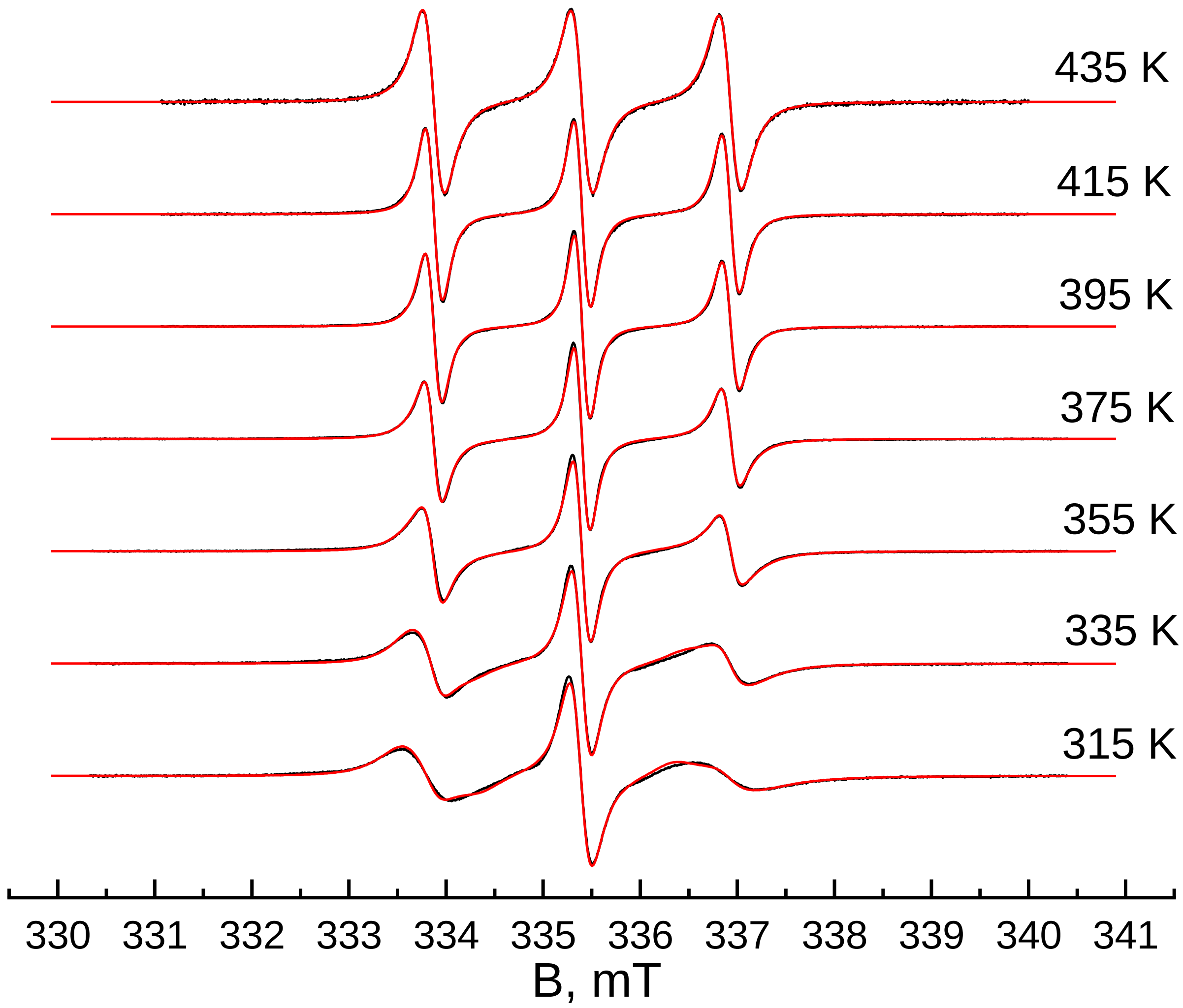
Supplementary Materials

Rotational mobility of TEMPO spin probe in polypropylene: EPR spectra simulation and calculation via approximated formulas

Natalia A. Chumakova [1,2] *, Tatiana S. Yankova [2], Alexander I. Kokorin [1,3,4]

[1] *N. N. Semenov Federal Research Center for Chemical Physics, Russian Academy of Science, Kosygin St. 4, Moscow, 119991, Russia.*
[2] *M. V. Lomonosov Moscow State University, Chemistry Department, Leninskiye Gory, 1/3, Moscow, 119991, Russia*
[3] *Plekhanov Russian University of Economics, Stremyanny per., 36, Moscow, 115093, Russia*
[4] *Infochemistry Scientific Center of ITMO University, Lomonosova str. 9, St. Petersburg 191002, Russia*

