Molecular Dynamics in a Blue Phase Liquid Crystal: A ^{1}H fast field-cycling NMR relaxometry study (Electronic Supplementary Information)

Anton Gradišek,[a‡] Tomaž Apih,[ab] Valentina Domenici,[c], Vladimira Novotna,[d] and Pedro José Sebastião[e]

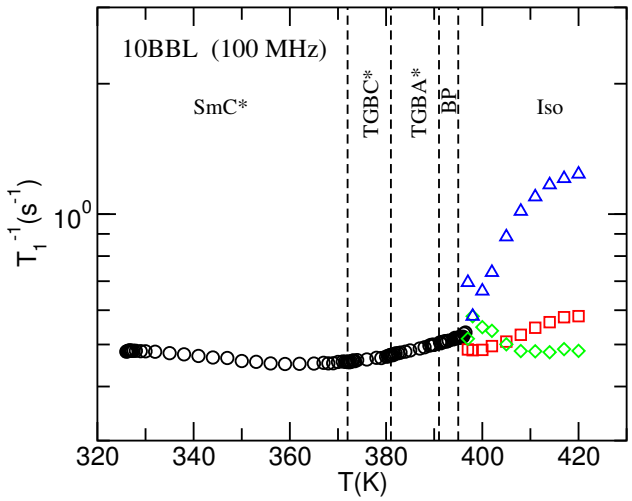

Fig. 1 Experimental spin-lattice relaxation results obtained as a function of temperature for the Larmor frequency of 100 MHz. In color are presented the values of the three relaxation rate components of the magnetization decay obtained in the isotropic phase.

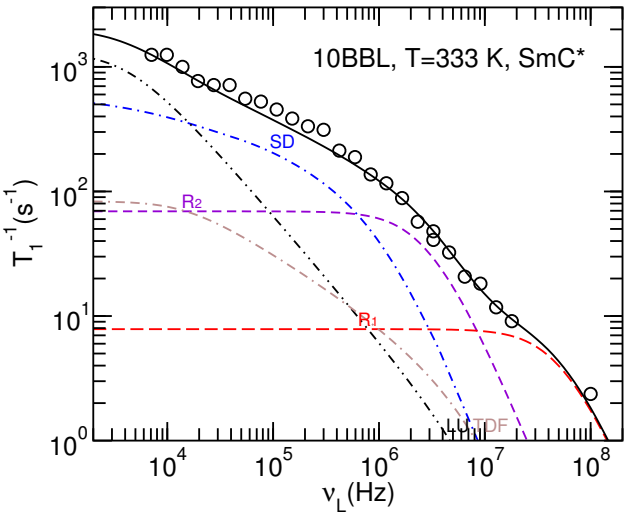

Fig. 2 Best global model fit results of the 10BBL experimental spin-lattice relaxation dispersion results obtained at 333 K in the SmC*, as explained in the paper's main text.

In Figure 1 are presented the T_1^{-1} results obtained as a function of temperature for the Larmor frequency 100 MHz. The analysis of the experimental results obtained in the isotropic phase were not considered in this study that is focused on the results obtained in the 10BBL mesophases.

The model fit to the experimental data was made using a non-linear least-square minimization procedure with a global minimum target for all experimental results. However, in view of the diverse relaxation mechanisms relevant for the spin-lattice relaxation in each mesophase the iterative global minimization procedure followed four steps. In each step the least square minimization of the T_1^{-1} model to experimental results of each mesophase was attempted taking into account the model fitting parameters obtained for the other mesophases.

In the following are presented the fit reports obtained for each mesophase, using the software package referred in the paper's main text. As it can be observed in addition to the T_1^{-1} temperature dependence presented in the paper's main text for three selected Larmor frequencies the global fit was performed taking into account additional T_1^{-1} data obtained for 4 MHz, 100 kHz, and 10 kHz.

In the case of the SmC* phase in addition to the T_1^{-1} dispersion fit at 353 K presented in the in Figure 5d) in the main text of this paper a fit of the T_1^{-1} dispersion obtained at 333 K is presented in Figure 2.

