Investigation of group 8 metallocenes @ *TASCA*

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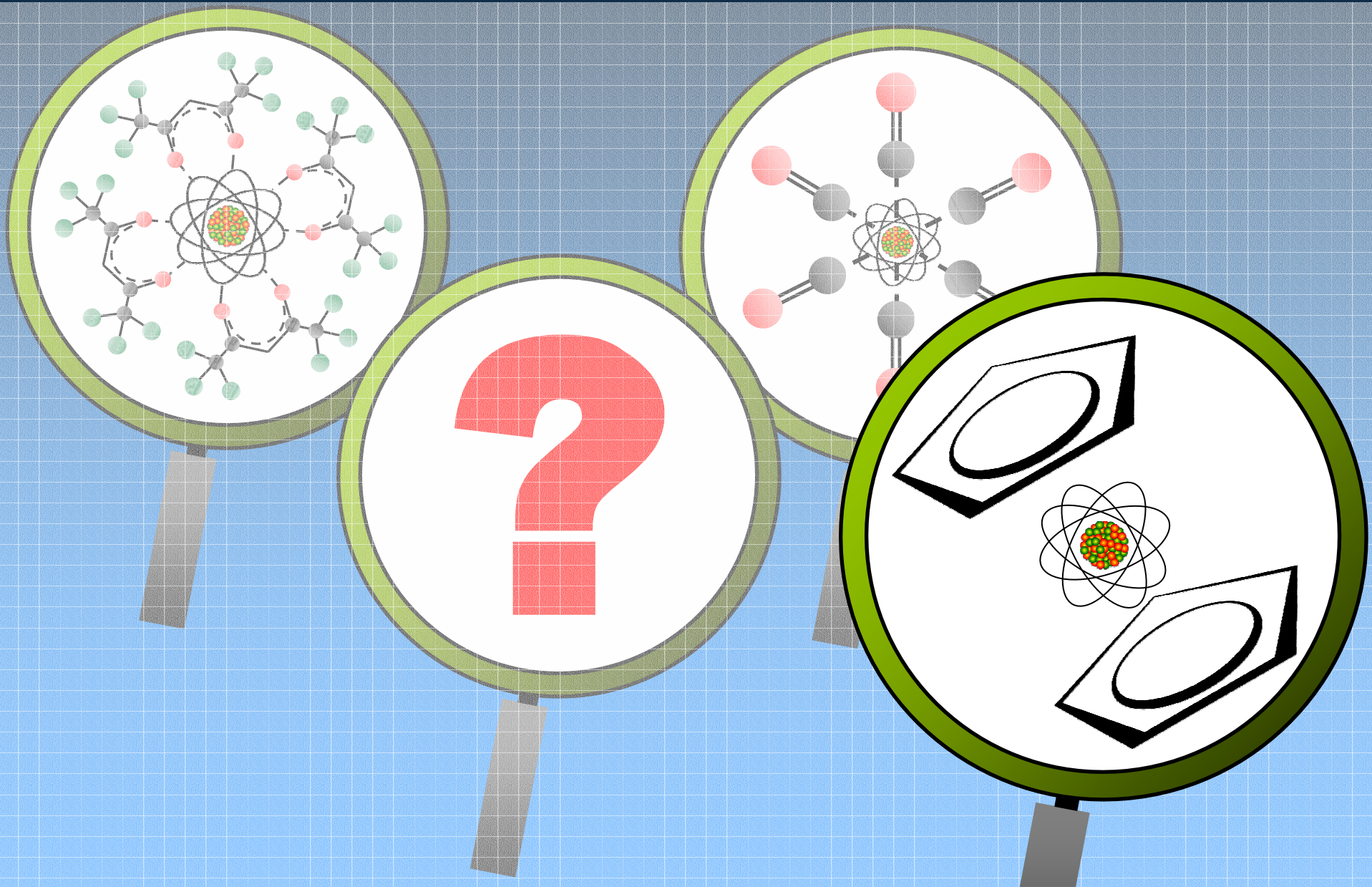
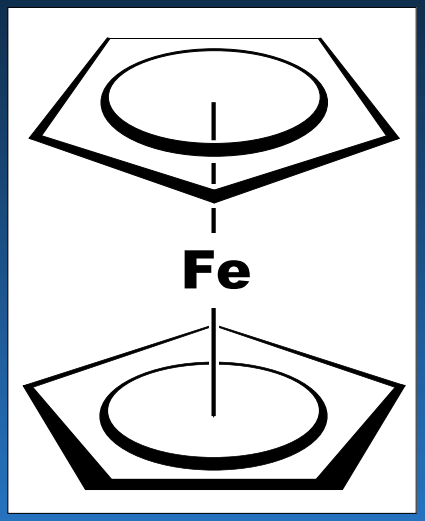
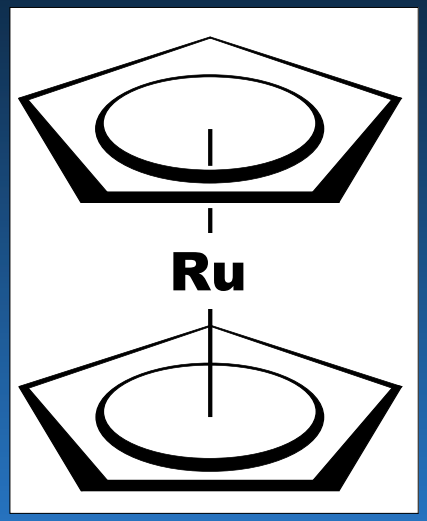
Presented on the 6th workshop on Recoil Separator for Superheavy Element Chemistry *TASCA 07*, September 28, 2007, DAVOS,

