

Supporting Information for:

On the explanations of the recovery of PLP-molar mass distribution at high laser frequencies: a simulation study

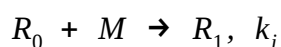
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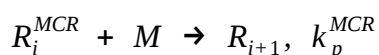
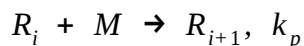
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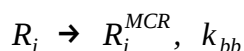
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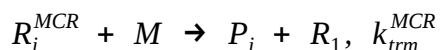
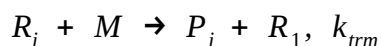
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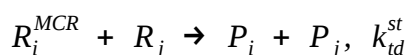
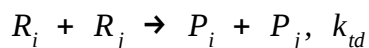
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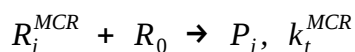
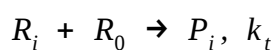
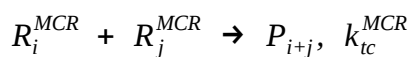
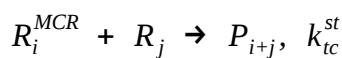
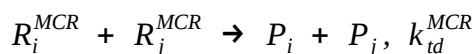


Chain transfer to monomer:

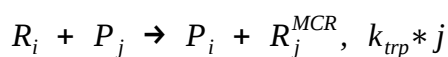


Termination:





Intermolecular transfer to polymer



Scheme SI.1. Kinetic mechanism of the BA polymerization. The rate coefficients are shown in left-hand side of the reaction. M: BA monomer; R_i : chain-end radical with length i ; R_i^{MCR} : MCR with length i ; P_i : dead polymer with length i . R_0 : radical generated in the laser pulse. k_{ti}^{st} is the geometrical average of the termination rates of the involved spices (e.g. $k_{tc}^{st} = \sqrt{k_{tc} * k_{tc}^{MCR}}$).

Table SI.1. Arrhenius parameters for the rate coefficients used for PLP simulation of BA.

Parameter	Frequency factor $L \text{ mol}^{-1} \text{ s}^{-1}$ or s^{-1}	Activation energy kJ mol^{-1}	Reference
$k_i = k_p$	2.21×10^7	17.9	1
k_t	1.3×10^{10}	8.4	2
k_{bb}	7.40×10^7	32.7	3
k_p^{MCR}	1.58×10^6	28.9	4
k_{trm}	2.88×10^5	32.6	5
k_{trm}^{MCR}	2.2×10^5	46.1	5
k_t^{MCR}	1.29×10^7	4.0	5
$^1\text{cd}_s$	0.1	---	6
$^2\text{cd}_t$	0.9	---	6
k_{trp}	2.48×10^3	27.7	7

¹ cd_s termination by disproportionation ratio of chain-end radicals.

² cd_t termination by disproportionation ratio of MCRs.

References

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