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fitteia Report

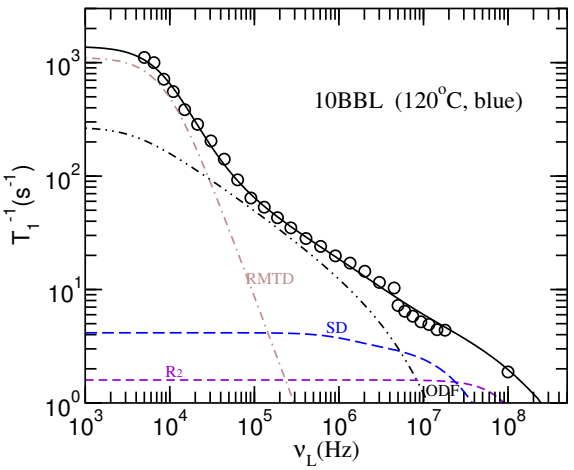
(internet based fitter service)

Subject	BBL, blue-fT-SDN
Date	Monday 22nd July, 2013, 18:10
Affiliation	pj.sebastiao@gmail.com 193.136.137.244
Abstract	Fit report produced with the fit results of function: z=BPPfT(x, y, a1, tau1, E1, Tref) + RdrfT(x, y, Adr, taudr, ED, Tref) + (y<1000.0) ? SDN11_2_DllDp2(x, d, n, tauD*exp(ED/8.31*(1.0/y-1.0/Tref)), 0.0) : SDN11_2_DllDp2(y, d, n, tauD*exp(ED/8.31*(1.0/x-1.0/Tref)), 0.0) + BPPfT(x, y, af, tauf, ER, Tref) + ODFNfT(x, y, fcm, fcM0, fcM1, Aodf0, Aodf1, Aodf2, Tref) to the 111 experimental points, considering 5 free parameters.

$tau1 = 1.96 \times 10^{-09}$ (fixed)
$a1 = 4.19 \times 10^{+08}$ (fixed)
$E1 = 68380$ (fixed)
$Adr = 3.0956 \times 10^{+07} \pm 8.7293 \times 10^{+05}$
$taudr = 3.83 \times 10^{-05}$ (fixed)
$fcm = 3172.2$ (fixed)
$fcM0 = 1.0201 \times 10^{+07} \pm 9.7814 \times 10^{+05}$
$fcM1 = 0$ (fixed)
$d = 5.6448$ (fixed)
$n = 6.76 \times 10^{+22}$ (fixed)

$tauD = 6.6307 \times 10^{-09} \pm 6.0563 \times 10^{-10}$
$ED = 54684$ (fixed)
$af = 8.81 \times 10^{+08}$ (fixed)
$tauf = 3.21 \times 10^{-10}$ (fixed)
$ER = 41475$ (fixed)
$Aodf0 = -21.738 \pm 1151.4$
$Aodf1 = 1011 \pm 64.358$
$Aodf2 = 0$ (fixed)
$Tref = 376$ (fixed)

$\chi^2[100000] = 66.0708$
$\chi^2[393] = 112.784$
$\chi^2[1 \times 10^{+08}] = 1.19465$
$\chi^2[1 \times 10^{+06}] = 37.9991$
$\chi^2[4 \times 10^{+06}] = 31.6175$
$\chi^2_t = 249.666$



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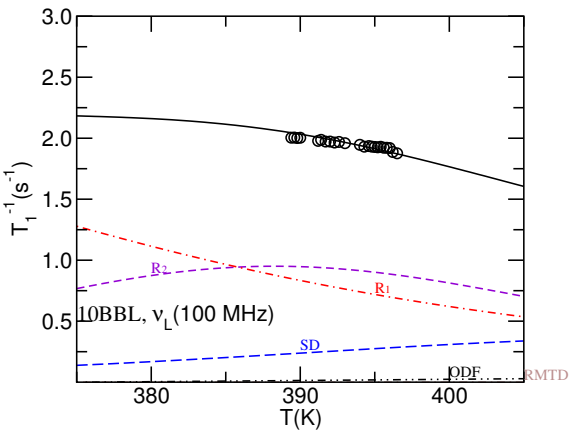

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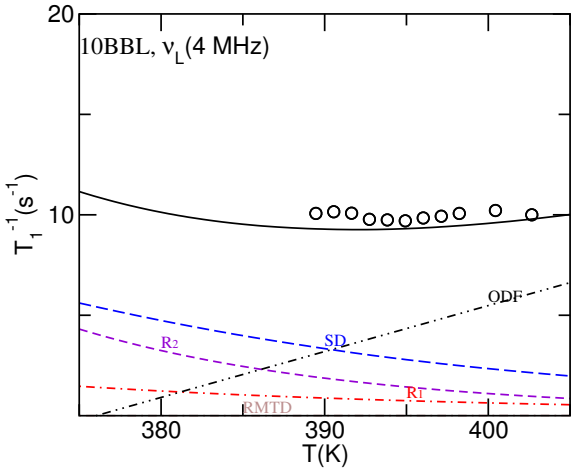

