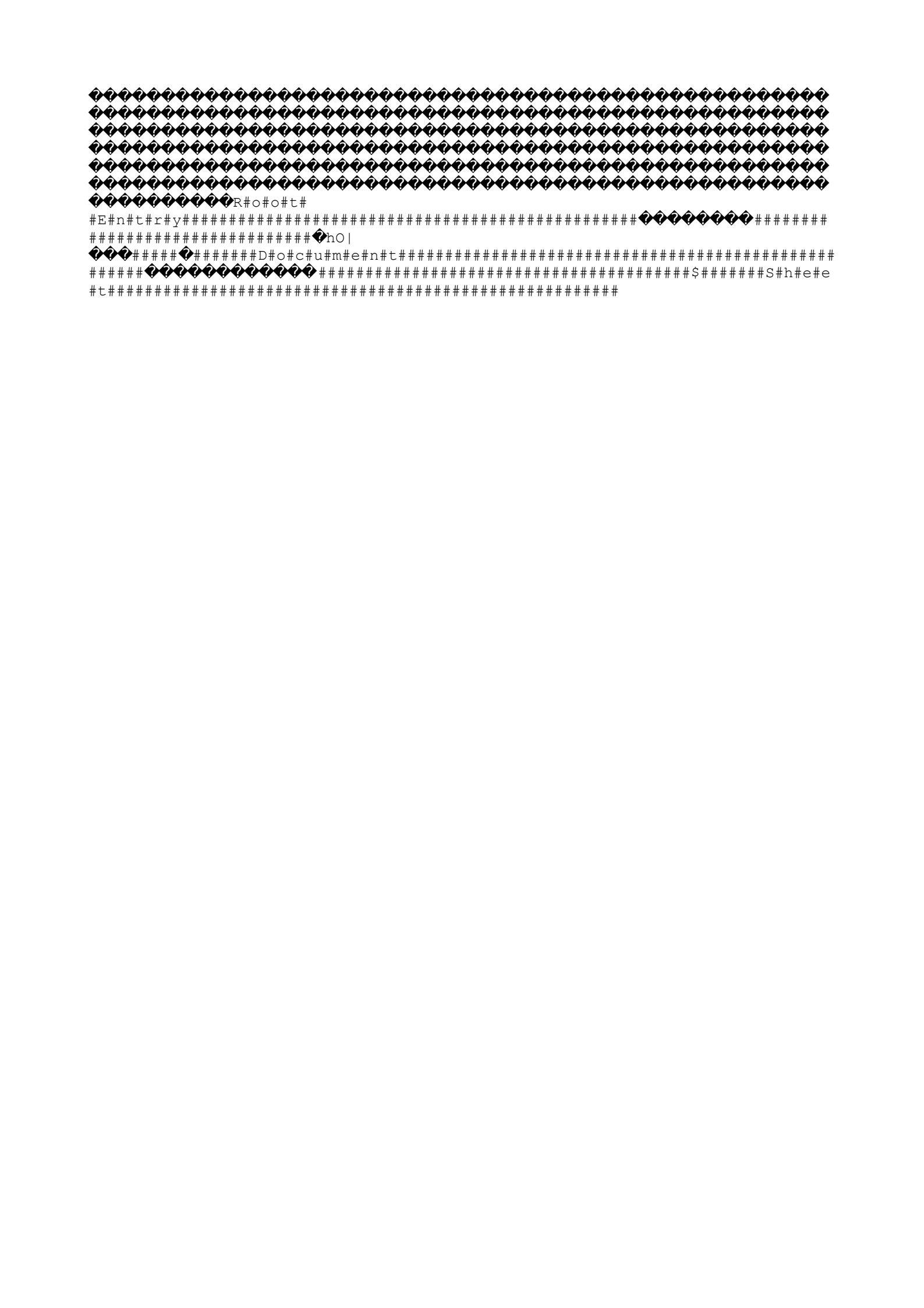
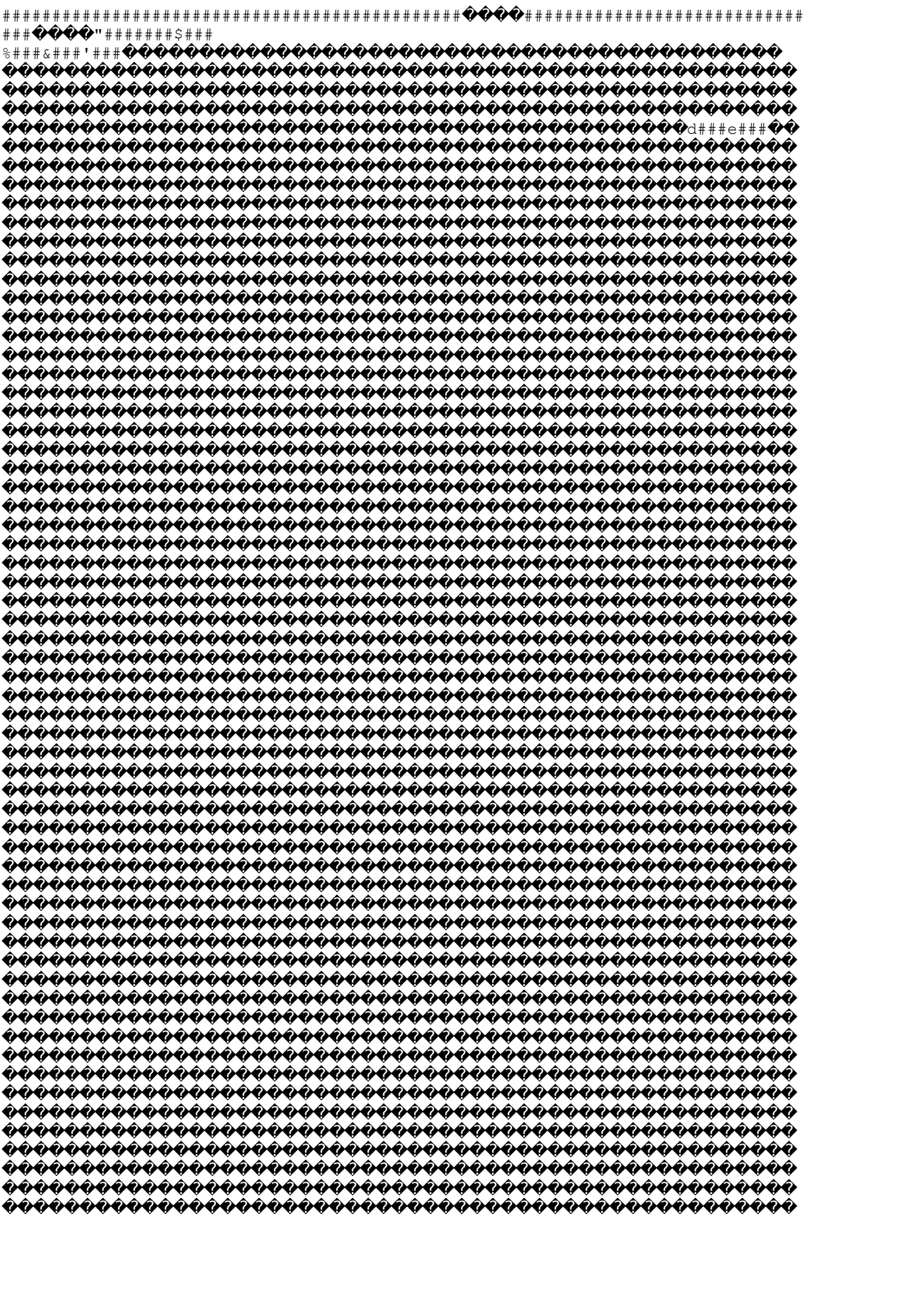


