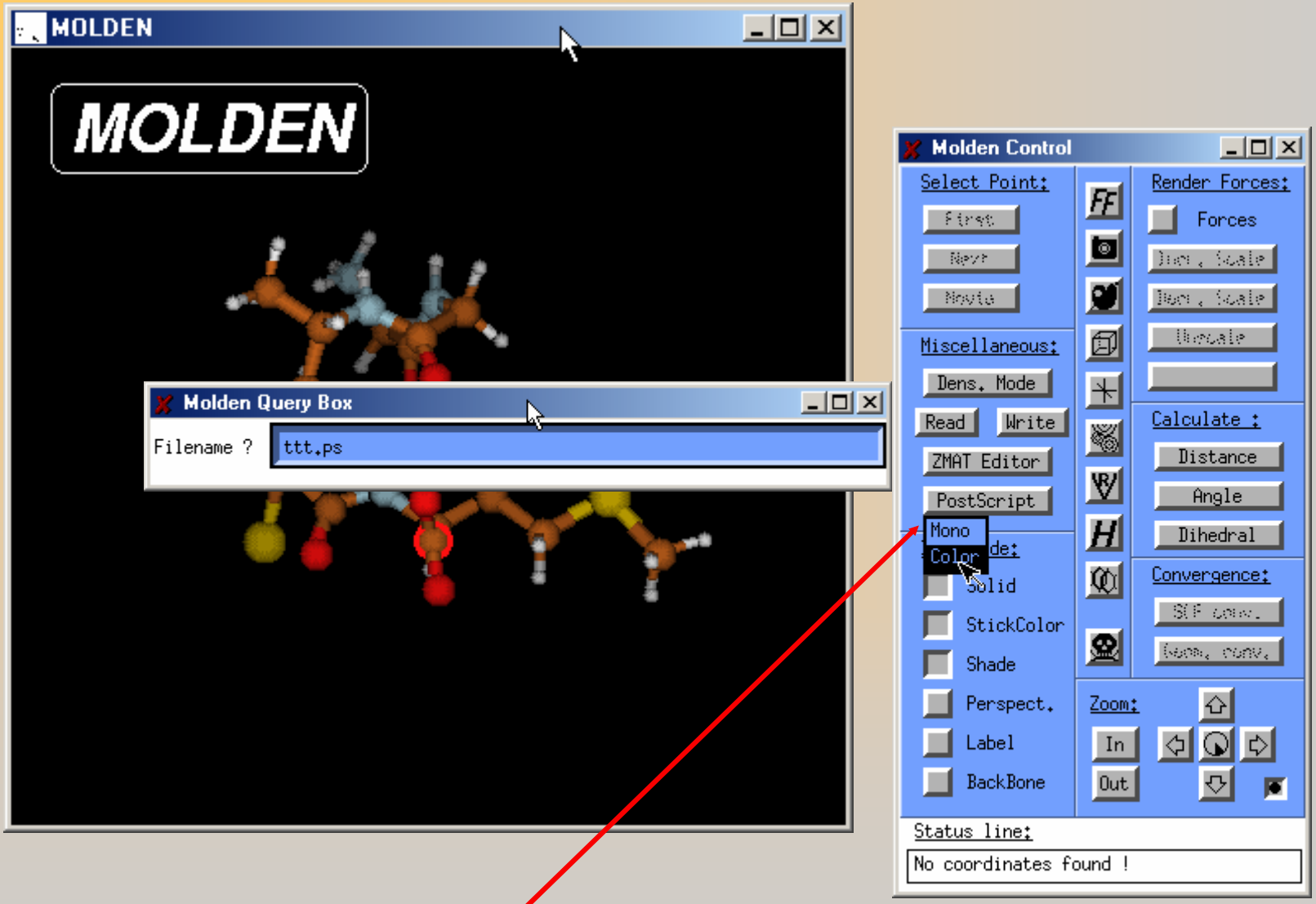


budowanie sekwencji aminokwasów – pełna macierz Z

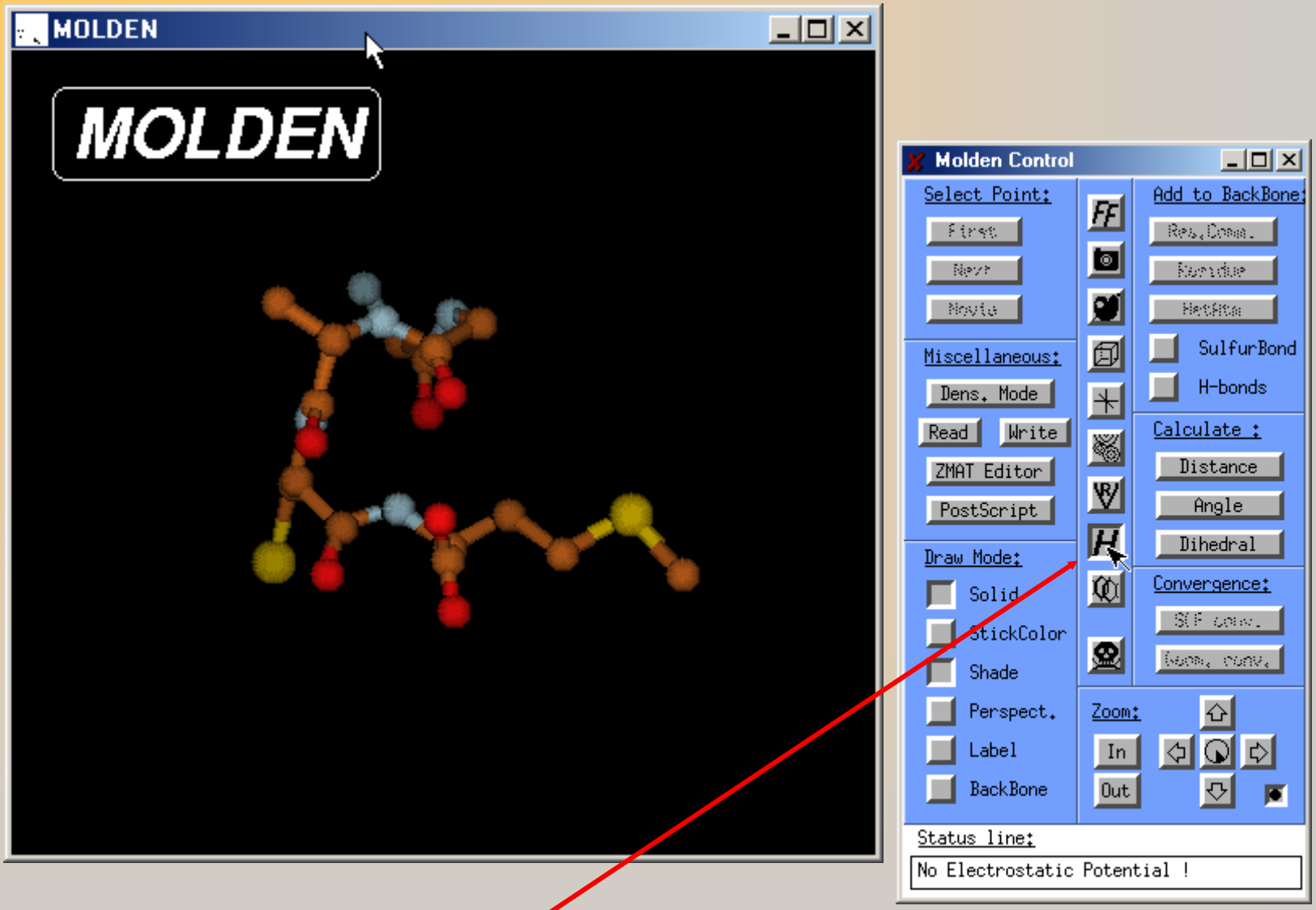

MOLDEN
MOLDEN
DiHedral
Close
1
-47.000000
0
4
180.000000
0
3
61.000000
0
1
120.342000
0
1
-120.342000
0
Full Z-Mat
Apply Changes to current Z-Mat
Cancel Non-Applied Changes
Delete Line
Add Line
Substitute atom by Fragment
New Z-mat
MapXYZ/Optimise
Set Status All Variables
New Z-mat from screen coordinates:
Reorder Z-matrix
Select by cursor
DeSelect
Apply Selection
Molden Control
Select Point:
First
Next
Movie
Render Forces:
Forces
Incr. Scale
Decr. Scale
THR
ILE
VAL
MET
ASP
ASN
PRO
ARG
HIS
PHE
TYR
TRP
PHI
-58.000
PSI
-47.000
Read
Close
Label
BackBone
In
Out
Status line:
Last point



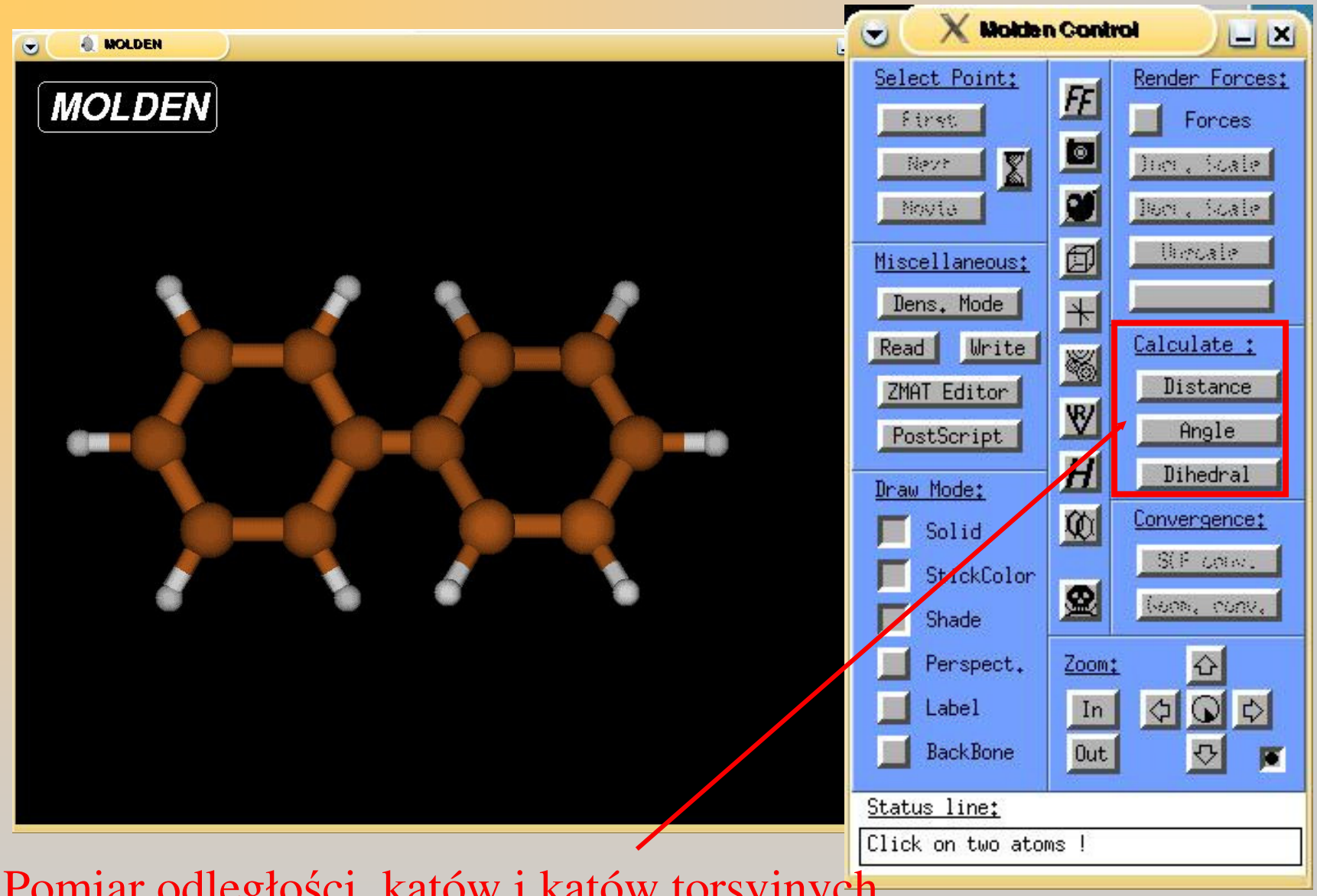
Zapis macierzy Z w pliku (format MOPACa)



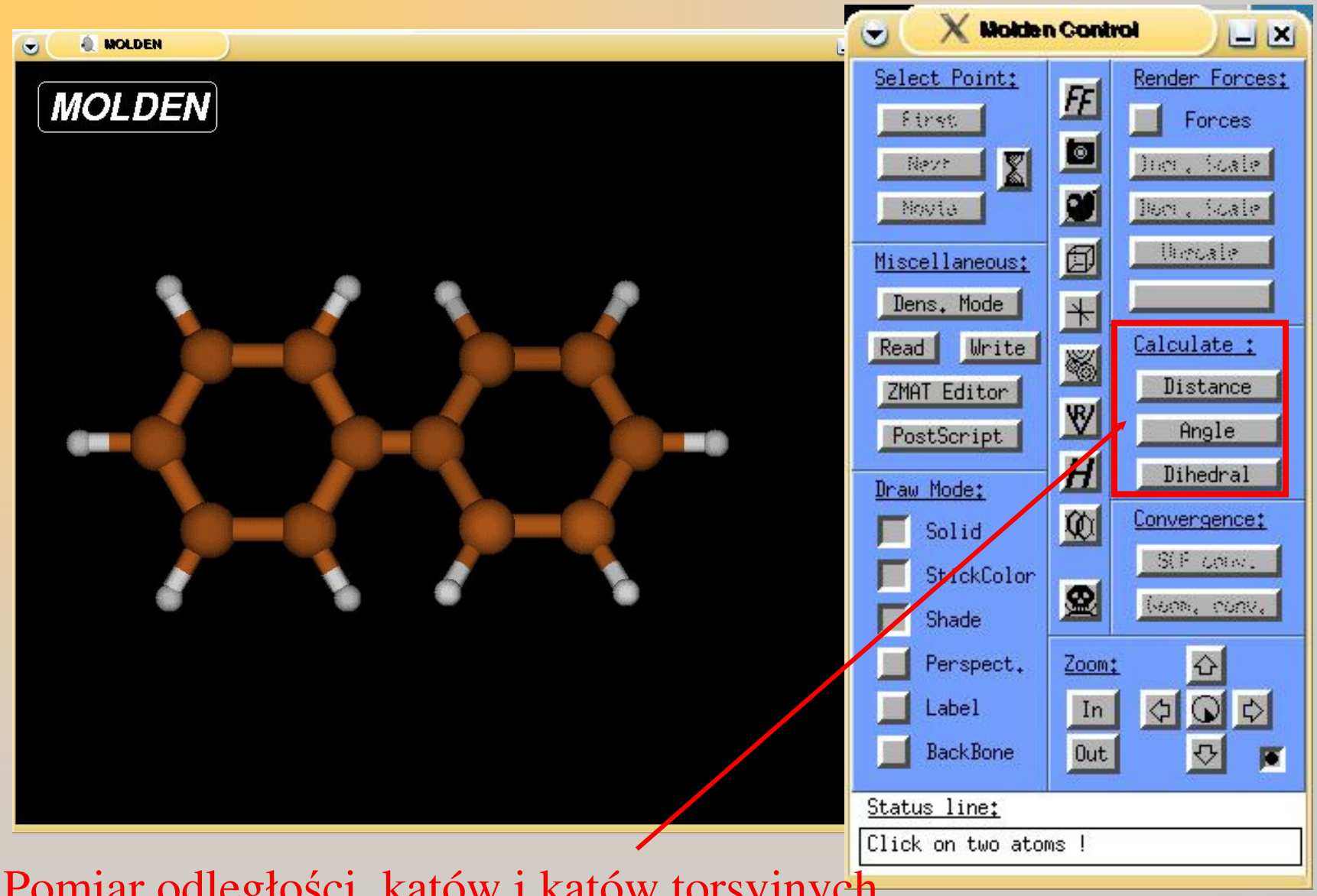
Zapis rysunku w pliku (postscript)