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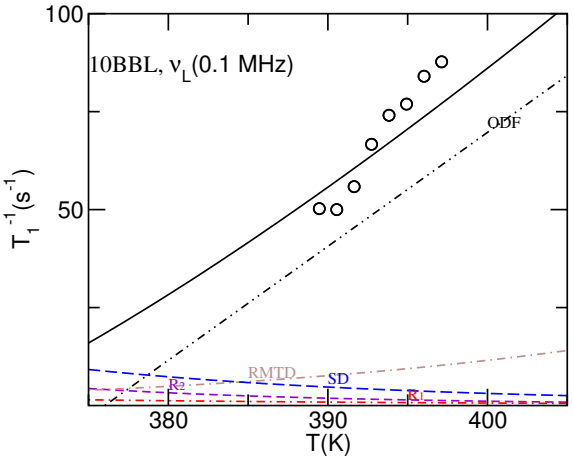

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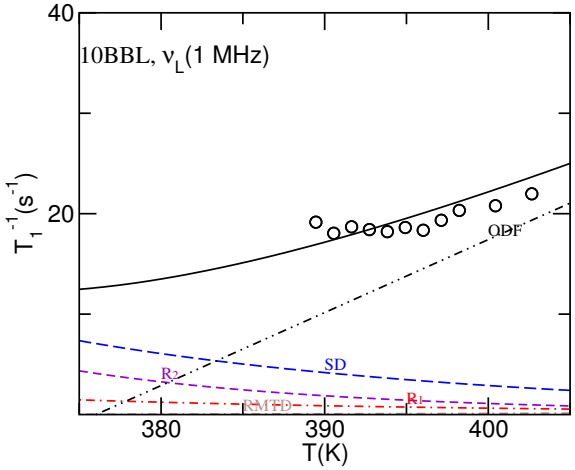


recta-4.pdf

fitteia Report

(internet based fitter service)

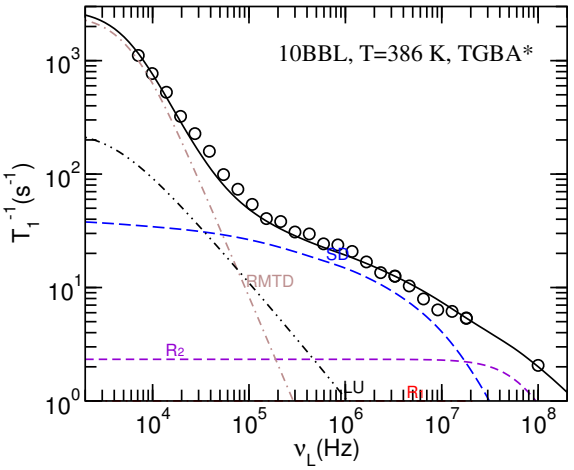
Subject	BBL, TGBA-fT
Date	Monday 3rd June, 2013, 23:09
Affiliation	pj.sebastiao@gmail.com 146.164.6.8
Abstract	Fit report produced with the fit results of function: z=BPPfT(x, y, a1, tau1, E1, Tref) + RdrfT(x, y, Adr, taudr, Edr, Tref) + SDSmA11_polifT(x, y, d, n, tauD, ED, Tref) + BPPfT(x, y, af, tauf, ER, Tref) + LUfT(x, y, Alu0, Alu1, Alu2, fcm, fcM, Tref) to the 224 experimental points, considering 6 free parameters.

$tau1 = 1.96 \times 10^{-09}$ (fixed)
$a1 = 4.19 \times 10^{+08}$ (fixed)
$E1 = 68364$ (fixed)
$Adr = 4.5756 \times 10^{+07} \pm 2.2544 \times 10^{+06}$
$taudr = 3.7643 \times 10^{-05} \pm 8.9938 \times 10^{-06}$
$Edr = 36254 \pm 25785$
$fcm = 3000$ (fixed)
$fcM = 1 \times 10^{+07}$ (fixed)
$d = 5$ (fixed)
$n = 6.76 \times 10^{+22}$ (fixed)

$tauD = 1.3143 \times 10^{-08} \pm 3.0538 \times 10^{-10}$
$ED = 65220$ (fixed)
$af = 8.81 \times 10^{+08}$ (fixed)
$tauf = 3.21 \times 10^{-10}$ (fixed)
$ER = 41475$ (fixed)
$Alu0 = 7.7451 \times 10^{+05} \pm 3.6348 \times 10^{+05}$
$Alu1 = -52182 \pm 33913$
$Alu2 = 8751$ (fixed)
$Tref = 376$ (fixed)