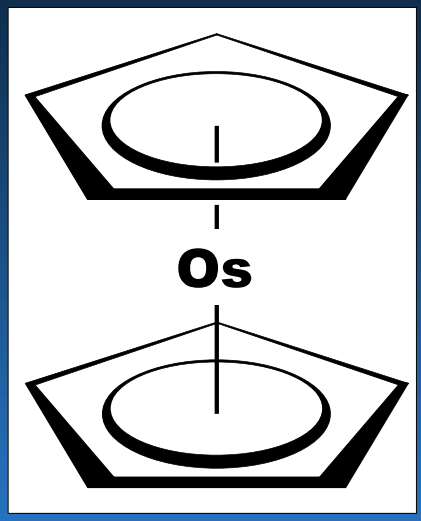
The Bigger Picture

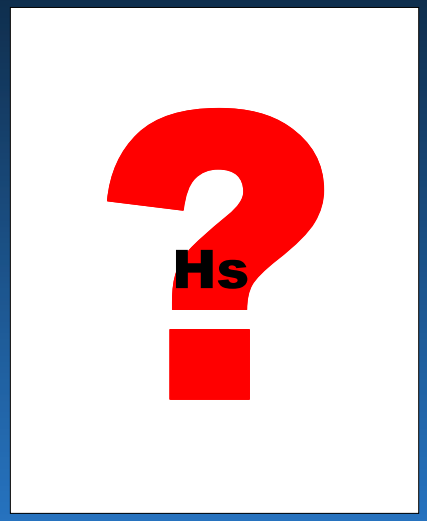


Why Hassocene? Science







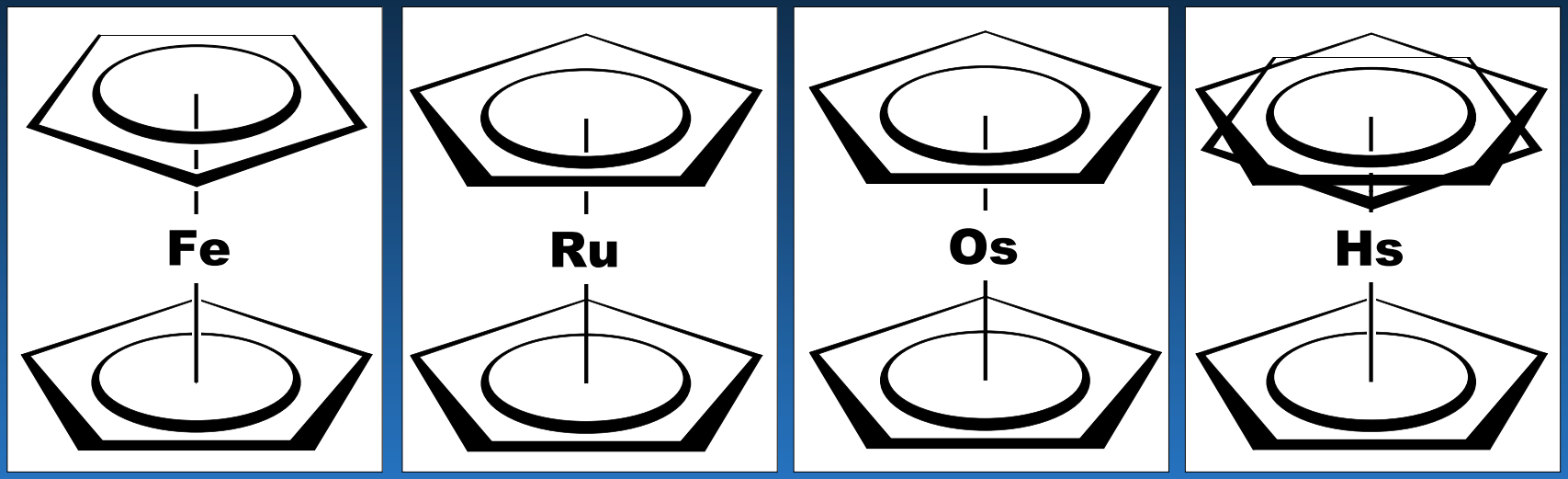


-Group 8 metallocenes: 18 electrons

-$Ru(Cp)_2$ is the most stable metallocene!

-Metal-ring bond strenght: Fe<Ru<Os

Why Hassocene? Science



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ΔH_{sub} [kJ/mol]	73.4±1.1	76-83	73-80	??

J.S. Chickos, W.E. Acree Jr., J. Phys. Chem. Ref. Data 31 (2002) 537

Why Hassocene? Science

- Metallocenes: metal in formal 2+ state (though, ring-metal bonding mainly covalent)

  → in contrast to past studies, where the metal was in its highest oxidation state

  → influence of relativistic effects better visible?

- Due to large number of $M(Cp)_2$: many effects studied systematically across the Periodic Table

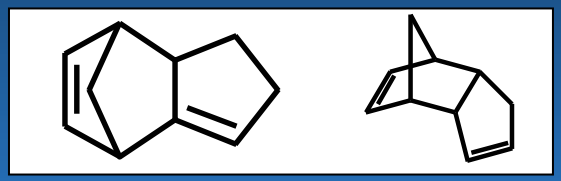
  (example: competing S-O splitting vs. Jahn-Teller following ionization)

- Highly symmetric systems with moderate number of atoms → fully relativistic 4c-DFT calculations planned