Atomy wodoru nie wyświetlane

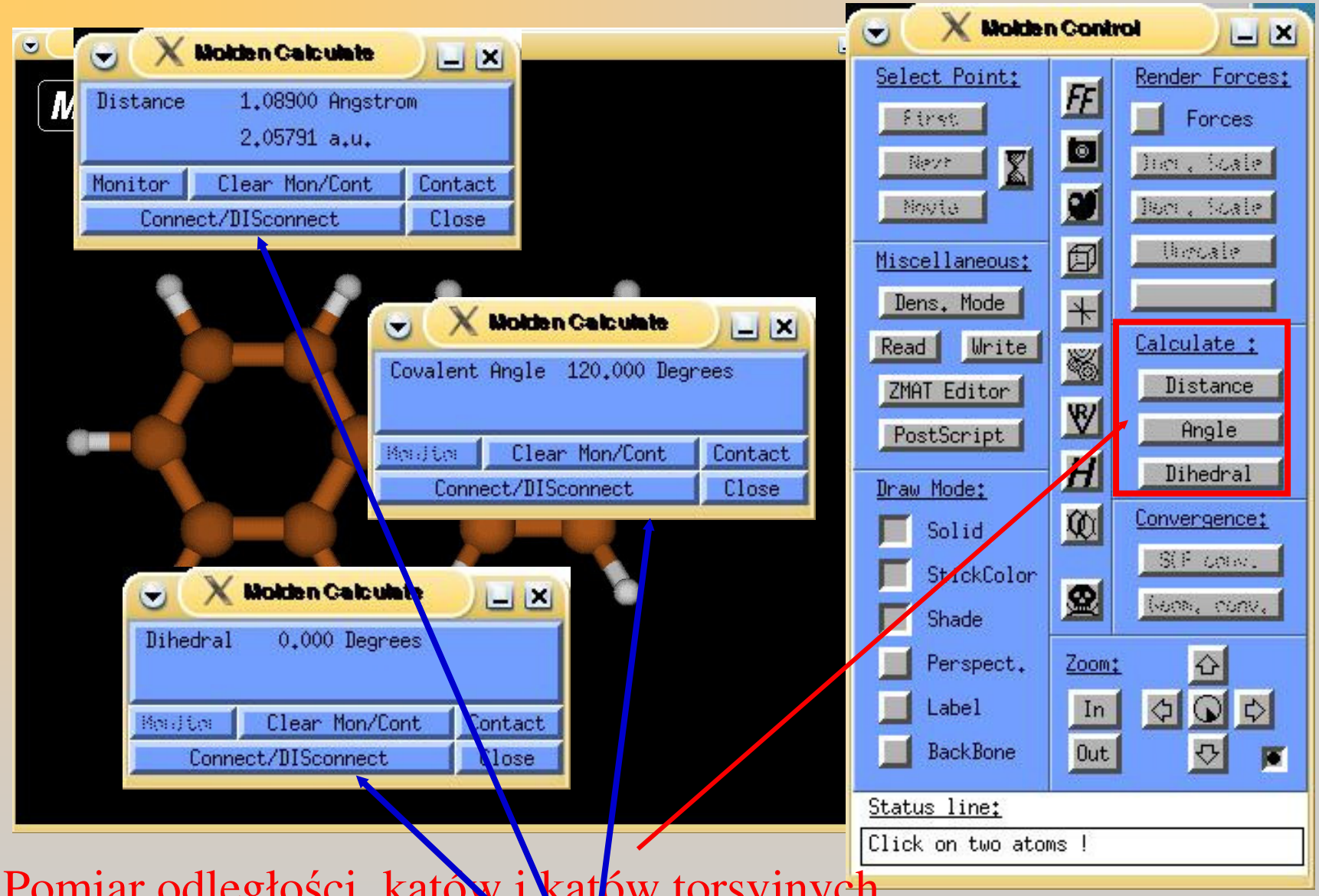


Pomiar odległości, kątów i kątów torsyjnych



Pomiar odległości, kątów i kątów torsyjnych

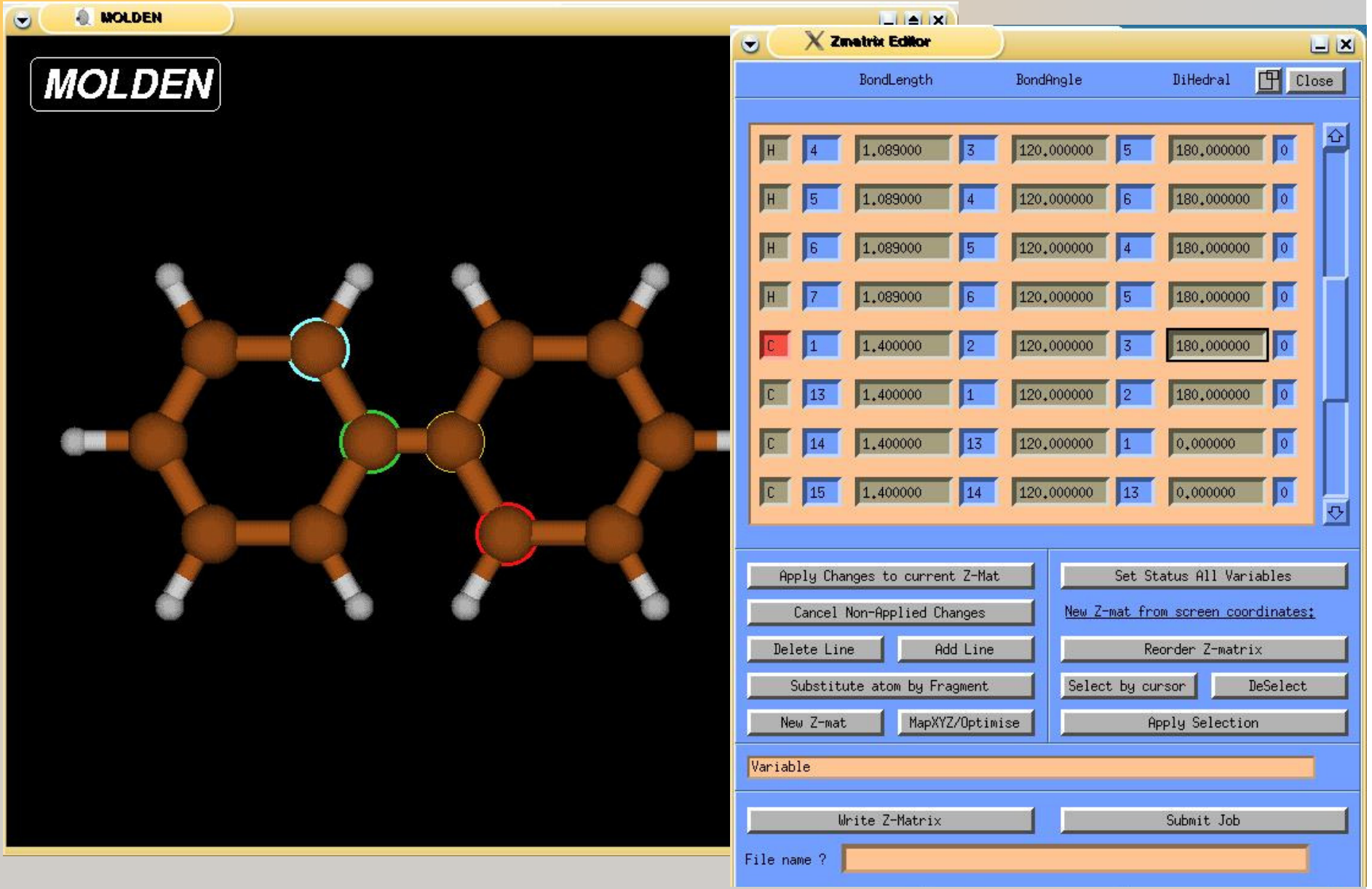
Po wybraniu odpowiedniego przycisku należy wskazać odpowiednio dwa, trzy lub cztery atomy (kliknając)