[1] N. N. Semenov Federal Research Center for Chemical Physics, Russian Academy of Science, Kosygin St. 4, Moscow, 119991, Russia.
[2] M. V. Lomonosov Moscow State University, Chemistry Department, Leninskiye Gory, 1/3, Moscow, 119991, Russia
[3] Plekhanov Russian University of Economics, Stremyanny per., 36, Moscow, 115093, Russia
[4] Infochemistry Scientific Center of ITMO University, Lomonosova str. 9, St. Petersburg 191002, Russia
* Correspondence: harmonic2011@yandex.ru; Tel.: (+79167974879)



435 K
415 K
395 K
375 K
355 K
335 K
315 K
330
331
332
333
334
335
336
337
338
339
340
341
B, mT

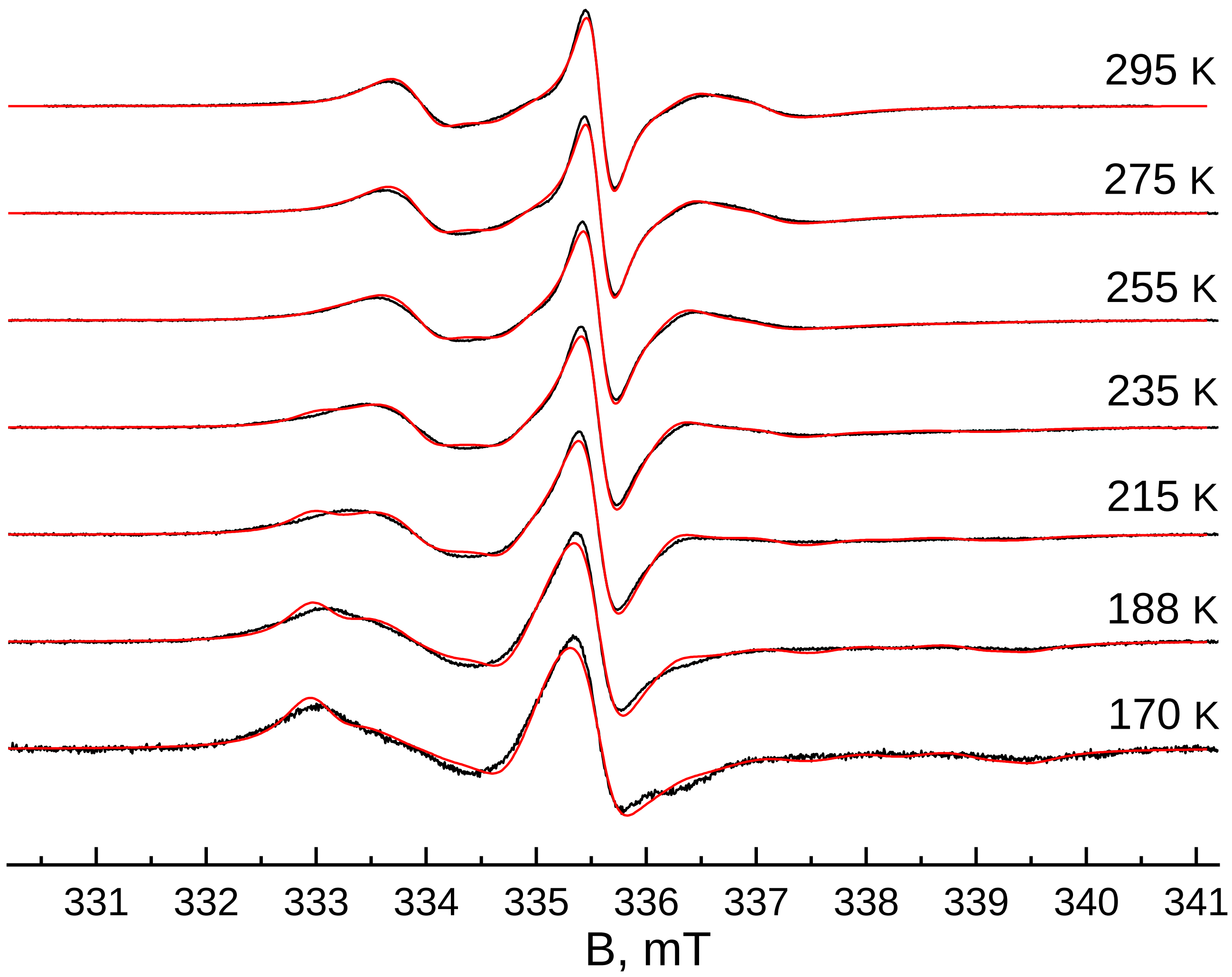


Figure S1. EPR spectra of TEMPO in PP (black lines) and the results of their simulation (red lines).

