Supporting Information for

Kinetics of Ga(NOTA) formation from weak Ga-citrate complexes

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Table S1 Protonation and stability constants of species involving Ga^{3+}, acetate, citrate and NOTA.

	OH^{-a}	acetate[a]	Citrate[b]	NOTA[c]
Log K_{1H}	-	4.49	5.70	11.61
Log K_{2H}	-	-	4.35	5.65
Log K_{3H}	-	-	2.91	3.17
Log β_{GaL}	-3.31	2.41	10.02	30.98
Log $\beta_{Ga(L)2}$	-6.76	-	15.3	-
Log $\beta_{Ga(L)3}$	-11.16	-	-	-
Log $\beta_{Ga(L)4}$	-17.17	-	-	-
Log β_{GaLH}	-	-	11.6	-
Log β_{GaLOH}	-	-	7.1	21.28
Log $\beta_{Ga2L(OH)2}$	-	-1.16	-	-

a M. Clausén, L.-O. Öhman, J. D. Kubicki, P. Persson *J. Chem. Soc., Dalton Trans.*, **2002**, 2559–2564. b Jackson, G. E.; Byrne, M. J.; *J. Nucl. Med.*, **1996**, *37*, 379.Clarke, E. T.; Martell, A. E.; *Inorg. Chim. Acta*, **1991**, *181*, 273–280. c. Clarke, E. T.; Martell, A. E.; *Inorg. Chim. Acta*, **1991**, *181*, 273–280.; Martell, A. E.; Motekaitis, R. J.; Clarke, E. T.; Delgado, R.; Sun, Y.; Ma, R.; *Supramol. Chem.* **1996**, *6*, 353.

Figure S1. Speciation diagrams of the gallium(III)-acetate system.

c_{Ga}= 4.0 mM, $c_{acetate}$= 100 mM.

The diagram was calculated using literature data (Table S1). However, in the kinetic experiments only in the presence of acetate (without citrate), no precipitation has been observed during the experiment.

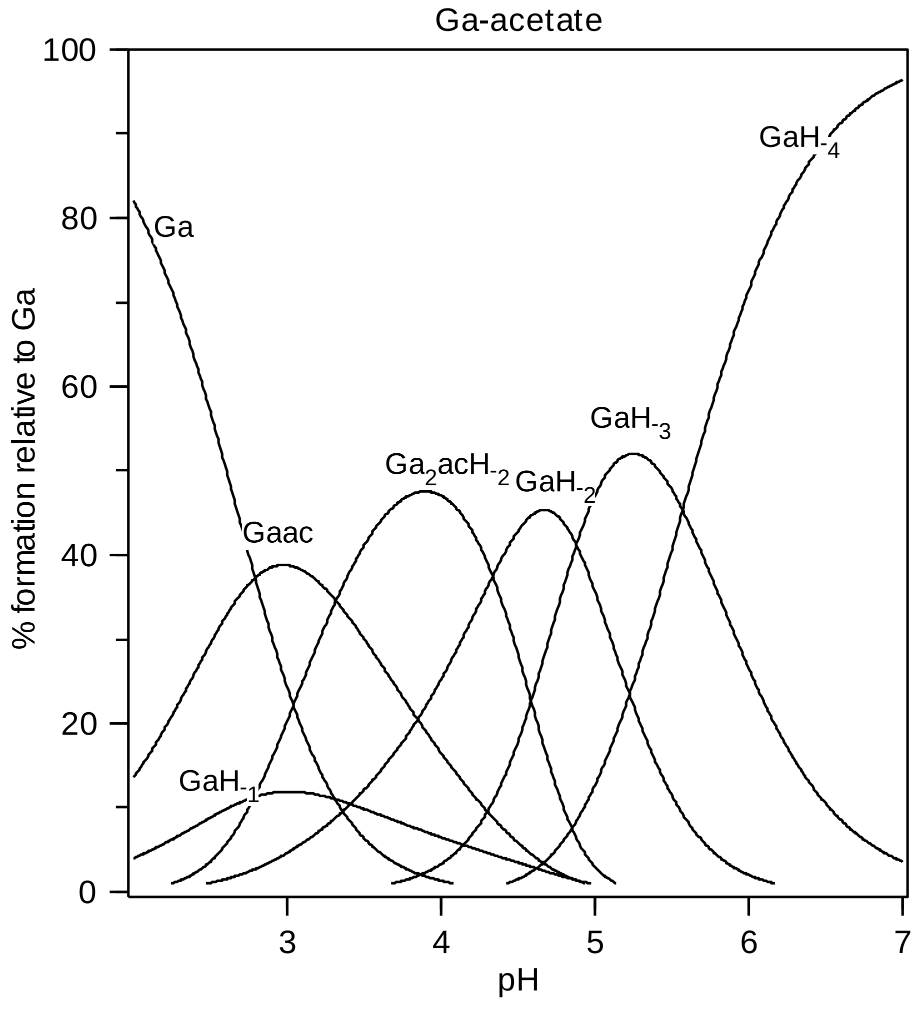

Figure S2 Speciation diagrams of the gallium(III)-citrate system.

c_{Ga}= 4.0 mM, $c_{citrate}$= 4.7 mM.