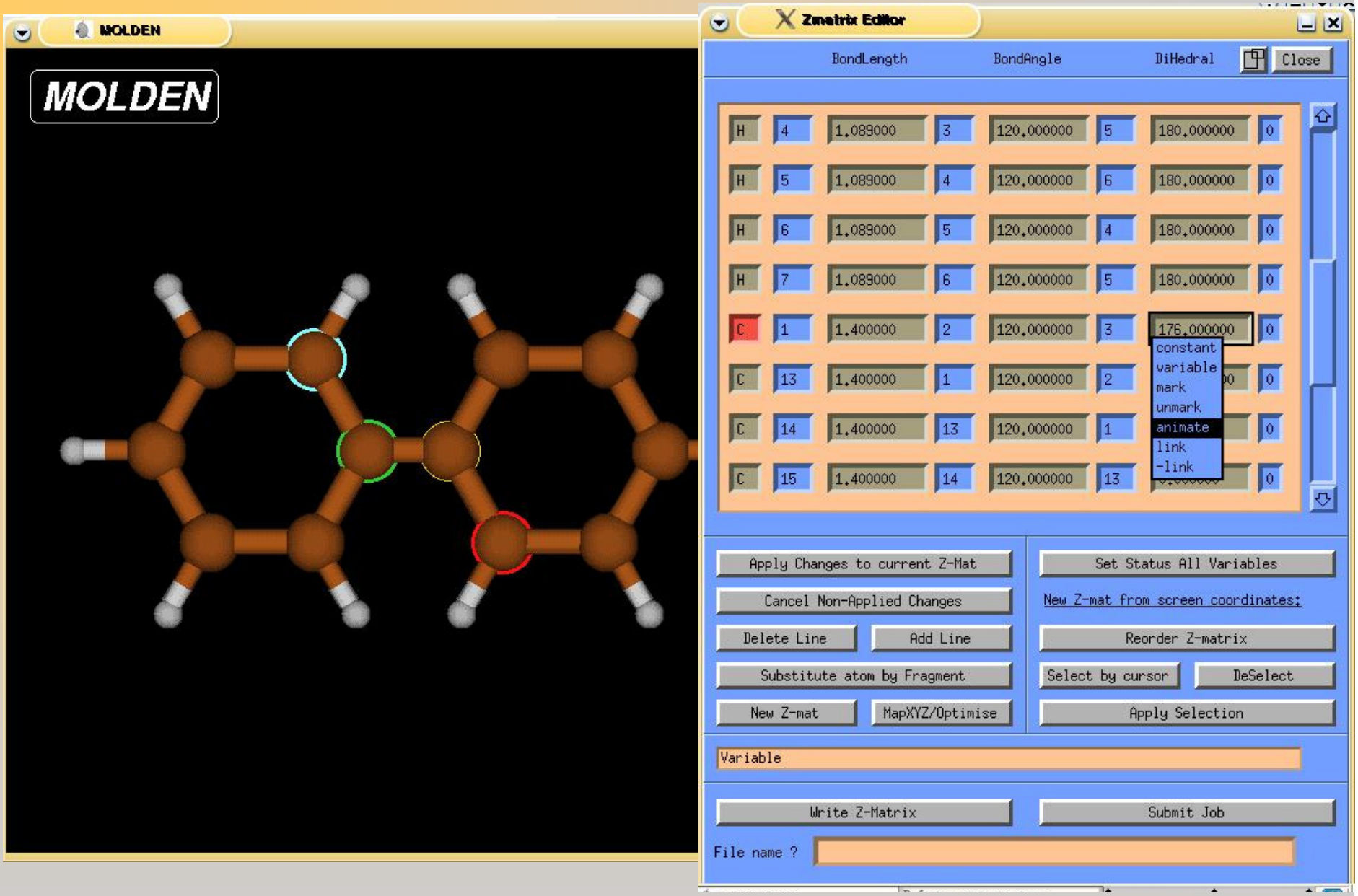
Pomiar odległości, kątów i kątów torsyjnych

