

# Supporting Materials Section

## **Intermediate Role of Gallium in Oxidic Glasses: Solid State NMR Structural Studies of the Ga<sub>2</sub>O<sub>3</sub>-NaPO<sub>3</sub> System**

Jinjun Ren<sup>a,b</sup> and Hellmut Eckert<sup>a,c\*</sup>

<sup>a</sup> Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstr. 30, D-48149 Münster, Germany

<sup>b</sup> Key Laboratory of Materials for High-Power Laser, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Science, Shanghai 201800, China

<sup>c</sup> Instituto da Física Sao Carlos Universidade de Sao Paulo, Sao Carlos, SP 13590, Brazil

AUTHOR INFORMATION

**Corresponding Author**

\*Email: [eckerth@uni-muenster.de](mailto:eckerth@uni-muenster.de)

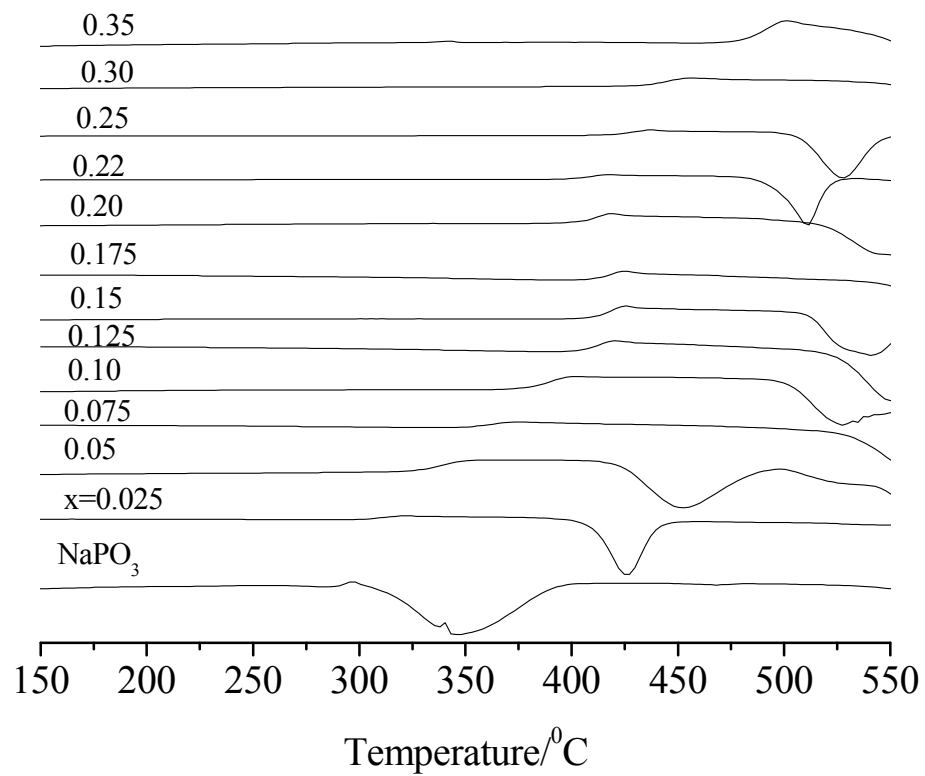
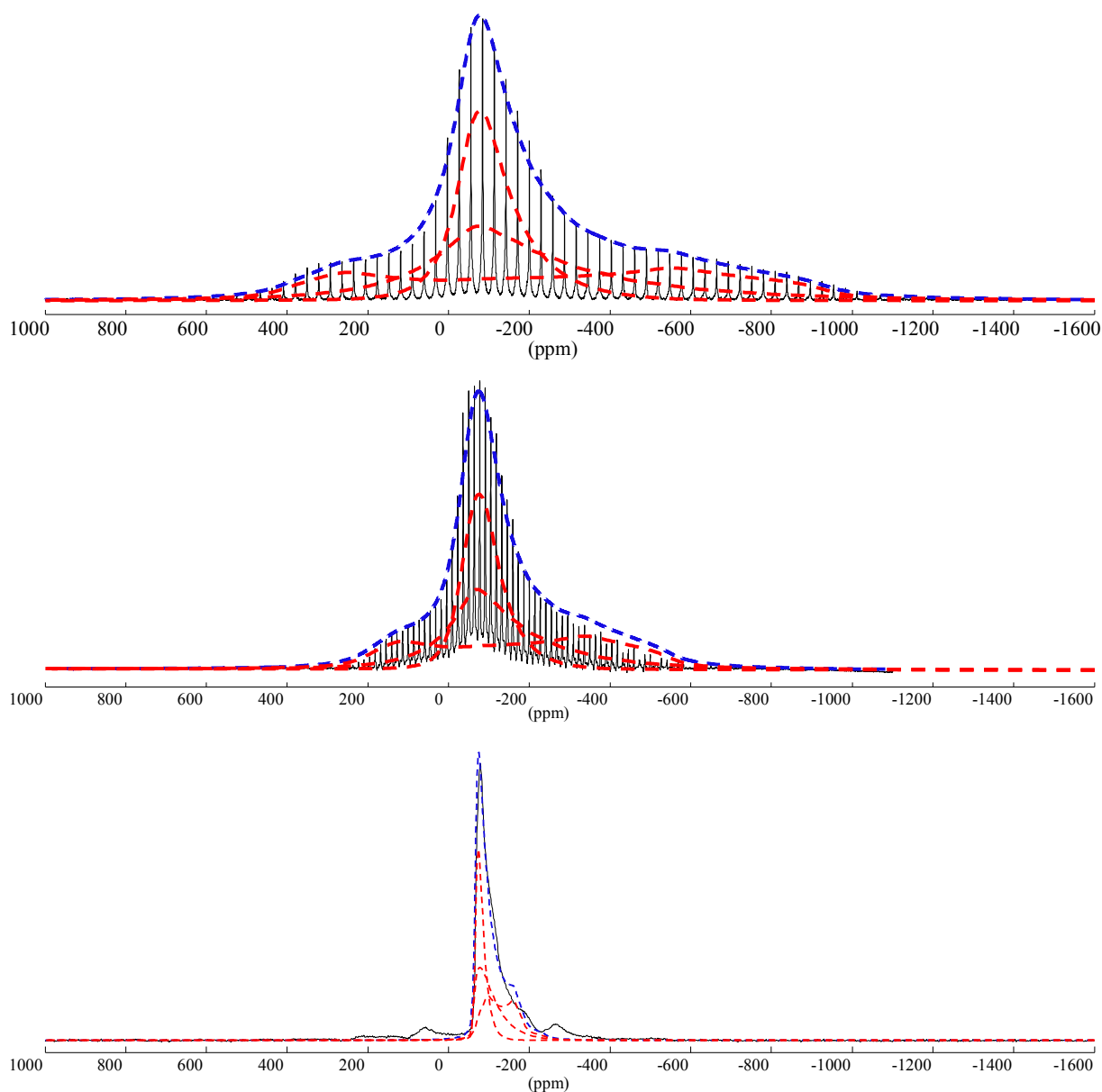
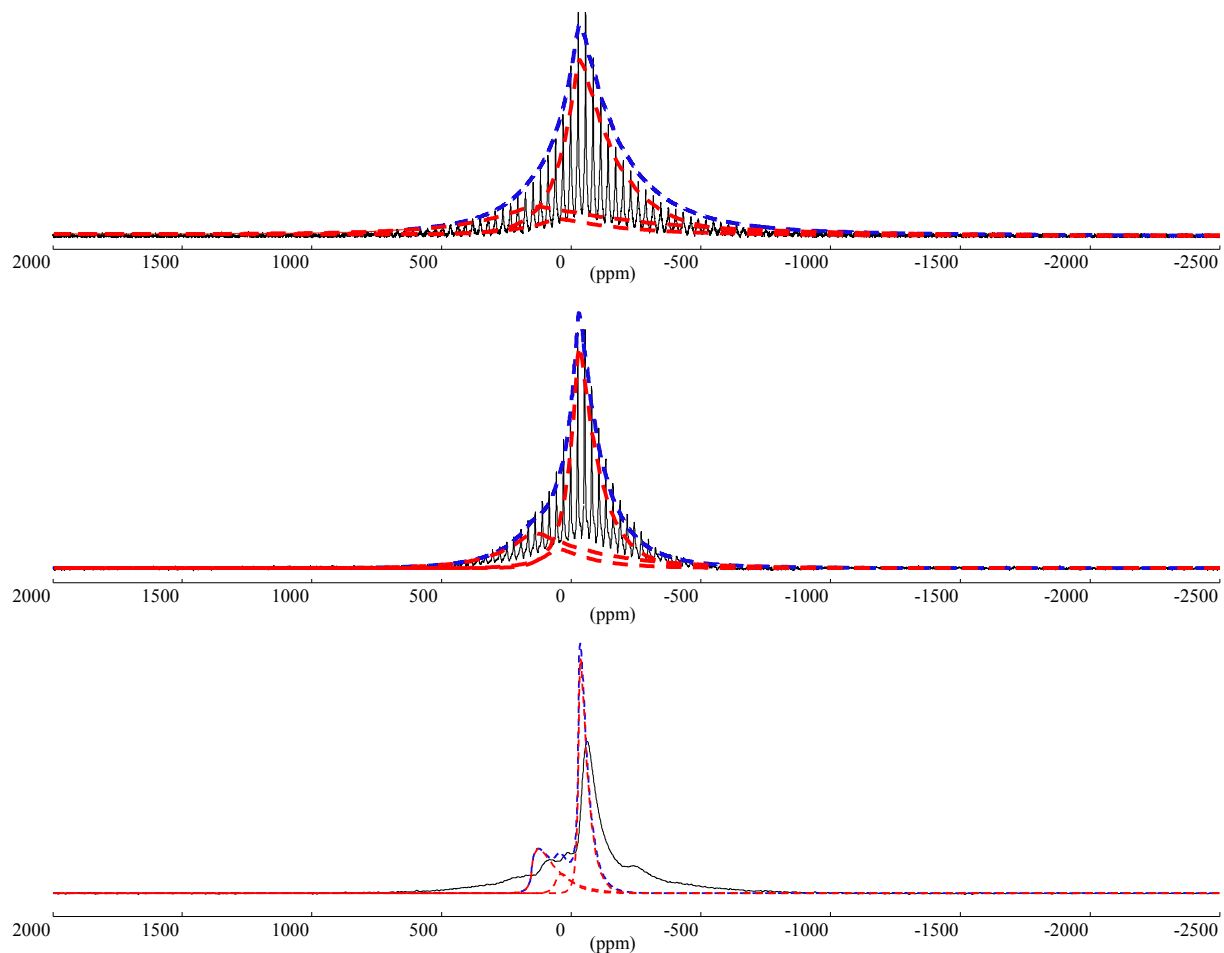