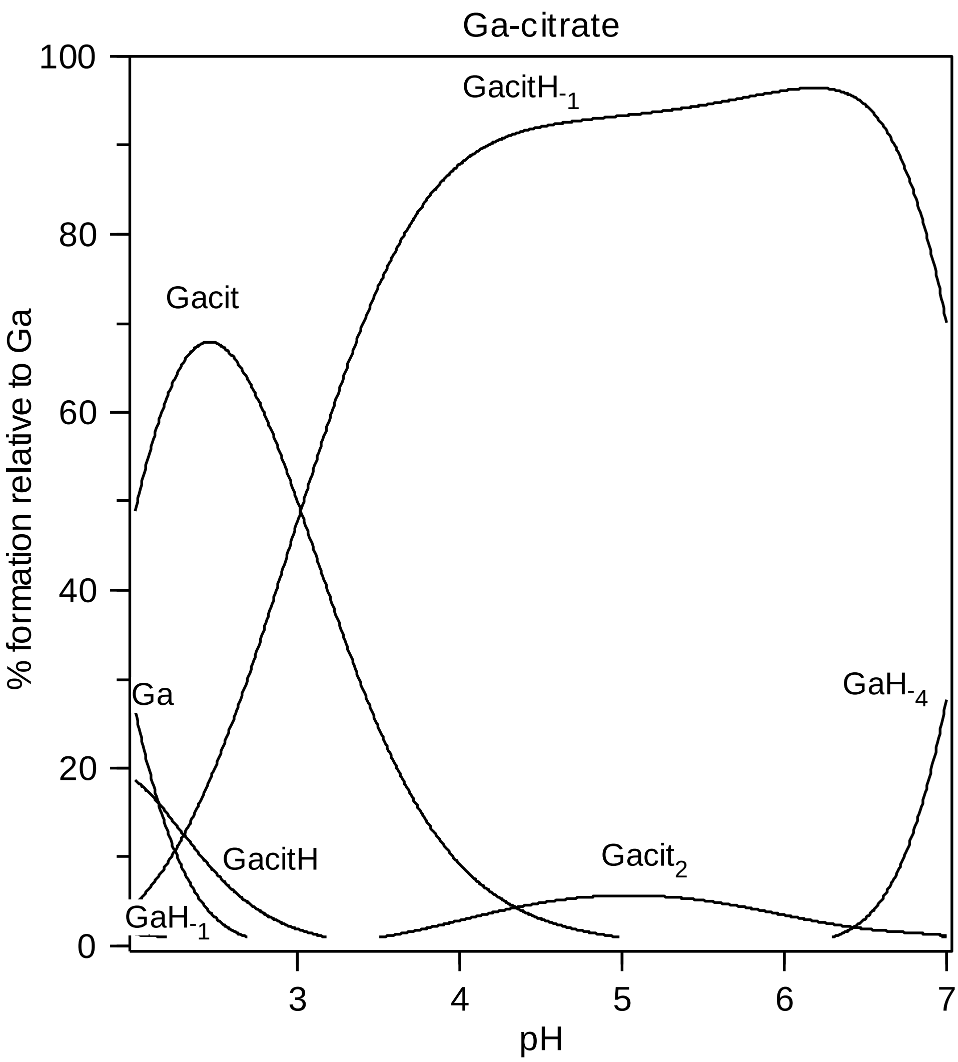

Figure S3. Speciation diagrams of the gallium(III)-citrate system.

c_{Ga}= 4.0 mM, $c_{citrate}$= 9.8 mM.