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

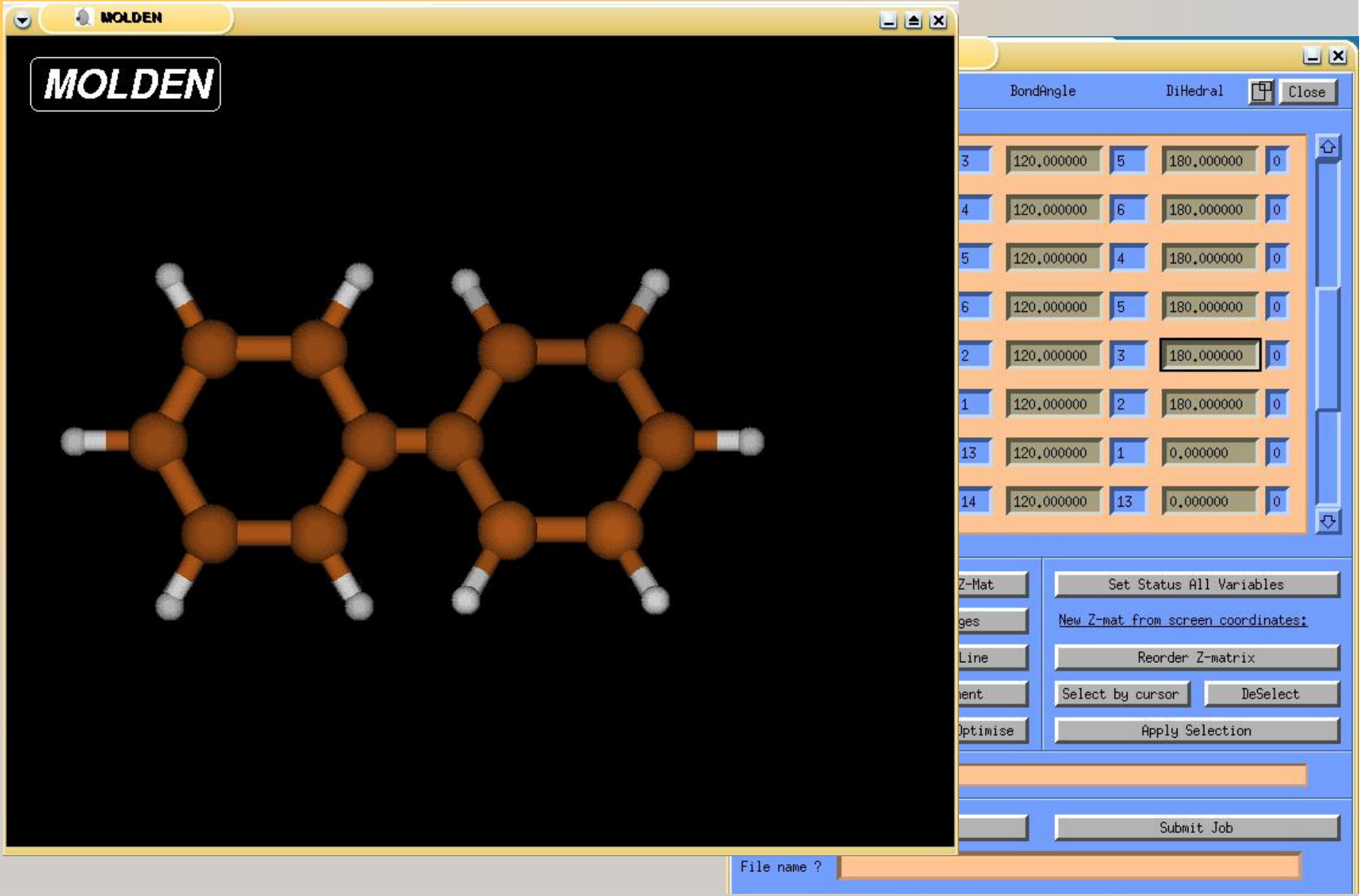
Pojawi się jedno z trzech okienek widocznych powyżej



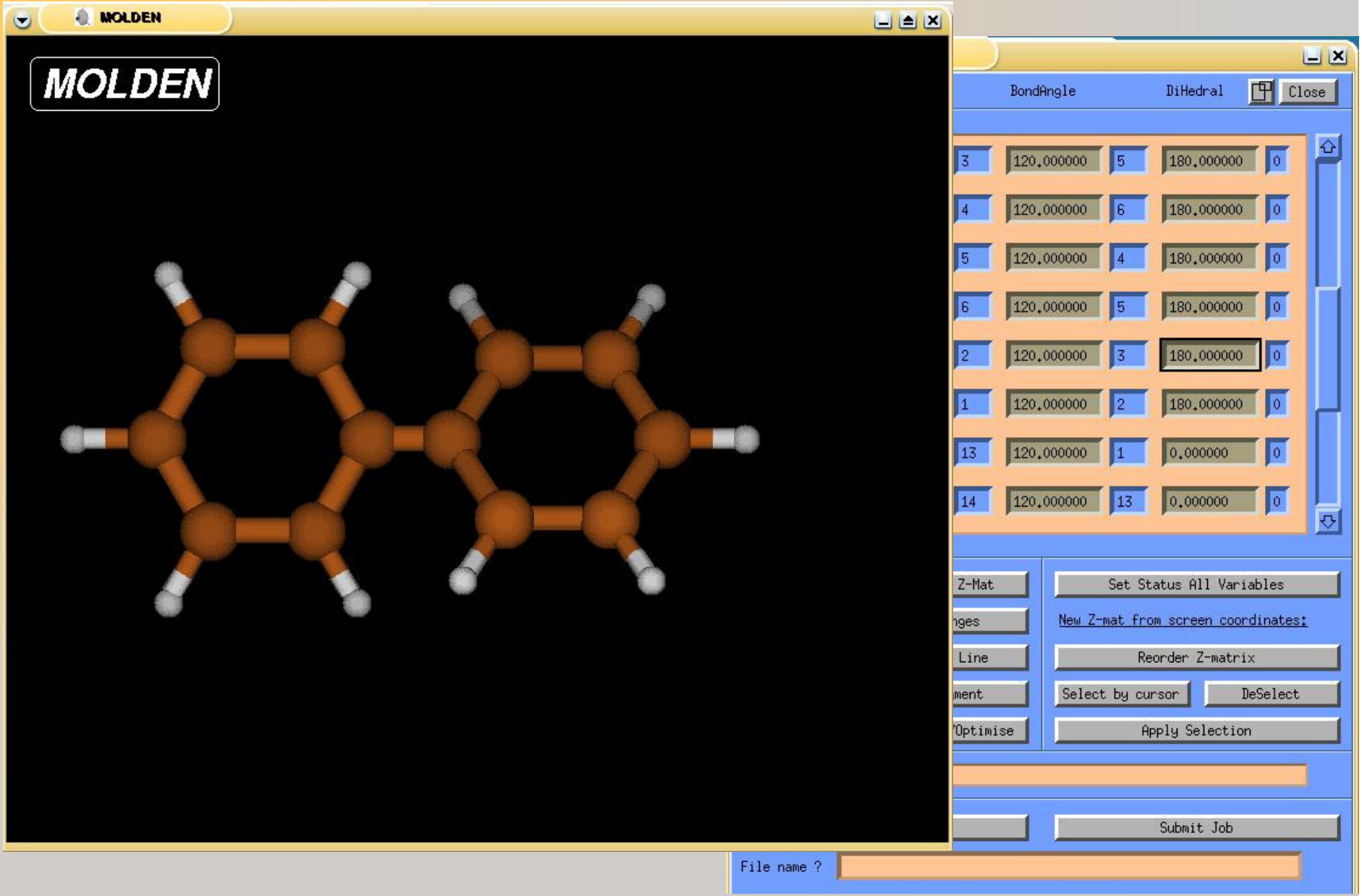
Zaznaczenie kątą w *edytorze macierzy Z* powoduje zaznaczenie atomów definiujacych kąt