Figure S1 DSC curves of  $x\text{Ga}_2\text{O}_3-(1-x)\text{NaPO}_3$  glasses



**Figure S2:**  $^{71}\text{Ga}$  static WURST-QCPMG spectrum at 7.05 T (top), static QCPMG spectrum at 9.4 T (middle) and 11.7 MAS-NMR spectrum (bottom) of crystalline  $\text{Ga}(\text{PO}_3)_3$ . The red dashed lines show the individual deconvolution components, simulated with the joint parameters of Table S2. The blue dashed curve indicates the overall simulated curve. The Figure demonstrates that a consistent simulation of field dependent static and MAS-NMR spectra can be achieved with this crystalline compound.



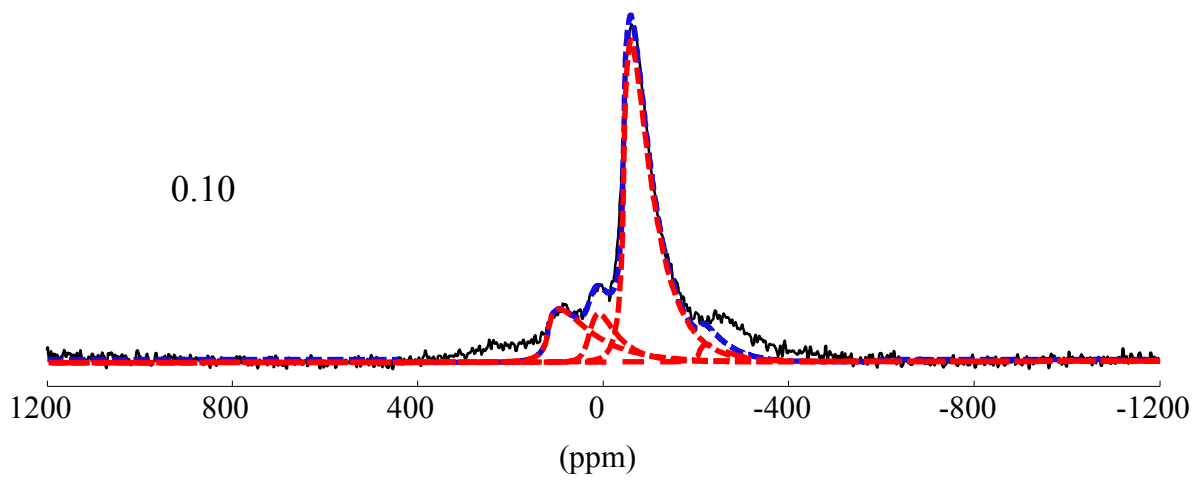
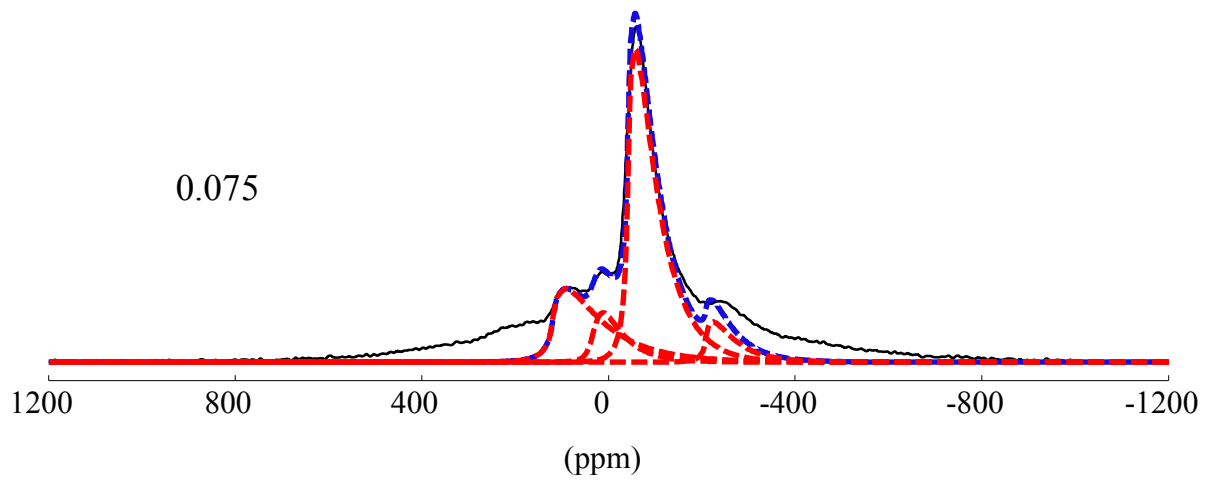
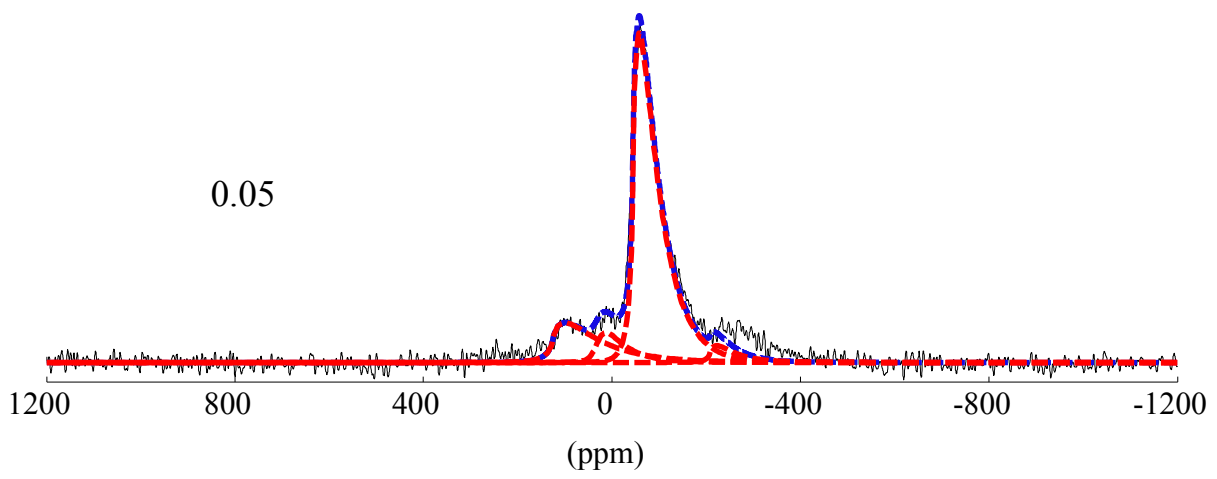
**Figure S3**  $^{71}\text{Ga}$  static WURST-QCPMG at 7.05 T (top), static QCPMG at 9.4 T (middle) and MAS-NMR spectrum (bottom: on the field of 11.7 T) spectra of a glass sample with  $x = 0.075$ . The red dashed curves show the individual deconvolution components, which were simulated with the joint fitting parameters listed in Table S2, using the Czjzek model. The blue dashed curve indicates the overall simulated curve. The Figure demonstrates that a consistent simulation of field dependent static and MAS-NMR spectra cannot be achieved with the glassy material.