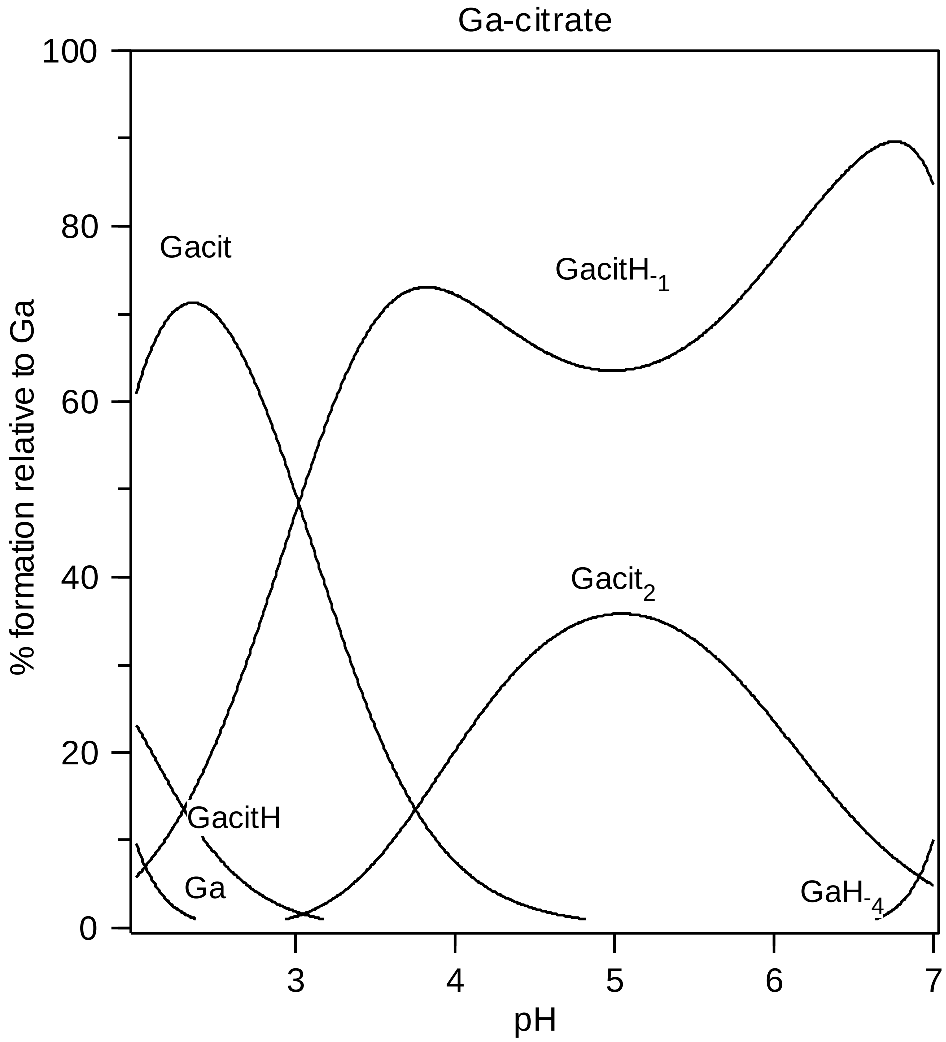

Figure S4. Speciation diagrams of the gallium(III)-citrate system.

c_{Ga}= 4.0 mM, $c_{citrate}$= 19.0 mM.

