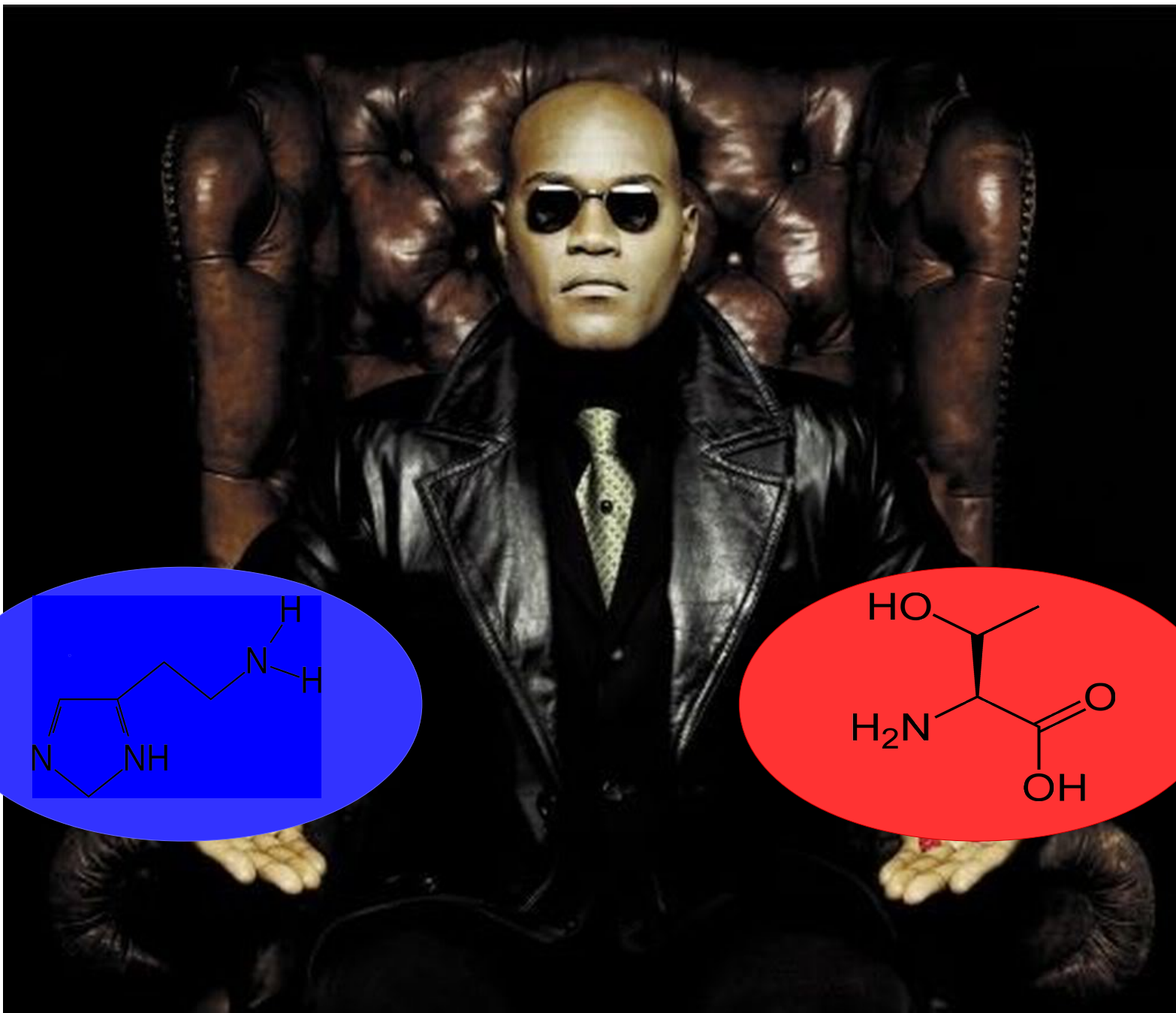


On the way to equilibrium structure of histamine

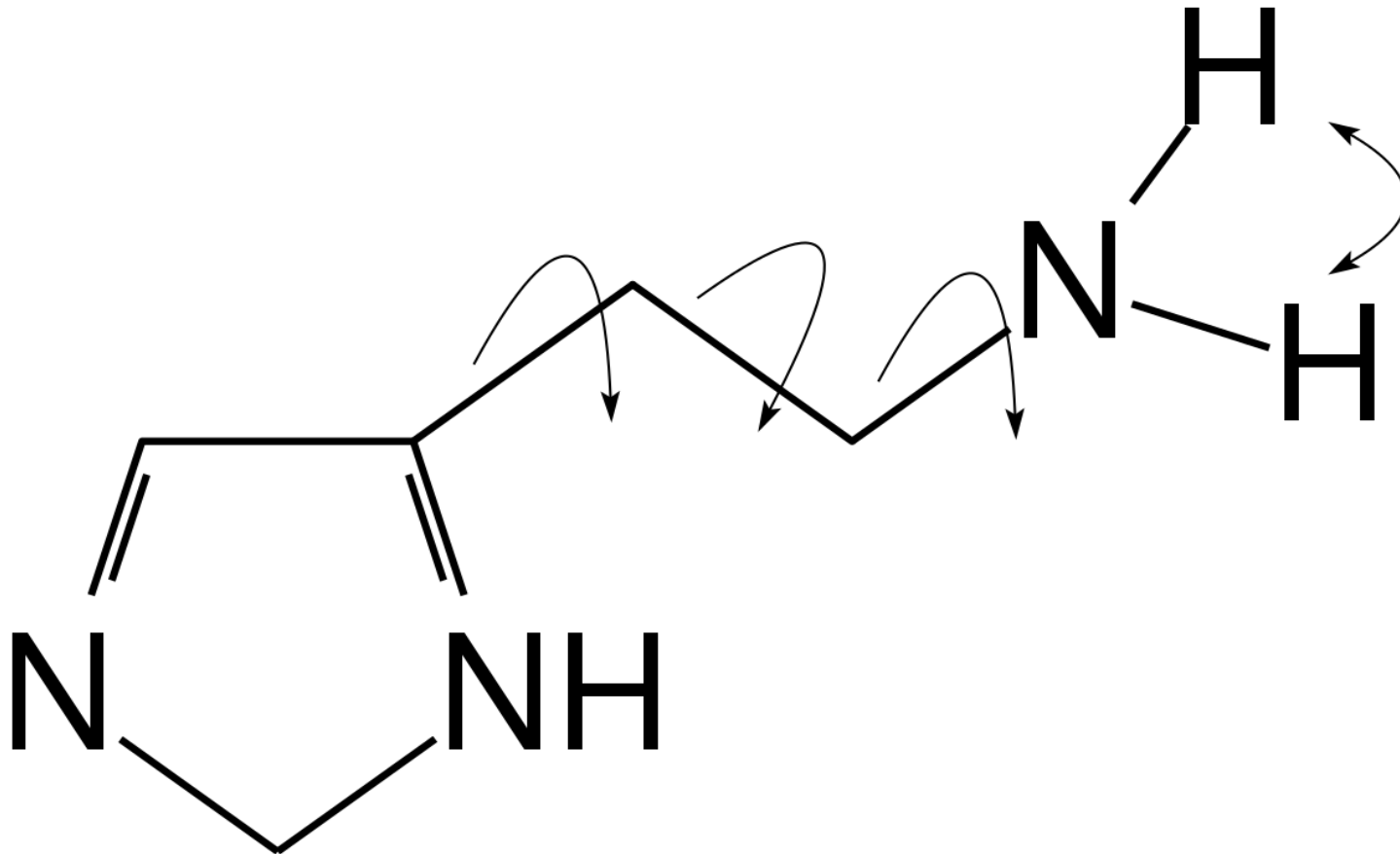


Denis Tikhonov

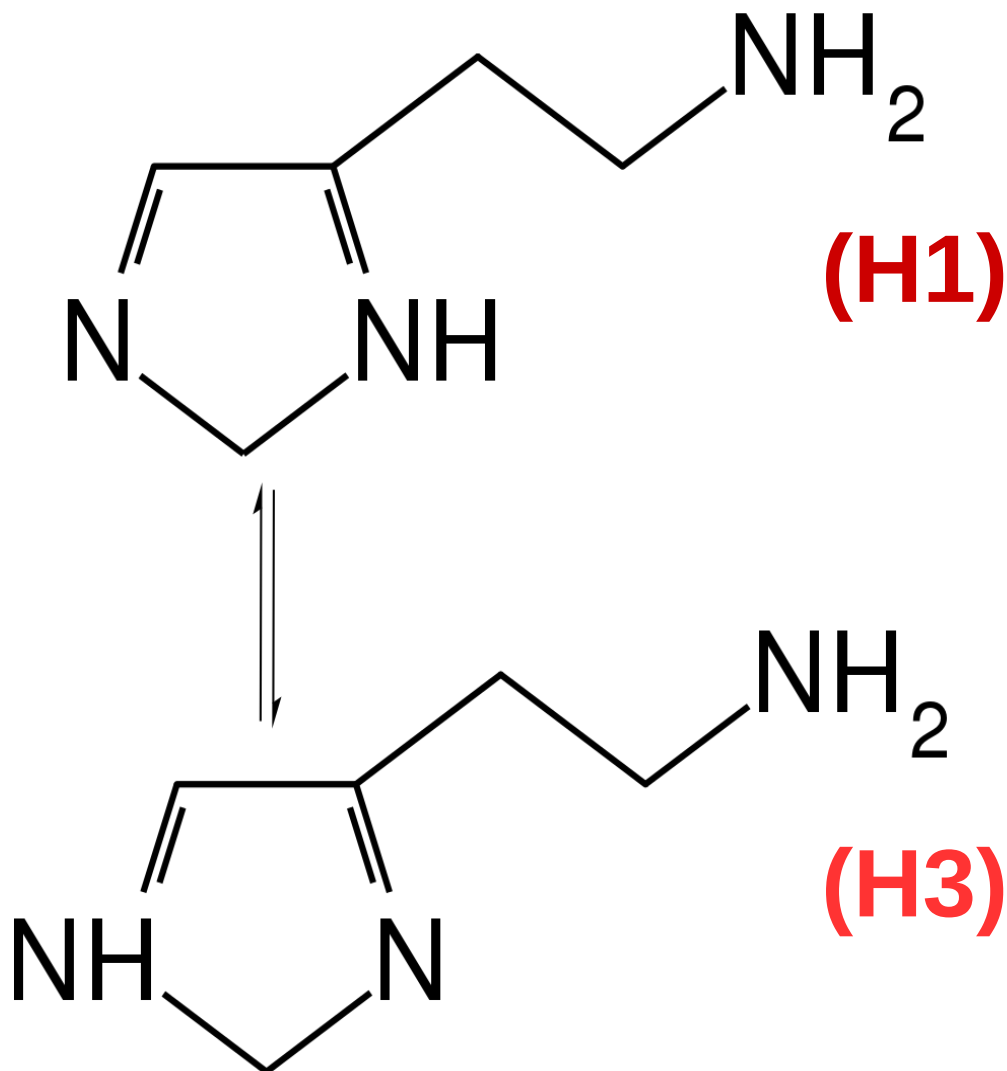
Projects for Ph.D. thesis



Histamine molecule



Tautomerism in histamine



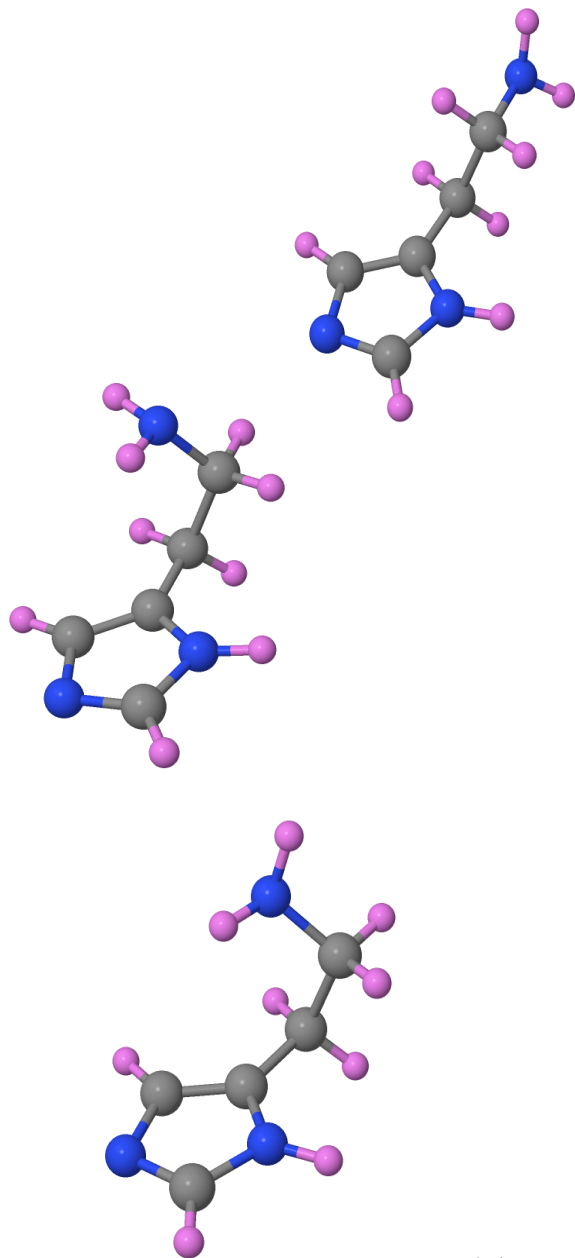
- Beat Vogelsanger, Peter D. Godfrey, and Ronald D. Brown \

J. Am. Chem. SOC. 1991, 113, 7864-7869

