

**Dr. Matthias Bechmann**  
Senior lecturer, Institute of  
Organic Chemistry

P +43-(0)732 2468 5412  
matthias.bechmann@jku.at

Office:  
**Alexandra Schinagl, BSc**  
Ext. 5400  
alexandra.schinagl@jku.at

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**Supervisor Review for the Bachelor:**  
**“Characterisation of Polydimethyl Siloxane (PDMS) by liquid-state NMR spectroscopy”**  
**by Solmaz Haddady Khelejan**

The thesis by Solmaz Haddady Khelejan “*Characterisation of Polydimethyl Siloxane (PDMS) by liquid-state NMR spectroscopy*” investigates the platinum catalysed polymerization of commercially available PDMS samples by <sup>1</sup>H nuclear magnetic resonance (NMR) spectroscopy methods. The basis for this thesis are the publications: (i) Mechanical characterisation of energy dissipation in silicone elastomer blends (R. Breuer, 2018); (ii) Solvent Compatibility of Poly(dimethylsiloxane)-Based Microfluidic Devices (J.N. Lee et al 2003); (iii) Understanding NMR Spectroscopy (J. Keeler 2015); (iv) Diffusion-Ordered Spectroscopy (G.A. Morris 2009). In these works the mechanical properties of PDMS are characterised, (i) & (ii). Further in (iii) & (iv) NMR methods are presented that can be used to characterise molecules in general with respect to their structure, size and quantity.

Ms Haddady Khelejan has applied a selection of these NMR methods to the task of analysing the mixture composition of the Base and Curing Agent versions of PDMS. The identification of the NMR resonances corresponding to the reactive sites during the PDMS polymerisation then allowed the monitoring of the polymerisation process in real time. This data was then analysed by an exponential fitting approach. The information here created is useful to further investigate the influence of PDMS composition on the mechanical properties of the PDMS polymer family.

Ms Haddady Khelejan has worked relatively independently. Due to the interdisciplinary character of this thesis, help was provided with the NMR measurements. She was able to extract NMR parameters from spectra by data analysis and evaluated the data series with respect to their time dependence. For data fitting she independently developed a python script for biexponential fitting. She has summarised the relevant primary literature and included relevant secondary literature for this thesis. From the methodological point of view there are a view open questions that

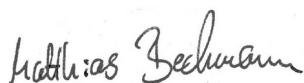
were not explored sufficiently. e.g. the  $^1\text{H}$  spectra have not been completely analysed or  $^{13}\text{C}$  or  $^{29}\text{Si}$  NMR were not considered. This might be partially excused due to the non-chemistry background of the writer.

In this thesis Ms Haddady Khelejan demonstrated that she can cite appropriate literature and explain her scientific approach and analyse and report her results.

**Shortcomings:** The work lacks clarity in some places. The biexponential formula and its application would gain from more substantiation. There are some inconsistencies in the citation method and formatting of references. The plots are acceptable and suitable but would profit from retouching and pruning. Discussion of plots could be a bit more extensive.

**Strength:** Overall the manuscript and the analysis of the results appear thorough. The plots are selected suitably to present the scientific problem and to show the results found by the author. The numeric methods used for the data fitting are sound and applicable for the problem at hand.

I can confidently state that Ms Solmaz Haddady Khelejan is worthy of obtaining a Bachelor of science title, given the work performed in this thesis



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