#############################y#J####h0|
####S#h#e#e#t#D#a#t#a###
##M#o#l#e
#c#u#l#e#s###
################y#J####h0|
####M#0#0#0#1###
##

#############################y#J####h0|
####M#o#l#e#c#u#l#e###
##########
###C#o#m#m#a#n#d#s#######
###

###I#n#p#u#t#############
###

###G#e#o#m#e#t#r#y###
###C#a#l#c#u#l#a#t#i#o#n#s###
###J#o#b#L#o#g###



```
[illegible]
[illegible]
[illegible]
```

```
RunProperty
 OPT HF 3-21G(*)
EndStep
CopyArchiveToPreviousArchive
RunPruneArchive
 OPT HF 3-21G(*)
EndStep
# Molecule Mode: 'Pending' [3]

CopyArchiveToPre OPT HF 3-21G(*)
M0001
0 1
84  -0.048114261  -0.908848861   0.000000000
 9  -1.190442366  -2.425734656   0.000000000
17   2.049310823  -1.887379009  -0.000000000
35   1.589456647   1.087511296  -0.000000000
53  -1.704250529   1.217498937  -0.000000000
ENDCART
ATOMLABELS
"Po1"
"F1"
"Cl1"
"Br1"
"I1"
ENDATOMLABELS
HESSIAN
   -4   16   15   14   17
    1    2    1
    1    3    1
    1    4    1
    1    5    1
ENDHESS
BEGINPROPIN
ENDPROPIN
BEGINPREFERENCES
 MM:CONF_SELECTION_RULE=2
ENDPREFERENCES
   1    4    1
    1    5    1
ENDHESS
BEGINPR[illegible]H[illegible]
```