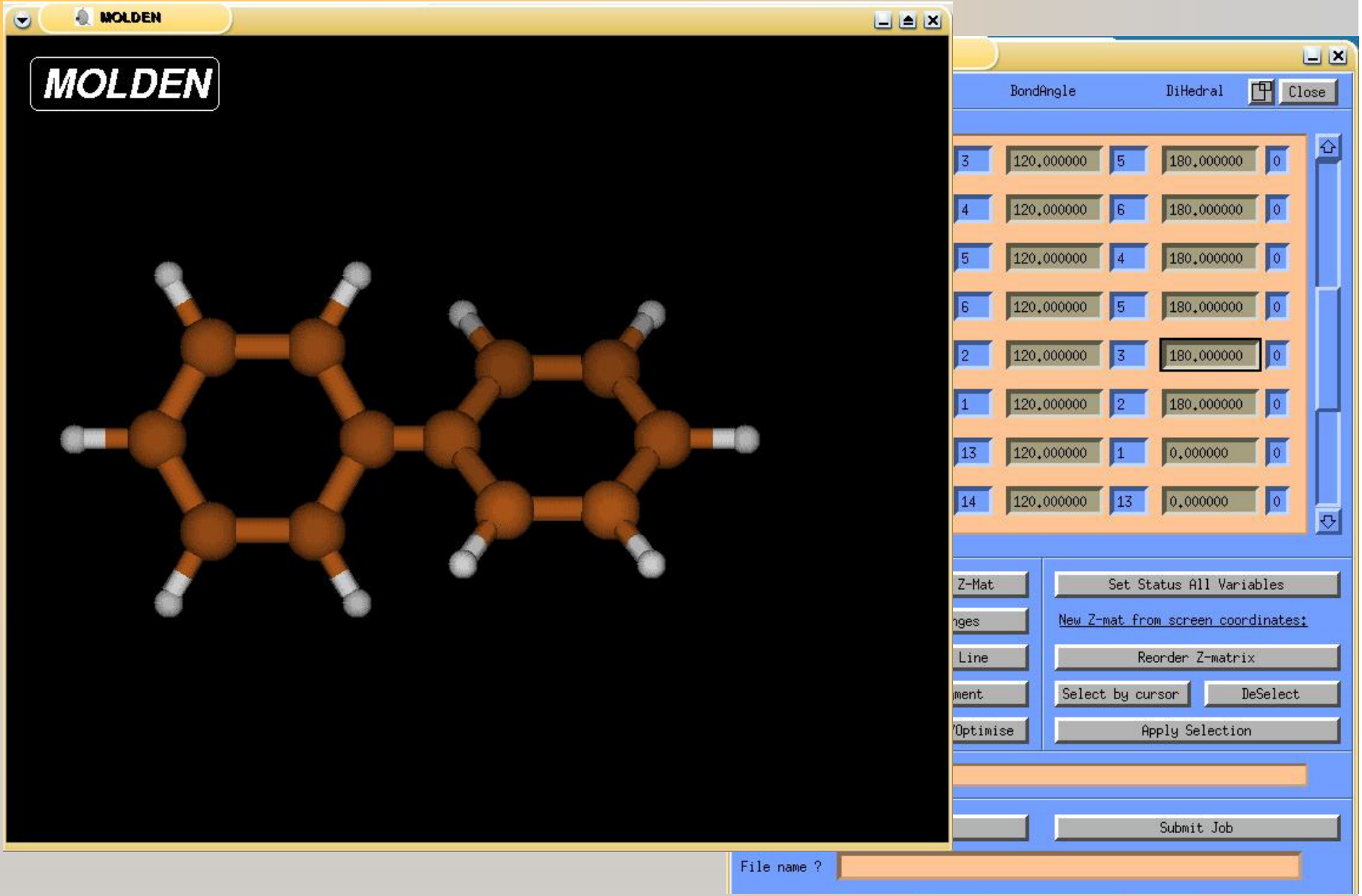
Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.



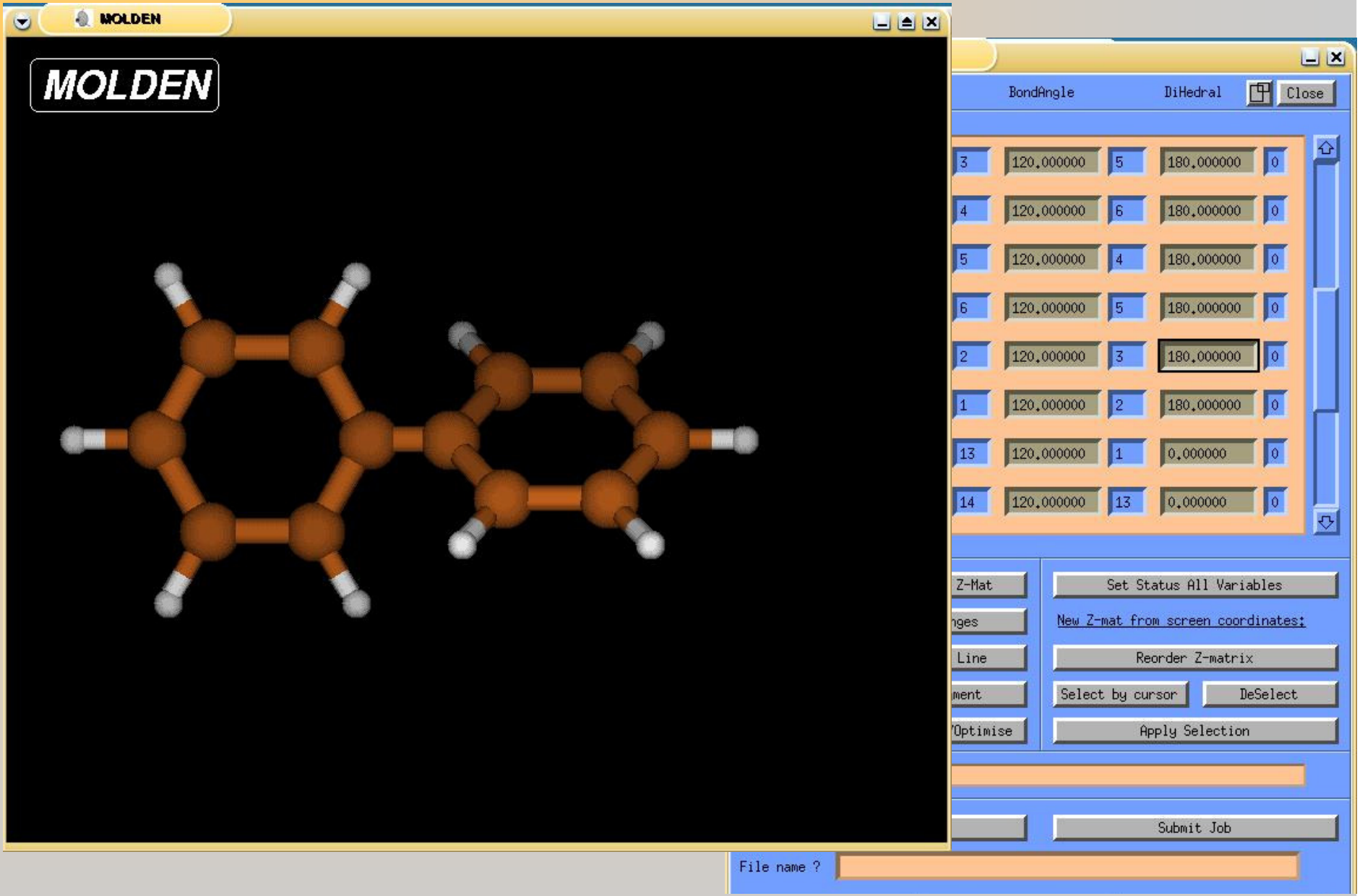
Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.