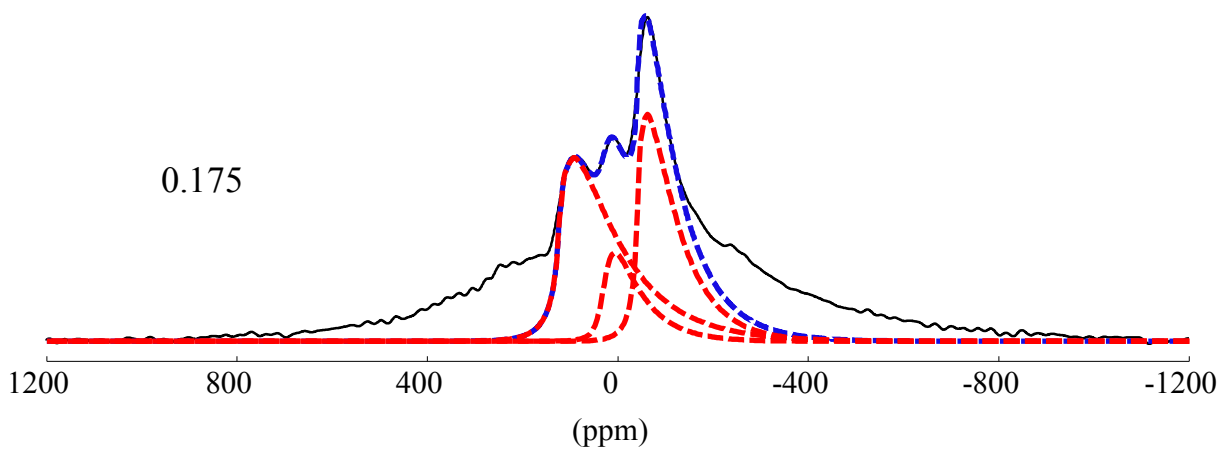
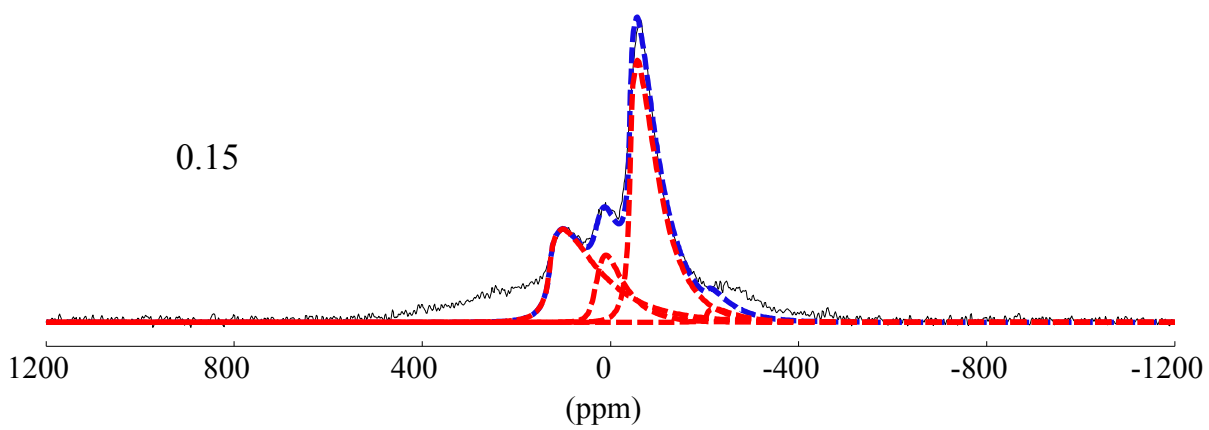
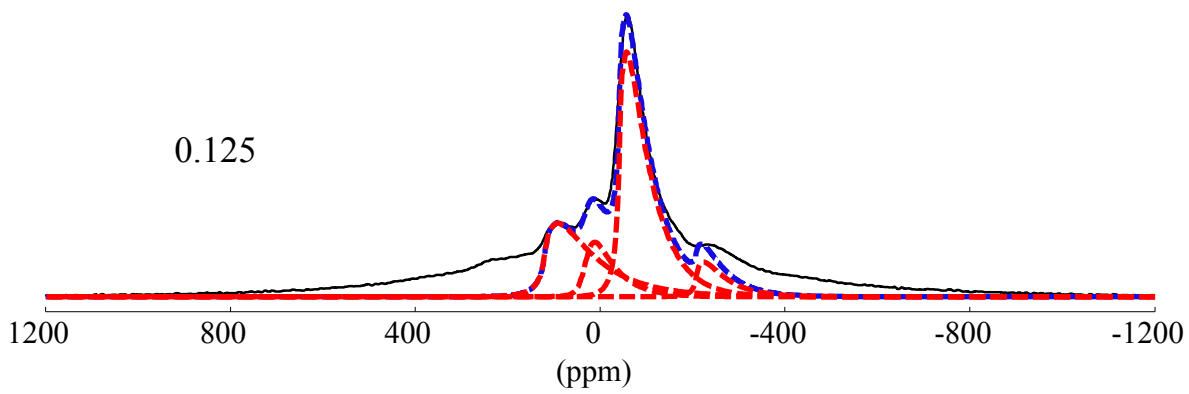
**Table S1:** Individual best-fit deconvolution parameters obtained for the  $^{71}\text{Ga}$  QCPMG spectrum at 9.4 T and of the static WURST-QCPMG spectrum at 7.05 T (in parentheses) measured on crystalline  $\text{Ga}(\text{PO}_3)_3$ .

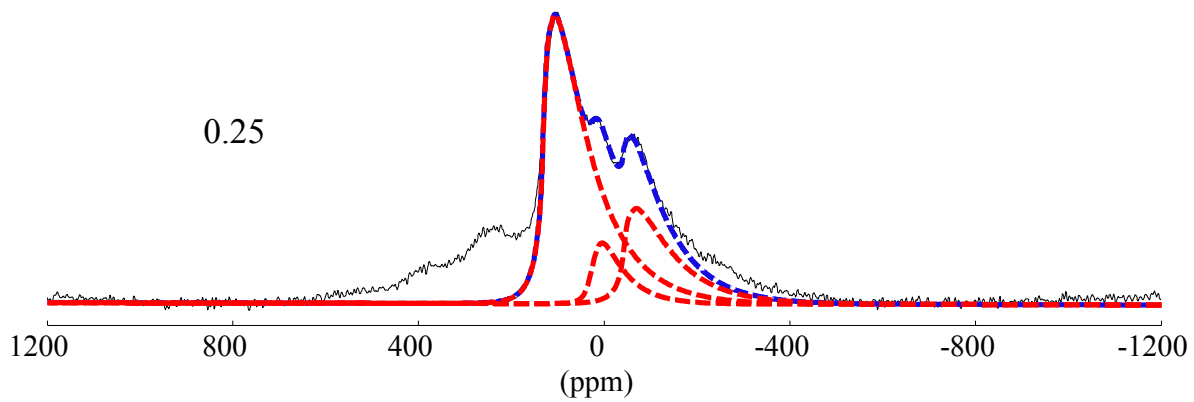
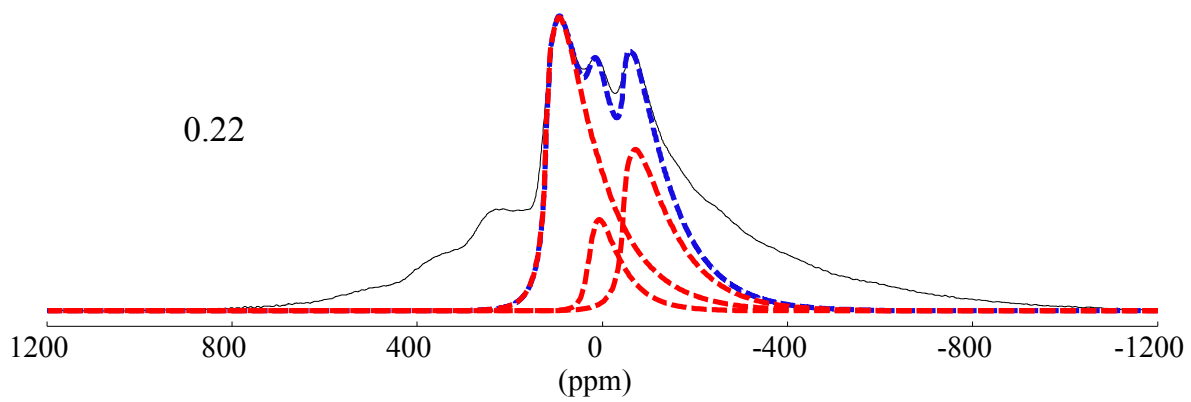
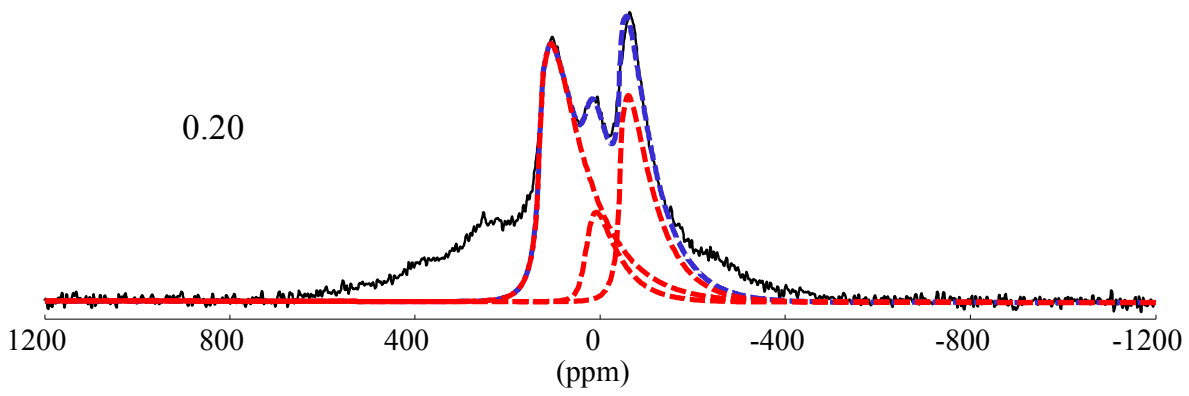
Peak position/ppm	$C_q/\text{MHz}$	$\eta_q$	Fraction/%
$\pm 5$ ppm	$\pm 0.2$ MHz	$\pm 0.2$	$\pm 3\%$
-64(-69)	3.5(3.5)	0.6(0.6)	30(33)
-59(-64)	5.9(6.1)	0.6(0.6)	33 (34)
-50(-60)	8.1(8.6)	0.3(0.3)	37(33)

