

Gaussian 03 input file (named something.com)

#N HF/3-21G OPT

HCl

0 1

Cl

H 1 B1

B1 1.6000000

Highlights from output file

Search for a local minimum.

Step number 1 out of a maximum of 20

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Second derivative matrix not updated -- first step.

The second derivative matrix:

```
          R1
          R1          0.13133
Eigenvalues --- 0.13133
```

RFO step: Lambda=-3.76445364D-02.

Linear search not attempted -- first point.

Maximum step size (0.300) exceeded in Quadratic search.

-- Step size scaled by 0.636

Iteration 1 RMS(Cart)= 0.14142136 RMS(Int)= 0.10000000

Iteration 2 RMS(Cart)= 0.07071068 RMS(Int)= 0.00000000

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000000

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	3.02356	-0.07975	0.00000	-0.30000	-0.30000	2.72356

Item	Value	Threshold	Converged?
Maximum Force	0.079755	0.000450	NO
RMS Force	0.079755	0.000300	NO
Maximum Displacement	0.150000	0.001800	NO
RMS Displacement	0.212132	0.001200	NO

Predicted change in Energy=-1.801673D-02

Search for a local minimum.

Step number 2 out of a maximum of 20

[deleted some lines]

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.72356	-0.05590	-0.31556	0.00000	-0.31556	2.40800
Item		Value	Threshold	Converged?		
Maximum Force		0.055903	0.000450	NO		
RMS Force		0.055903	0.000300	NO		
Maximum Displacement		0.157779	0.001800	NO		
RMS Displacement		0.223133	0.001200	NO		

Predicted change in Energy=-1.368229D-02

[Skipped Step Number 3]

Search for a local minimum.

Step number 4 out of a maximum of 20

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Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.44507	-0.00022	-0.00073	0.00000	-0.00073	2.44434
Item		Value	Threshold	Converged?		
Maximum Force		0.000219	0.000450	YES		
RMS Force		0.000219	0.000300	YES		
Maximum Displacement		0.000364	0.001800	YES		
RMS Displacement		0.000514	0.001200	YES		

Predicted change in Energy=-7.488106D-08

Optimization completed.

-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.2939	-DE/DX = -0.0002	!
