



FACULTY OF SCIENCE  
Charles University

## Report on defence of dissertation thesis

Academic year: 2023/2024

**Student's name and surname:** Priyam Bharadwaz  
**Student's ID:** 49552142

**Type of the study programme:** doctoral  
**Study programme:** Modelling of Chemical Properties on Nano- and Biostructures  
**Study ID:** 646990

**Title of the thesis:** Chemical reactivity through the lens of traditional and non-traditional concepts

**Thesis department:** Department of Physical and Macromolecular Chemistry (2600)

**Language of the thesis:** English  
**Language of defence:** English

**Supervisor:** RNDr. Martin Srnec, Ph.D.  
**Reviewer(s):** RNDr. Jan Heyda, Ph.D.  
doc. Mgr. Michal Straka, Ph.D.

**Date of defence:** 18.09.2024    **Venue of defence:** Praha  
**Attempt:** regular

**Course of the examination:**

- chairman Pavel Jungwirth introduced Priyam Bharadwaz
- PJ asked supervisor MS to comment Priyams personality
- PJ asked PB for the presentation of her PhD work (25 min)
- PJ asked the first reviewer M. Straku for providing review + questions related to work
- PJ asked the second reviewer J. Heydu for providing review + questions related to work
- PJ opened the discussion including the members of the committee
  - oJ. Pittner: 1) questions on the relativistic effects in case of Ni complexes.
  - o 2) question on multireference character of Ni complexes.
  - oJiráček: question of MCR vs. methyltransferase (MCR: methyl reductase
  - oObšil: question on alternative pathways for methane production
  - oGrajciar: question on other non-TST cases in chemistry
- PJ asked questions from public
- closed part of defense: evaluation

<b>Result of defence:</b>	pass (P)	
<b>Chair of the board:</b>	Jungwirth Pavel, prof. Mgr., CSc., DSc. (present)	.....
<b>Committee members:</b>	Cwiklik Lukasz (present)	.....
	Grajciar Lukáš, doc. RNDr., Ph.D. (present)	.....
	Jiráček Jiří, RNDr., CSc. (present)	.....
	Kolafa Jiří, prof. RNDr., CSc. (present)	.....
	Obšil Tomáš, prof. RNDr., Ph.D. (present)	.....
	Pittner Jiří, doc. Dr. rer. nat., DSc. (present)	.....