Table S1. Rotational characteristics of TEMPO in PP.

T,K	τ_x (s)	τ_y (s)	τ_z (s)	$\langle\tau_c\rangle$ (s)	σ_x	σ_y	σ_z	$\langle\sigma\rangle$	Libr, isotrop	h_G (G)	h_L (G)	$\tau_c^*(1)$ (s)	$\tau_c^*(2)$ (s)	$\tau_c^*(3)$ (s)	$\tau_c^*(4)$ (s)
435	$2.5\cdot10^{-11}$			$2.5\cdot10^{-11}$	$0.70^{\#}$			$0.70^{\#}$	–	$0.8^{\#}$	1.7	$2.58\cdot10^{-11}$	$2.20\cdot10^{-11}$	$2.55\cdot10^{-11}$	$2.41\cdot10^{-11}$
425	$3.3\cdot10^{-11}$			$3.3\cdot10^{-11}$	$0.70^{\#}$			$0.70^{\#}$	–	$0.8^{\#}$	1.4	$3.24\cdot10^{-11}$	$5.72\cdot10^{-11}$	$3.32\cdot10^{-11}$	$4.40\cdot10^{-11}$
415	$4.25\cdot10^{-9}$	$1.53\cdot10^{-11}$	$2.09\cdot10^{-10}$	$4.26\cdot10^{-11}$	$0.70^{\#}$			$0.70^{\#}$	–	$0.8^{\#}$	1.1	$4.29\cdot10^{-11}$	$1.31\cdot10^{-10}$	$4.21\cdot10^{-11}$	$8.41\cdot10^{-11}$
405	$7.15\cdot10^{-8}$	$2.02\cdot10^{-11}$	$3.58\cdot10^{-10}$	$5.74\cdot10^{-11}$	$0.70^{\#}$			$0.70^{\#}$	–	$0.8^{\#}$	0.9	$6.31\cdot10^{-11}$	$2.34\cdot10^{-10}$	$6.10\cdot10^{-11}$	$1.43\cdot10^{-10}$
395	$1.67\cdot10^{-7}$	$3.09\cdot10^{-11}$	$5.31\cdot10^{-10}$	$8.76\cdot10^{-11}$	$0.70^{\#}$			$0.70^{\#}$	–	$0.8^{\#}$	0.8	$7.05\cdot10^{-11}$	$3.54\cdot10^{-10}$	$6.72\cdot10^{-11}$	$2.03\cdot10^{-10}$
385	$1.7\cdot10^{-7\,\#}$	$4.68\cdot10^{-11}$	$7.72\cdot10^{-10}$	$1.32\cdot10^{-10}$	$0.70^{\#}$			$0.70^{\#}$	–	$0.8^{\#}$	0.7	$9.43\cdot10^{-11}$	$5.00\cdot10^{-10}$	$8.45\cdot10^{-11}$	$2.84\cdot10^{-10}$
375	$1.7\cdot10^{-7\,\#}$	$5.65\cdot10^{-11}$	$1.24\cdot10^{-9}$	$1.62\cdot10^{-10}$	0.75			$0.70^{\#}$	–	$0.8^{\#}$	0.7	$1.23\cdot10^{-10}$	$6.66\cdot10^{-10}$	$1.13\cdot10^{-10}$	$3.77\cdot10^{-10}$
365	$1.7\cdot10^{-7\,\#}$	$7.31\cdot10^{-11}$	$1.59\cdot10^{-9}$	$2.10\cdot10^{-10}$	0.71			$0.70^{\#}$	–	$0.8^{\#}$	0.6	$1.56\cdot10^{-10}$	$9.10\cdot10^{-10}$	$1.37\cdot10^{-10}$	$5.08\cdot10^{-10}$
355	$1.7\cdot10^{-7\,\#}$	$1.08\cdot10^{-10}$	$2.03\cdot10^{-9}$	$3.08\cdot10^{-10}$	0.68			$0.70^{\#}$	–	$0.8^{\#}$	0.7	$2.24\cdot10^{-10}$	$1.25\cdot10^{-9}$	$1.92\cdot10^{-10}$	$7.05\cdot10^{-10}$
345	$1.7\cdot10^{-7\,\#}$	$2.43\cdot10^{-10}$	$4.31\cdot10^{-9}$	$6.88\cdot10^{-10}$	$0.70^{\#}$			$0.70^{\#}$	27°	$0.8^{\#}$	0.8	$3.58\cdot10^{-10}$	$1.84\cdot10^{-9}$	$3.09\cdot10^{-10}$	$1.05\cdot10^{-9}$
335	$1.7\cdot10^{-7\,\#}$	$3.92\cdot10^{-10}$	$6.41\cdot10^{-9}$	$1.11\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	28°	$0.8^{\#}$	0.9	$5.23\cdot10^{-10}$	$2.53\cdot10^{-10}$	$5.05\cdot10^{-10}$	$1.46\cdot10^{-10}$
325	$1.7\cdot10^{-7\,\#}$	$5.46\cdot10^{-10}$	$7.47\cdot10^{-9}$	$1.52\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	25°	$0.8^{\#}$	0.9	$7.76\cdot10^{-10}$	$3.26\cdot10^{-10}$	$8.25\cdot10^{-10}$	$1.94\cdot10^{-10}$