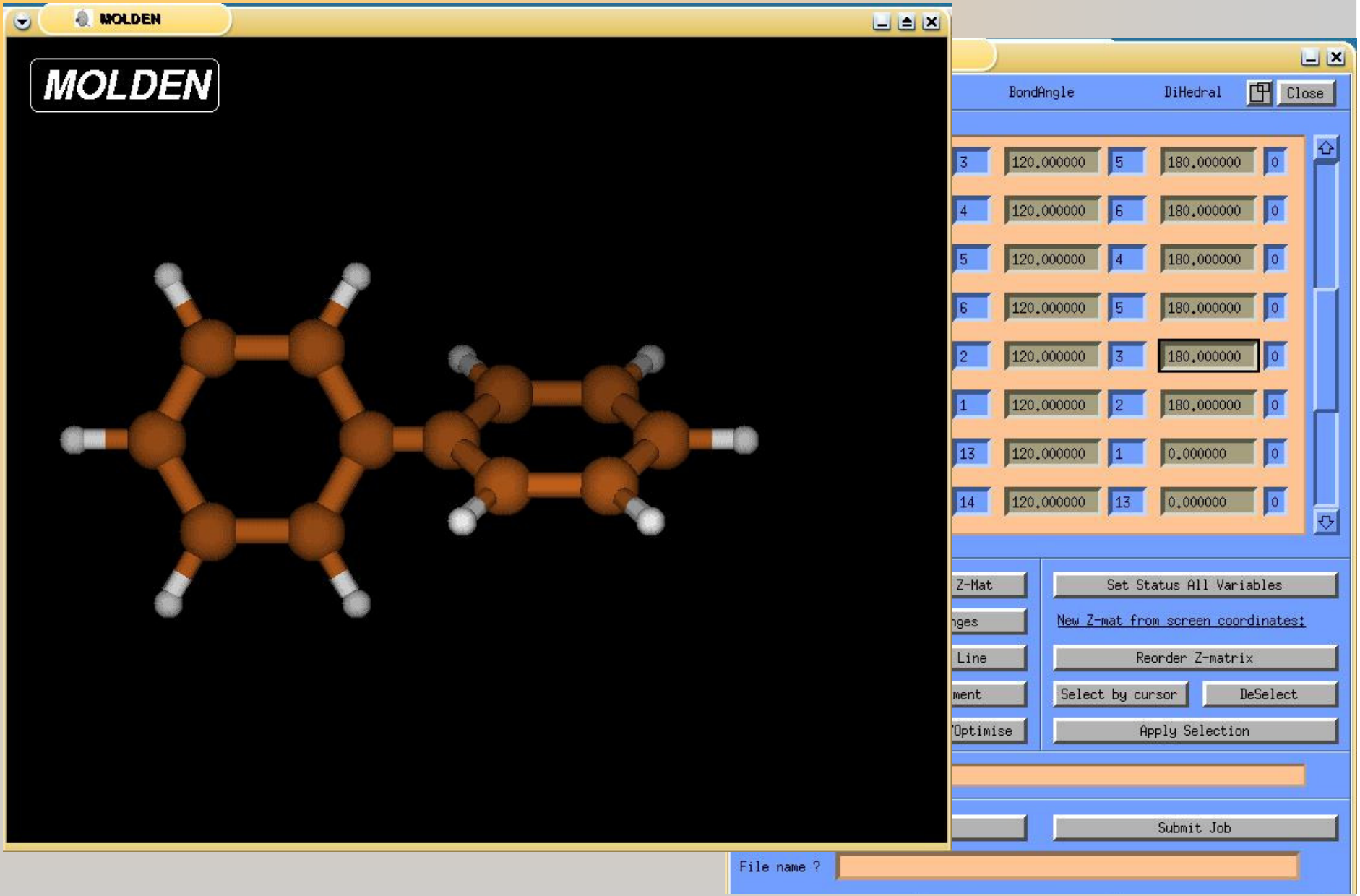
Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.



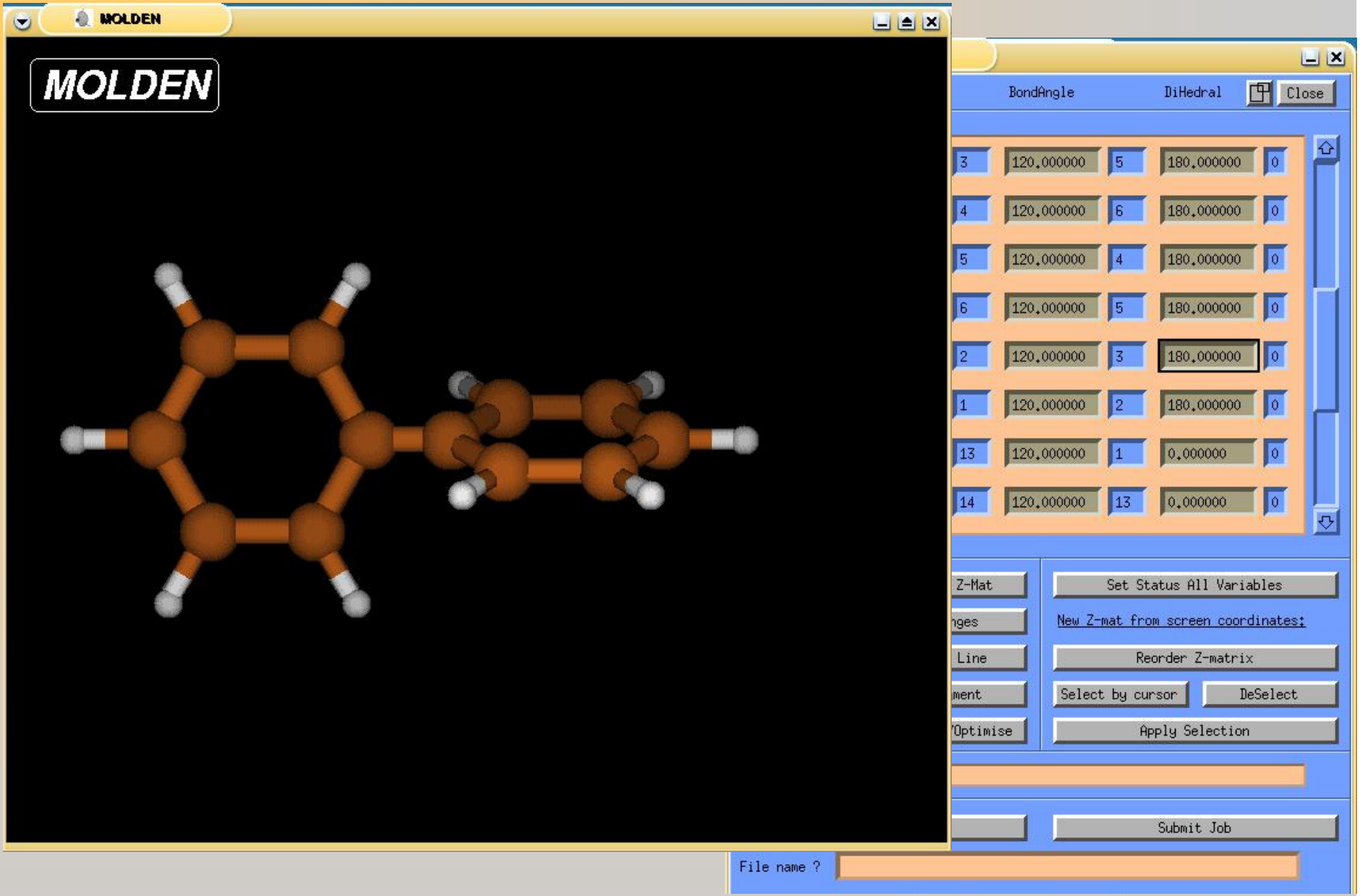
Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.



