

Research Overview:

The Excel files in this database are presented in supplement to the work reported by Hall et al. (see "Citation for Dataset" for complete reference) at the University of Michigan in Ann Arbor, MI and at the Illinois Institute of Technology in Chicago, IL. This research is supported by the National Science Foundation, under grants DMR 1403335 and 1707640. In summary, Hall et al. investigates the successes and failures of current tube theory in predicting the rheology of star-linear 1,4-polybutadiene blends. In addition, this study provides a vast assortment of star-linear blend datasets to help assess and develop predictive theories. The excel files featured in this database are the raw data, included both master curves and unshifted plots, of the 1,4-polybutadiene blends presented in Hall et al.

Methods:

The small amplitude oscillatory shear (SOAS) G' and G'' rheology data for the star-linear blends in this database were measured using the Rheometric Scientific ARES-LS and RMS-800 rheometers at temperatures ranging from 25°C to -100°C, using liquid nitrogen as a cooling agent. The TA Orchestrator v7.2.0.4 software was used to horizontally and vertically shift the G' and G'' data to create master curves at reference temperature 25°C. Please note that the applied vertical shifting (b_T) was in proportion to changes in temperature. Density changes with temperature were within around 7%, and were usually ignored in generating the master curves. Example master curves both using, and ignoring, density changes with temperature are shown in Figure S29 in the Supplemental Information of Hall et al. (see "Citation for Dataset" for complete reference).

Please note that select star-linear 1,4-polybutadiene blends reported in Hall et. al. were borrowed from literature for analysis. Details concerning these blends are shown below in File Inventory.

File Inventory:

The 29 Excel files (listed below) in this database contain the 1,4-polybutadiene datasets that were freshly tested via rheology and analyzed with the TA Orchestrator software, as described above, and the 1,4-polybutadiene datasets borrowed from literature. Please note that the files containing the borrowed star-linear blends from literature report the citation. Also note that the reference temperature of all master curve data is 25°C. The temperatures of the unshifted G' and G'' used to generate the master curves are labelled in the Excel files.

24.5KS-7.5KL blends

- Reports the G' and G'' linear rheology for the 24KS-7.5KL 1,4-polybutadiene blends with star volume fractions 0.5, 0.2 and 0.1
- These blends were borrowed from the literature (Shivokhin et al. "Understanding Constraint Release in Star/Linear Polymer Blends." *Macromolecules* **2014**, 47, 2451-2463)
- This star "24.5KS" has 3 arms with a molecular weight of 24.5 kDa per arm

24KS-13.3KL (80%S- 20%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 24KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.8
- This star "24KS" has 4 arms with a molecular weight of 24 kDa per arm

24KS-13.3KL (40%S- 60%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 24KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.4
- This star "24KS" has 4 arms with a molecular weight of 24 kDa per arm

24KS-13.3KL (20%S- 80%L) blend

- Reports the G' and G'' linear rheology for the 24KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.2
- This star "24KS" has 4 arms with a molecular weight of 24 kDa per arm

24KS-13.3KL (10%S- 90%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 24KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.1
- This star "24KS" has 4 arms with a molecular weight of 24 kDa per arm

24KS-58KL blends

- Reports the G' and G'' linear rheology for the 24KS-58KL 1,4-polybutadiene blends with star volume fractions 0.8, 0.6, 0.4, 0.2 and 0.1
- These blends were borrowed from the literature (Desai et al. "Challenging Tube and Slip-Link Models: Predicting the Linear Rheology of Blends of Well-Characterized Star and Linear 1,4-Polybutadienes." *Macromolecules* **2016**, 49 (13), 4964-4977)
- This star "24KS" has 4 arms with a molecular weight of 24 kDa per arm

25.3KS-73KL blends

- Reports the G' and G'' linear rheology for the 25.3KS-73KL 1,4-polybutadiene blends with star volume fractions 0.9, 0.6, 0.3 and 0.1
- This star "25.3KS" has 4 arms with a molecular weight of 25.3 kDa per arm

24KS-210KL blends

- Reports the G' and G'' linear rheology for the 24KS-210KL 1,4-polybutadiene blends with star volume fractions 0.8, 0.6, 0.4, 0.2 and 0.1
- This star "24KS" has 4 arms with a molecular weight of 24 kDa per arm

25.3KS-260KL blends

- Reports the G' and G'' linear rheology for the 25.3KS-260KL 1,4-polybutadiene blends with star volume fractions 0.8, 0.6, 0.4, 0.2 and 0.05
- This star "25.3KS" has 4 arms with a molecular weight of 25.3 kDa per arm

42.3KS-105KL blends

- Reports the G' and G'' linear rheology for the 42.3KS-105KL 1,4-polybutadiene blends with star volume fractions 0.75, 0.5, 0.3, 0.2 and 0.1
- These blends were borrowed from the literature (Struglinski et al. "Effects of Polydispersity on the Linear Viscoelastic Properties of Entangled Polymers. 3. Experimental Observations on Binary Mixtures of Linear and Star Polybutadienes." *Macromolecules* **1998**, 21, 783-789)
- This star "42.3KS" has 3 arms with a molecular weight of 42.3 kDa per arm

44KS-13.3KL (90%S-10%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 44KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.9
- This star "44KS" has 4 arms with a molecular weight of 44 kDa per arm

44KS-13.3KL (80%S-20%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 44KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.8
- This star "44KS" has 4 arms with a molecular weight of 44 kDa per arm

44KS-13.3KL (60%S-40%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 44KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.6
- This star "44KS" has 4 arms with a molecular weight of 44 kDa per arm

