

Supporting information

to

A theoretical study of hydrogen abstraction reactions in guanosine and uridine

by

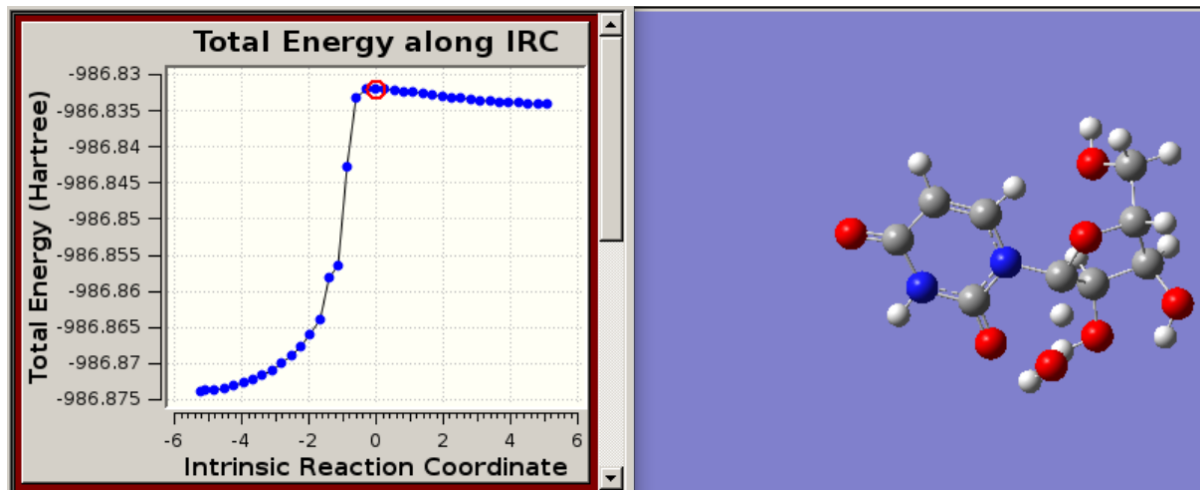
Kasper Frølund Schaltz and Stephan P. A. Sauer

Department of Chemistry, University of Copenhagen, DK-2100 Copenhagen Ø,
Denmark

Intrinsic Reaction Coordinate plots – Uridine

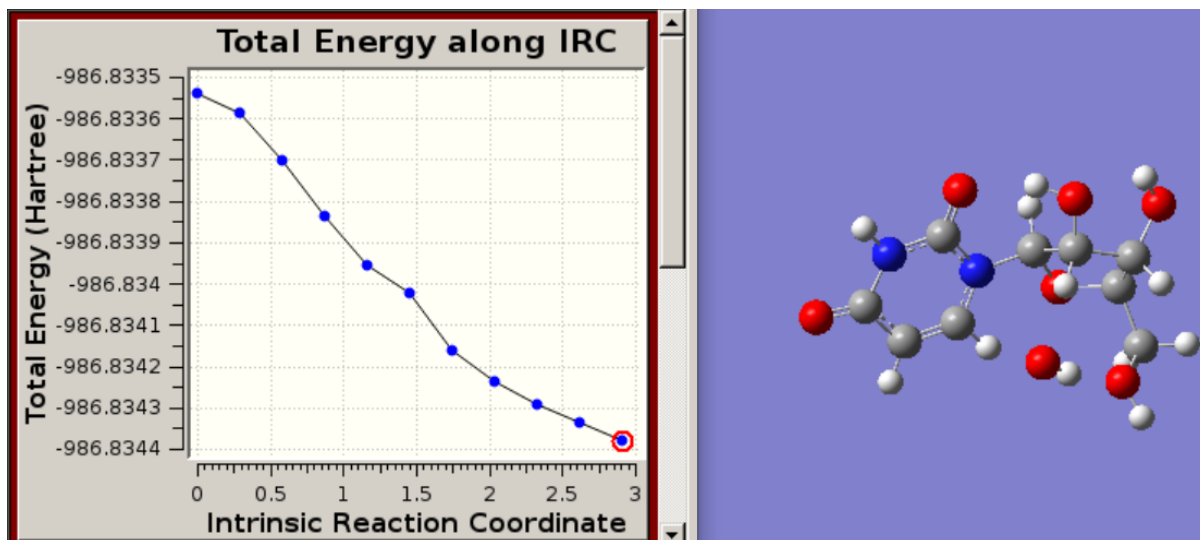
C1

Forward and reverse:

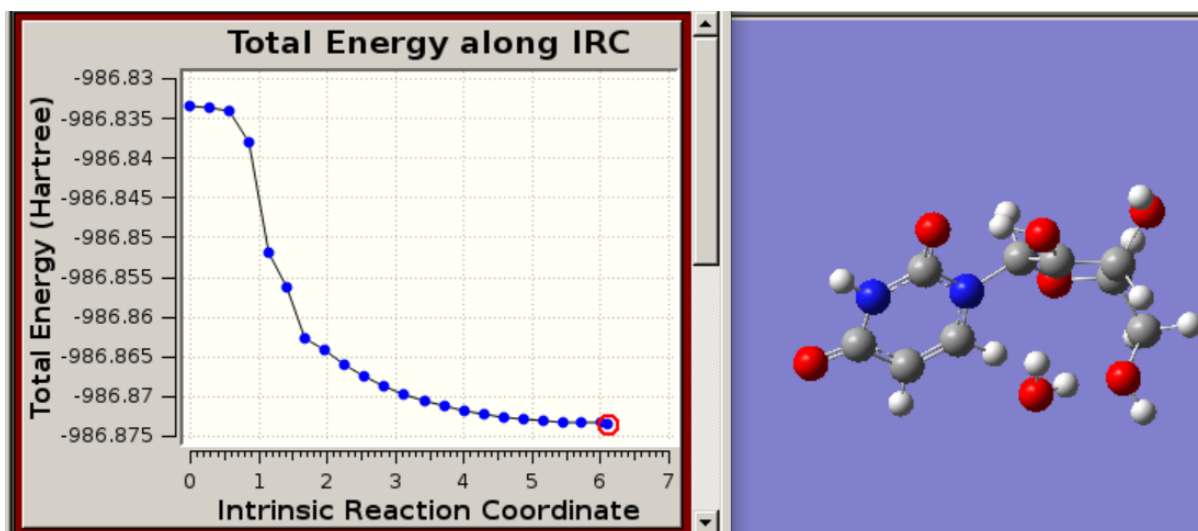


C2

Reverse:

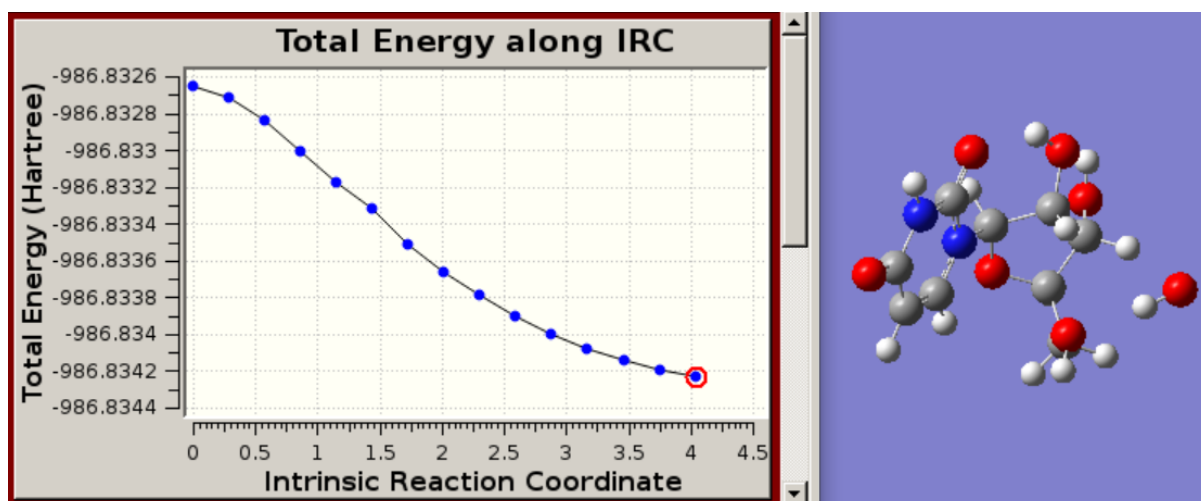


Forward:

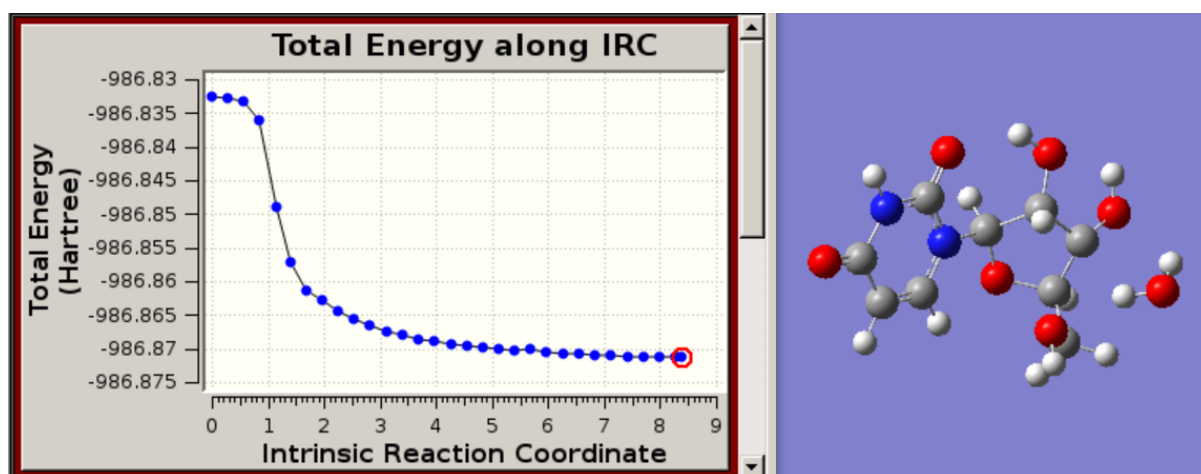


C3

Reverse:

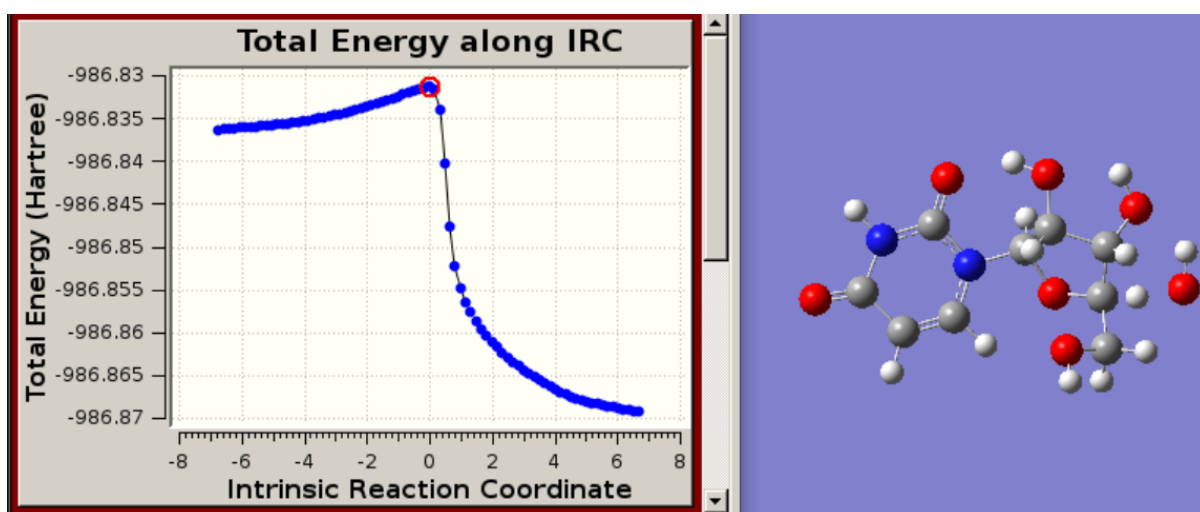


Forward:



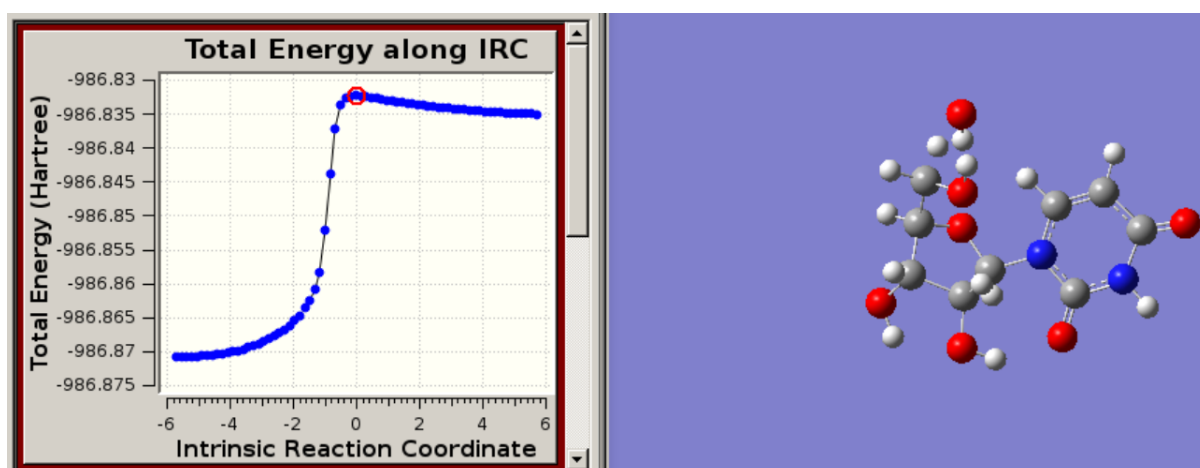
C4

Reverse and forward:



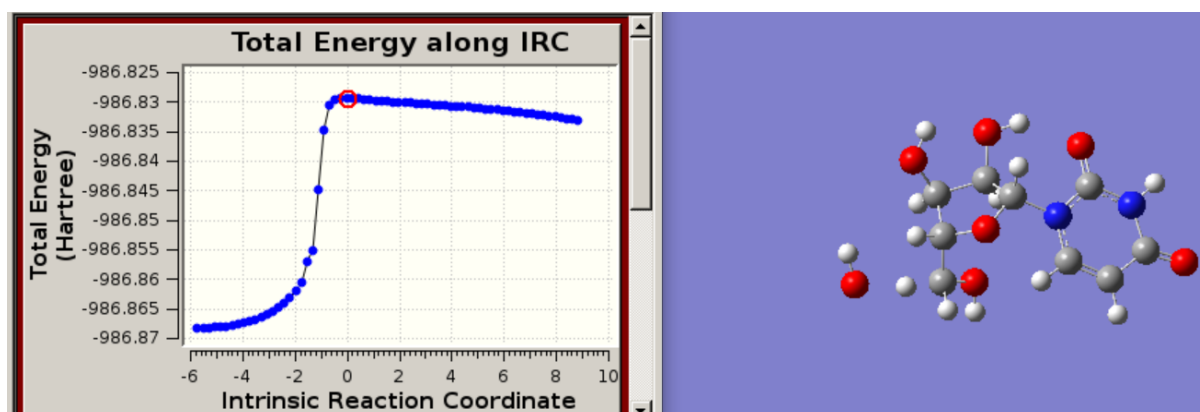
C5_HO

Forward and reverse:



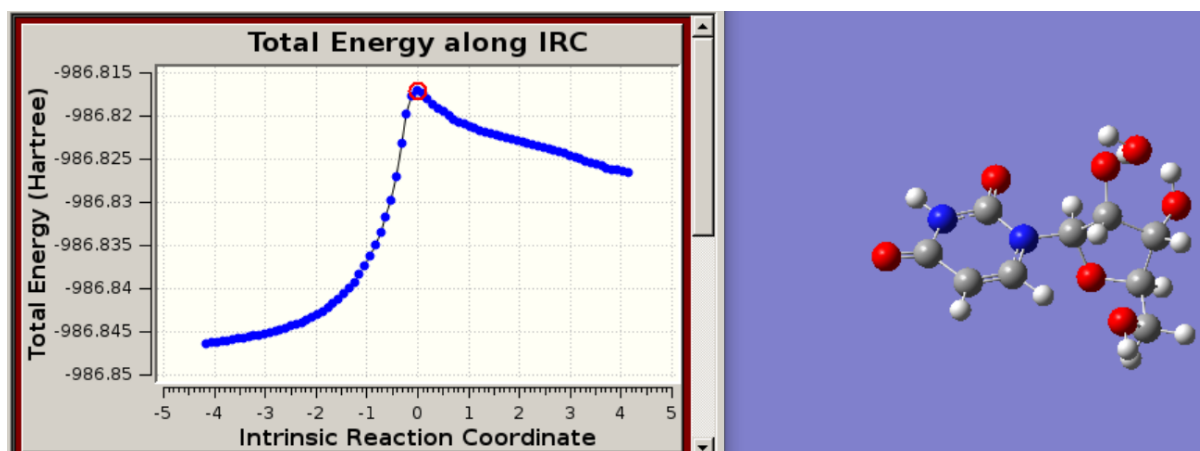
C5_HC

Forward and reverse



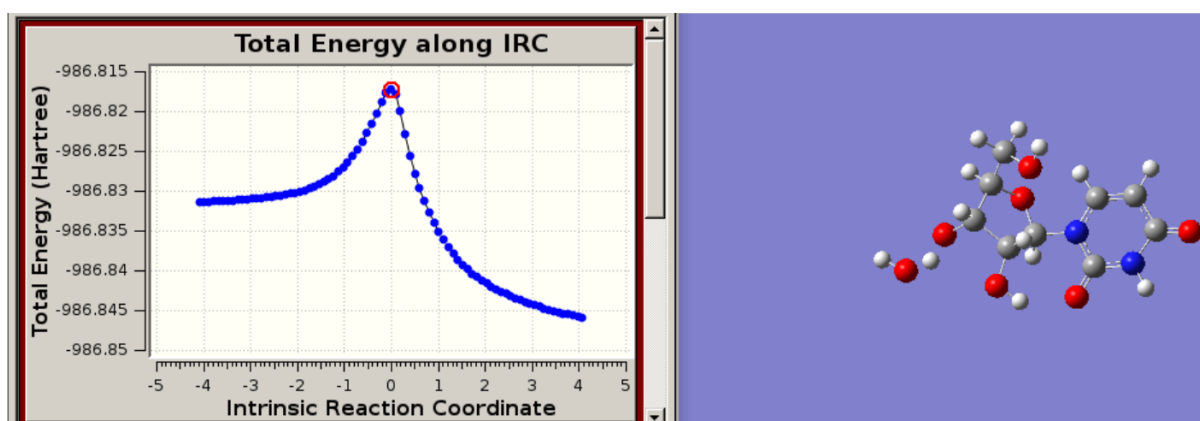
O2

Forward and reverse:



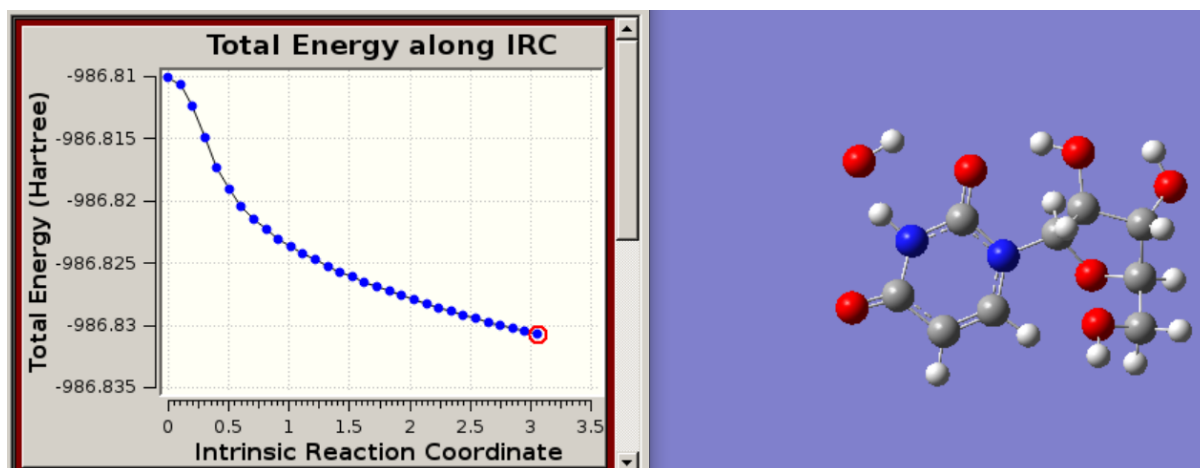
O3

Reverse and forward:

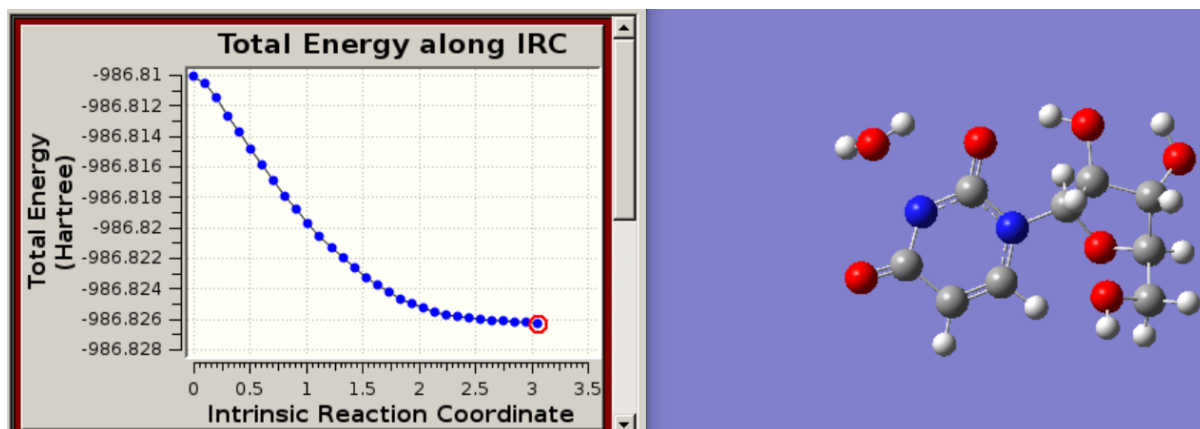


H3

Reverse:

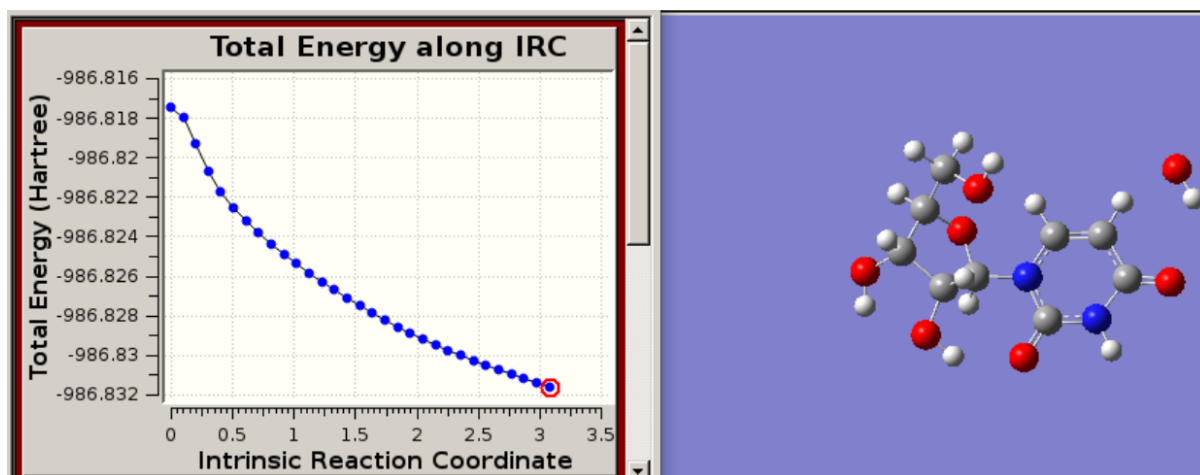


Forward:

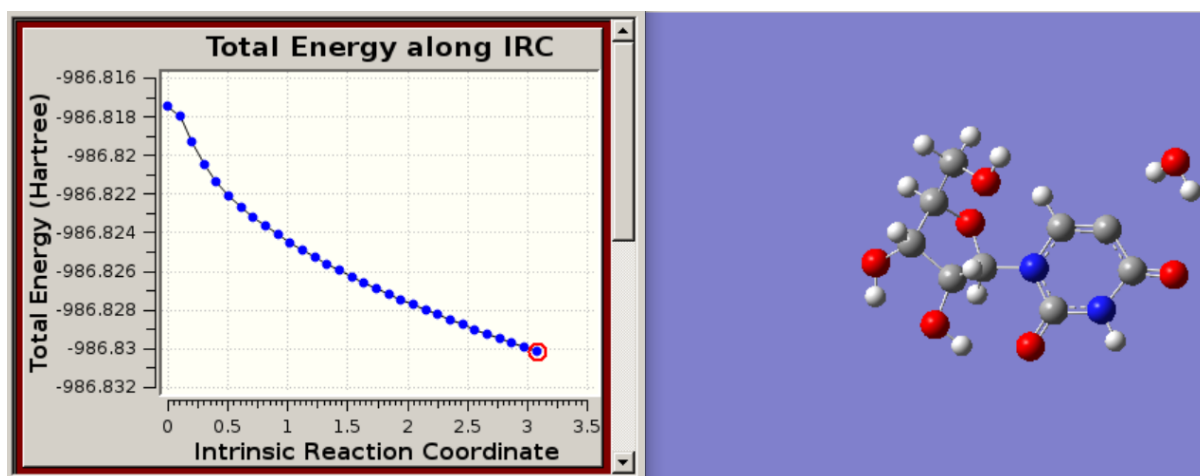


H5

Reverse:

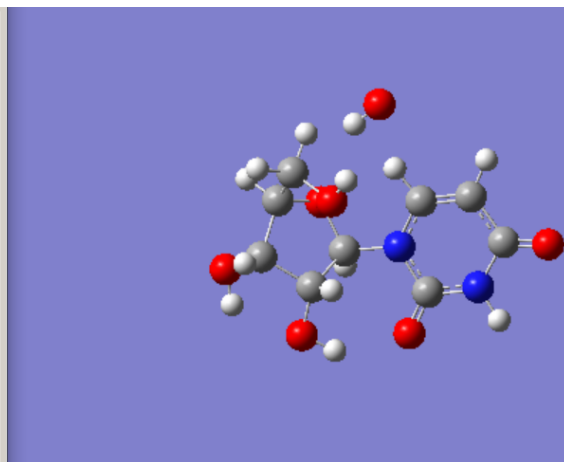
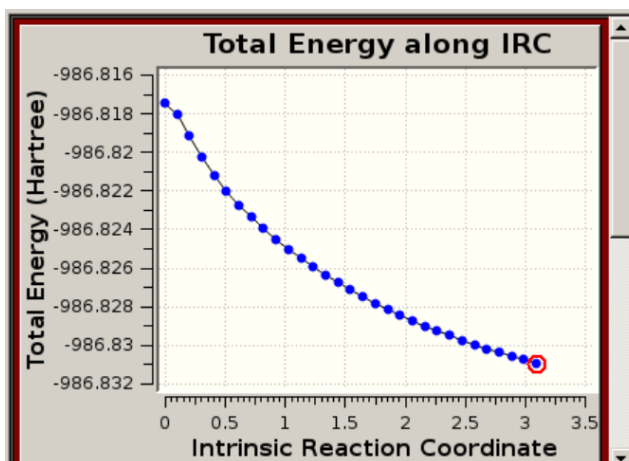