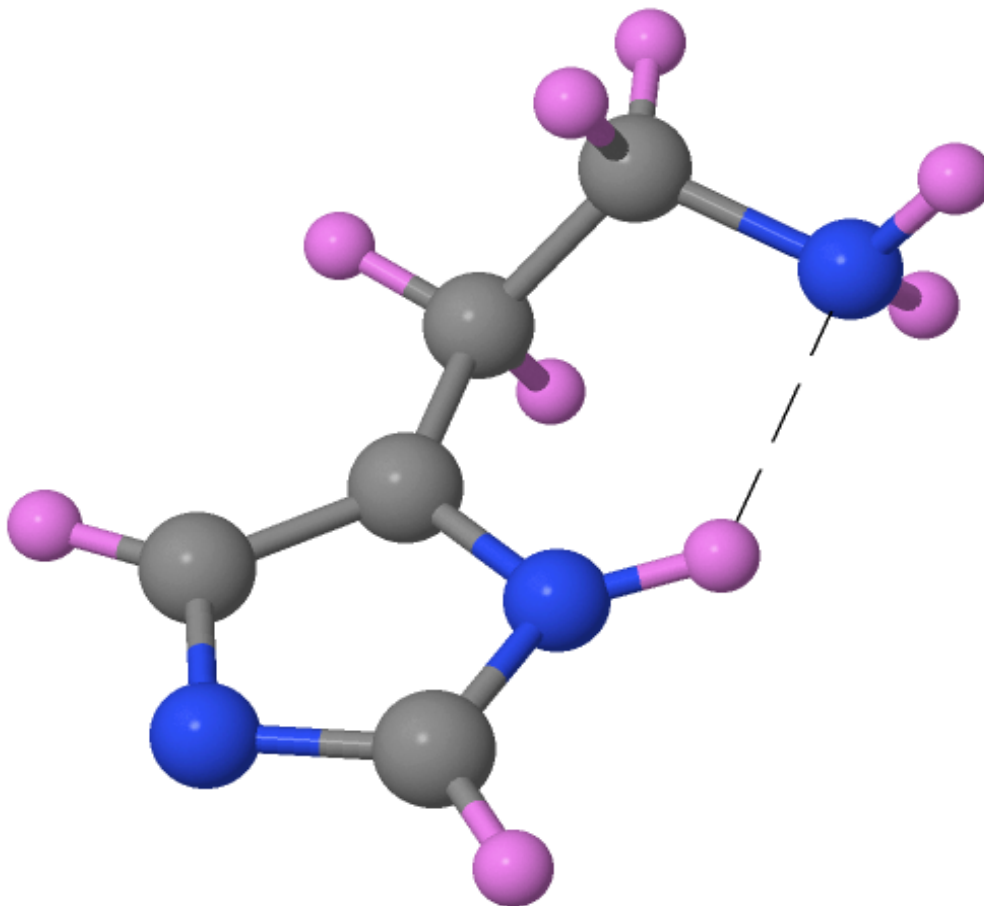
- Peter D. Godfrey and Ronald D. Brown \

J. Am. Chem. Soc. 1998, 120, 10724-10732

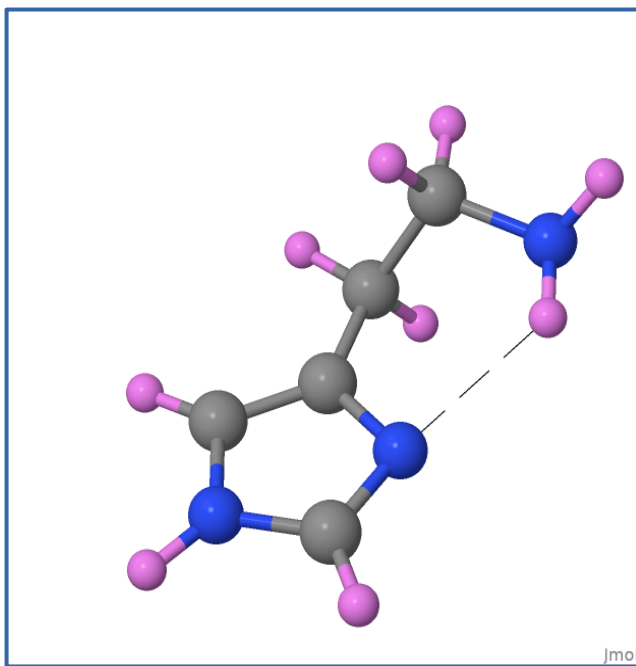
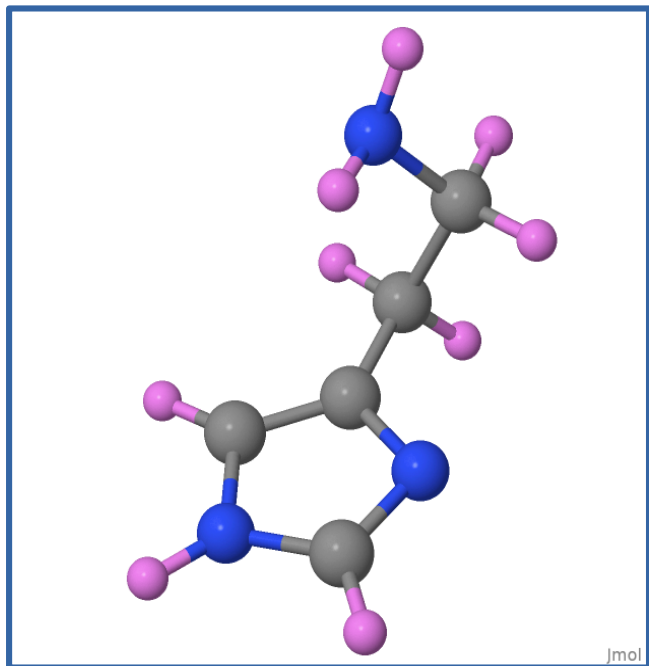
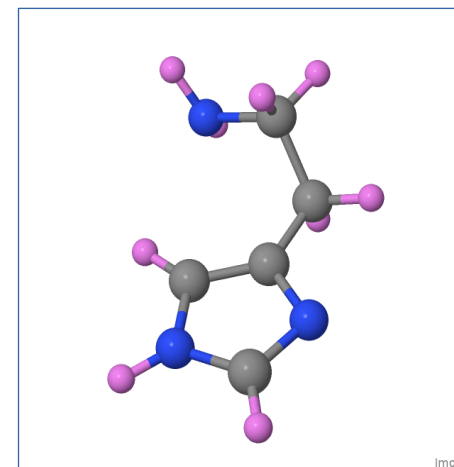
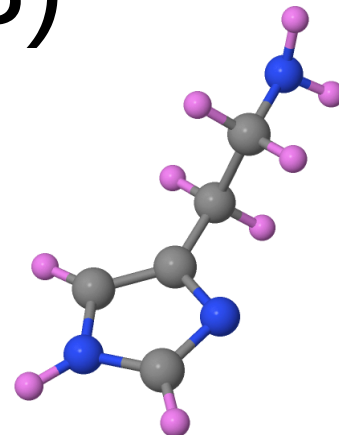
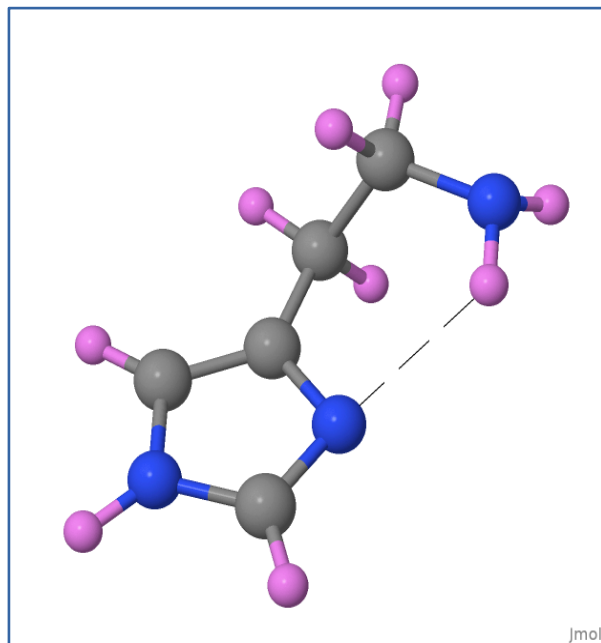
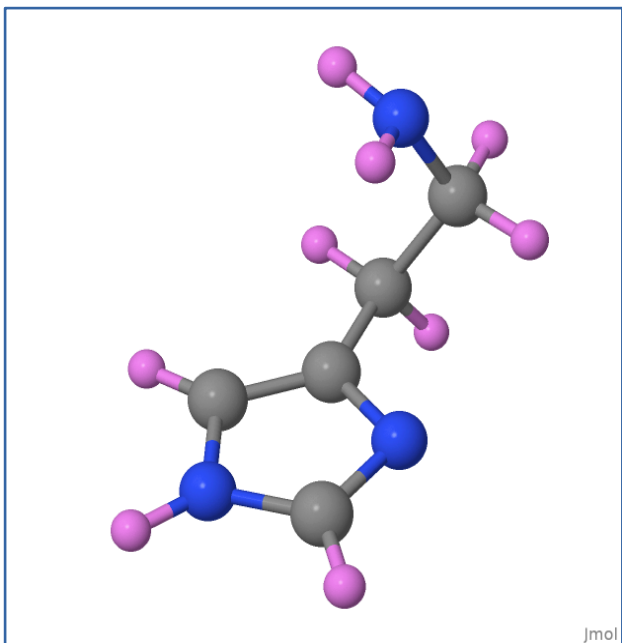
Histamine conformers (H1)



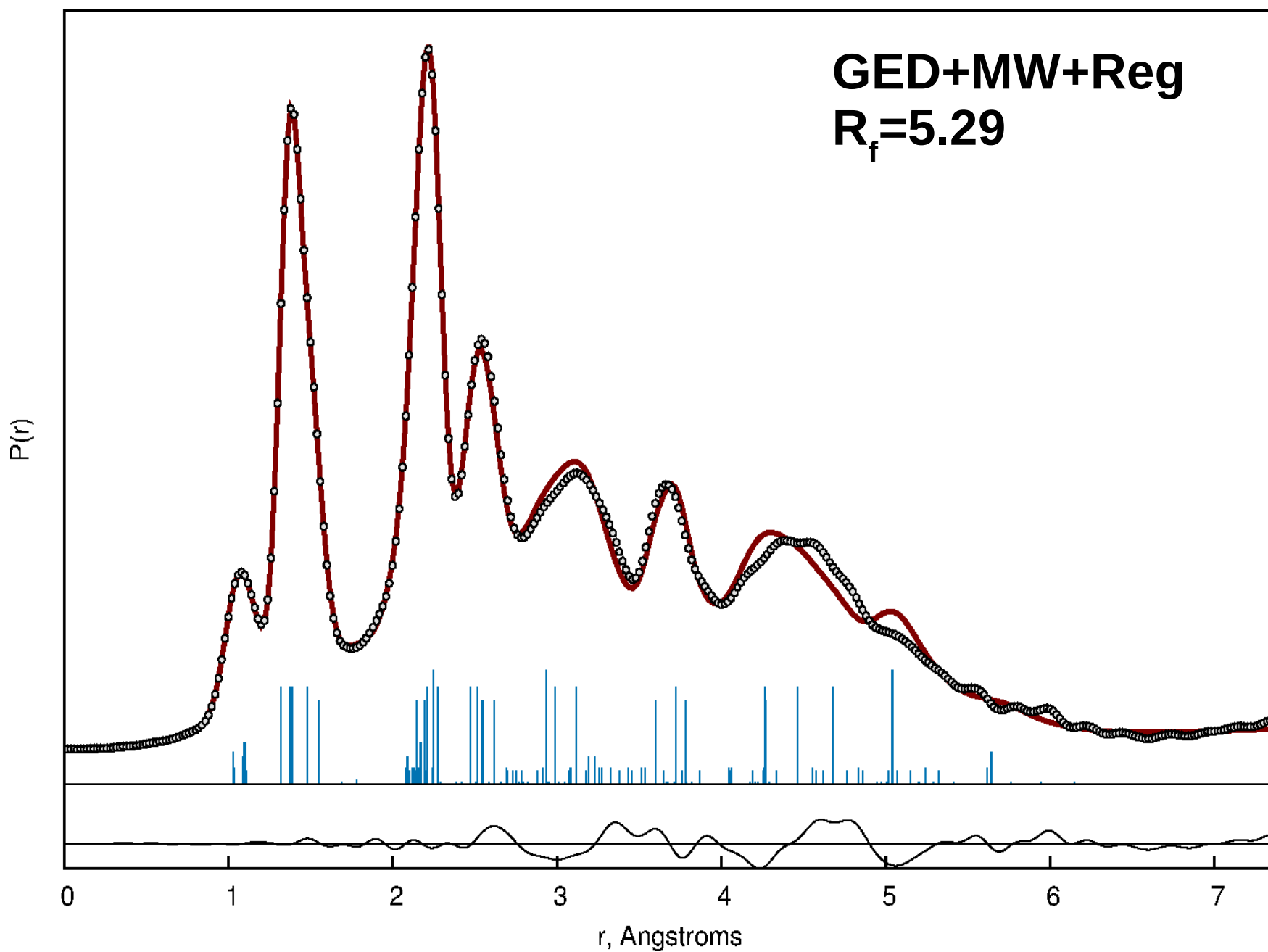
92.2 %



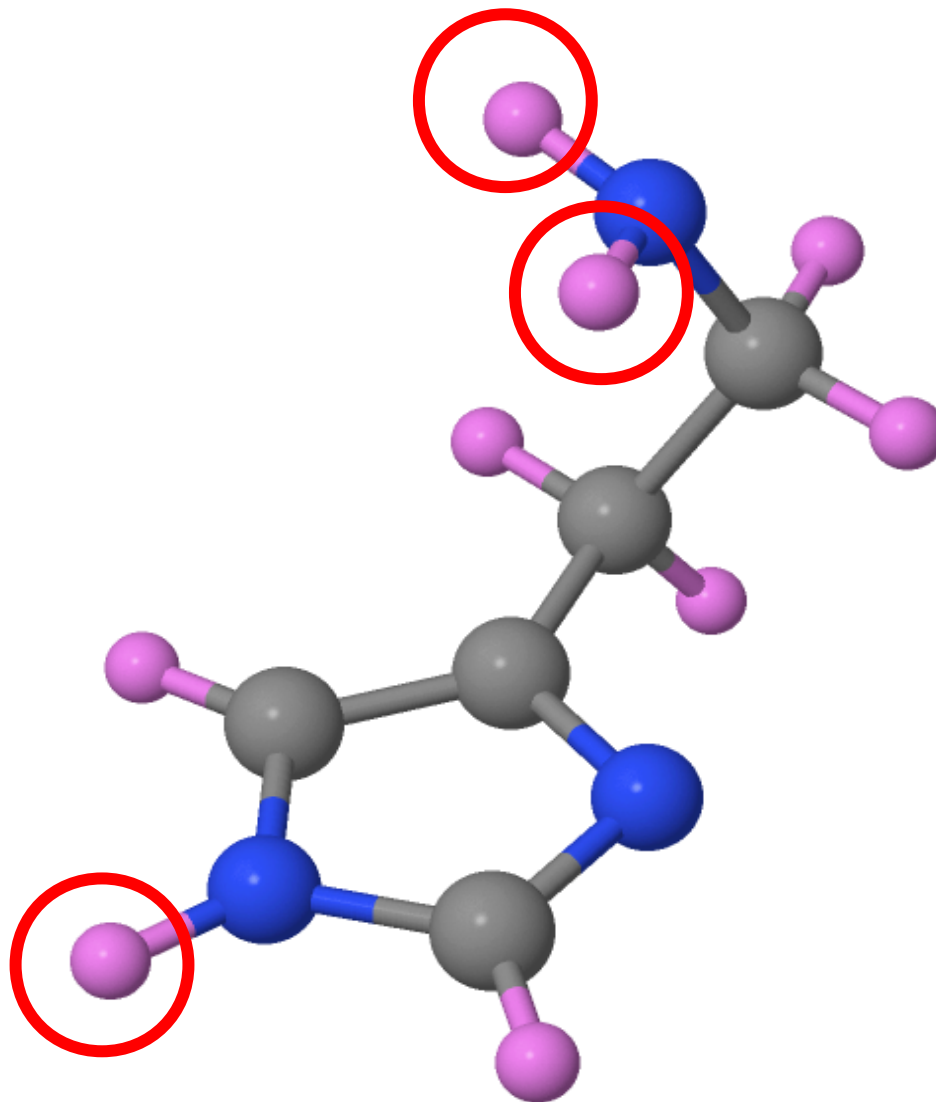
Histamine conformers (H3)



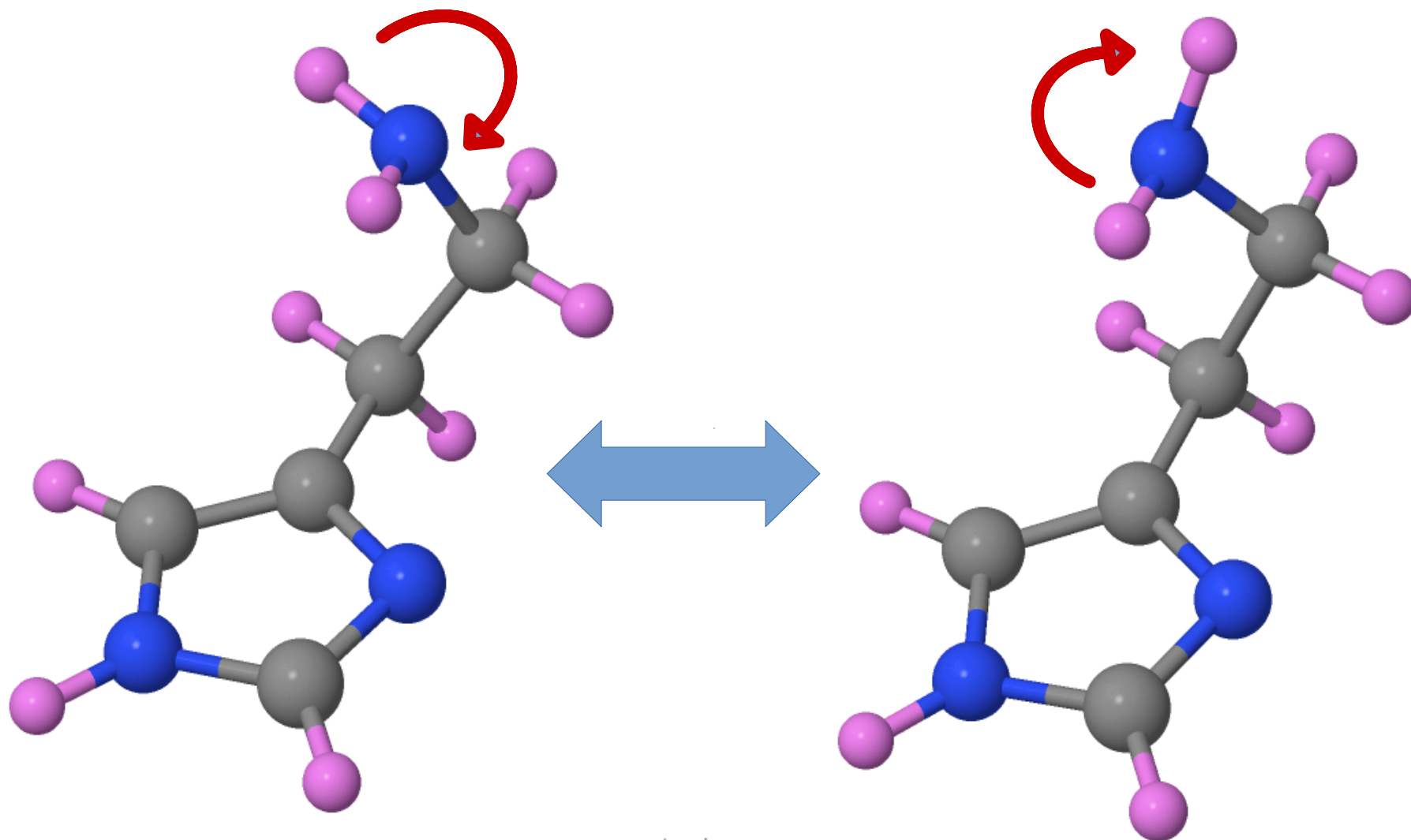
Single conformer GED analysis



Problematic hydrogens (H3)



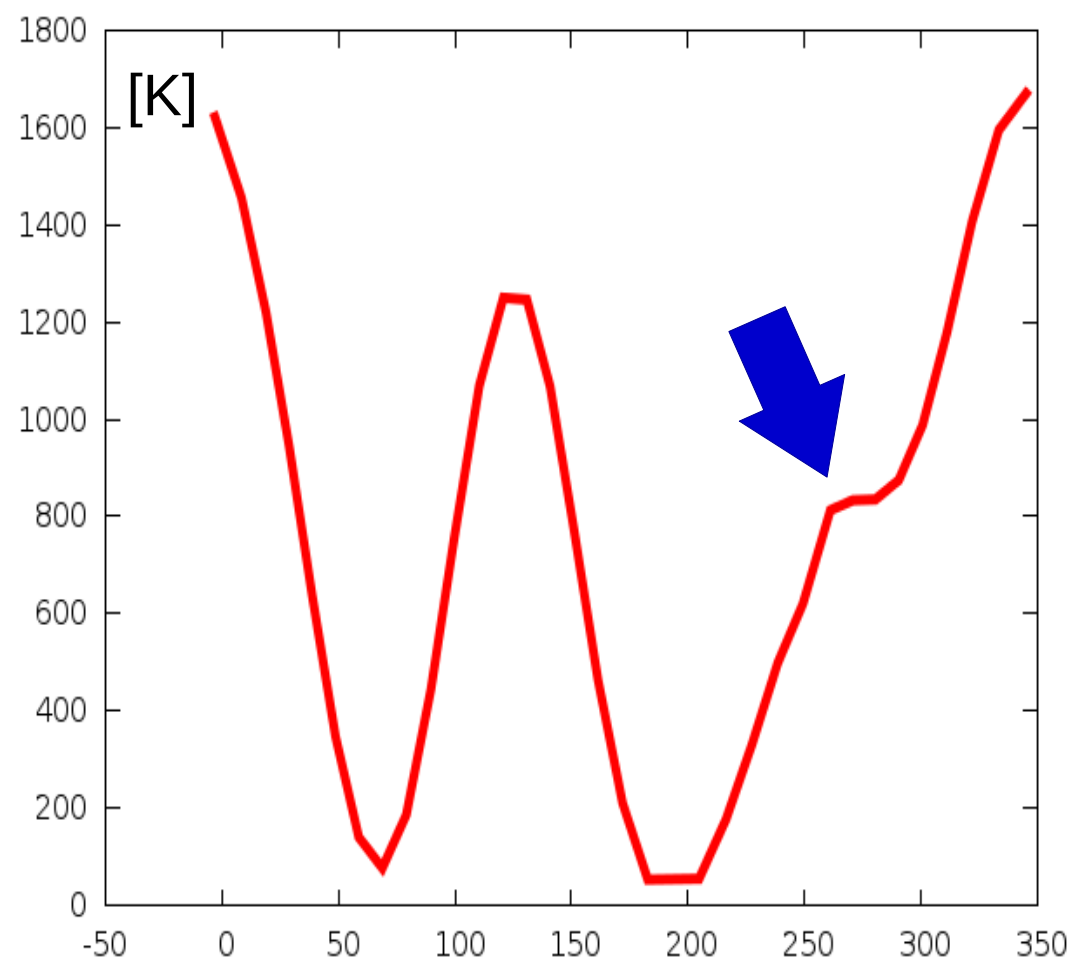
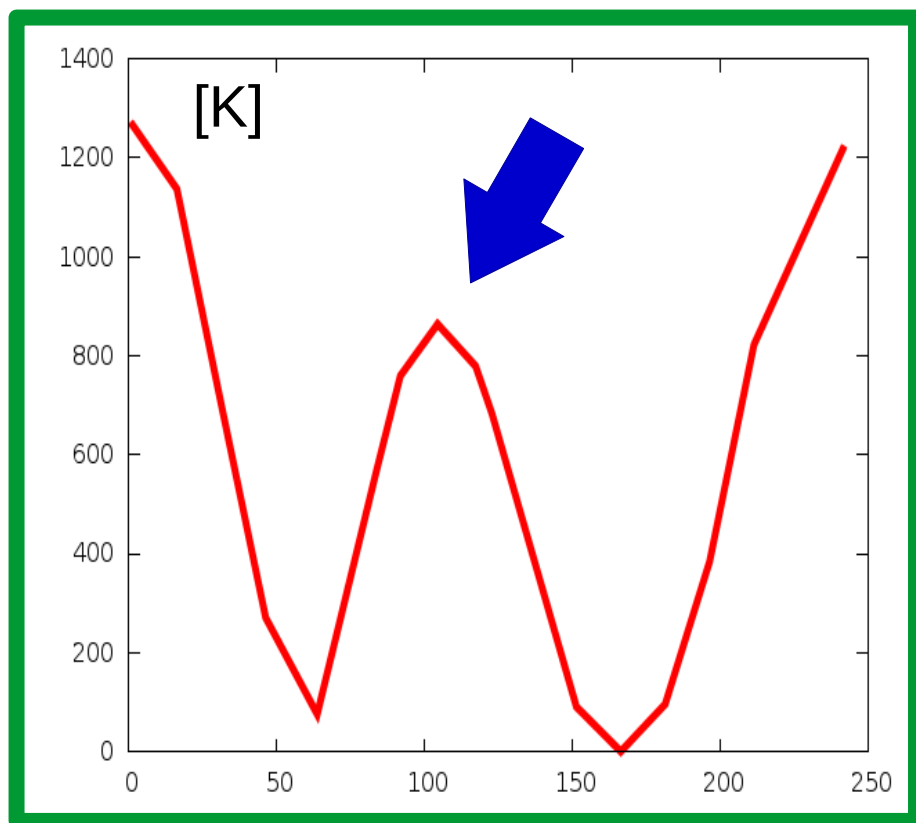
Problematic hydrogens: the source



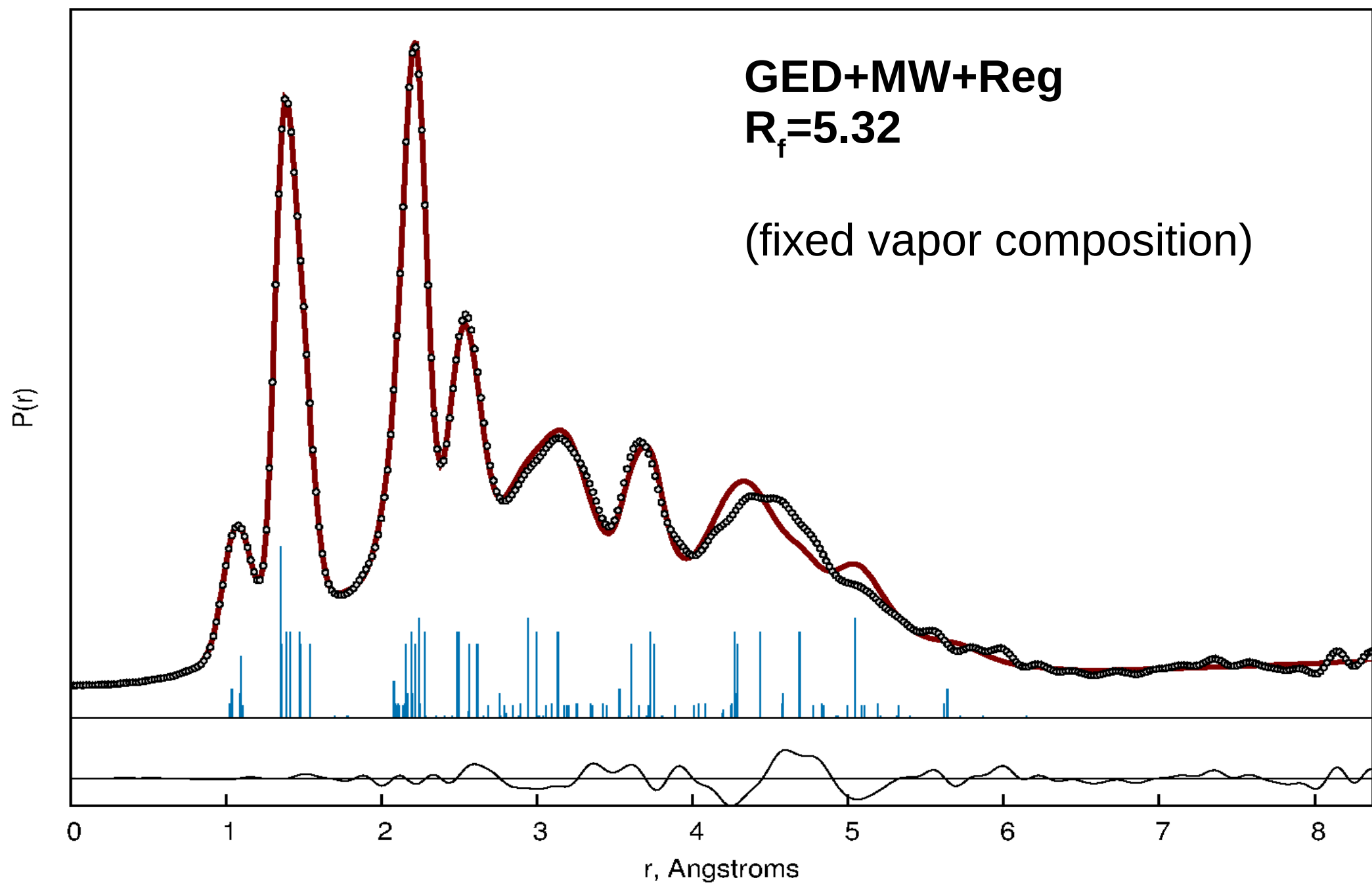
Jmol

Jmol

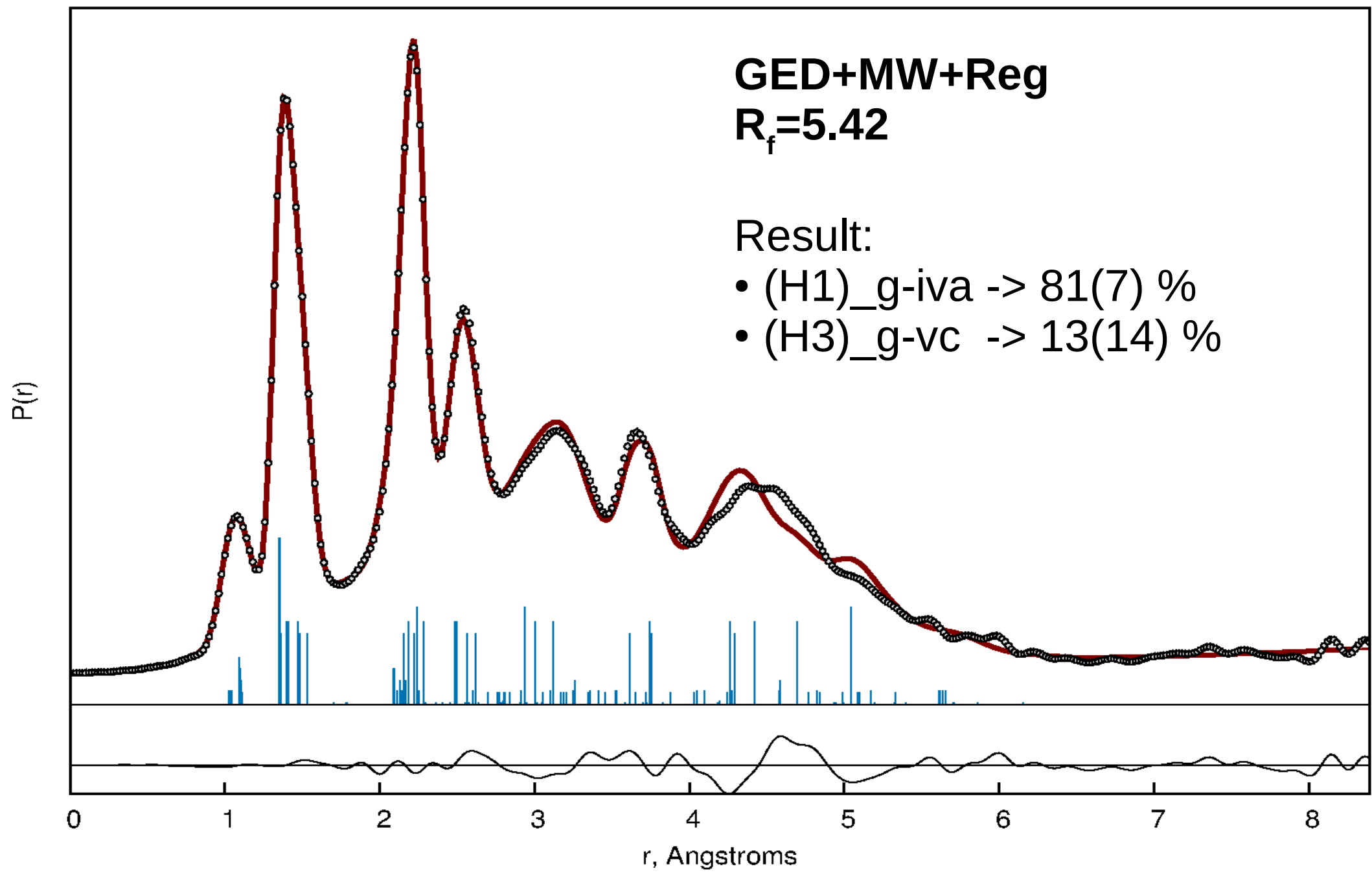
Inversion vs. Internal rotation



5 conformers GED analysis

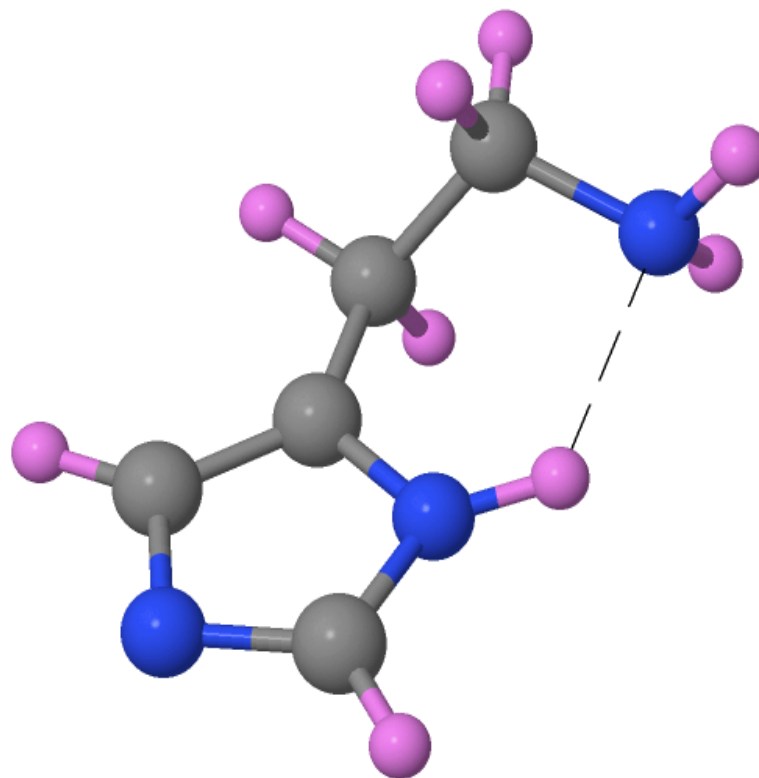
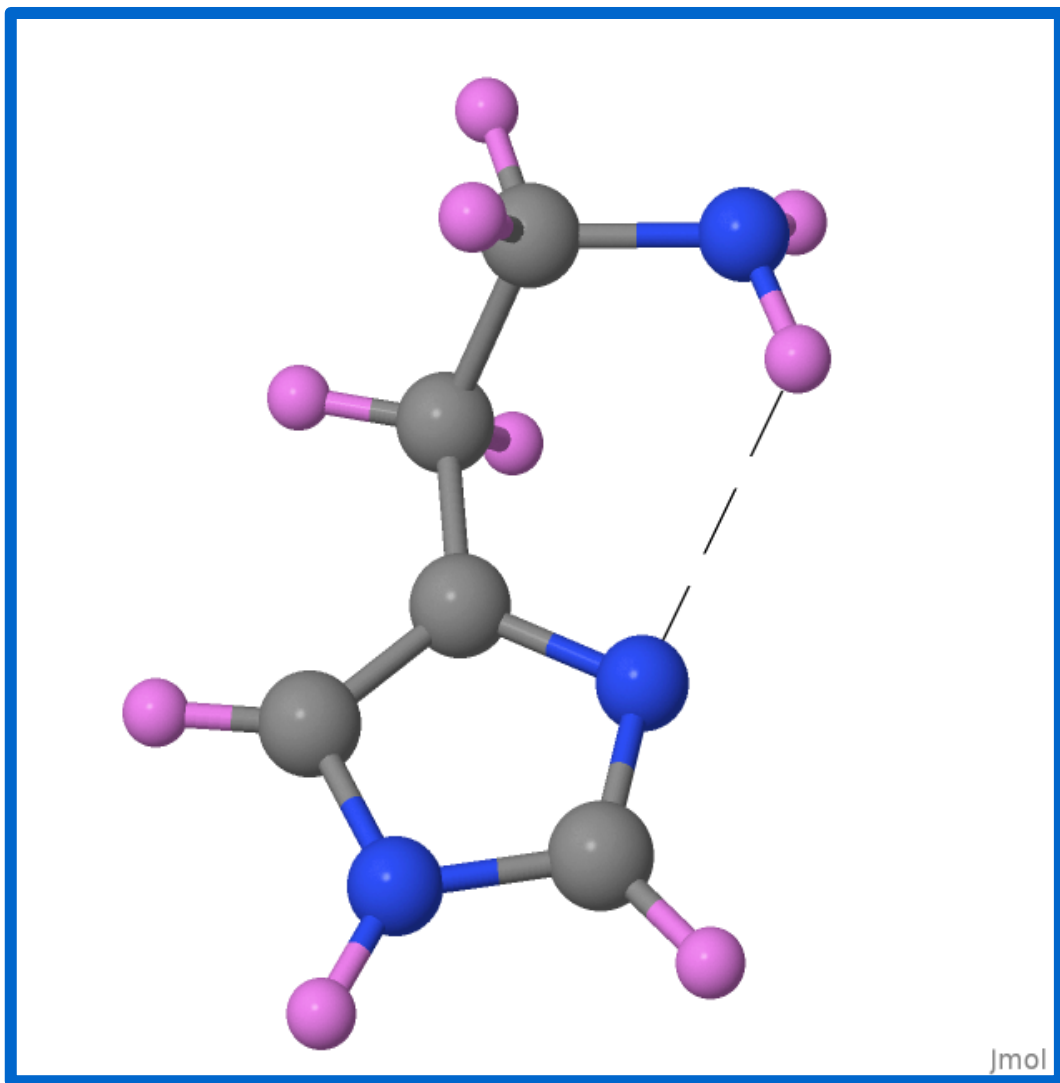


5 conformers GED analysis



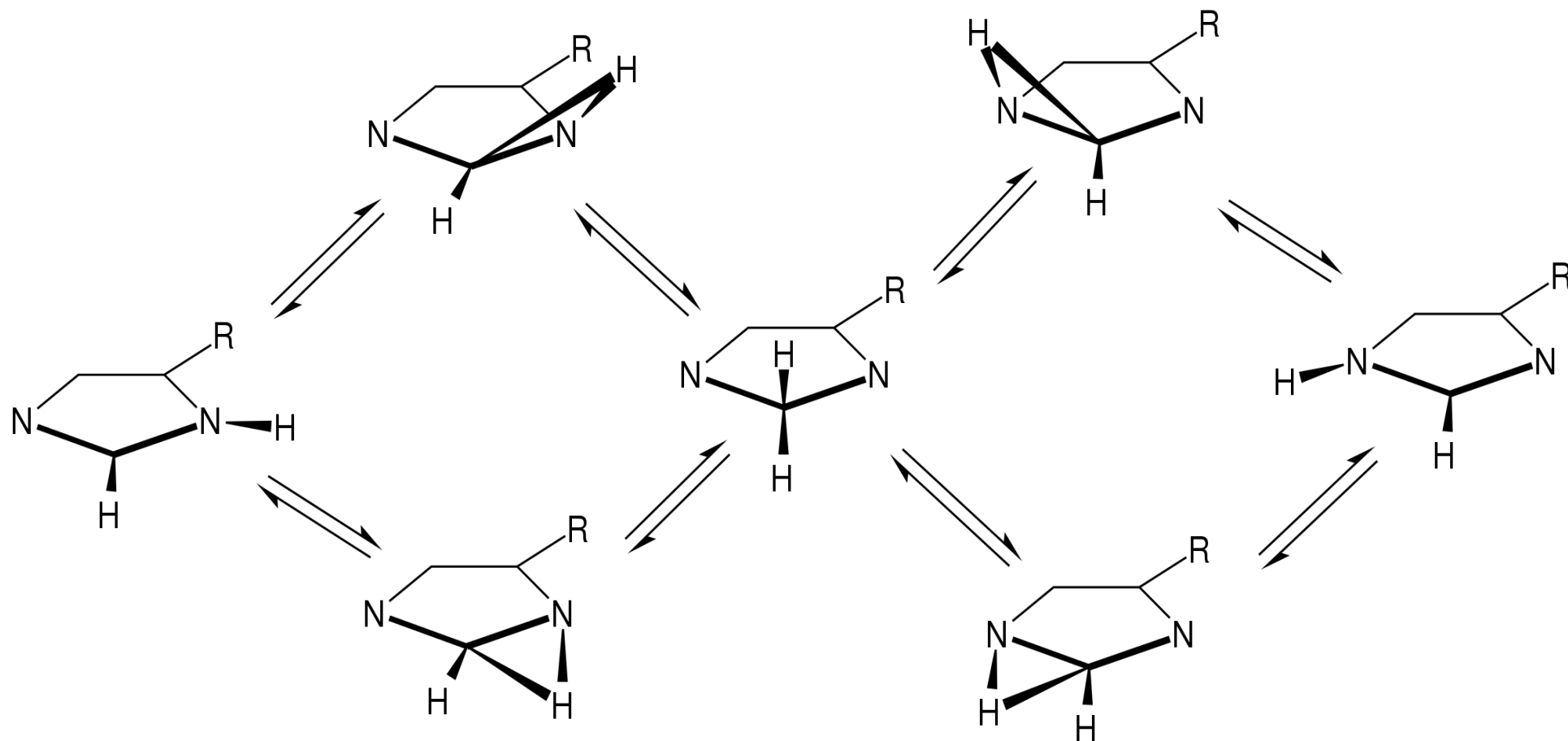
Is the system even at the
equilibrium?

Aqueous solution vs. gas



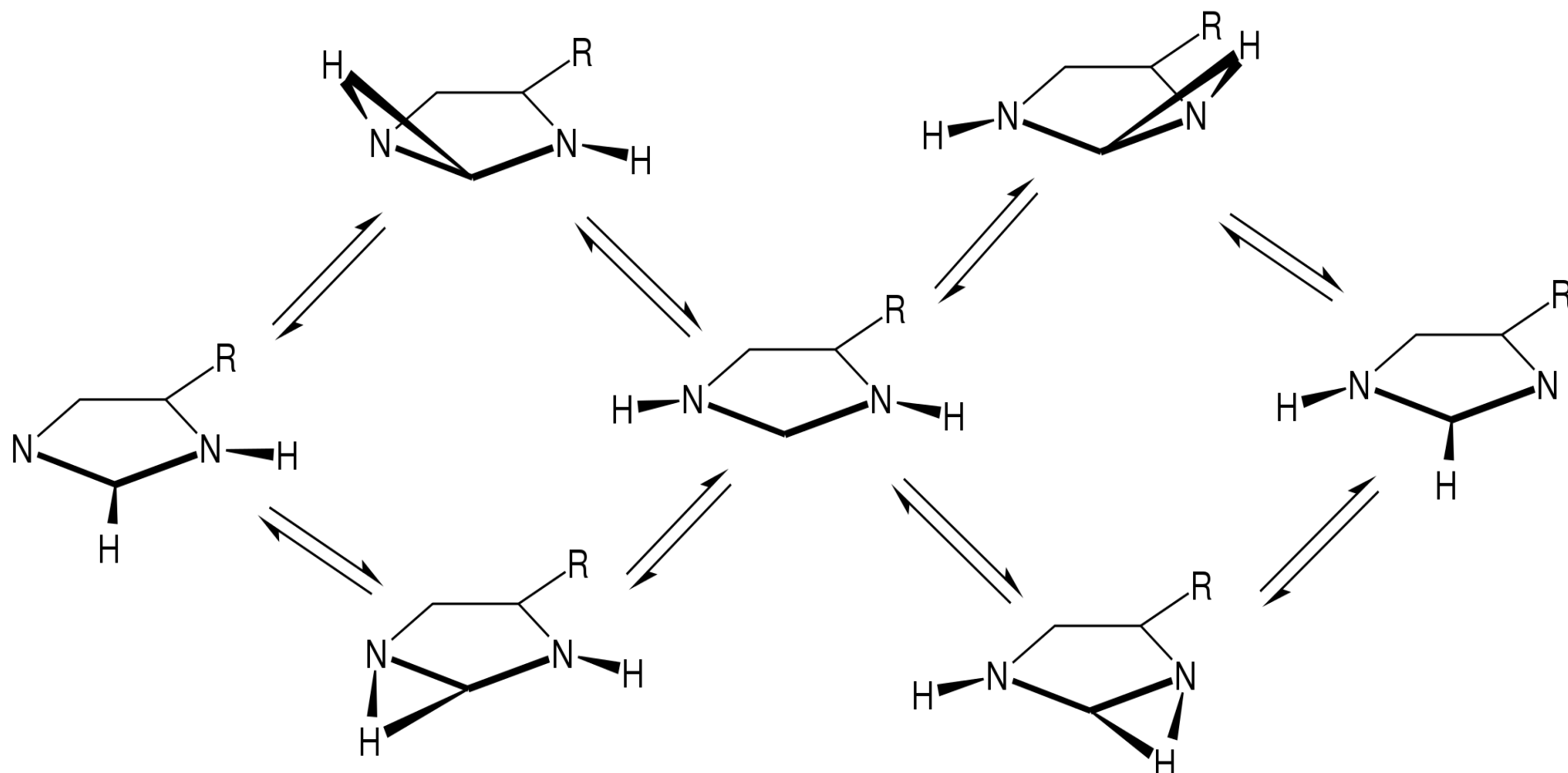
F. Javier Ramirez, Inaki Tunon, Juan A. Collado, and Estanislao Silla //
J. AM. CHEM. SOC. 2003, 125, 2328-2340

Mechanism of tautomerisation in gas: first guess



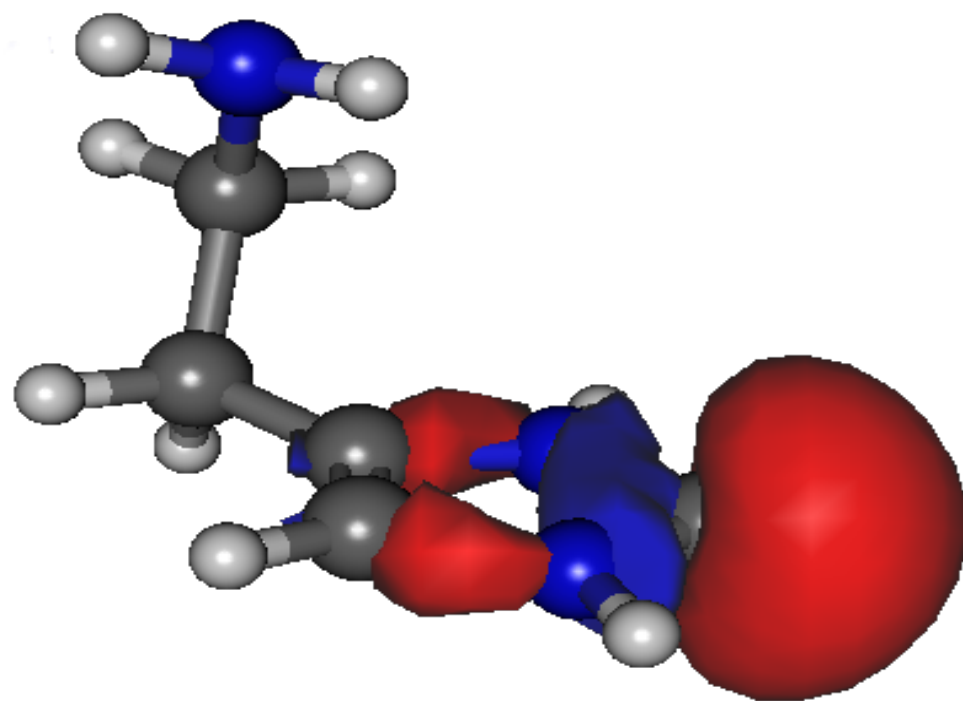
Yu.A. Borisov, N.P. Vorob'eva, I.A. Abronin, A.F. Kolomiets //Bulletin of the
Academy of Sciences of the USSR, Division of chemical science
December 1988, Volume 37, Issue 12, pp 2504-2507

Mechanism of tautomerisation in gas: second guess

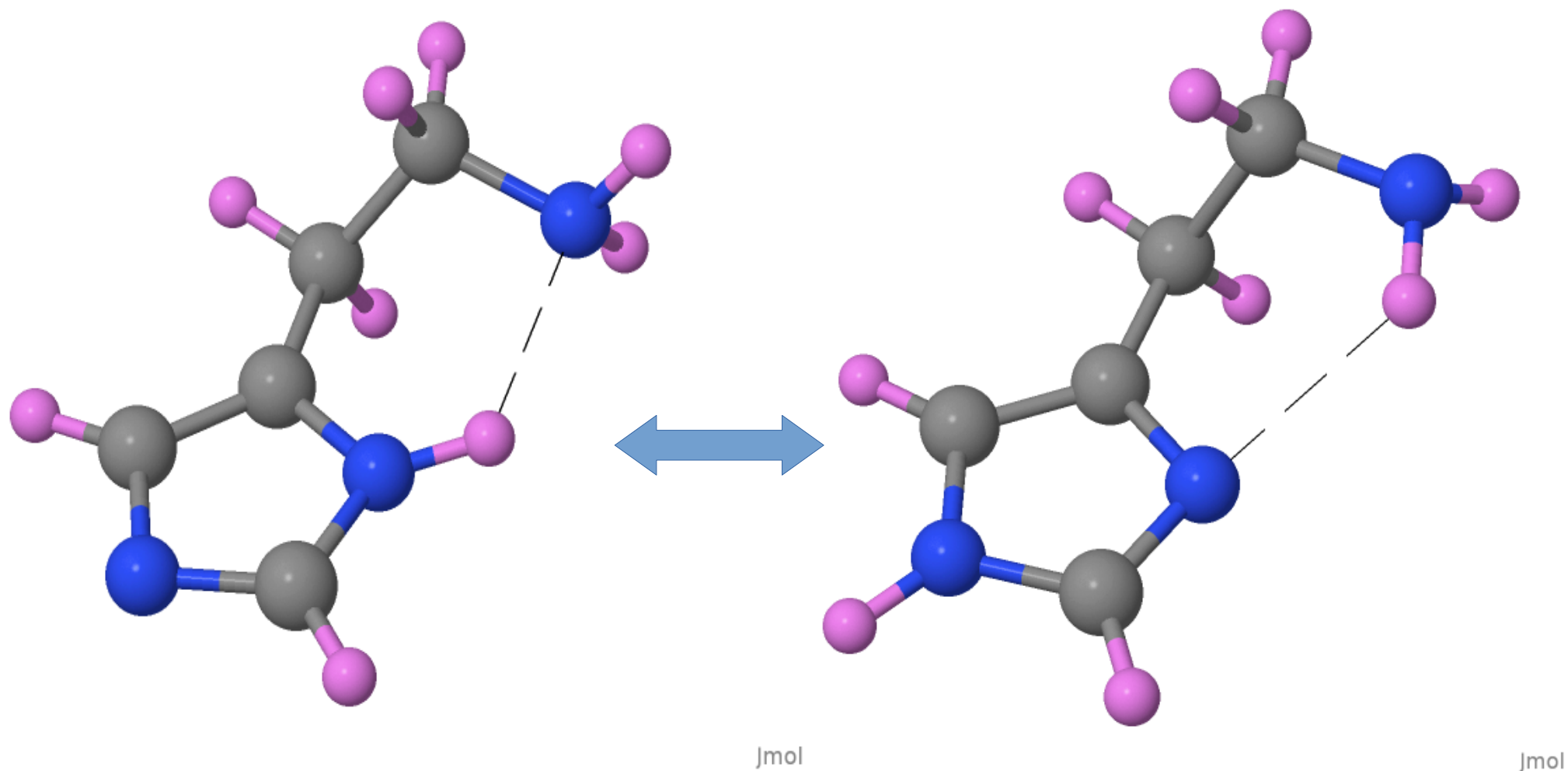


Yu.A. Borisov, N.P. Vorob'eva, I.A. Abronin, A.F. Kolomiets //Bulletin of the
Academy of Sciences of the USSR, Division of chemical science
December 1988, Volume 37, Issue 12, pp 2504-2507

