

## IUPAC Subcommittee on “Modeling of Polymerization Kinetics and Processes”

Minutes of meeting held during 29<sup>th</sup> Australasian Polymer Symposium, Hobart, February 12, 2007

### Attendees:

Michal Buback (chair)	Atsushi Kajiwara
Christopher Barner-Kowollik	Bert Klumperman
Patrice Castignolles	Kris Matyjaszewski
Michelle Coote	Graeme Moad
Hans Heuts	Greg Russell

Minutes prepared by Michael Buback and Greg Russell.

1. Minutes from Il Ciocco meeting (September 2006) approved.
2. Greg Russell unanimously elected as new head of the subcommittee, starting immediately after the IUPAC General Assembly to be held 4 – 12 August 2007 in Turin, attendance of which will be Michael Buback’s last duty as subcommittee chair.
3. New members: Shiping Zhu and Denis Bertin were recommended, and to this end they will be contacted in due course.
4. Task-group reports were made as follows, with the resulting actions as indicated:
  - Hans Heuts, Greg Russell and Michael Buback on task-group 2000 – 028 – 1 – 400 (“Critically evaluated termination rate coefficients for free-radical polymerization. 1. Current status, evaluation of experimental methods, data for styrene and methyl methacrylate”, chaired by Greg Russell)  
Action: Hans to prepare first draft of paper on styrene and MMA by the end of June 2007.
  - Atsushi Kajiwara on task-group 2002 – 053 – 1 – 400 (“Establishment of quantitative reliability of electron spin resonance techniques for polymerization kinetics”, chaired by Bunichiro Yamada)  
Action: Bunichiro to submit paper on vinyl pivalate  $k_p$  as soon as possible.
  - Michael Buback on task-group 2004 – 034 – 1 – 400 (“Critically evaluated propagation rate coefficients for free-radical polymerization of water-soluble monomers polymerized in the aqueous phase”, chaired by Igor Lacík)  
Action: None.
  - Michael Buback, Chris Barner-Kowollik, Michelle Coote, Bert Klumperman and Graeme Moad on task-group 2004 – 040 – 1 – 400 (“Towards a holistic mechanistic model for reversible addition fragmentation chain transfer (RAFT) polymerizations: Dithiobenzoates as mediating agents”, chaired by Philipp Vana)  
Action: A meeting of this task-group will take place in Göttingen in September 2007 while Chris B-K is visiting Germany.

5. New projects: The following is a list of suggestions that have been discussed either in the recent past and/or in Hobart, with some being considered more plausible (as IUPAC projects) than others:

- $k_p$  for PEG-ylated MMA (suggested by Kris Matyjaszewski)
- Depropagation
- Combination to disproportionation ratios
- Chain transfer rate coefficients: benchmark values
- Copolymerization: reactivity ratios
- Copolymerization: propagation rate coefficients (models, etc.)
- Chain-length-dependent termination: benchmark values (there are now quite a few systems where the same  $k_t^{i,i}$  values have been found by different groups using different methods)
- Termination: benchmark values for conversion variation (e.g. MMA? MAA?)
- ATRP: current situation on mechanisms; benchmark rate coefficients
- NMP: benchmark rate coefficients
- Initiation: survey of reliable initiator decomposition and initiator efficiency data
- Primary radical addition
- Quantum-chemical calculation of RP rate coefficients: guidelines

6. Next Meetings:

- Definitely the 236<sup>th</sup> ACS Natl. Mtg. in Philadelphia, 17 – 22 Aug. 2008 (Kris M is organizing a symposium at this meeting).
- If there is enough interest then a meeting could also be held at the 2008 World Polymer Congress in Taipei (Taiwan) (worryingly, a few quick Google searches failed to unearth the dates for this congress!).