**Table S2.** Joint fitting parameters of the  $^{71}\text{Ga}$  static WURST-QCPMG spectra at 7.05 T, the static QCPMG spectra at 9.4 T for crystalline  $\text{Ga}(\text{PO}_3)_3$  and for a glass sample with composition  $x=0.075$ .

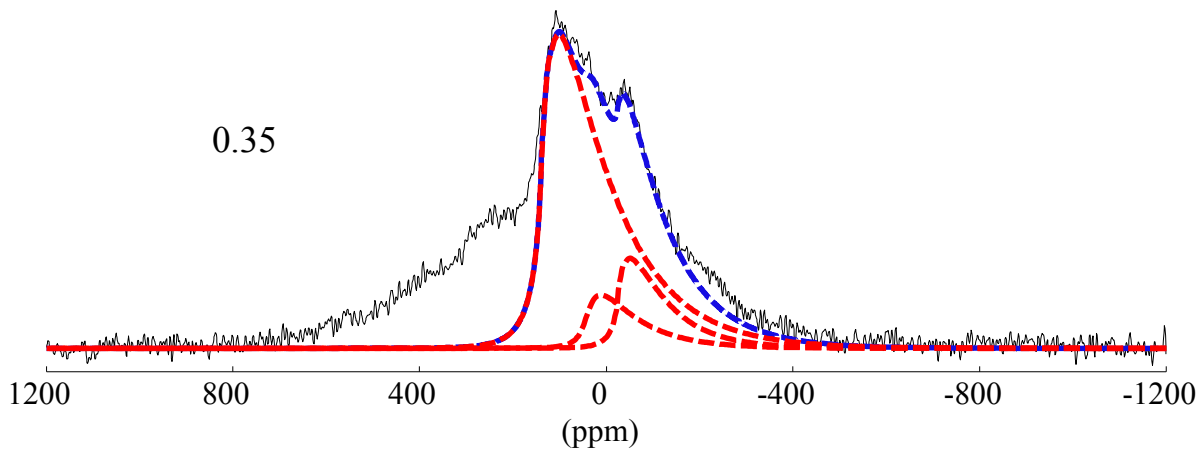
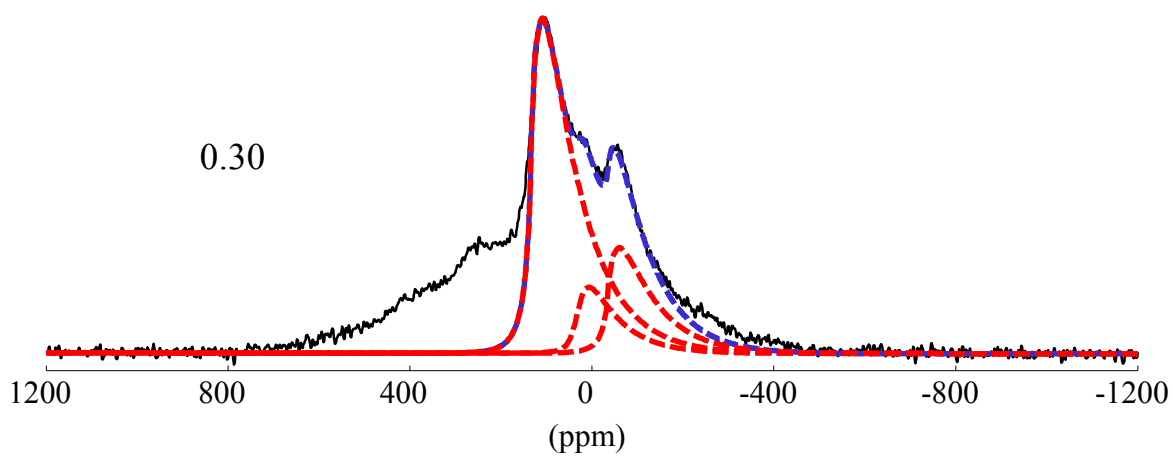
Sample	Peak position/ppm	$C_q/\text{MHz}$	$\eta_q$	Fraction/%
$\text{Ga}(\text{PO}_3)_3$	-66	3.5	0.6	34
	-62	6.0	0.6	34
	-55	8.3	0.3	32
0.075	-28	4.6	0.6	30
	57	6.0	0.6	9.5
	154	8.1	0.6	60