$\chi^2[386] = 259.879$
$\chi^2[1 \times 10^{+06}] = 17.4151$
$\chi^2[1 \times 10^{+08}] = 2.73594$
$\chi^2_t = 359.804$

$\chi^2[100000] = 10.9764$
$\chi^2[4 \times 10^{+06}] = 25.7939$
$\chi^2[40000] = 43.0034$



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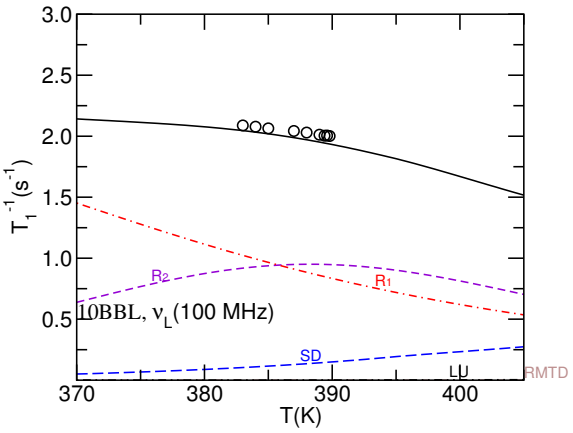

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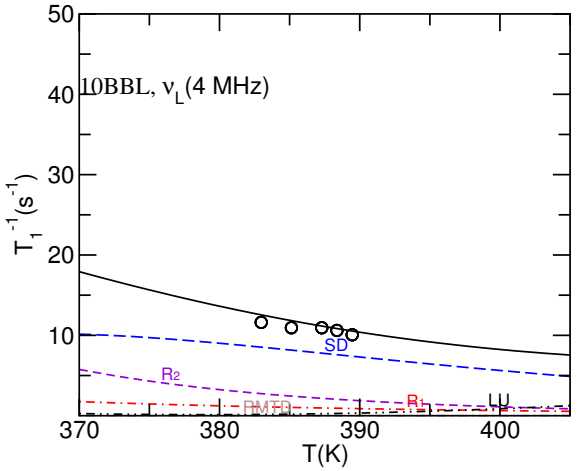

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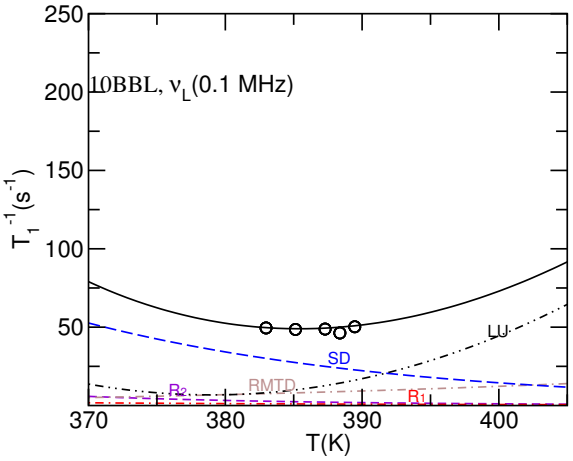

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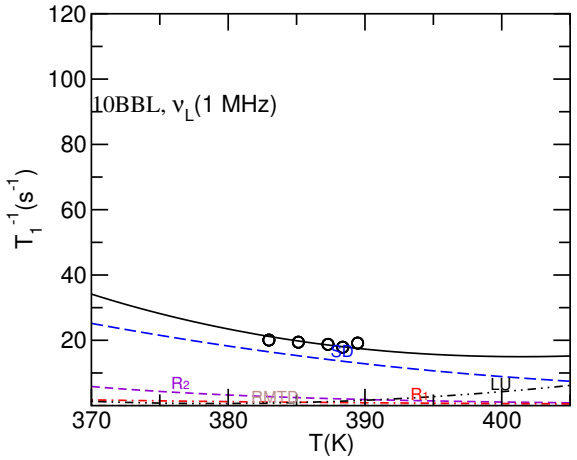

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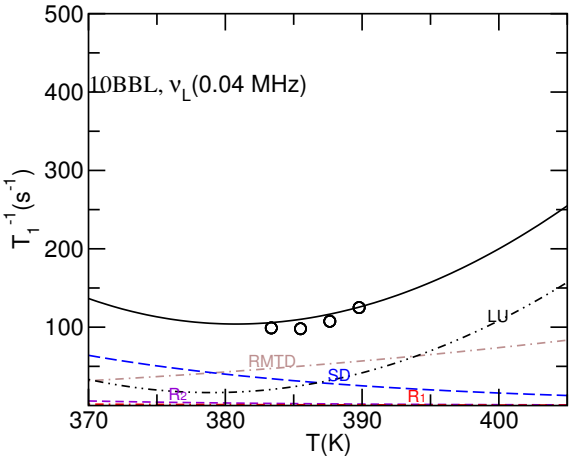