315	$1.7\cdot10^{-7\,\#}$	$5.44\cdot10^{-10}$	$9.06\cdot10^{-9}$	$2.05\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	25°	$0.8^{\#}$	0.9	$1.01\cdot10^{-9}$	$3.97\cdot10^{-9}$	$1.06\cdot10^{-9}$	$2.39\cdot10^{-9}$
305	$1.7\cdot10^{-7\,\#}$	$8.68\cdot10^{-10}$	$9.86\cdot10^{-9}$	$2.38\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	21°	$0.8^{\#}$	0.8	$1.14\cdot10^{-9}$	$4.45\cdot10^{-9}$	$1.28\cdot10^{-9}$	$2.69\cdot10^{-9}$
295	$1.7\cdot10^{-7\,\#}$	$9.80\cdot10^{-10}$	$9.98\cdot10^{-9}$	$2.66\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	19°	$0.8^{\#}$	0.8	$1.29\cdot10^{-9}$	$4.78\cdot10^{-9}$	$1.52\cdot10^{-9}$	$2.92\cdot10^{-9}$
285	$1.7\cdot10^{-7\,\#}$	$1.03\cdot10^{-9}$	$1.03\cdot10^{-8}$	$2.79\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	20°	$0.8^{\#}$	0.8	$1.44\cdot10^{-9}$	$5.02\cdot10^{-9}$	$1.68\cdot10^{-9}$	$3.11\cdot10^{-9}$
275	$1.7\cdot10^{-7\,\#}$	$1.16\cdot10^{-9}$	$1.05\cdot10^{-8}$	$3.11\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	17°	$0.8^{\#}$	0.8	$1.56\cdot10^{-9}$	$5.47\cdot10^{-9}$	$1.82\cdot10^{-9}$	$3.39\cdot10^{-9}$
265	$1.7\cdot10^{-7\,\#}$	$1.39\cdot10^{-9}$	$1.05\cdot10^{-8}$	$3.65\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	15°	$0.8^{\#}$	0.8	$1.81\cdot10^{-9}$	$5.92\cdot10^{-9}$	$2.21\cdot10^{-9}$	$3.73\cdot10^{-9}$
255	$1.7\cdot10^{-7\,\#}$	$1.54\cdot10^{-9}$	$1.02\cdot10^{-8}$	$3.99\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	10°	$0.8^{\#}$	0.7	$2.30\cdot10^{-9}$	$6.66\cdot10^{-9}$	$2.86\cdot10^{-9}$	$4.34\cdot10^{-9}$
245	$1.7\cdot10^{-7\,\#}$	$1.69\cdot10^{-9}$	$1.09\cdot10^{-8}$	$4.35\cdot10^{-9}$	$0.70^{\#}$			$0.70^{\#}$	<1°	$0.8^{\#}$	0.8	$2.78\cdot10^{-9}$	$7.34\cdot10^{-9}$	$3.56\cdot10^{-9}$	$4.91\cdot10^{-9}$
235	$1.7\cdot10^{-7\,\#}$	$2.44\cdot10^{-9}$	$8.55\cdot10^{-9}$	$5.63\cdot10^{-9}$	1.27	1.02	0.39	0.89	–	$0.8^{\#}$	0.7	$3.48\cdot10^{-9}$	$8.22\cdot10^{-9}$	$4.61\cdot10^{-9}$	$5.70\cdot10^{-9}$
225	$1.7\cdot10^{-7\,\#}$	$2.91\cdot10^{-9}$	$8.05\cdot10^{-9}$	$6.33\cdot10^{-9}$	1.14	1.11	0.33	0.86	–	$0.8^{\#}$	0.7	$5.17\cdot10^{-9}$	$1.01\cdot10^{-8}$	$7.24\cdot10^{-9}$	$7.50\cdot10^{-9}$
215	$1.7\cdot10^{-7\,\#}$	$3.59\cdot10^{-9}$	$9.47\cdot10^{-9}$	$7.69\cdot10^{-9}$	0.96	1.31	0.37	0.88	–	$0.8^{\#}$	1.0	$5.66\cdot10^{-9}$	$1.07\cdot10^{-8}$	$8.54\cdot10^{-8}$	$8.02\cdot10^{-9}$
207	$1.7\cdot10^{-7\,\#}$	$4.79\cdot10^{-9}$	$1.08\cdot10^{-8}$	$9.75\cdot10^{-9}$	1.21	1.27	0.26	0.91	–	$0.8^{\#}$	1.0	$6.45\cdot10^{-9}$	$1.14\cdot10^{-8}$	$1.02\cdot10^{-8}$	$8.80\cdot10^{-9}$