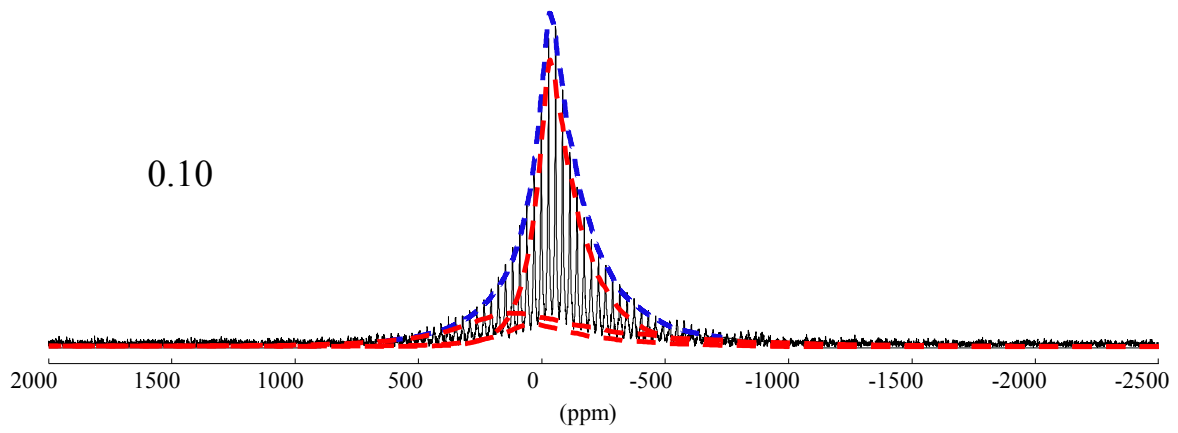
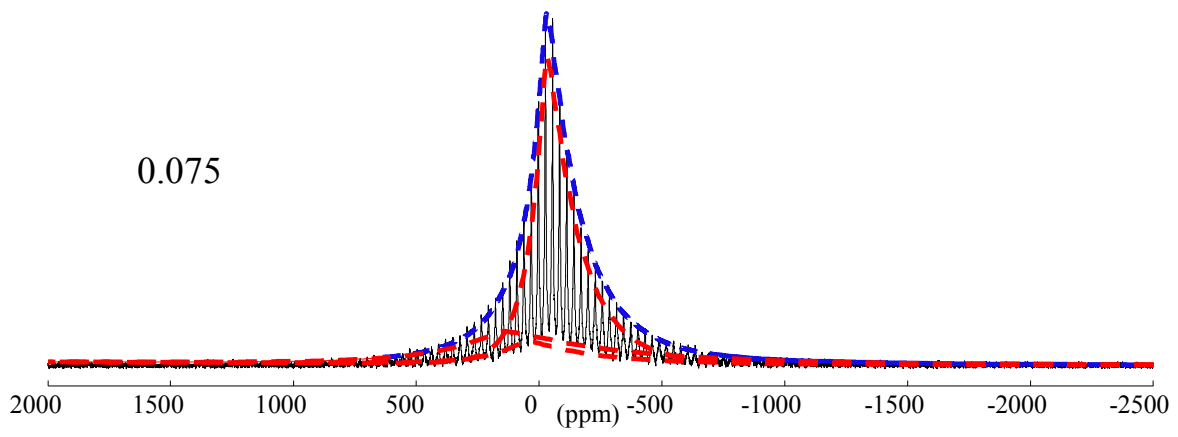
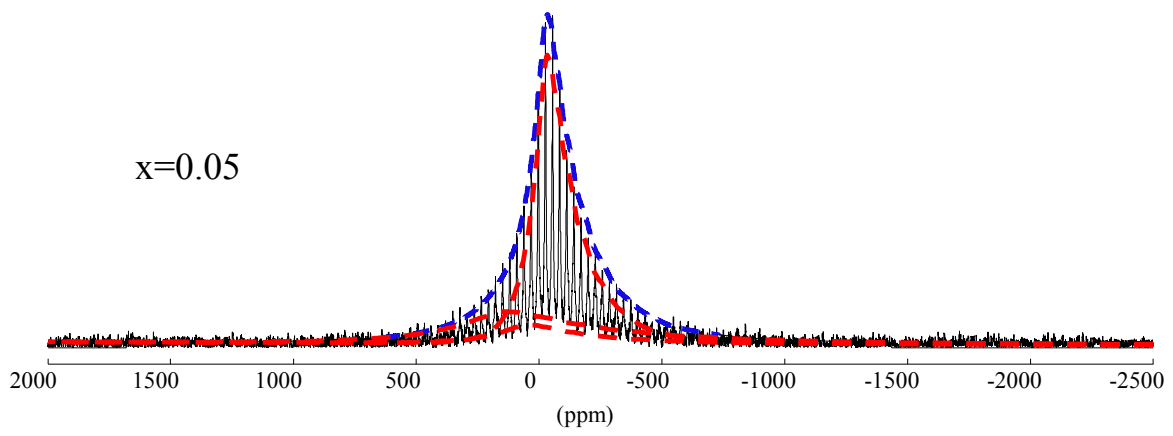