TGBA-6.pdf

fitteia Report

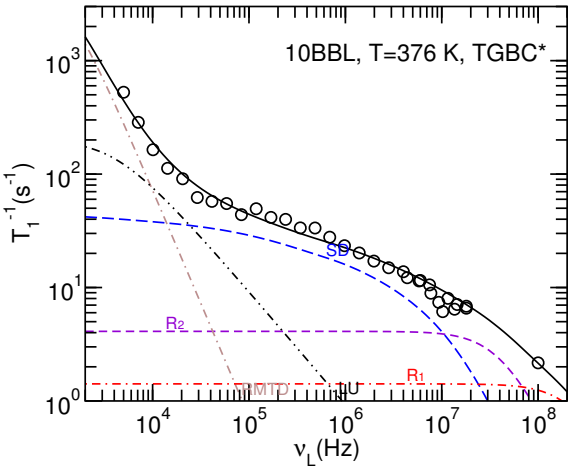
(internet based fitter service)

Subject	BBL, TGBC-fT
Date	Monday 3rd June, 2013, 23:07
Affiliation	pj.sebastiao@gmail.com 146.164.6.8
Abstract	Fit report produced with the fit results of function: z=BPPfT(x, y, a1, tau1, E1, Tref) + RdrfT(x, y, Adr, taudr, Edr, Tref) + SDSmA11_polifT(x, y, d, n, tauD, ED, Tref) + BPPfT(x, y, af, tauf, ER, Tref) + LUfT(x, y, Alu0, Alu1, Alu2, fcm, fcM, Tref) to the 328 experimental points, considering 6 free parameters.

$tau1 = 1.96 \times 10^{-09}$ (fixed)
$a1 = 4.19 \times 10^{+08}$ (fixed)
$E1 = 68384$ (fixed)
$Adr = 2.0938 \times 10^{+07} \pm 1.1202 \times 10^{+06}$
$taudr = 0.00014603 \pm 1.1799 \times 10^{-05}$
$Edr = 4.9119 \times 10^{+05} \pm 28478$
$fcm = 3000$ (fixed)
$fcM = 1.95 \times 10^{+08}$ (fixed)
$d = 5$ (fixed)
$n = 6.76 \times 10^{+22}$ (fixed)

$tauD = 8.53 \times 10^{-09}$ (fixed)
$ED = 65220$ (fixed)
$af = 8.81 \times 10^{+08}$ (fixed)
$tauf = 3.21 \times 10^{-10}$ (fixed)
$ER = 41475$ (fixed)
$Alu0 = 9.3018 \times 10^{+05} \pm 39142$
$Alu1 = 14167 \pm 14492$
$Alu2 = 8768.8 \pm 3220.6$
$Tref = 376$ (fixed)

$\chi^2[100000] = 13.6567$
$\chi^2[4 \times 10^{+06}] = 1.95884$
$\chi^2[1 \times 10^{+08}] = 4.38659$
$\chi^2[40000] = 93.0998$
$\chi^2[1 \times 10^{+06}] = 34.3994$
$\chi^2[376] = 349.53$
$\chi^2[10000] = 21.5592$
$\chi^2_t = 518.591$



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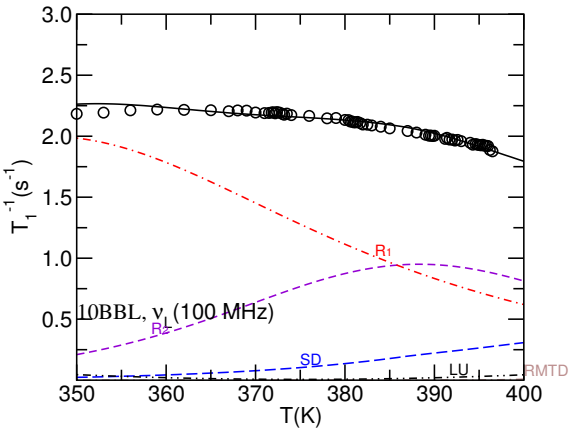