Ph##`#P##  ####M0001########2###Po1#####T#########sn####n#5J#X6p#w9#
##1###F1##### #########m?<K

```
UD  g#  #:,9###2###Cl1###############H #d#@V#I2   ~uQW.###2#
##Br1#######O#######p#jn?#:>rf?
2R#   ###1###I1#####5#  #######5#3D?h*z?`*<{
######Bond4#################  ######Bond2#################
######Bond1#################  ######Bond7#################E
######Bond4#################  ##########  OPT HF 3-21G(*)
##########  ##########Bond7###################V##@##############?
###1###C2#######
```

 #########"###OPT HF 3-21G(*) ################Lx?
VYWSPARTAN STUDENT MECHANICS PROGRAM: PC/x86 131

Frequency Calculation

Adjusted 4 (out of 15) low frequency modes

Reason for exit: Successful completion
Mechanics CPU Time : .22
Mechanics Wall Time: .61
SPARTAN STUDENT Quantum Mechanics Program: (PC/x86) Release 131jv4

Job type: Geometry optimization.
Method: RHF
Basis set: 3-21G(*)
Number of shells: 27
Number of basis functions: 105
Multiplicity: 1

SCF model:
A restricted Hartree-Fock SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Optimization:

Step	Energy	Max Grad.	Max Dist.
1	-10041.504449	0.422632	0.200062
2	-10041.654302	0.263479	0.204056
3	-10041.746280	0.176288	0.233177
4	-10041.796240	0.123556	0.217135
5	-10041.834115	0.083216	0.189805
6	-10041.857724	0.058851	0.231229
7	-10041.874485	0.044648	0.211683
8	-10041.889393	0.032338	0.241651
9	-10041.902265	0.026997	0.164772
10	-10041.914040	0.032507	0.256651
11	-10041.924186	0.019293	0.225378
12	-10041.932396	0.019228	0.222777
13	-10041.938300	0.015778	0.214447
14	-10041.942309	0.015402	0.218411
15	-10041.945252	0.011528	0.197310
16	-10041.947440	0.008832	0.187985
17	-10041.948742	0.004623	0.066531
18	-10041.948905	0.001943	0.016293
19	-10041.948937	0.001527	0.046562
20	-10041.948999	0.001161	0.011763

Error Occured: Maximum optimization cycles reached
See verbose output for more information

Reason for exit: Maximum optimization cycles reached
Quantum Calculation CPU Time : 4:31.03
Quantum Calculation Wall Time: 4:40.21
###################### Spartan Properties Archive 117

PROP STRING INITIAL_KEYWORDS 3 BEGIN
"OPT"
"HF"
"3-21G(*)"

```
END
PROP STRING CALCULATION_VERSION = " 131j_ST"
PROP STRING CALCULATION_TARGET = "PC/x86"
PROP STRING CALCULATION_CPUTARGET = "P2"
PROP STRING INTERNAL_BUILD_DATE = "Mar 27 2009"
PROP STRING CALC_MACHINEHOSTNAME = "STO15523"
PROP STRING CALC_START_TIMESTAMP = "Wed May 05 18:07:44 2010"
PROP STRING CALC_START_TIMESTAMP2 = "2010-05-05 18:07:44.452"
PROP STRING CALCULATION_EXE_PATH = "C:\PROGRAM
FILES\WAVEFUNCTION\SPARTANSTV412\P2"
PROP STRING CALCULATION_EXE_TIME = "2009-09-02 16:45"
PROP VALUE:STATIC ORIGINAL_ATOM_COUNT =       5.000000000
PROP VALUE:BYATOM:STATIC ORIGINAL_COORDS 5  3 BEGIN
       0.00000000      0.00000000    1.0000000000   -1.3830000000
0.00000000    1.0000000000
       0.00000000      0.00000000    2.7720000000    2.1320000000
0.00000000    1.0000000000
       0.00000000      0.00000000   -0.5310000000
END
################################################y######Normal exit.#No
Message Returned  #C:\PROGRAM
FILES\WAVEFUNCTION\SPARTANSTV412\P2\WFStrt.exe#M0001##}###.#######{######Norm
al exit.#Successful completion  #C:\PROGRAM
FILES\WAVEFUNCTION\SPARTANSTV412\P2\WFMech.exe#M0001#############################Ab
normal exit.#Maximum optimization cycles reached  #C:\PROGRAM
FILES\WAVEFUNCTION\SPARTANSTV412\P2\WFQM.exe#M0001##F############################A
bnormal exit.#Maximum optimization cycles reached  #C:\PROGRAM
FILES\WAVEFUNCTION\SPARTANSTV412\P2\WFQM.exe#M0001##F##########################
################################################################################
################################################################################
################################################################
```