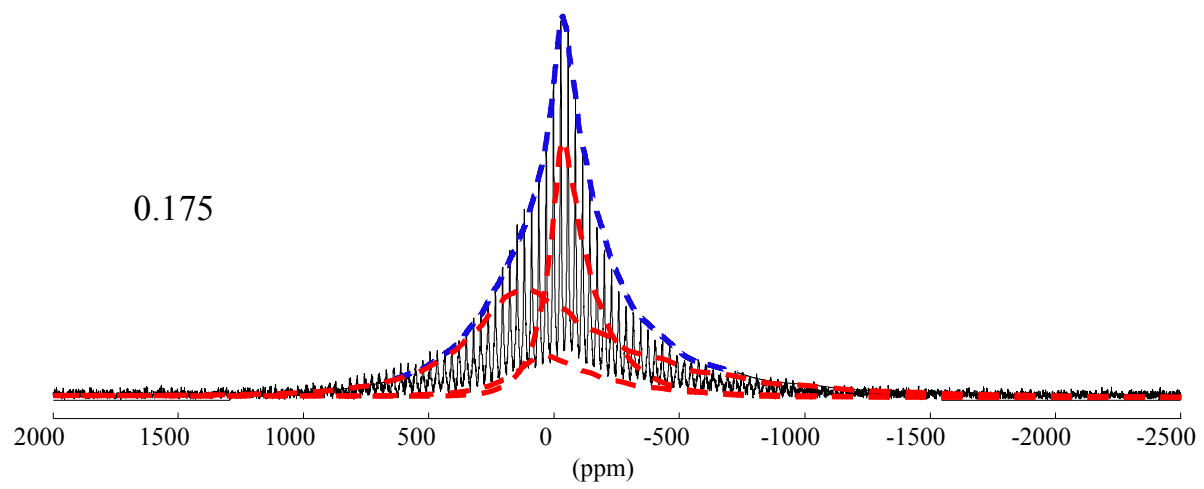
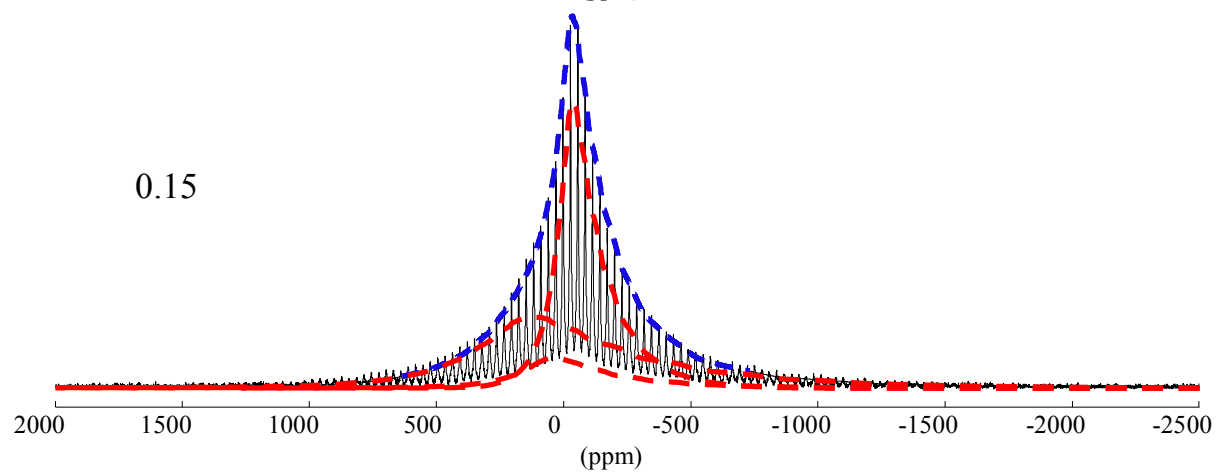
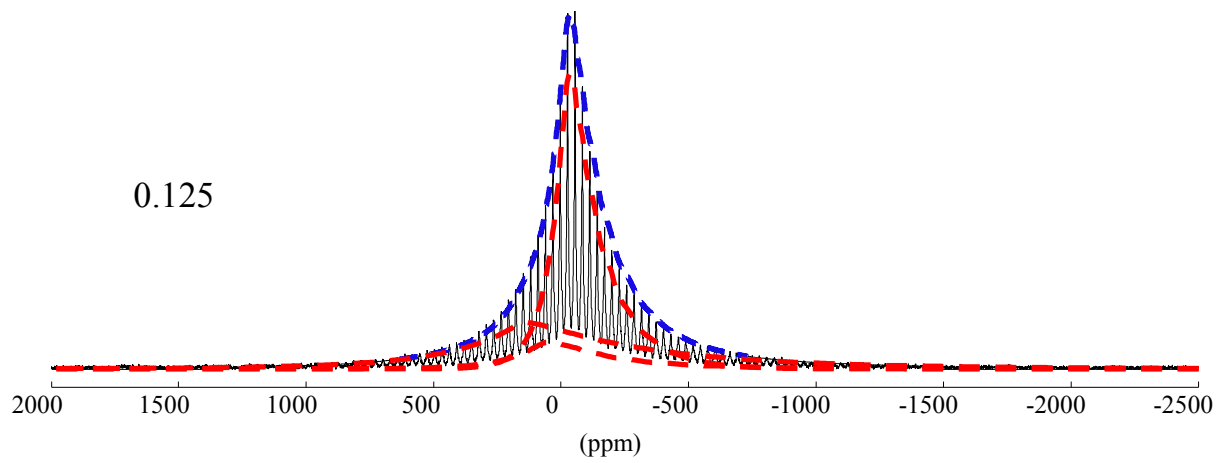