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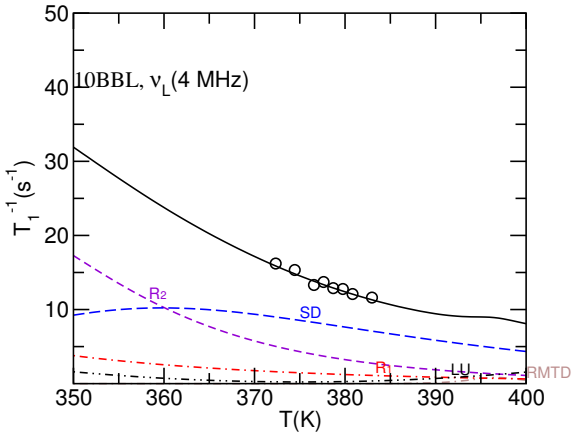

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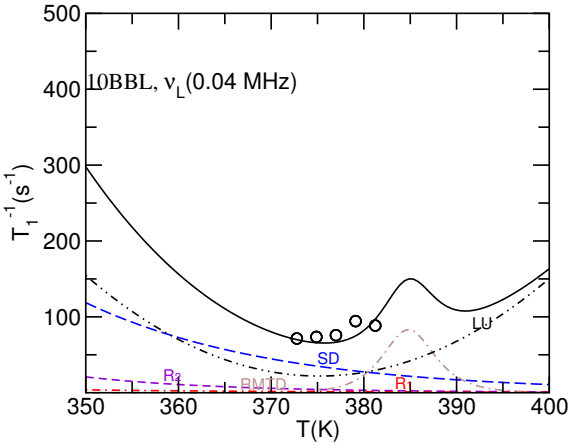

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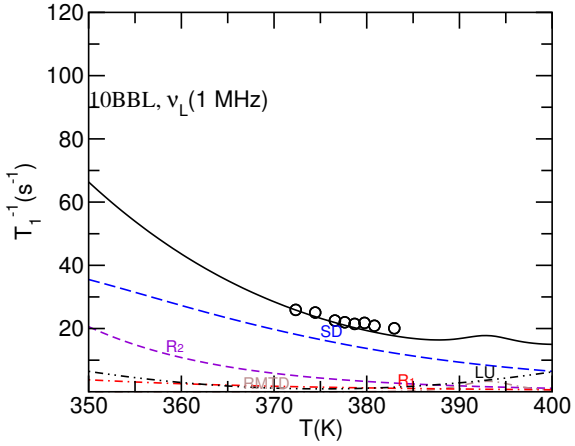

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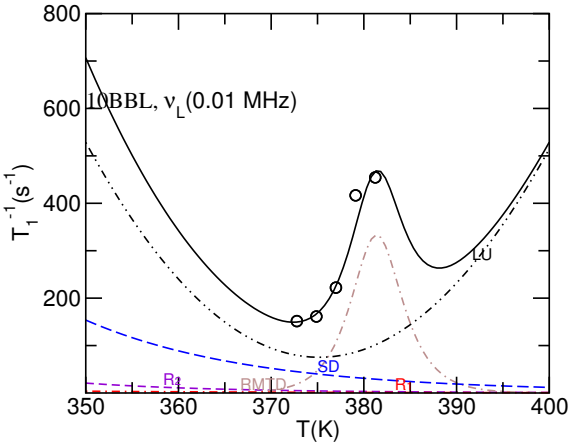

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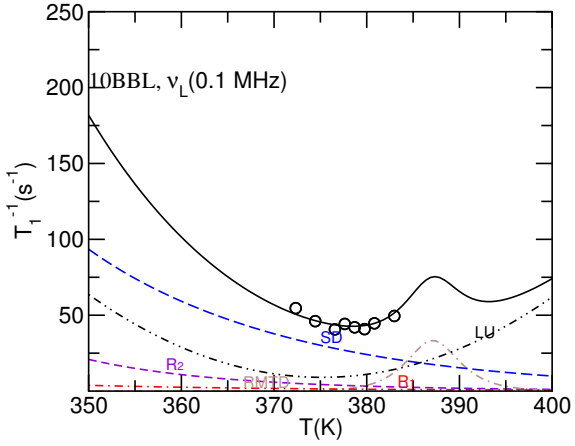


TGBC-5.pdf

fitteia Report

(internet based fitter service)