44KS-13.3KL (40%S-60%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 44KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.4
- This star "44KS" has 4 arms with a molecular weight of 44 kDa per arm

44KS-13.3KL (20%S-80%L) blend

- Reports the G' and G'' linear rheology, including master curves and unshifted data, for the 44KS-13.3KL 1,4-polybutadiene blend with a star volume fraction of 0.2
- This star "44KS" has 4 arms with a molecular weight of 44 kDa per arm

47KS-73KL blends

- Reports the G' and G'' linear rheology for the 47KS-73KL 1,4-polybutadiene blends with star volume fractions 0.8, 0.6, 0.4, 0.2 and 0.1
- This star "47KS" has 4 arms with a molecular weight of 47 kDa per arm

47KS-260KL blends

- Reports the G' and G'' linear rheology for the 47KS-73KL 1,4-polybutadiene blends with star volume fractions 0.8, 0.6, 0.4 and 0.2
- This star "47KS" has 4 arms with a molecular weight of 47 kDa per arm

7.5KL pure

- Reports the G' and G'' linear rheology for the linear 7.5 kDa 1,4-polybutadiene borrowed from literature (Shivokhin et al. "Understanding Constraint Release in Star/Linear Polymer Blends." *Macromolecules* **2014**, 47, 2451-2463)

13.3KL pure

- Reports the G' and G'' linear rheology for the linear 13.3 kDa 1,4-polybutadiene

58KL pure

- Reports the G' and G'' linear rheology for the linear 58 kDa 1,4-polybutadiene borrowed from the literature (Desai et al. "Challenging Tube and Slip-Link Models: Predicting the Linear Rheology of Blends of Well-Characterized Star and Linear 1,4-Polybutadienes." *Macromolecules* **2016**, 49 (13), 4964-4977)

73KL pure

- Reports the G' and G'' linear rheology for the linear 73 kDa 1,4-polybutadiene

105KL pure

- Reports the G' and G'' linear rheology for the linear 105 kDa 1,4-polybutadiene borrowed from the literature (Struglinski et al. "Effects of Polydispersity on the Linear Viscoelastic Properties of Entangled Polymers. 3. Experimental Observations on Binary Mixtures of Linear and Star Polybutadienes." *Macromolecules* **1998**, 21, 783-789)

210KL pure

- Reports the G' and G'' linear rheology for the linear 210 kDa 1,4-polybutadiene

260KL pure

- Reports the G' and G'' linear rheology for the linear 260 kDa 1,4-polybutadiene

24KS pure

- Reports the G' and G'' linear rheology for the four-arm star 1,4-polybutadiene with a molecular weight of 24 kDa per arm
- Data are borrowed from the literature (Desai et al. "Challenging Tube and Slip-Link Models: Predicting the Linear Rheology of Blends of Well-Characterized Star and Linear 1,4-Polybutadienes." *Macromolecules* **2016**, 49 (13), 4964-4977)

24.5KS pure

- Reports the G' and G'' linear rheology for the three-arm 1,4-polybutadiene with an arm molecular weight of 24.5 kDa per arm
- Data are borrowed from the literature (Shivokhin et al. "Understanding Constraint Release in Star/Linear Polymer Blends." *Macromolecules* **2014**, 47, 2451-2463)

25.3KS pure

- Reports the G' and G'' linear rheology for the four-arm star 1,4-polybutadiene with a molecular weight of 25.3 kDa per arm

42.3KS pure

- Reports the G' and G'' linear rheology for the three-arm 1,4-polybutadiene with a molecular weight of 42.3 kDa per arm
- Data borrowed from the literature (Struglinski et al. "Effects of Polydispersity on the Linear Viscoelastic Properties of Entangled Polymers. 3. Experimental Observations on Binary Mixtures of Linear and Star Polybutadienes." *Macromolecules* **1998**, 21, 783-789)

44KS pure

- Reports the G' and G'' linear rheology for the four-arm star 1,4-polybutadiene with a molecular weight of 44 kDa per arm

47KS pure

- Reports the G' and G'' linear rheology for the four-arm star 1,4-polybutadiene with a molecular weight of 47 kDa per arm

Definition of Terms and Variables:

- The file names listed above utilize the following terminology: "K" represents "kDa," whereas "S" and "L" respectively represent "Star" and "Linear" backbone architecture

- The numbers listed as part of the file names are the molecular weights of the polymers measured by Gel Permeation Chromatography (GPC). The exception to this is the "105KL," which has a GPC molecular weight of 100 kDa.
- The star polymers shown in the files are referenced by their arm molecular weights.
- In the files, G' and G'' respectively represent the elastic and viscous moduli, which are both measured in Pascal
- In the files, "Freq" represents the "Frequency," which is measured in radians/second
- In the files, all temperature readings are conducted in Celsius "C"

Use and Access:

- The files listed in this database may be accessed by Microsoft Excel or a similar software that can read datasheets.
- The files can be used and manipulated for research purposes
- Credit for files used in a journal publication or any public works can be given using the "Citation for Dataset" shown below.

Citation for Dataset:

Hall, R.; Desai, P.S; Kang, B-G; Huang, Q.; Lee, S.; Chang, T.; Venerus, D.C.; Ntetsikas, K.; Polymeropoulos, G.; Hadjichristidis, N.; Larson, R.G. Assessing the Range of Validity of Current Tube Models Through Analysis of a Comprehensive Set of Star-Linear 1,4-Polybutadiene Polymer Blends. *Macromolecules* **2019** (currently under review)