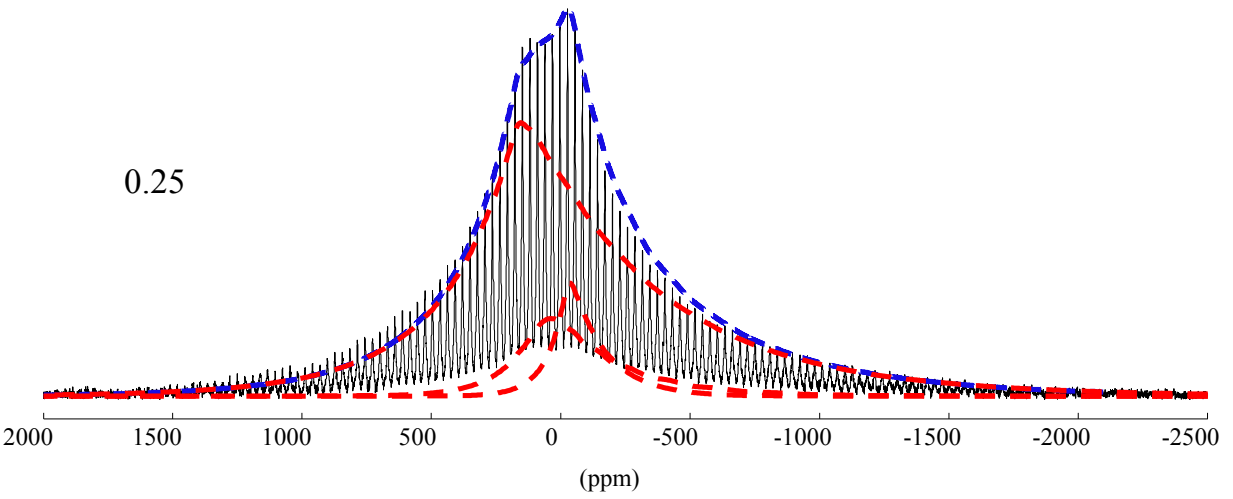
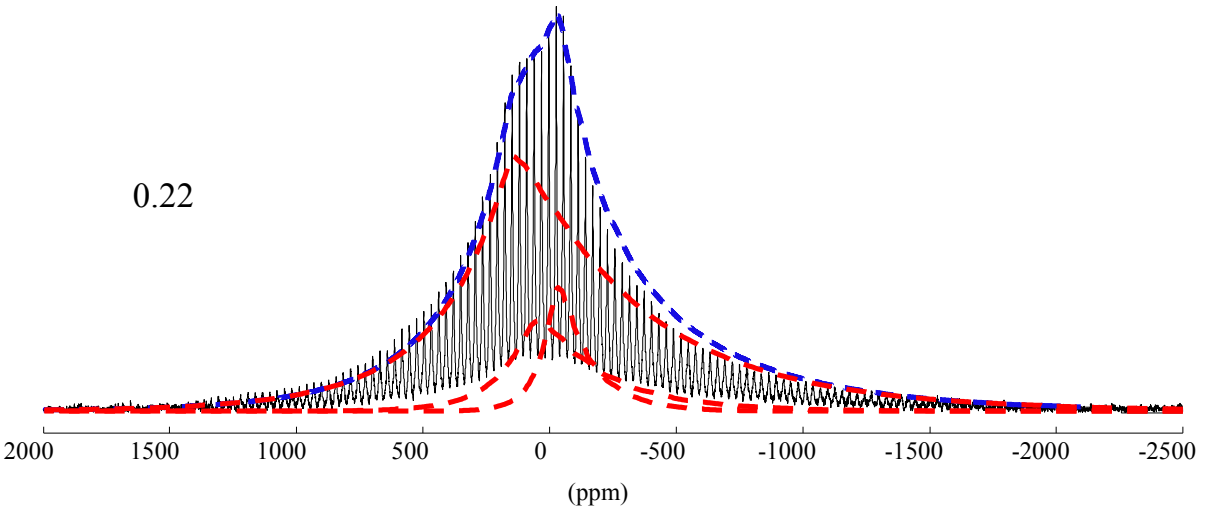
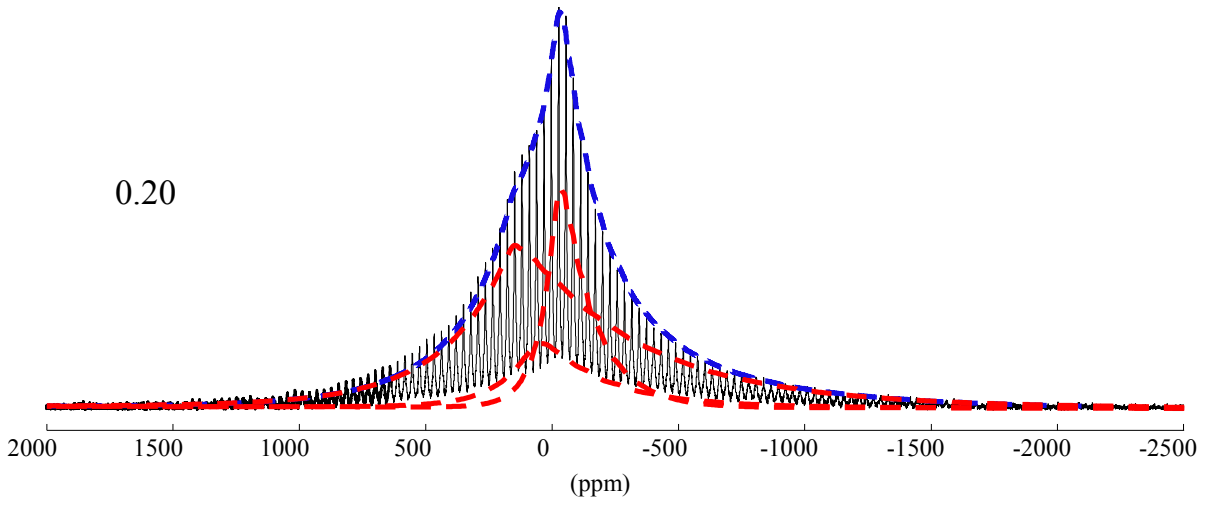