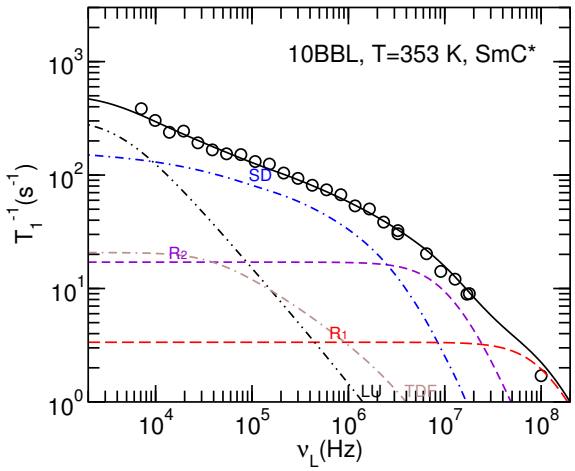
Subject	BBL, SmC-fT-properTDF
Date	Monday 3rd June, 2013, 23:02
Affiliation	pj.sebastiao@gmail.com 146.164.6.8
Abstract	Fit report produced with the fit results of function: z=BPPfT(x, y, a1, tau1, E1, Tref) + SDSmA11_polifT(x, y, d, n, tauD, ED, Tref) + BPPfT(x, y, af, tauf, ER, Tref) + LUfT(x, y, Alu0, Alu1, Alu2, fcm, fcM, Tref) + ODFNfT(x, y, ftcm0, ftcM, Aodf0, Aodf1, ftcm1, 366.0) to the 458 experimental points, considering 7 free parameters.

$tau1 = 1.96 \times 10^{-09}$ (fixed)
$a1 = 4.19 \times 10^{+08}$ (fixed)
$E1 = 68364$ (fixed)
$fcm = 3172.2$ (fixed)
$fcM = 1 \times 10^{+07}$ (fixed)
$d = 5$ (fixed)
$n = 6.76 \times 10^{+22}$ (fixed)
$tauD = 8.53 \times 10^{-09}$ (fixed)
$ED = 65200$ (fixed)
$af = 8.81 \times 10^{+08}$ (fixed)
$tauf = 3.21 \times 10^{-10}$ (fixed)

$ER = 41475$ (fixed)
$Alu0 = 1.8362 \times 10^{+06} \pm 1.0938 \times 10^{+05}$
$Alu1 = 1.5136 \times 10^{+05} \pm 12287$
$Alu2 = 6039.8 \pm 357.15$
$Tref = 376$ (fixed)
$Aodf0 = 242.65 \pm 321.1$
$Aodf1 = -321.89 \pm 37.304$
$ftcm1 = 1000 \pm 738.44$
$ftcm0 = 45769 \pm 9073.2$
$ftcM = 1 \times 10^{+07}$ (fixed)

$\chi^2[333] = 192.96$
$\chi^2[1 \times 10^{+06}] = 43.6518$
$\chi^2[1 \times 10^{+08}] = 5.61443$
$\chi^2[40000] = 46.1677$
$\chi^2_t = 510.462$

$\chi^2[100000] = 48.5068$
$\chi^2[4 \times 10^{+06}] = 30.1934$
$\chi^2[10000] = 52.9344$
$\chi^2[353] = 90.4336$



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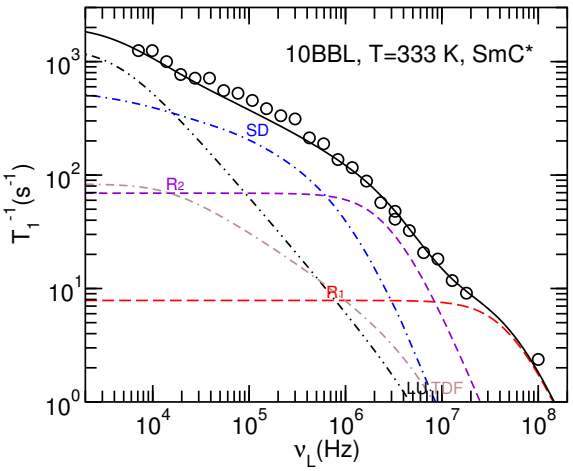

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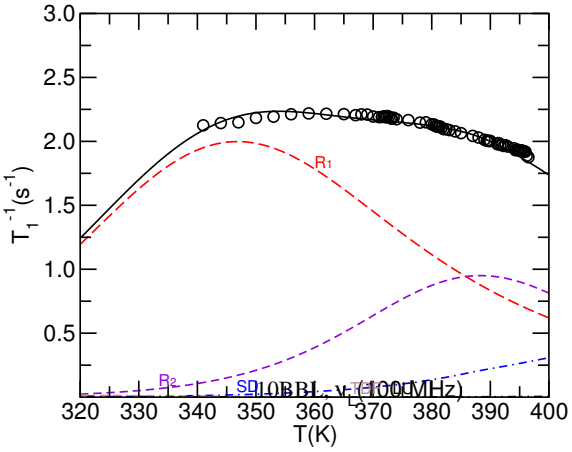

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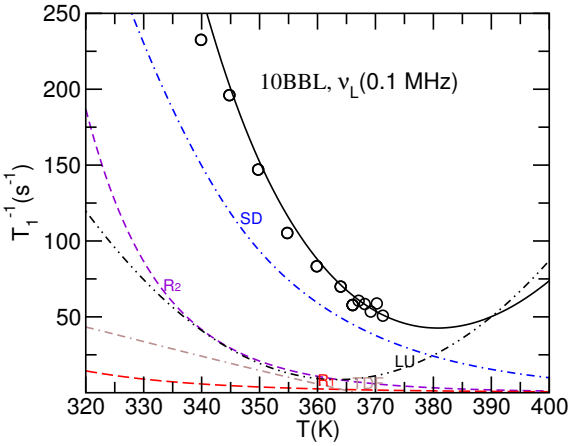

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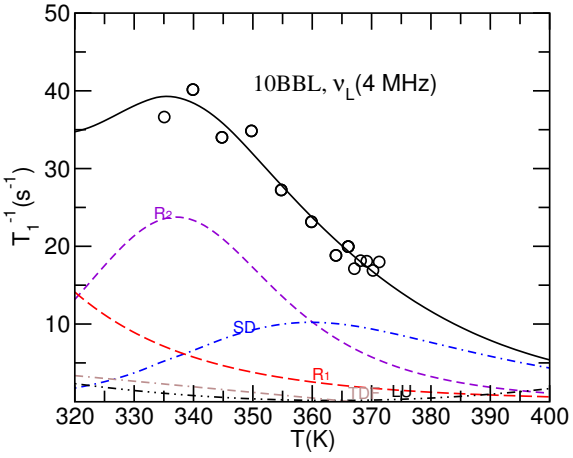

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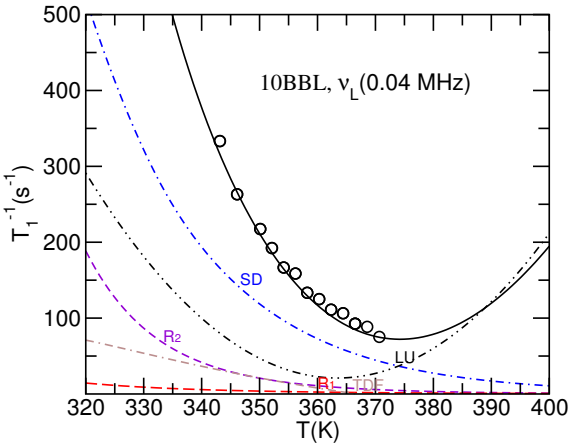

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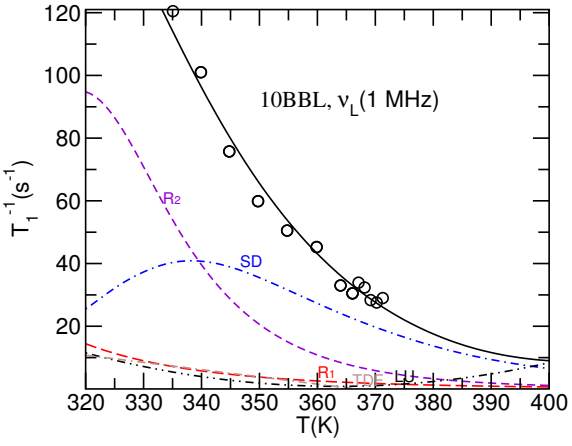
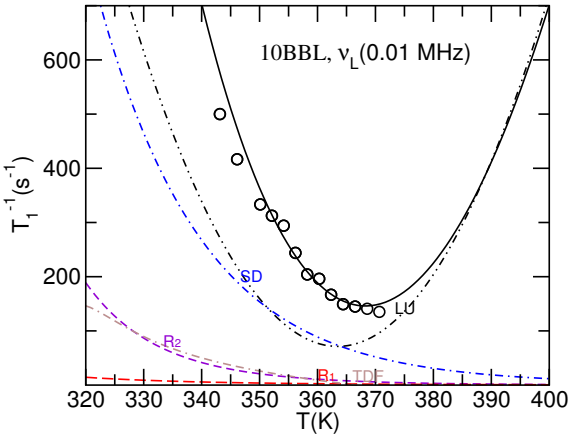


SmC-5.pdf



SmC-8.pdf