Forward:

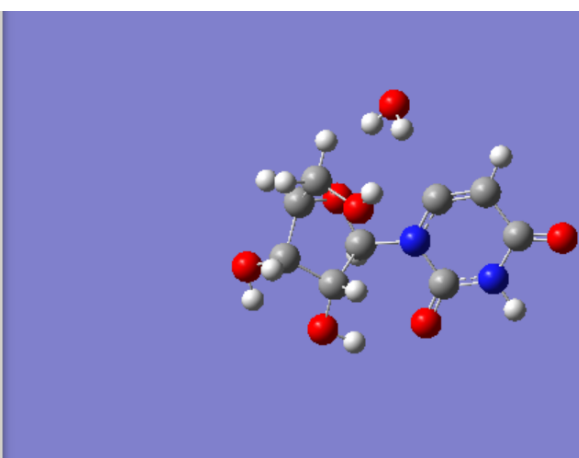
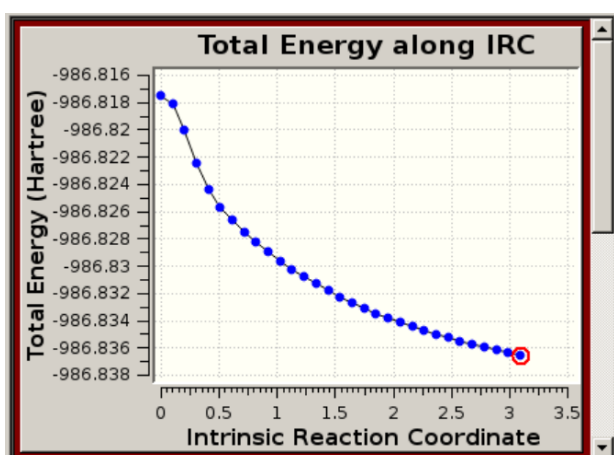


H6

Reverse:



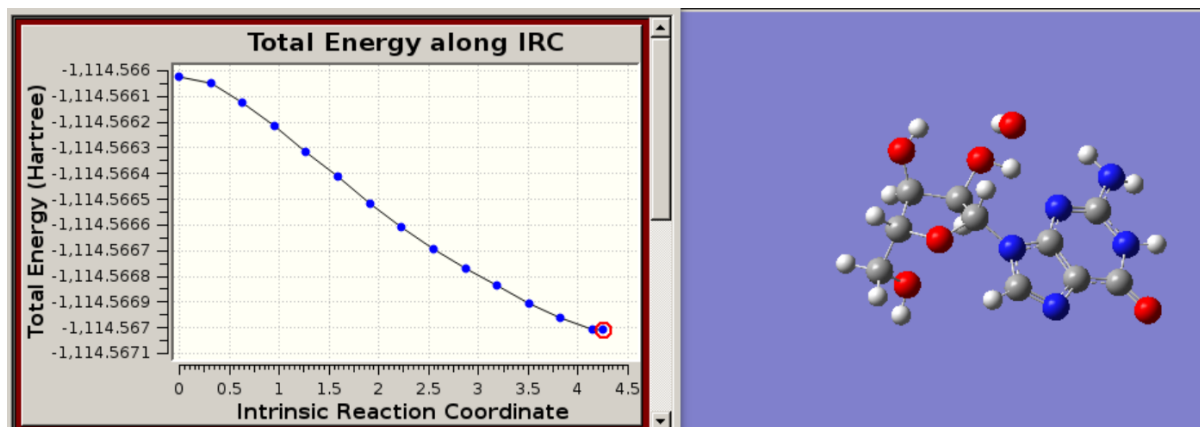
Forward:



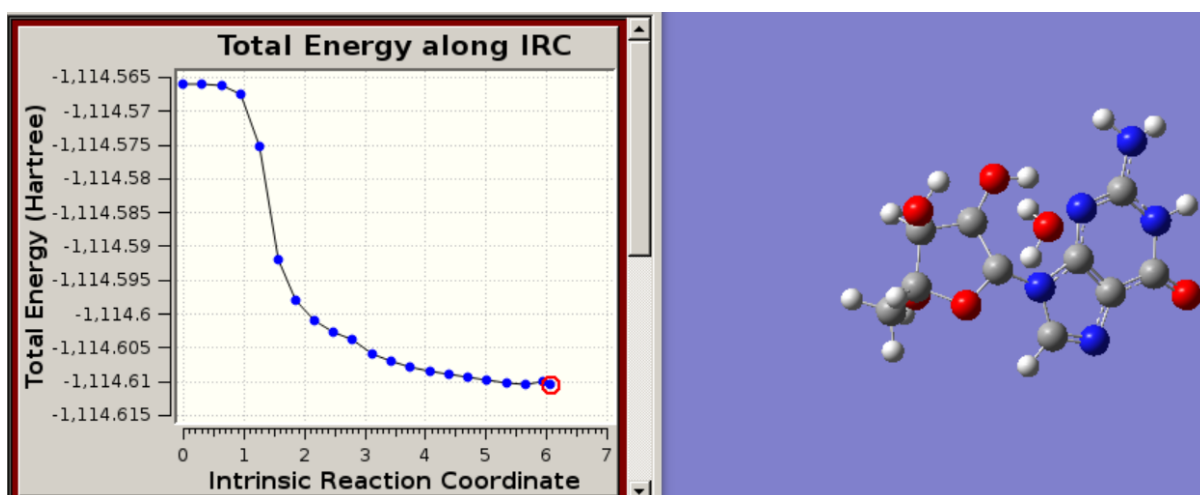
Intrinsic Reaction Coordinate plots – Guanosine

C1

Reverse:

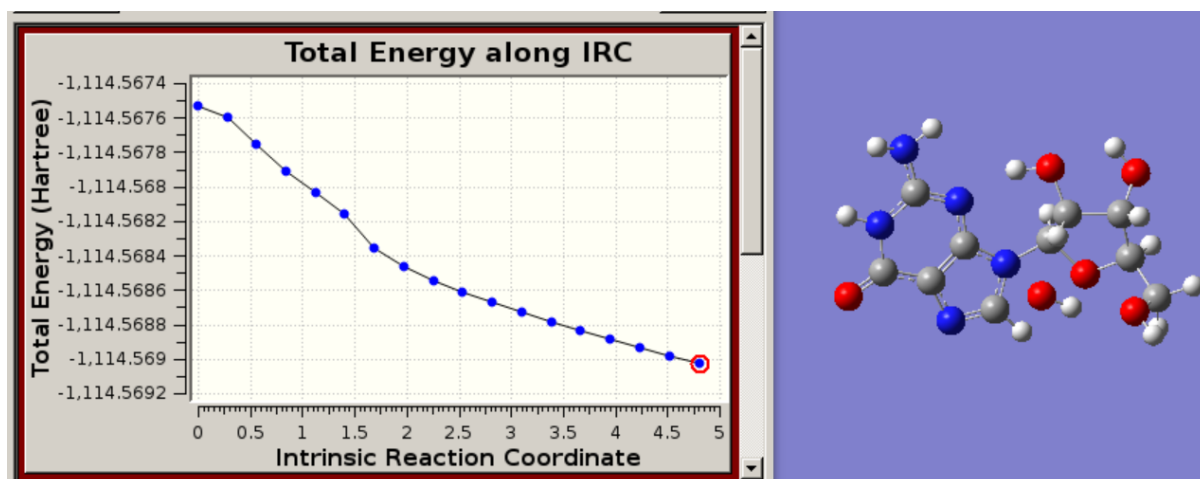


Forward:

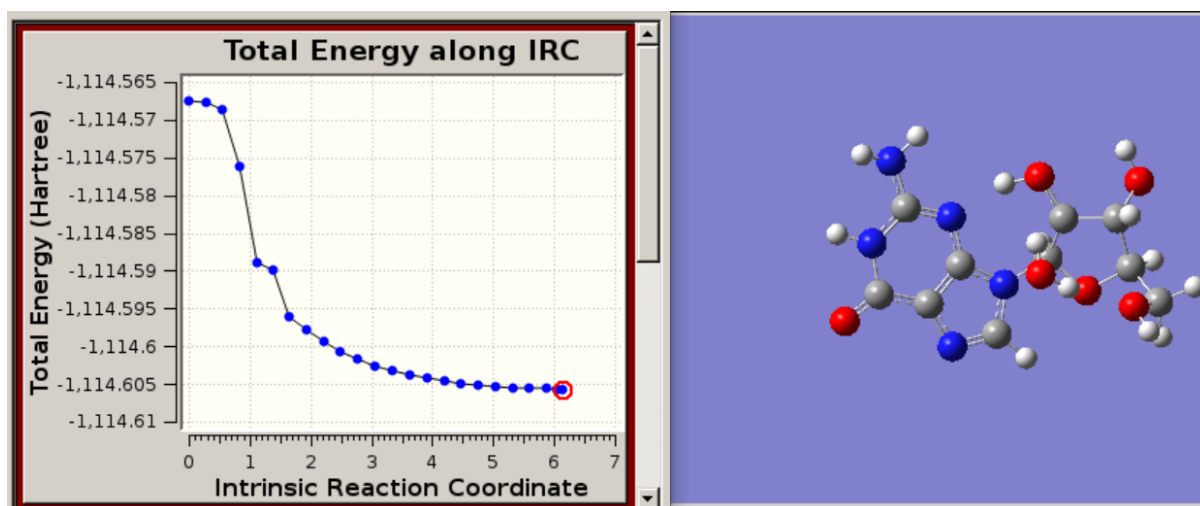


C2

Reverse:

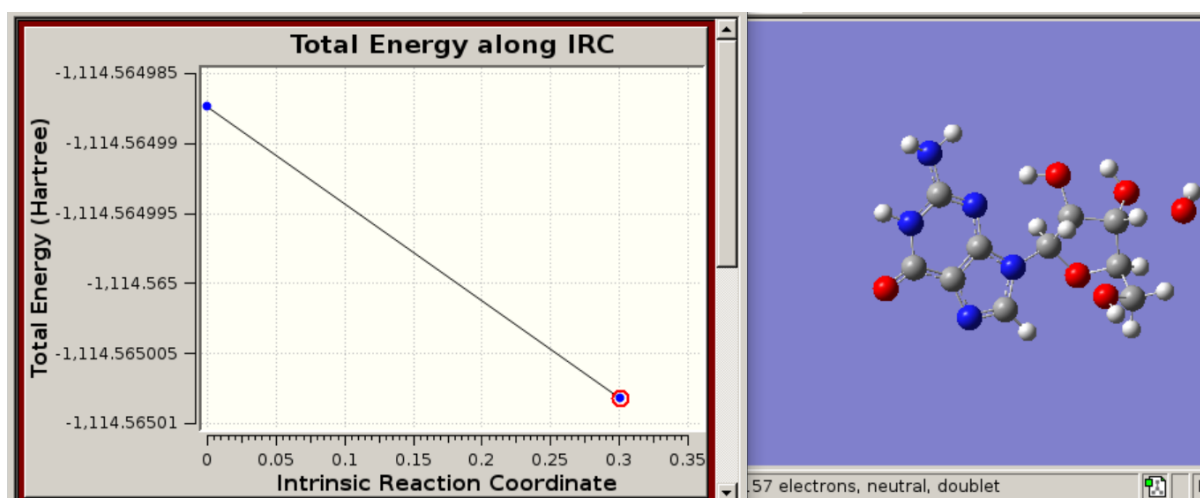


Forward:

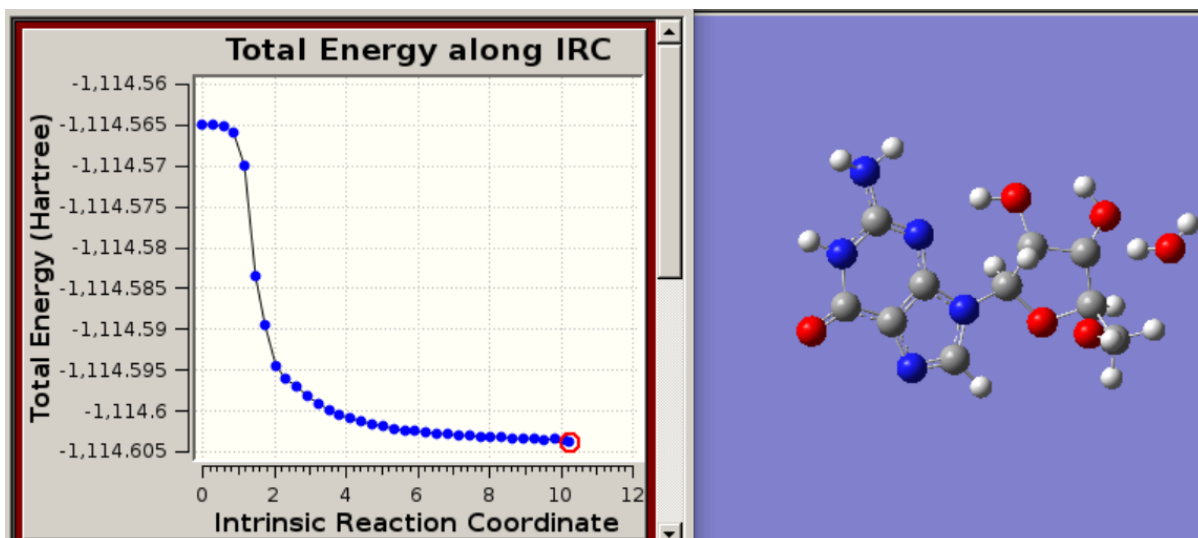


C3

Reverse:

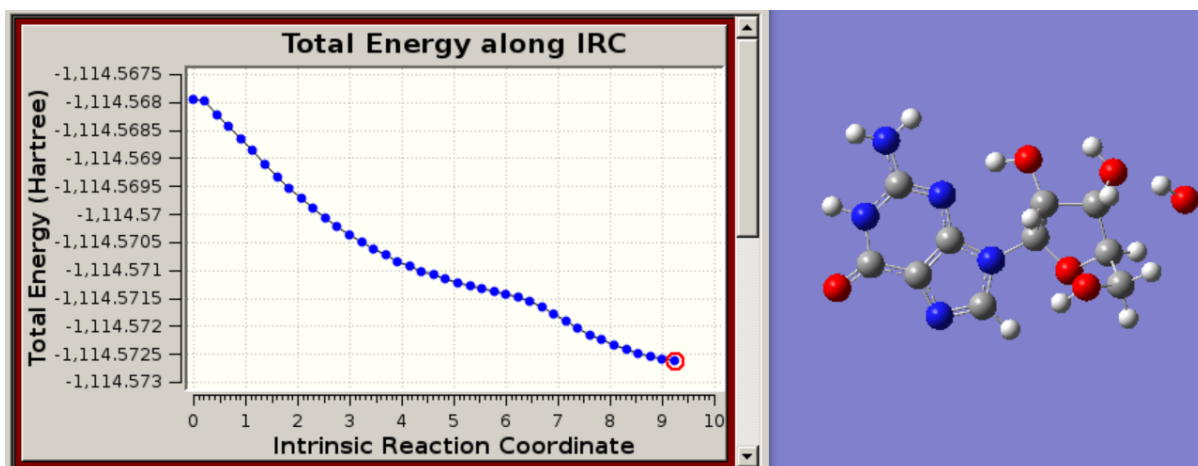


Forward:

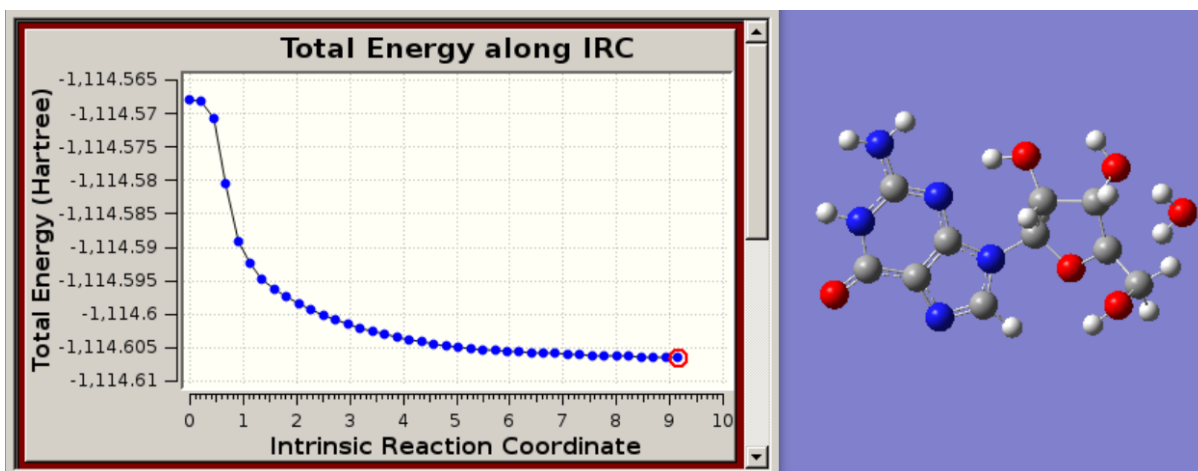


C4

Reverse:

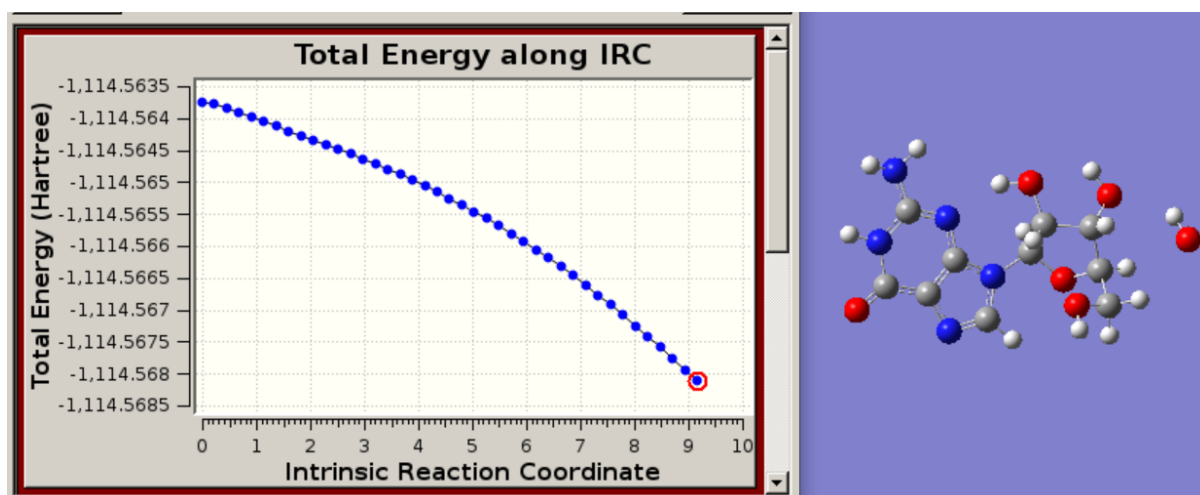


Forward:

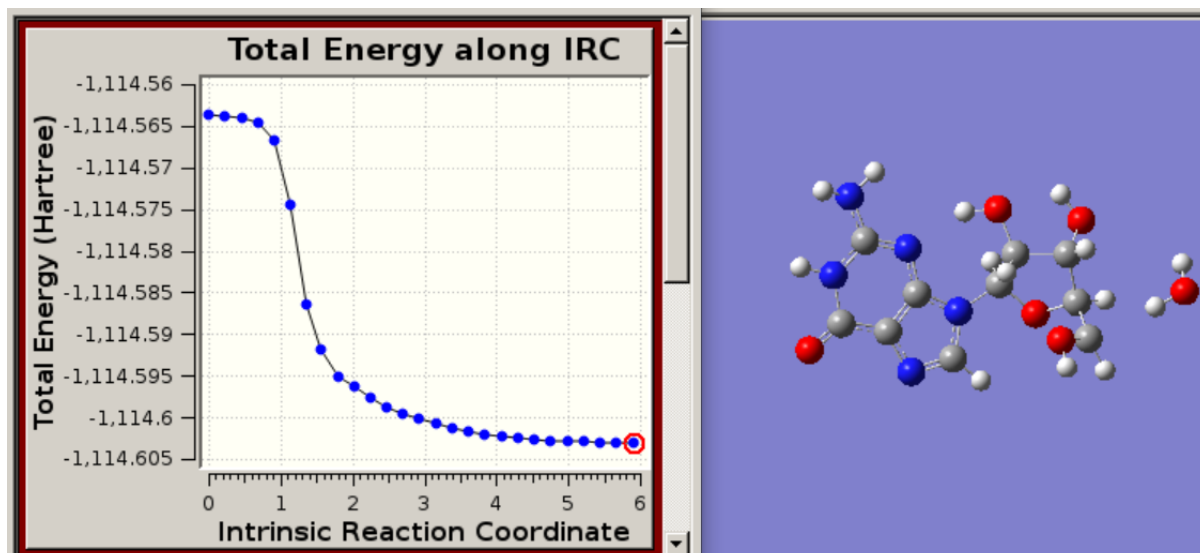


C5_HC

Reverse:

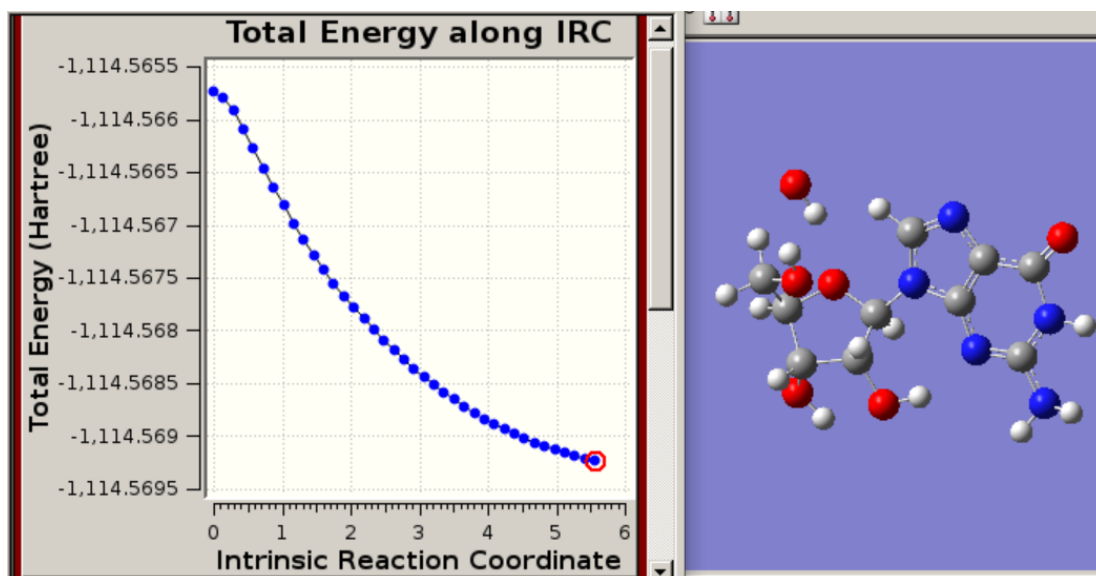


Forward:

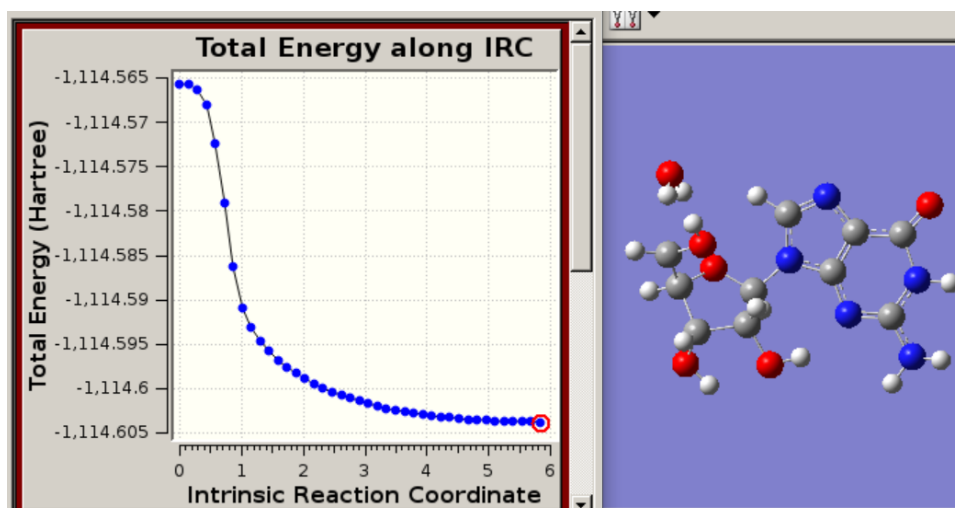


C5_HO

Reverse:

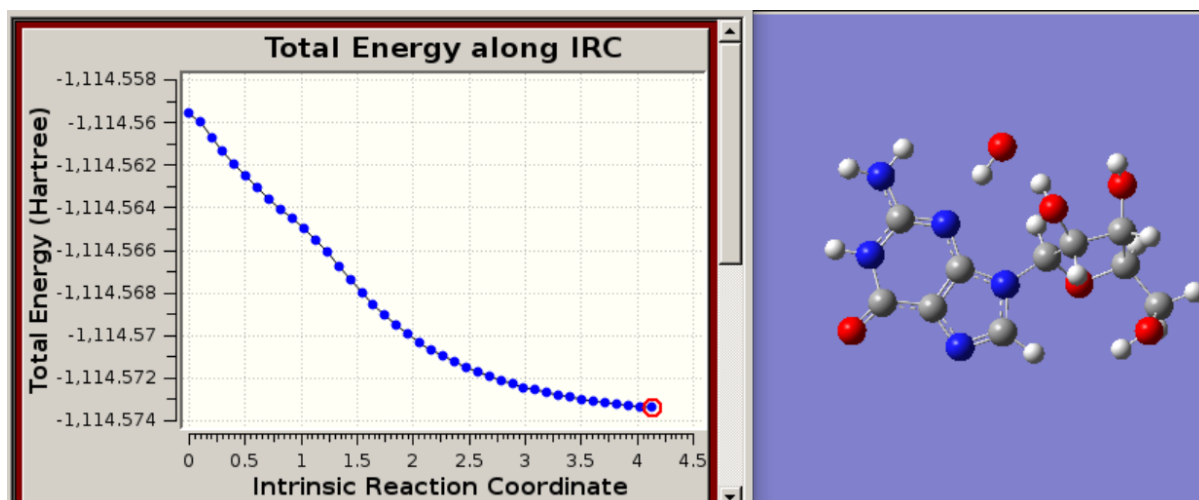


Forward:

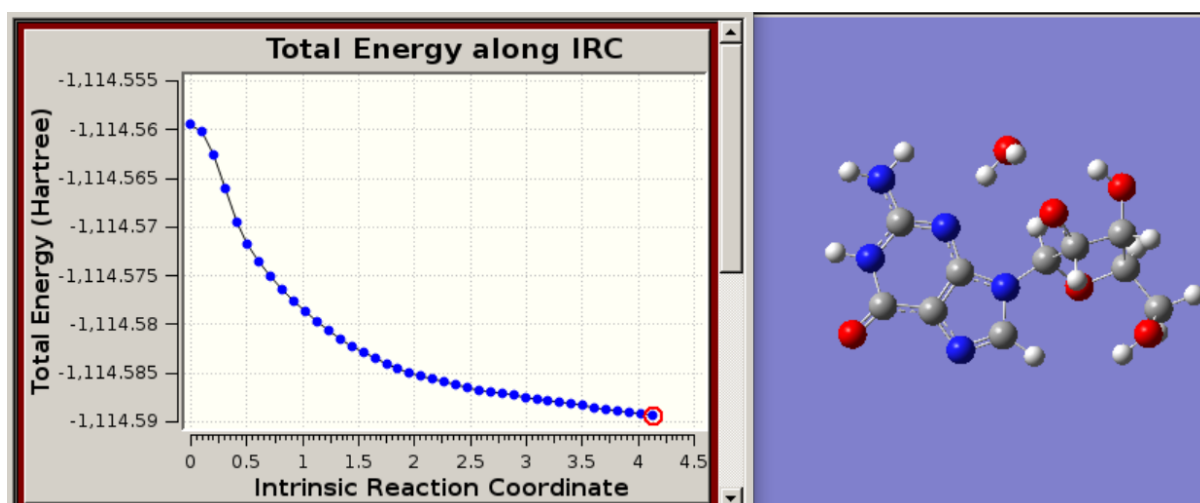


O2

Reverse:

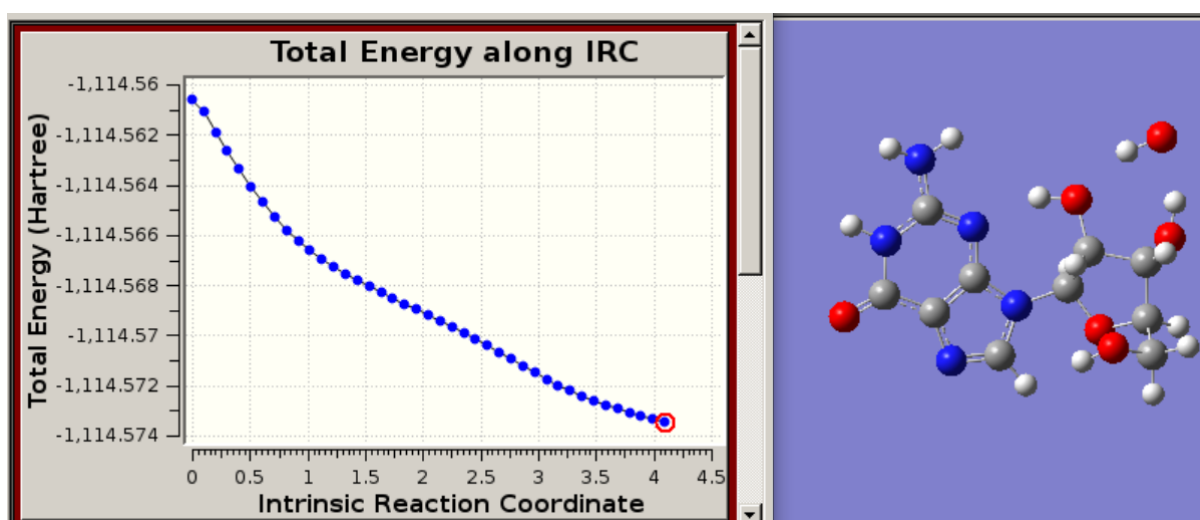


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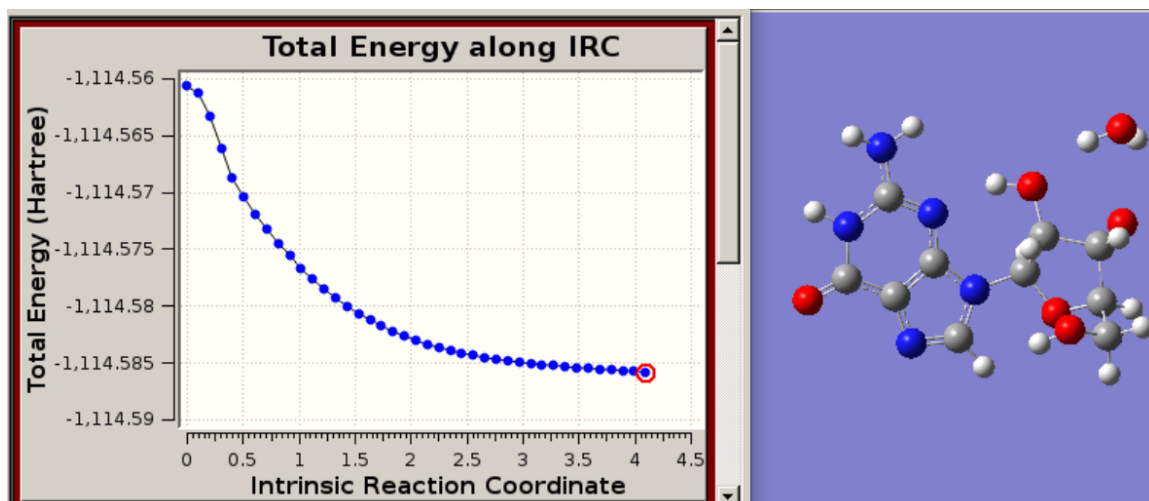


03

Reverse:

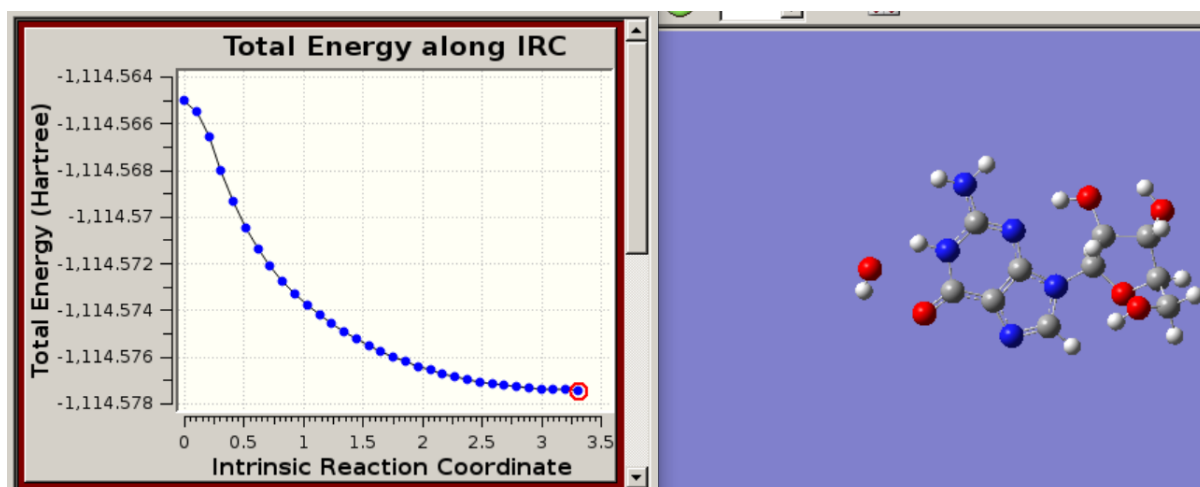


Forward:

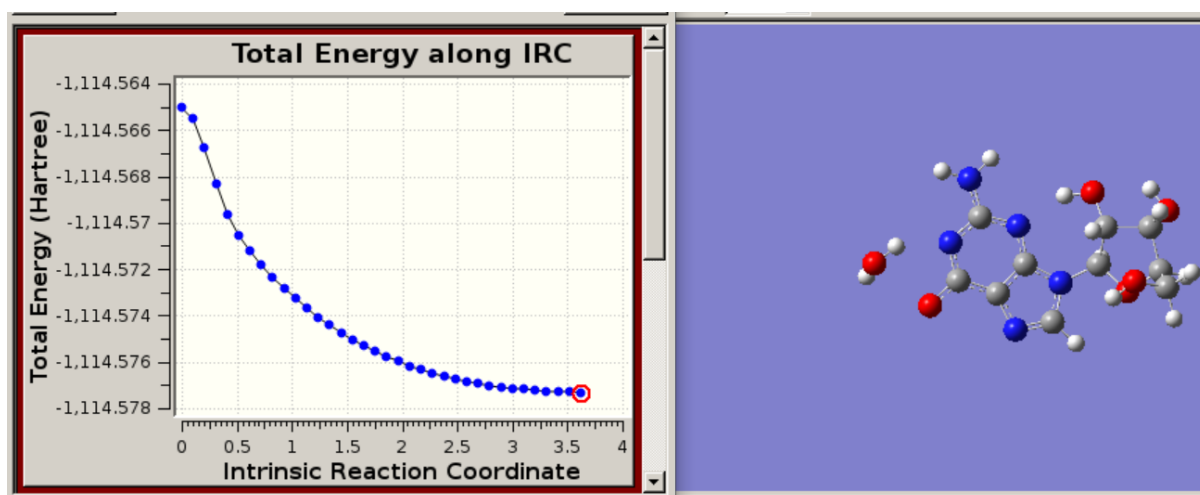


H1

Reverse:

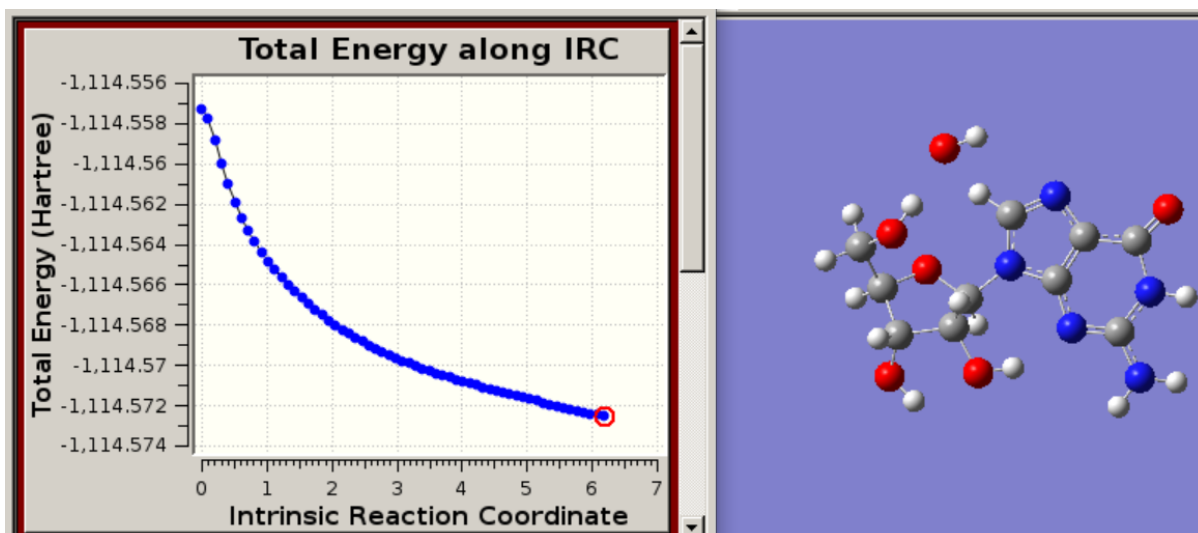


Forward:

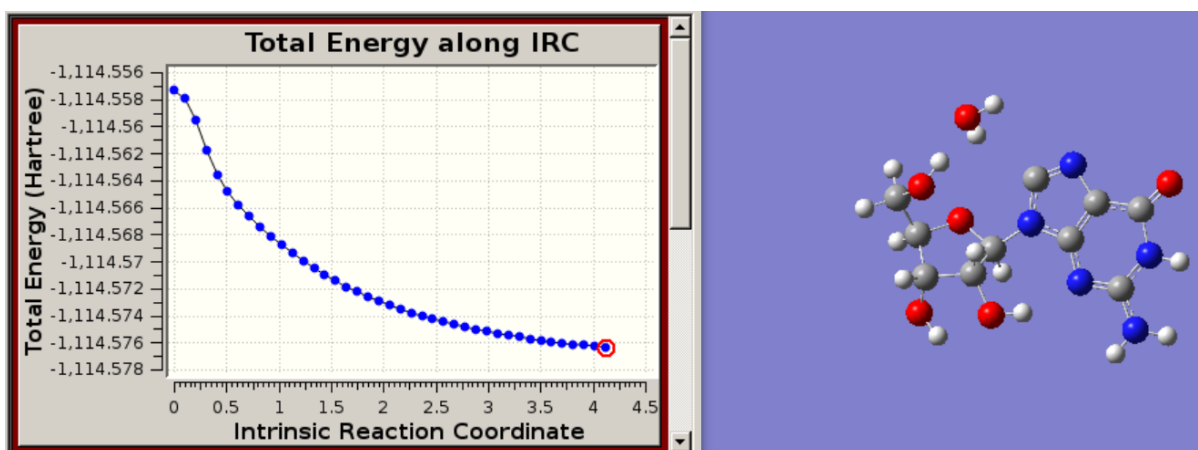


H8

Reverse:

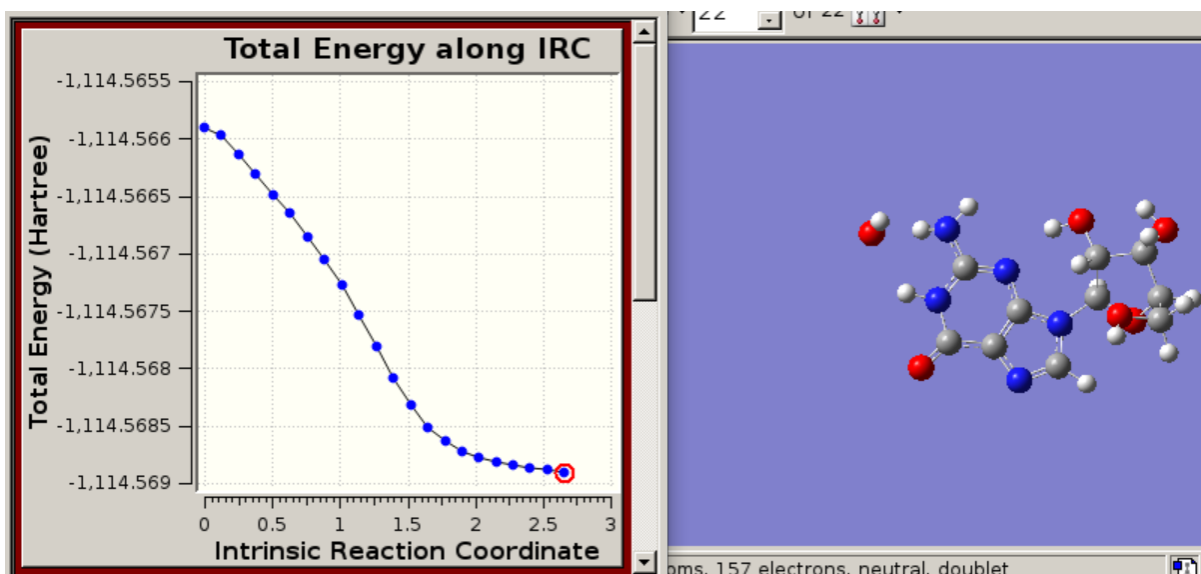


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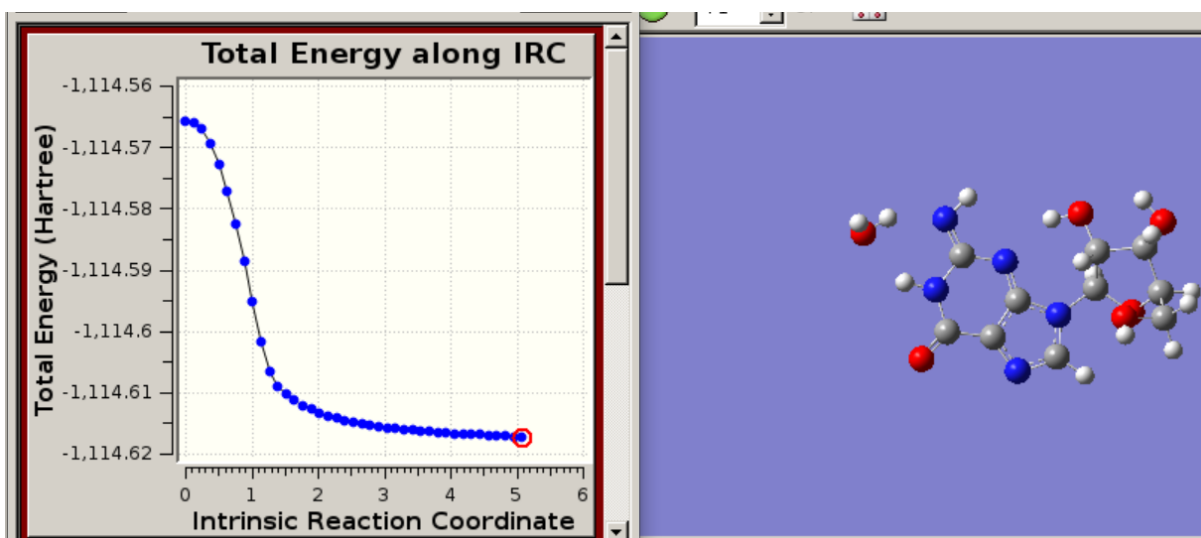


H21

Reverse:

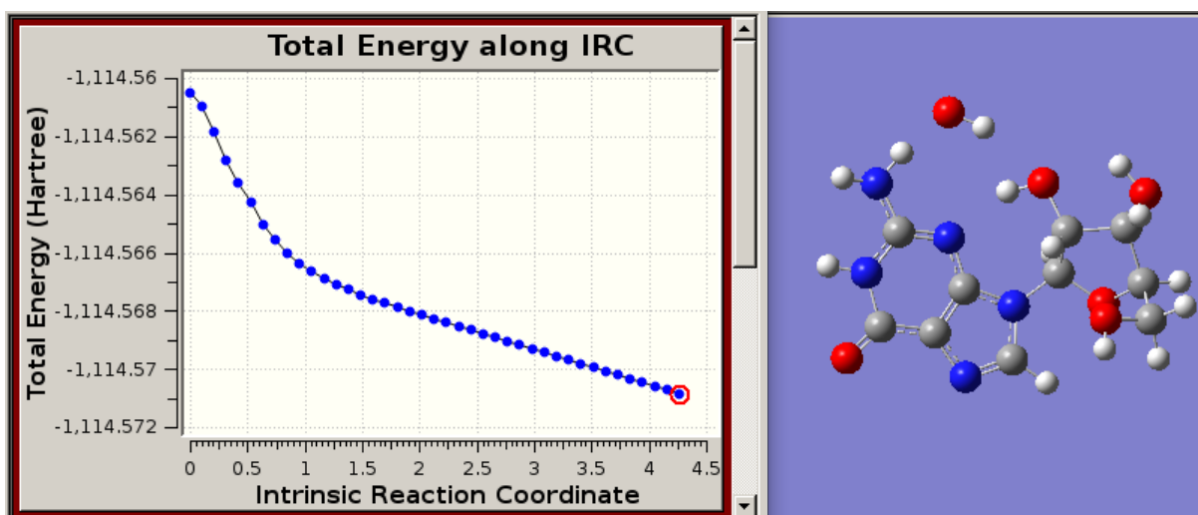


Forward:



H22

Reverse:



Forward:

