

Supporting info for

## Realistic modeling of Ruthenium Catalyzed Transfer Hydrogenation

Jan-Willem Handgraaf<sup>1</sup> and Evert Jan Meijer\*

van 't Hoff Institute for Molecular Sciences,  
Universiteit van Amsterdam, Nieuwe Achtergracht 166,  
1018 WV Amsterdam, The Netherlands

\*To whom correspondence should be addressed:  
E-mail: ejmeijer@science.uva.nl.

### Movie 1: Constraint released at $Q = 0.1 \text{ \AA}$

Movie 1 shows how the simulation evolves with the constraint released, starting from an initial configuration of the constrained simulation near the transition state ( $Q = -0.1 \text{ \AA}$ ). The total simulation time is 1.2 ps and every frame is 0.85 fs. Reacting molecules are shown in ball-stick representation. Green, red, blue, cyan and white indicate ruthenium, oxygen, nitrogen, carbon, and hydrogen nuclei, respectively. Hydrogen bonds are indicated by yellow dotted lines. Initially, the substrate (formaldehyde), tries to react with the catalyst complex and abstract the Ru-bound hydride. However, a complete transfer of the hydride only occurs when simultaneously the substrate abstracts a proton from a hydrogen bonded solvent molecule at 0.69 ps. The resulting product (methanol) diffuses slowly into solution. The methoxide that is formed after the proton transfer tries to react with the amine-moiety of the ligand by abstracting a proton. However, this reaction does not occur. Instead, the methoxide receives a proton from a hydrogen-bonded solvent molecule that in turn receives a proton from another second solvent molecule. In doing so the proton migrates through the solution. Note that the methoxide is stabilized by hydrogen-bonding interactions.

### Movie Details

Movie formats:

Movie 1.mpg (MPEG-1, 6 Mb, 25 frames per second)

Total run time:

~ 1.5 minute

---

<sup>1</sup>Present address: Soft Matter Chemistry, Leiden Institute of Chemistry, Universiteit Leiden, Einsteinweg 55, 2333 CC Leiden, The Netherlands. E-mail: j.w.handgraaf@chem.leidenuniv.nl.