198	$1.7\cdot10^{-7\,\#}$	$6.24\cdot10^{-9}$	$1.30\cdot10^{-8}$	$1.23\cdot10^{-8}$	1.20	1.39	0.23	0.94	–	$0.8^{\#}$	1.2	$7.76\cdot10^{-9}$	$1.29\cdot10^{-8}$	$1.38\cdot10^{-8}$	$1.02\cdot10^{-8}$
188	$1.7\cdot10^{-7\,\#}$	$8.77\cdot10^{-9}$	$1.53\cdot10^{-8}$	$1.62\cdot10^{-8}$	1.06	1.56	0.16	0.93	–	$0.8^{\#}$	1.5	$6.94\cdot10^{-9}$	$1.16\cdot10^{-8}$	$1.39\cdot10^{-8}$	$9.17\cdot10^{-9}$
179	$1.7\cdot10^{-7\,\#}$	$1.20\cdot10^{-8}$	$1.67\cdot10^{-8}$	$2.01\cdot10^{-8}$	0.95	1.69	0.12	0.92	–	$0.8^{\#}$	1.7	$6.13\cdot10^{-9}$	$1.06\cdot10^{-8}$	$1.19\cdot10^{-8}$	$8.23\cdot10^{-9}$
170	$1.7\cdot10^{-7\,\#}$	$1.71\cdot10^{-8}$	$1.77\cdot10^{-8}$	$2.48\cdot10^{-8}$	0.87	1.83	<0.10	0.90	–	$0.8^{\#}$	1.9	$6.52\cdot10^{-9}$	$1.09\cdot10^{-8}$	$1.28\cdot10^{-8}$	$8.59\cdot10^{-9}$

τ_x, τ_y, and τ_z are rotational correlation times corresponding to the molecular axes X, Y, and Z of TEMPO (see Fig.1b in the main text); $\langle\tau_c\rangle$ is the averaged rotational correlation time $\langle\tau_c\rangle = (\tau_x + \tau_y + \tau_z)/3$; $\tau_c^*(1)$, $\tau_c^*(2)$, $\tau_c^*(3)$, and $\tau_c^*(4)$ are rotational correlation times calculated by empirical formulas (1), (2), and (3) (see the main text); σ_x, σ_y, and σ_z are the widths of lognormal distribution of the rotational diffusion coefficients $D_{rot}=1/(6\cdot\tau_c)$ corresponding to the axes X, Y, and Z; $\langle\sigma\rangle$ is the averaged distribution width $\langle\sigma\rangle = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$; Libr is the amplitude of quasilibrations [1] *(isotropic value); h_G and h_L are the contributions of Gauss and Lorentz functions into the Voigt function describing the individual line shape.*

1. Chernova, D.A.; Vorobiev, A.K. Molecular Mobility of Nitroxide Spin Probes in Glassy Polymers. Quasi-libration Model. *J. Polym. Sci. Part B Polym. Phys.* **2009**, *47*, 107–120, doi:10.1002/polb.21619.