

Introduction

1

Administration

🗣️ Everything is on the Wiki

🗣️ Help!

- ⌘ Student Demonstrator in the tutorial room 12-1 and 2-4
- ⌘ Staff member around 2-3 **available via e-mail during lab hours**

really, everything!

2

Administration

🗣️ Everything is on the Wiki

🗣️ Help!

- ⌘ Student Demonstrator in the tutorial room 12-1 and 2-4
- ⌘ Staff member around 2-3 **available via e-mail during lab hours**

🗣️ Timetable

- ⌘ On the wiki
- ⌘ Manage your time!!

a problem last year
rough timings on the wiki
ask a staff member

3

Administration

🗣️ Everything is on the Wiki

🗣️ Help!

- ⌘ Student Demonstrator in the tutorial room 12-1 and 2-4
- ⌘ Staff member around 2-3 **available via e-mail during lab hours**

🗣️ Timetable

- ⌘ On the wiki
- ⌘ Manage your time!!
- ⌘ Module 1 5pm fri week 2
- ⌘ Module 2 5pm tues week 4
- ⌘ Module 3 5pm fri week 5

4

Administration

Everything is on the Wiki

Help!

- * Student Demonstrator in the tutorial room 12-1 and 2-4
- * Staff member around 2-3 **available via e-mail during lab hours**

Timetable

- * On the wiki
- * Manage your time!!
- * Module 1 5pm fri week 2
- * Module 2 5pm tues week 4
- * Module 3 5pm fri week 5

penalty for late hand-in
penalty applies only to late material
hand in what you can on-time

your hand-in will be acknowledged
if you don't get a reply within 1
working day see the module
supervisor ASAP

5

Administration

Everything is on the Wiki

Help!

- * Student Demonstrator in the tutorial room 12-1 and 2-4
- * Staff member around 2-3 **available via e-mail during lab hours**

Timetable

- * On the wiki
- * Manage your time!!
- * Module 1 5pm fri week 2
- * Module 2 5pm tues week 4
- * Module 3 5pm fri week 5

Report is a wiki

- * Write-up as you go

6

Administration

Everything is on the Wiki

Help!

- * Student Demonstrator in the tutorial room 12-1 and 2-4
- * Staff member around 2-3 **available via e-mail during lab hours**

Timetable

- * On the wiki
- * Manage your time!!
- * Module 1 5pm fri week 2
- * Module 2 5pm tues week 4
- * Module 3 5pm fri week 5

Report is a wiki

- * Write-up as you go

Feedback via e-mail

You are Unwell / cannot hand in on time

- * See me, early is MUCH better than late

7

Award

ACS 2009 Award in Organometallic Chemistry

- * Odile Eisenstein
- * Theoretical and computational chemist



8

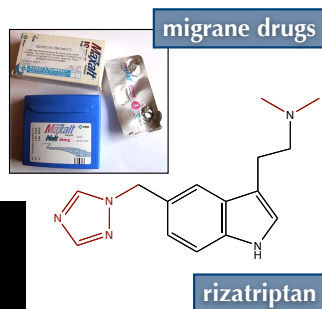
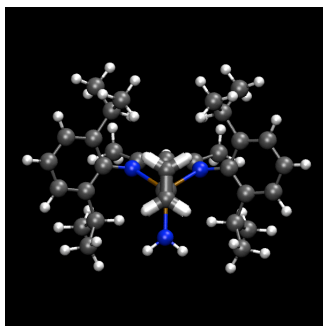
Research

Ca catalysts for hydroamination

- ⌘ key step in synthesizing alkaloids
- ⌘ rizatriptan is an alkaloid, it is used to block the serotonin receptor in the brain

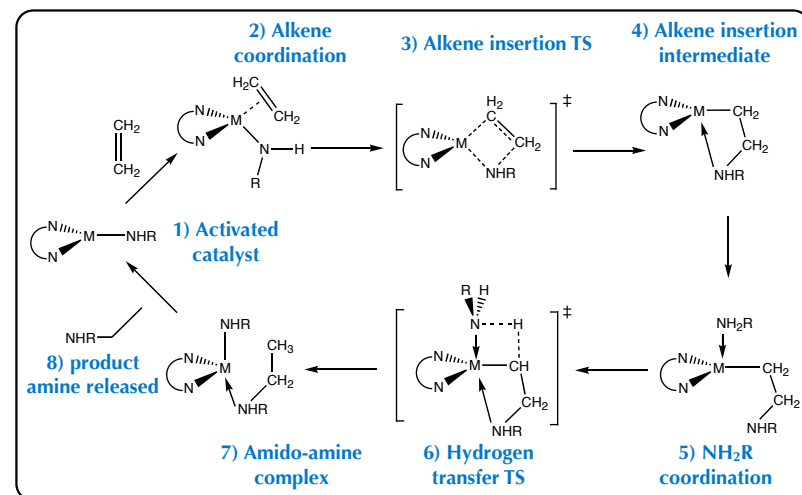
Catalyst

- ⌘ computed:



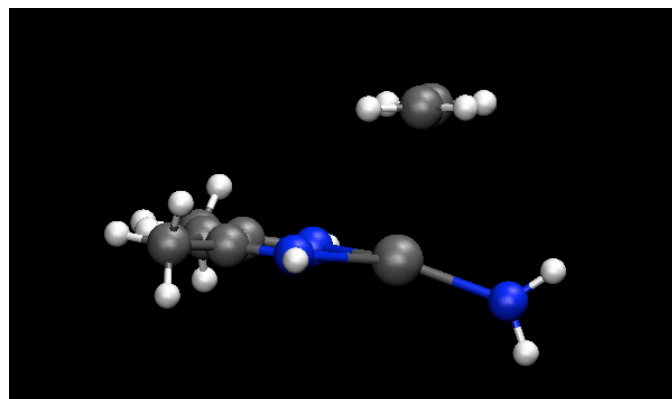
9

Catalytic Cycle



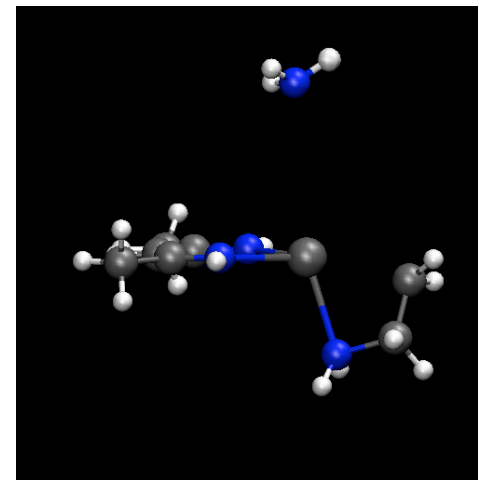
10

Alkene Insertion



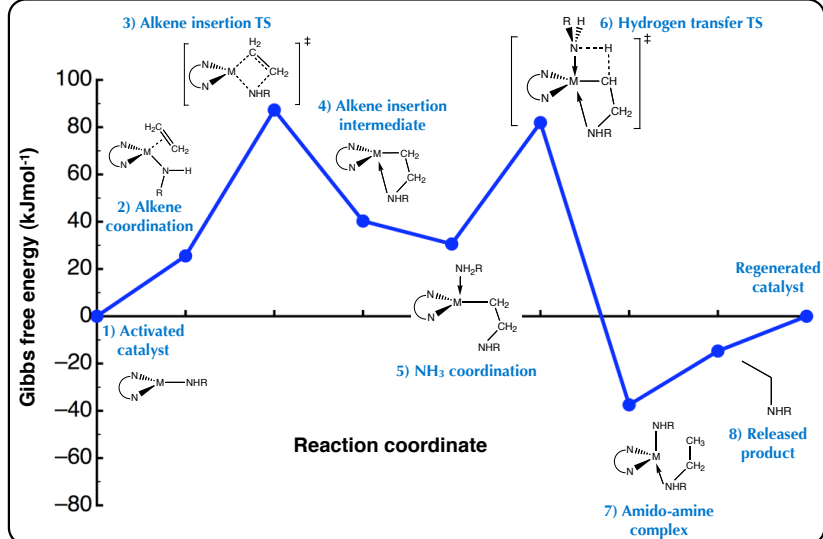
11

H-transfer



12

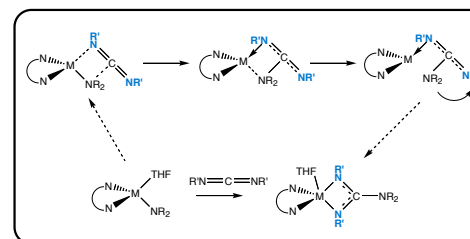
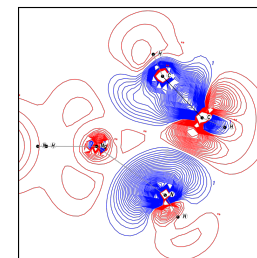
Energy Profile



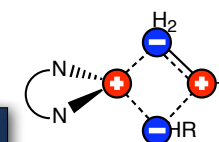
13

Useful Application

- cyclise amines but need to improve the reaction
- need to lower the energy of TS. **HOW?**
- look at the TS: stabilise the charge
- use 1,3-dialkyl substituted carbodiimide
- greater than 95% conversion at room temp in $\approx 30\text{min}$



Dr Mike Hill (Bath)



14