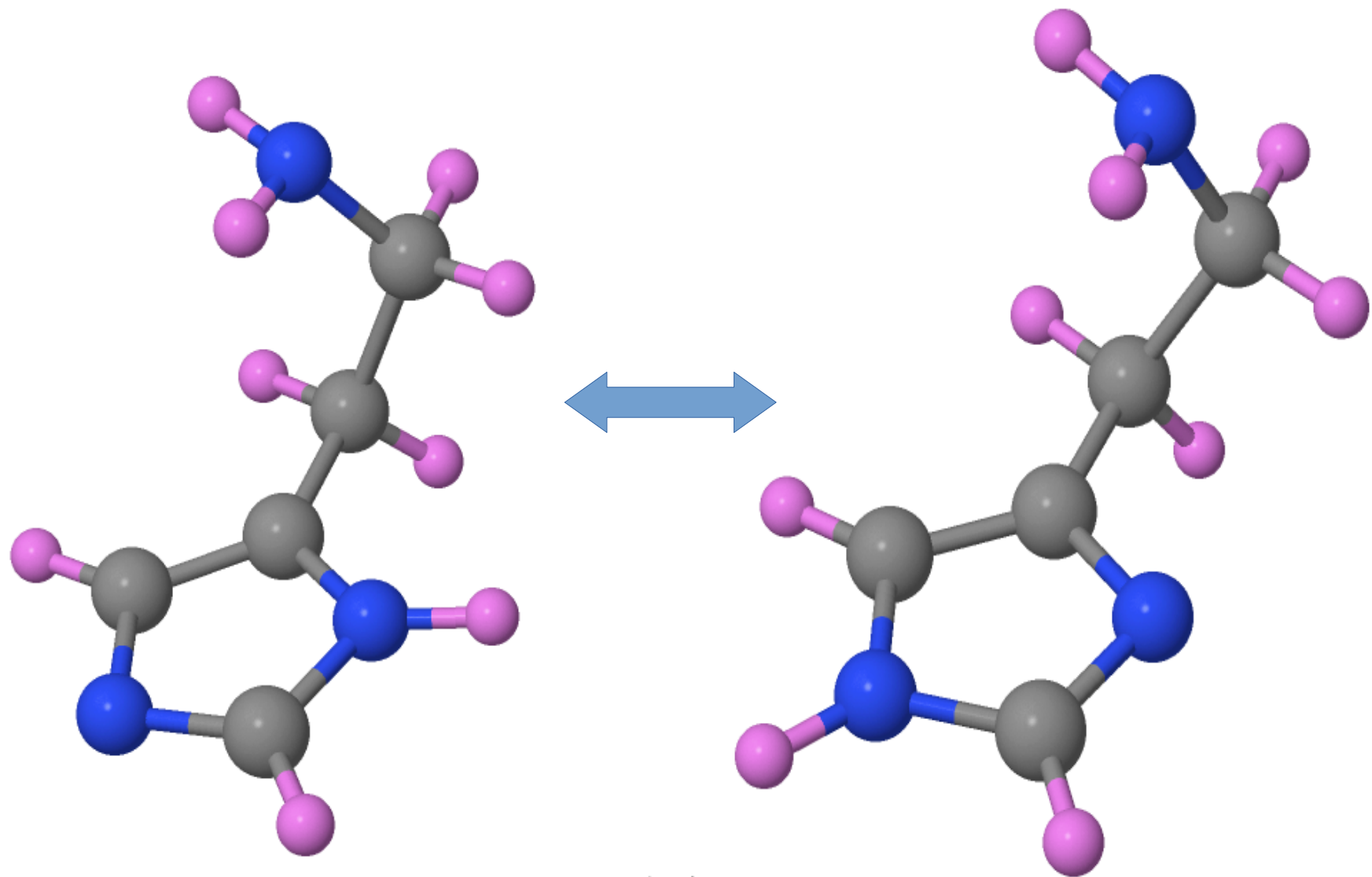
Intermediate electronic structure



Theoretical calculations

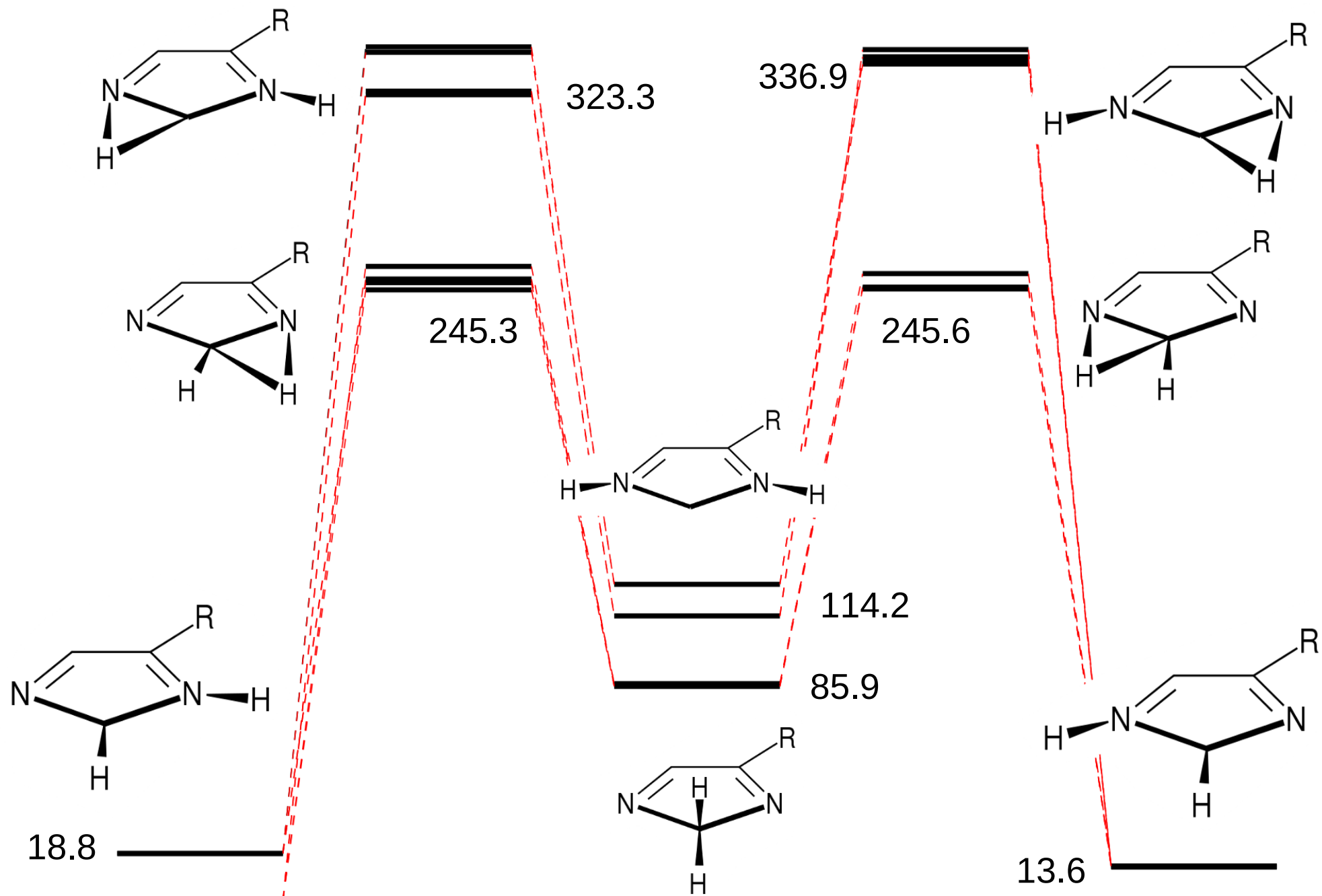


Theoretical calculations



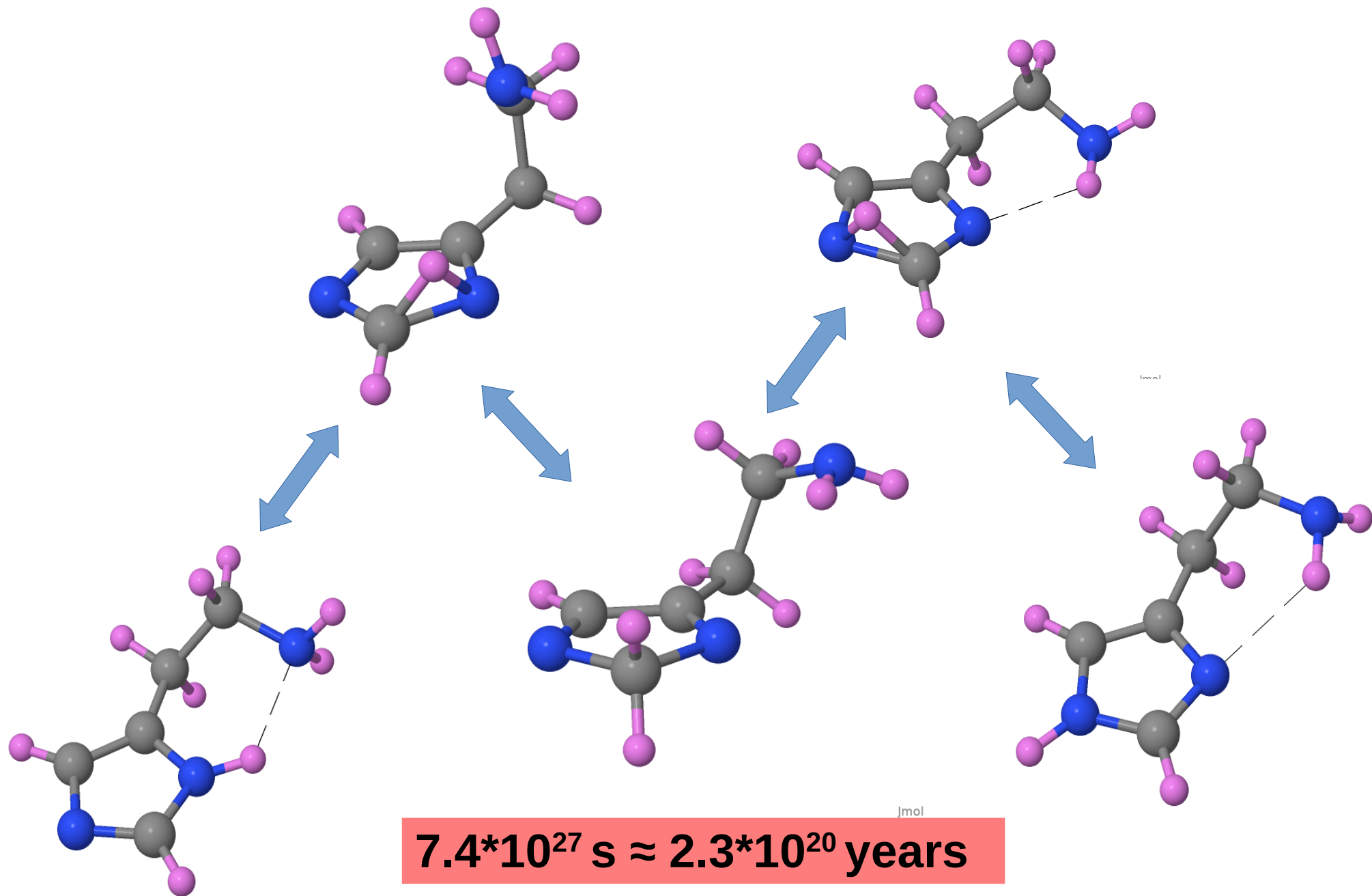
Jmol

Jmol



Note: [kJ/mol]

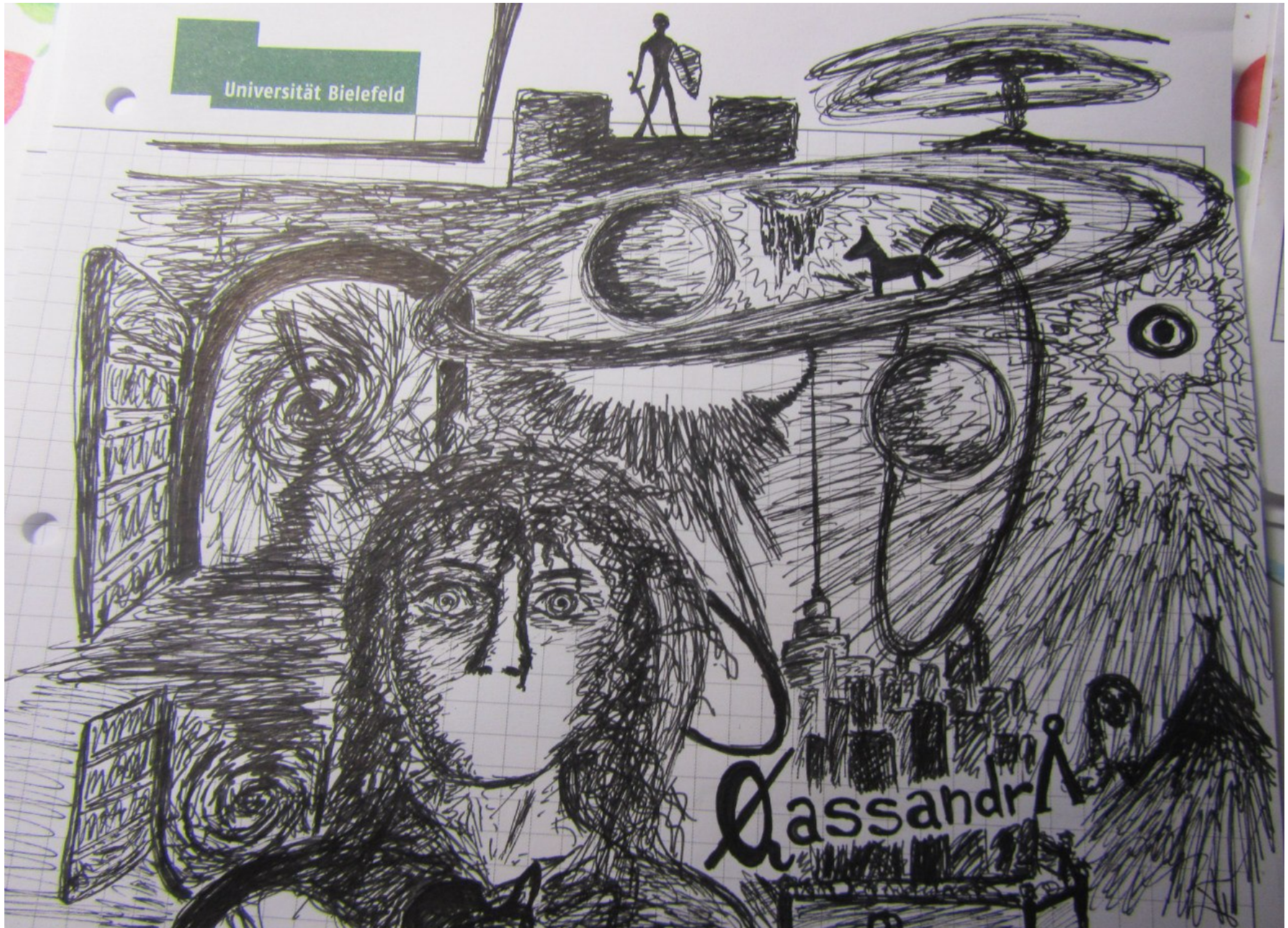
The fastest of the reactions?



Conclusions

- The tautomeric distribution for histamine is probably not the equilibrium one...
(@ the experiment conditions)

Introducing Qassandra v. i1.0



Thank You for Your Attention!

P.S. hoping for lots of questions