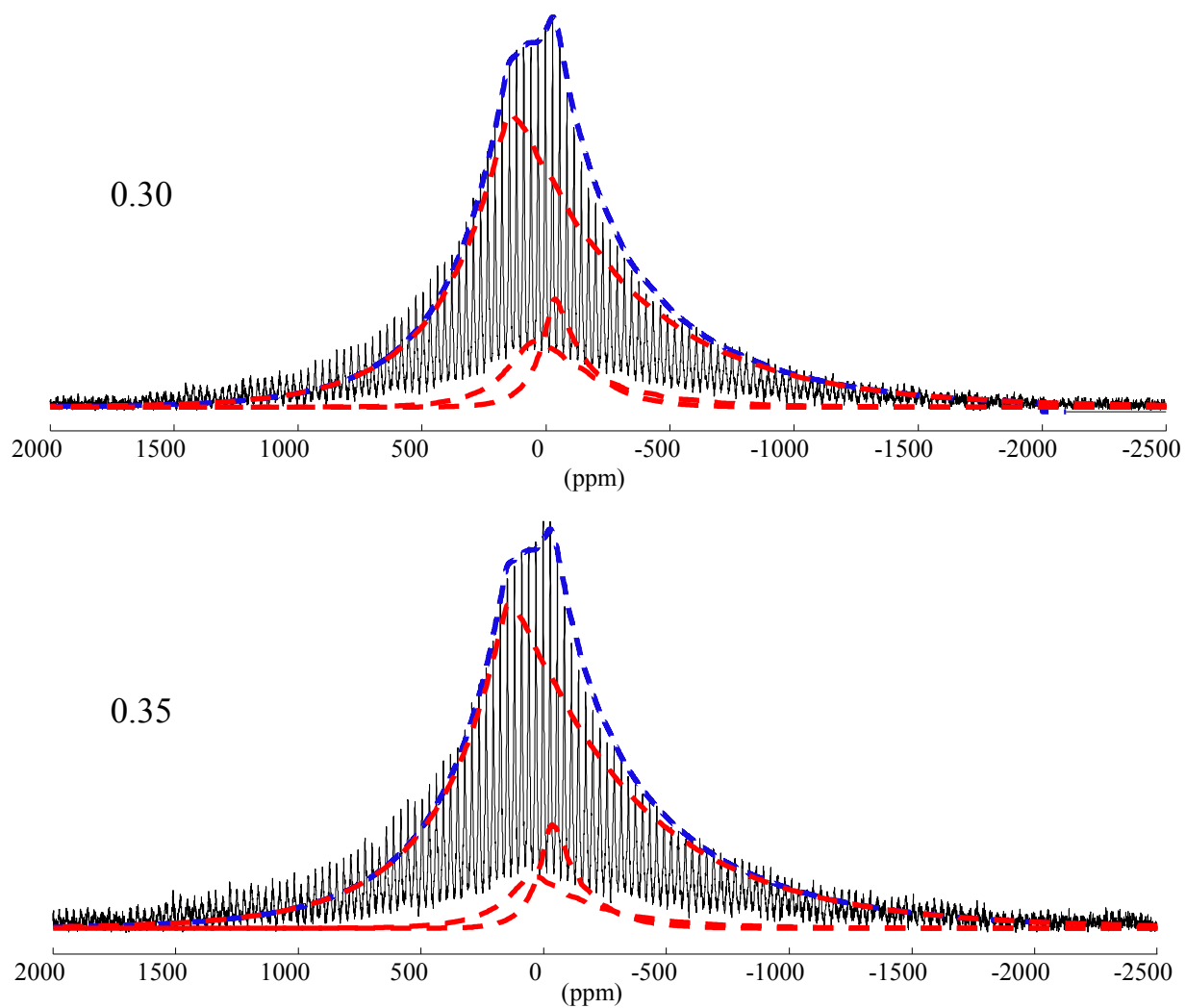


**Figure S4**  $^{71}\text{Ga}$  MAS NMR spectra at 11.7 T of  $(\text{NaPO}_3)_{1-x}(\text{Ga}_2\text{O}_3)_x$  glasses. Lineshape fits (red curves) to individual components; blue curves are the overall fitting results.









**Figure S5:** static  $^{71}\text{Ga}$  WURST-QCPMG NMR spectra at 7.05 T of  $(\text{NaPO}_3)_{1-x}(\text{Ga}_2\text{O}_3)_x$  glasses. Lineshape fits (red curves) to individual components; blue curves are the overall fitting results.