Supplementary information file

1. RooPositron is a computer program that fits positron lifetime spectra with different models. Program is written in C++ language and utilizes CERN ROOT libraries. The outstanding features of RooPositron are following: open-source code, any researcher can contribute; ability to add custom fitting models that correspond to meaningful physical parameters; in-depth control of the convolution operation properties; fitting models support calculation of indirect parameters. Program comes with a detailed `readme` file that covers installation, usage and adding custom models. RooPositron is hosted on GitHub (https://github.com/petrstepanov/roopositron).

2. Comparison between two 3-exp deconvolutions of the measured LT spectra when τ_1 was fixed to 125 ps (the p-Ps lifetime in vacuum) and when it is considered as a "common-free" parameter for each gas bubbling.

Table 1. Parameters of the 3-exponential decomposition of the LT spectra of the initially aerated isooctane, cyclohexane, isopropanol and water, and also after their bubbling with argon, oxygen and air at room temperature. The deviations of the values corresponding to "no bubbling" and "air bubbling" characterize experimental uncertainty of the data (τ_1 = 125 ps – fixed, $\lambda_o = 1/\tau_3$).

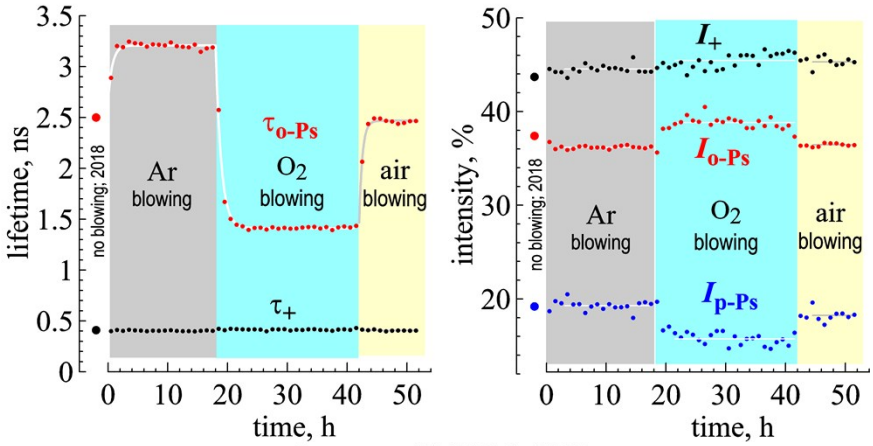
Liquid	I_1, %	τ_1, ns	I_2, %	τ_2, ns	I_3, %	τ_3, ns	$\lambda_o = 1/\tau_3$, ns^{-1}
Isooctane							
– Ar bubbling	22	0.125	35.1	0.44	42.9	4.03	0.248
– air bubbling	19.6	0.125	36.8	0.44	43.6	2.52	0.397
– no bubbling	20.1	0.125	35.4	0.44	44.6	2.55	0.39
– O_2 bubbling	15.8	0.125	33.3	0.47	51	1.11	0.90
Cyclohexane							
– Ar bubbling	19.3	0.125	44.55	0.404	36.2	3.21	0.312
– air bubbling	18.25	0.125	45.3	0.407	36.45	2.47	0.405
– no bubbling	19.2	0.125	43.7	0.41	37	2.5	0.40
– O_2 bubbling	15.74	0.125	45.44	0.415	38.8	1.41	0.71
Isopropanol							
– Ar bubbling	13.56	0.125	63.8	0.41	22.64	3.75	0.267
– no bubbling	13.3	0.125	63.9	0.41	22.8	3.1	0.323
– O_2 bubbling	11.45	0.125	65.0	0.41	23.53	1.86	0.538
Water							
– Ar bubbling	14.6	0.125	59.3	0.377	26.1	1.814	0.551
– air bubbling	14.2	0.125	59.76	0.377	26.0	1.81	0.552
– no bubbling	12.8	0.125	60.3	0.374	27	1.776	0.563
– O_2 bubbling	16.6	0.125	59.8	0.37	26.6	1.73	0.578

Below is the results of the fit when τ_1 was considered as a "common free" parameter for each gas bubbling:

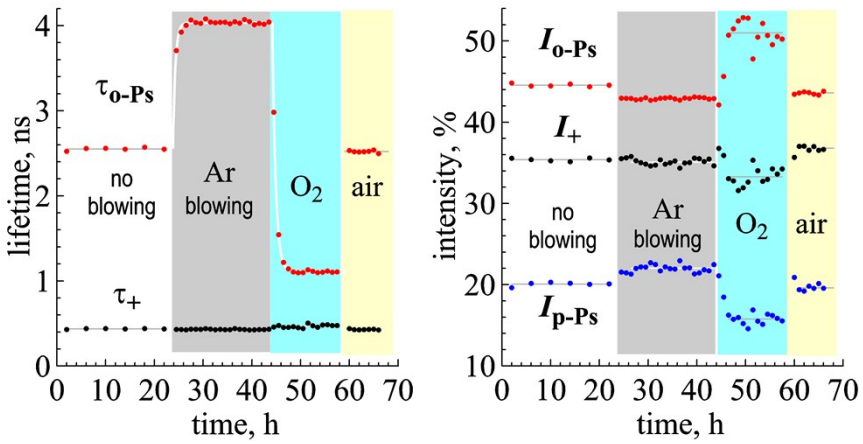
Liquid	I_1, %	τ_1, ps	I_2, %	τ_2, ns	I_3, %	τ_3, ns	$\lambda_o = 1/\tau_3$, ns^{-1}
Isooctane							
– Ar bubbling	24.6	148(1)	32.3(1)	0.45(1)	43.1(1)	4.01(1)	0.249
– air bubbling	21.8	145(1)	34.4(2)	0.45(1)	43.8(1)	2.51(1)	0.398
– before bubbling	22.6	149(1)	32.7(1)	0.46(1)	44.7(1)	2.546(3)	0.393
– O_2 bubbling	14	116(3)	31(1)	0.43(1)	55(2)	1.077(6)	0.929
Cyclohexane							
– Ar bubbling	25	165(2)	38.9(4)	0.44(1)	36.1(4)	3.26(4)	0.307
– air bubbling	23.9	165(2)	40.1(4)	0.45(1)	36.1(4)	2.515(40)	0.398
– O_2 bubbling	17.4	141(2)	44.3(4)	0.43(1)	38.4(4)	1.42(4)	0.703
Isopropanol							
– Ar bubbling	21.7	194(3)	56(1)	0.44(2)	22.5(1)	3.75(10)	0.267
– before bubbling	21	193(3)	56(1)	0.44(2)	22.5(10)	3.2(1)	0.313
– O_2 bubbling	16	173(4)	61(1)	0.43(2)	22.9(8)	1.905(10)	0.525
Water							
– Ar bubbling	31	213(4)	44(4)	0.44(2)	25(4)	1.833(16)	0.546
– air bubbling	25	194(3)	49(1)	0.42(2)	25.5(1)	1.802(15)	0.555
– O_2 bubbling	27	200(3)	47(4)	0.42(1)	26(3)	1.746(14)	0.573

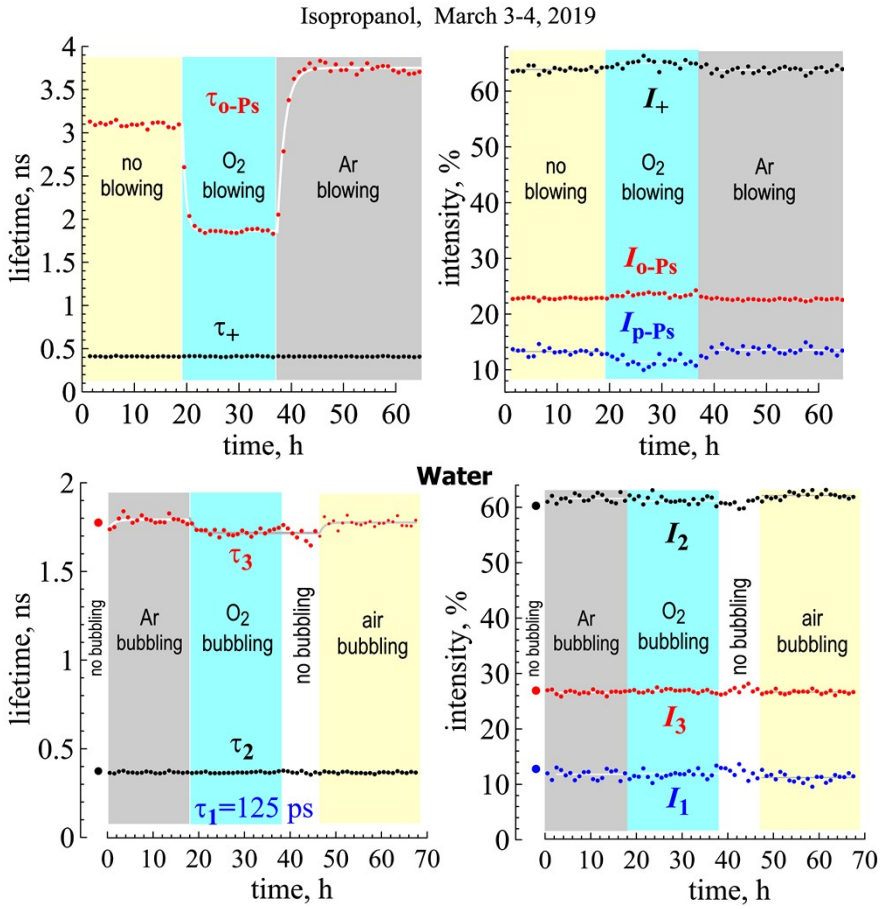
Results of the 3-exp fit when τ_1 was fixed to 125 ps (former pictures):