How Hassocene? Technical

Cp trivia

Cp is commercially available, it's cheap, comes in dimeric form



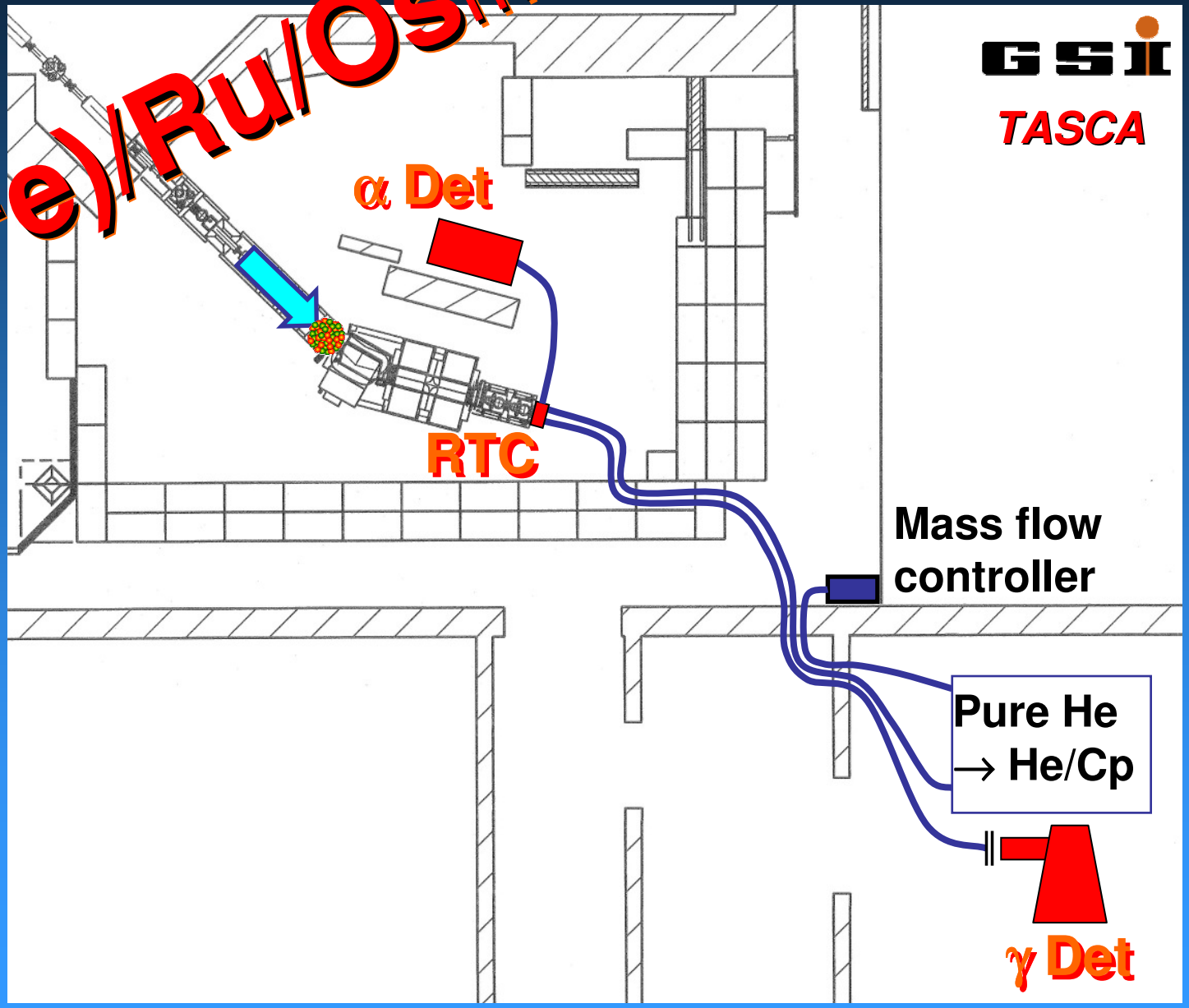
For synthesis, the monomeric form is needed

→ Cracking (usually: thermal cracking @ T>180°C, or at lower temp. with catalyst)

Once cracked, it dimerizes within hours @ room temperature (Diels-Alder-reaction)

→ On-line cracking+distillation!!

Where ~~Hassene~~ (Fe)/Ru/Os moeene?



When Hassocene? Timeline

Early 2008:

Submit proposal to G-PAC, requesting beamtime for preparation experiments with lighter homologs

(Hopefully…) later in 2008:

Start with several rather short (3-5 shifts) runs as soon as beamtime is available

Hassocene

- If $Hs(Cp)_2$ is stable, preseparation should make its investigation possible
- Relatively high volatility expected
- 4c-DFT calculations to be carried out in our group
- Interesting science
- Experiments with $Fe/Ru/Os(Cp)_2$ should start in 2008