Electronic supplementary materials *Mendeleev Commun.*, 2025, **35**, 739–742

Molecular dynamics simulation of the electrical conductivity of α,ω-bis(3-aminopropyl)polydimethylsiloxane

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Table S1. Molecular mass distribution of various α,ω-bis(3-aminopropyl)polydimethylsiloxane molecules containing *n* dimethylsiloxane units, in the APDMS850 mixture.

Number of units *n*	Number of molecules
2	2
3	4
4	9
5	14
6	19
7	22
8	22
9	20
10	16
11	12
12	8
13	5
14	3
15	2
16	1

Derivation of equation for isothermal compressibility

Let us assume that dependency of the simulation cell volume V on pressure p can be described by means of the linear combination of two exponential functions:

$$V = V(p) = v_1 e^{-\beta_1 (p-p_0)} + v_2 e^{-\beta_2 (p-p_0)} + V_{inf} \,, \tag{S1}$$

where p_0 is the value of pressure under normal conditions. It is not difficult to notice that:

$$\lim_{p\to\infty} V(p) = V_{inf} \,, \tag{S2}$$

$$V(p_0) = v_1 + v_2 + V_{inf} = V_0 \,, \tag{S3}$$

that is, at infinitely high pressure the cell volume tends to the value of V_{inf}, which acquires the meaning of the simulation cell volume, achievable at the ultimate compression, while the sum of V_{inf} and the v_1 and v_2 coefficients is equal to the equilibrium volume of the simulation cell V_0 at standard pressure. On the basis of equation S3, one can obtain an equation for the isothermal compressibility dependency on pressure:

$$\kappa(p) = -\frac{1}{V}\left(\frac{dV}{dp}\right)_{T=const},$$

$$\kappa(p) = \frac{\beta_1 v_1 e^{-\beta_1 (p-p_0)} + \beta_2 v_2 e^{-\beta_2 (p-p_0)}}{v_1 e^{-\beta_1 (p-p_0)} + v_2 e^{-\beta_2 (p-p_0)} + V_{inf}} \,. \tag{S4}$$

The isothermal compressibility calculated in such a way tends to zero at infinitely high pressure:

$$\lim_{p\to\infty} \kappa(p) = 0\,, \tag{S5}$$

which is to be expected. Let us accept the $\kappa(p)$ value at standard pressure p_0 as an estimate of the isothermal compressibility coefficient κ_T:

$$\kappa_T = \kappa(p_0) = \frac{\beta_1 v_1 + \beta_2 v_2}{v_1 + v_2 + V_{inf}}\,. \tag{S6}$$

Derivation of equation for concentration of silyl and silanol ions

Let us assume that the molecular mass distribution of PDMS1250 obeys the Poisson distribution along with APDMS850. Then the λ parameter for PDMS1250 is estimated to be 14.7, which allows us to calculate the molar concentrations C_k of polydimethylsiloxane molecules $PDMS_k$ of different lengths k in it. Let us further assume that the equilibrium constant K for dissociation of the polysiloxane chain into $PDMS_i^-$ and $PDMS_j^+$ ion pair is the same for polydimethylsiloxane molecules of any size. Then the following is valid:

$$K = \frac{[PDMS_i^-][PDMS_j^+]}{[PDMS_k]},\ i + j = k\,. \tag{S7}$$

Denote concentrations of silyl and silanol ions as a_k:

$$[PDMS_i^-] = \left[PDMS_j^+\right] = a_k\,. \tag{S8}$$

Sum of silyl or silanol ion concentration and concentration of corresponding polydimethylsiloxane molecules $PDMS_k$ is equal to C_k, concentration of polydimethylsiloxane molecules $PDMS_k$ in the absence of dissociation:

$$a_k + [PDMS_k] = C_k\,. \tag{S9}$$

Thence equation S7 can be expressed using a_k and C_k values:

$$K = \frac{a_k^2}{C_k - a_k} \tag{S10}$$

and transformed into quadratic equation

$$a_k^2 = KC_k - Ka_k, \tag{S11}$$

$$a_k^2 + Ka_k - KC_k = 0\,, \tag{S12}$$

which is solvable for each a_k and C_k:

$$\Delta = K^2 + 4KC_k,\ a_k^2 = \frac{1}{2}\left(\sqrt{K^2 + 4KC_k} - K\right). \tag{S13}$$

Topologies, cells and GROMACS run parameters files

Topologies, cells and GROMACS run parameters files, used for calculation of physicochemical characteristics of APDMS850, are available in ZENODO repository https://doi.org/10.5281/zenodo.15276451.