Cyclohexane. March 1-2, 2019



Isooctane, 25-27 Feb. 2019





Below there is a comparison of the fitting parameters (see Table 3) when p-Ps lifetime is fixed to 125 ps and to 160 ps:

Table 3. Parameters of the model Eqs. (5-10) obtained as a result of fitting of the LT spectra of liquids with different O_2 contents, $\tau_+ = 1/\lambda_+$, $\tau_{po} = 1/\lambda_{po}$, $\lambda_{qf} = \lambda_+$, $\lambda_b = 20$ ns^{-1}, $\lambda_{2\gamma} = 8$ ns^{-1}.

Liquid	$\lambda_+ = \lambda_{qf}$; τ_+ ns^{-1}; ns	λ_{po}; τ_{po} ns^{-1}; ns	P_{qf}	k_{opc}, M^{-1}s^{-1}	k_{ox}, M^{-1}s^{-1}	$k_{opc}/4 + k_{ox}$, M^{-1}s^{-1}
Isooctane	2.37 0.42	0.25 4.0	0.63	$9.7 \cdot 10^{10}$	$2.4 \cdot 10^{10}$	$4.8 \cdot 10^{10}$
Cyclohexane	2.52 0.40	0.32 3.1	0.53	$10.7 \cdot 10^{10}$	$1.1 \cdot 10^{10}$	$3.75 \cdot 10^{10}$
Isopropanol	2.50 0.40	0.27 3.7	0.34	$9.3 \cdot 10^{10}$	$0.5 \cdot 10^{10}$	$2.83 \cdot 10^{10}$
Water	2.40 0.41	0.55 1.81	0.48	$1.8 \cdot 10^{10}$	$1.3 \cdot 10^{10}$	$1.75 \cdot 10^{10}$

The following data correspond to p-Ps lifetime equal to **160 ps** (all other parameters are same):

Table 3. Parameters of the model Eqs. (5-10) obtained as a result of fitting of the LT spectra of liquids with different O_2 contents, $\lambda_{qf} = \lambda_+$, $\lambda_b = 20$ ns^{-1}, $\lambda_{2\gamma} = 1/0.16$ ns^{-1} (in accordance with the magnetic quenching experiments [11, 12]).

Liquid	$\lambda_+ = \lambda_{qf}$; $\tau_+ = 1/\lambda_+$ ns^{-1} ; ns	λ_{po} ; $\tau_{po} = 1/\lambda_{po}$ ns^{-1} ; ns	P_{qf}	k_{opc}, M^{-1}s^{-1}	k_{ox}, M^{-1}s^{-1}	$k_{opc}/4 + k_{ox}$, M^{-1}s^{-1}
Isooctane	2.430(1) 0.412	0.252(1) 3.968	0.639(2)	$9.62(9) \cdot 10^{10}$	$2.37(3) \cdot 10^{10}$	$4.78(5) \cdot 10^{10}$
Cyclohexane	2.568(2) 0.389	0.320(3) 3.125	0.542(1)	$12.6(2) \cdot 10^{10}$	$1.02(4) \cdot 10^{10}$	$4.17(5) \cdot 10^{10}$
Isopropanol	2.509(1) 0.399	0.276(2) 3.622	0.340(2)	$9.8(1) \cdot 10^{10}$	$0.35(5) \cdot 10^{10}$	$2.82(5) \cdot 10^{10}$
Water	2.516(8) 0.397	0.556(1) 1.799	0.451(3)	$1(1) \cdot 10^{10}$	$1.1(4) \cdot 10^{10}$	$1.3(8) \cdot 10^{10}$

Statistical uncertainties of the fitting parameters are indicated in parenthesis.