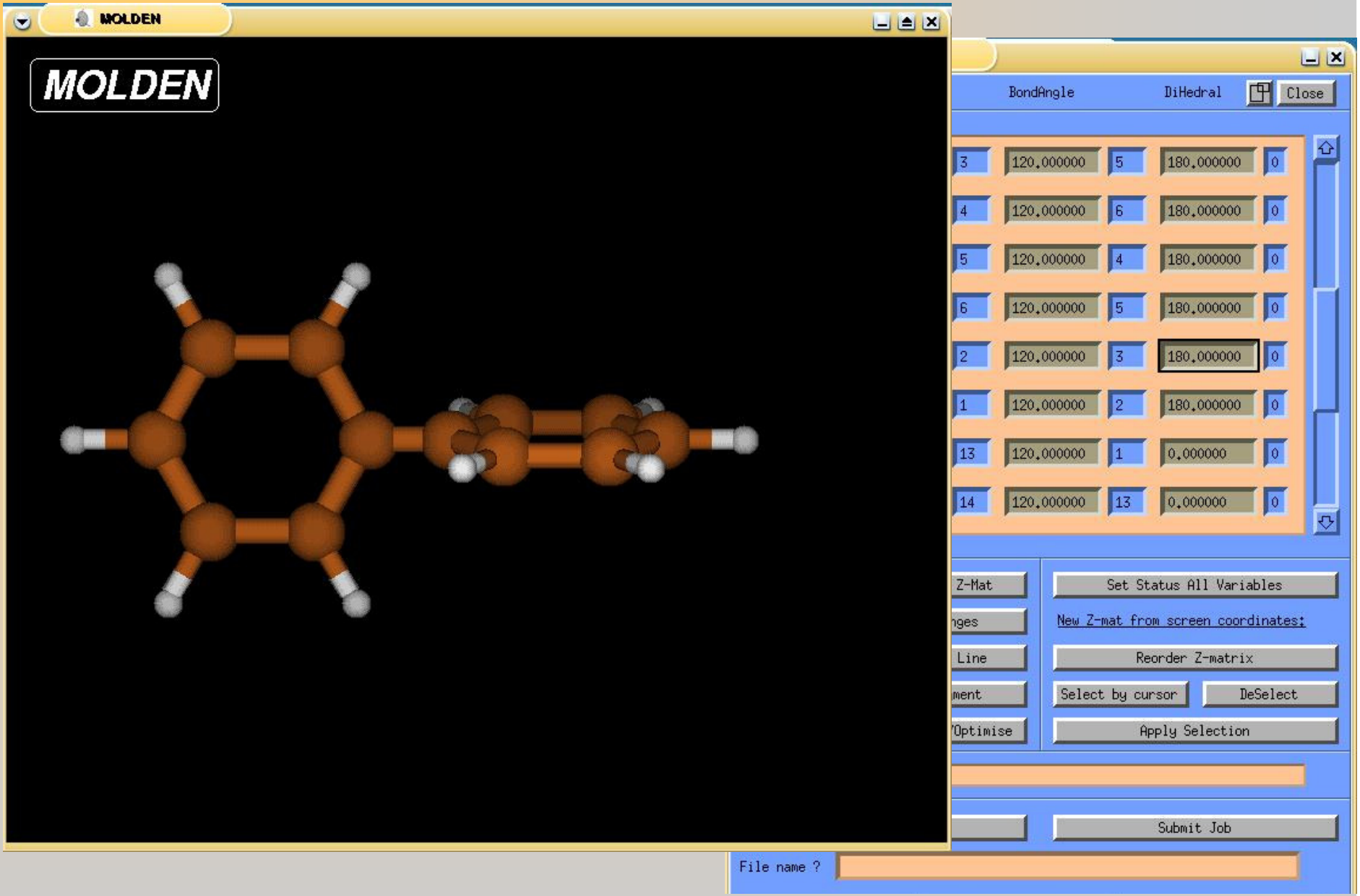
Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.



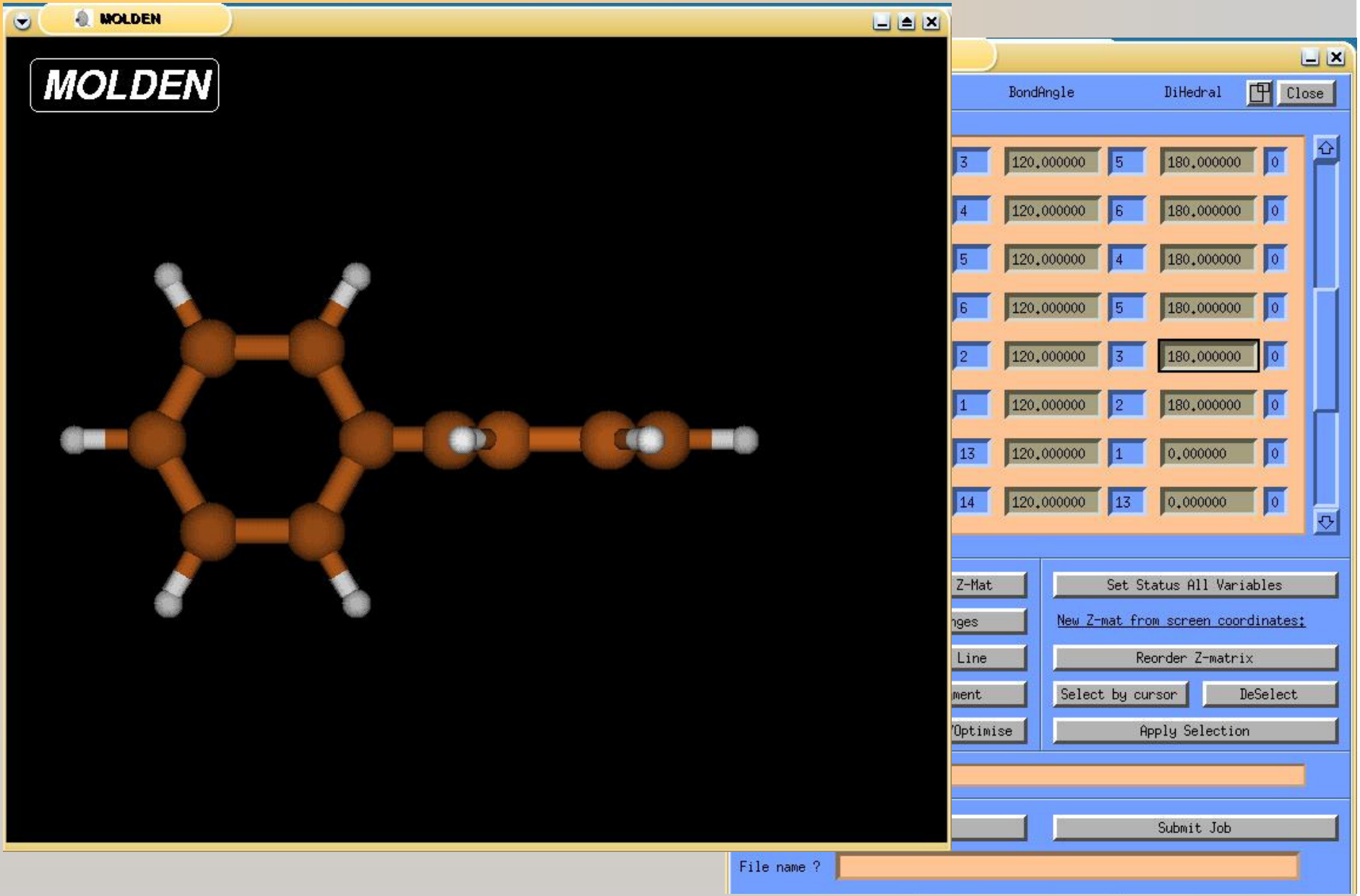
Opcja *animate* uruchamia animację ilustrującą zmiany geometrii wraz ze zmianą wybranego kąta.



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



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



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

cdn