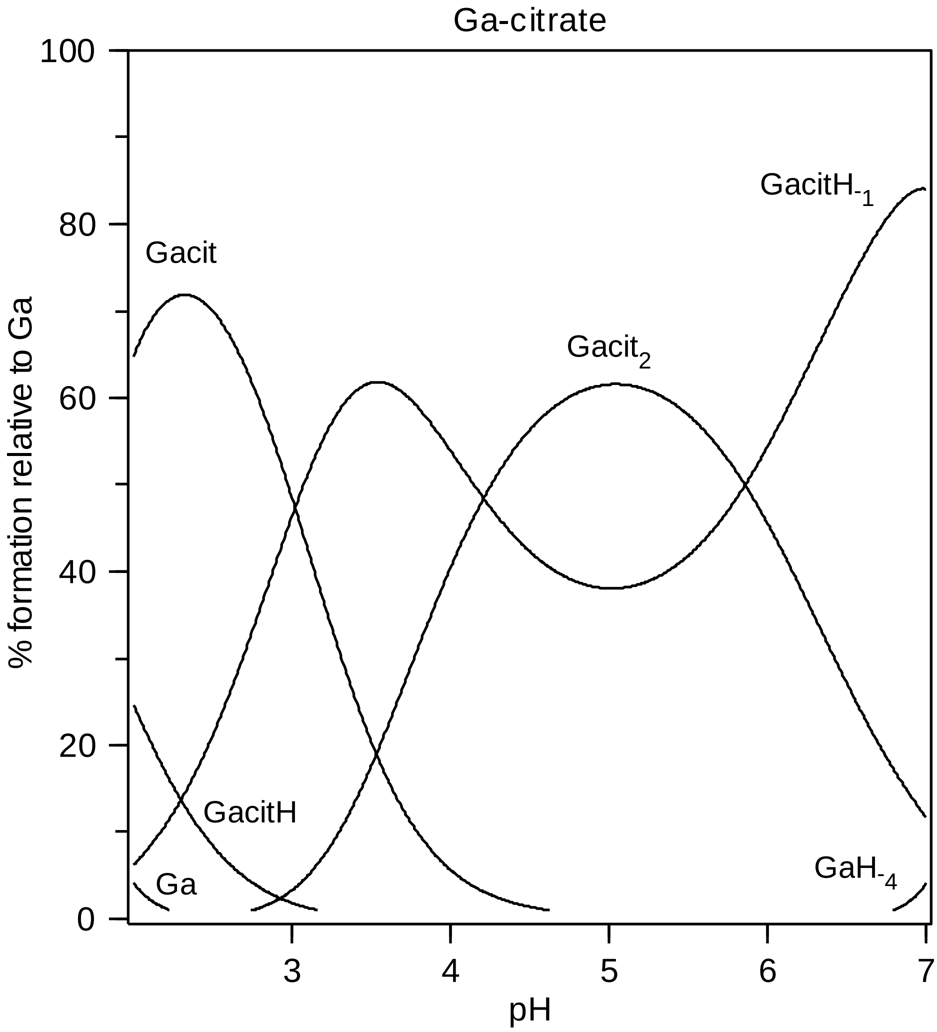

Figure S5. Speciation diagrams of the gallium(III)-citrate-acetate system.

c_{Ga}= 4.0 mM, $c_{citrate}$= 4.7 mM, $c_{acetate}$= 100 mM,

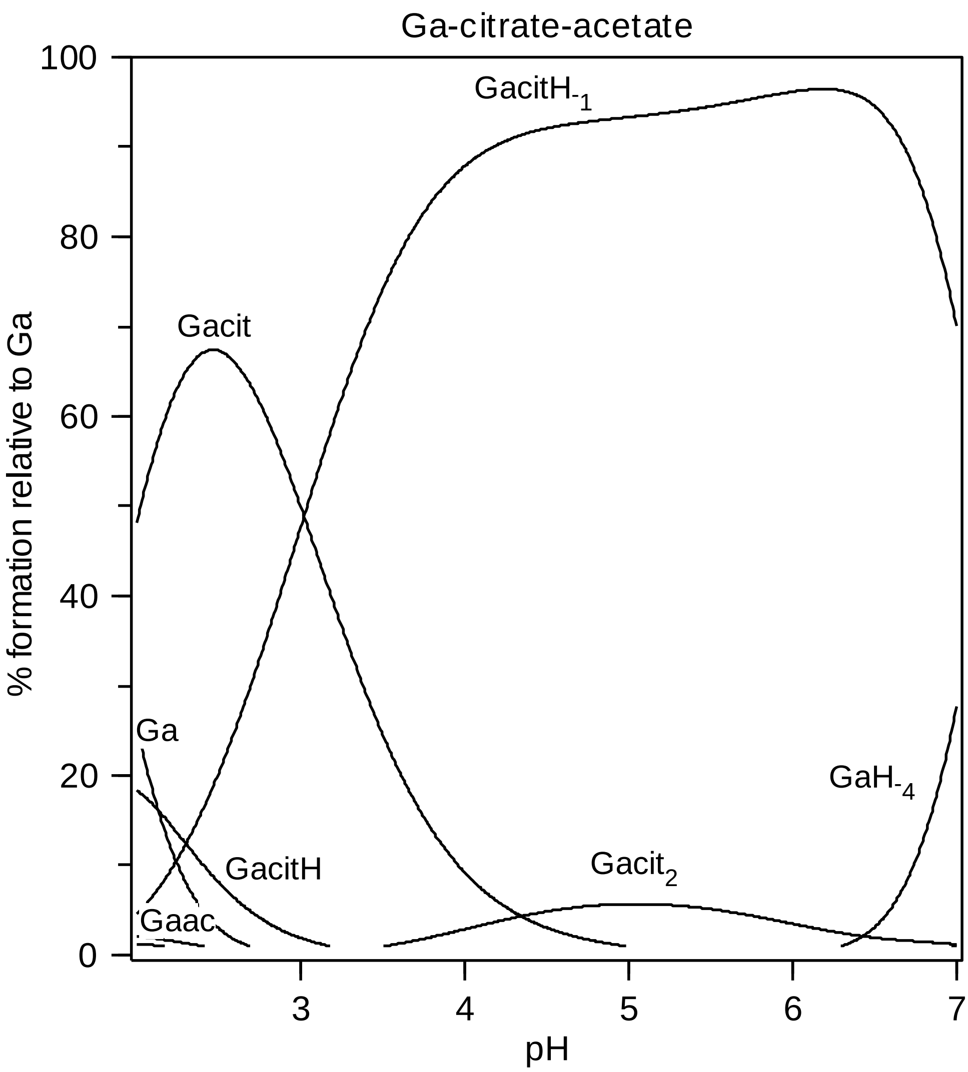

Figure S6. Speciation diagrams of the gallium-citrate-NOTA system.

c_{Ga}= 4.0 mM, c_{citrate}= 19 mM, c_{NOTA}= 4.0 mM.

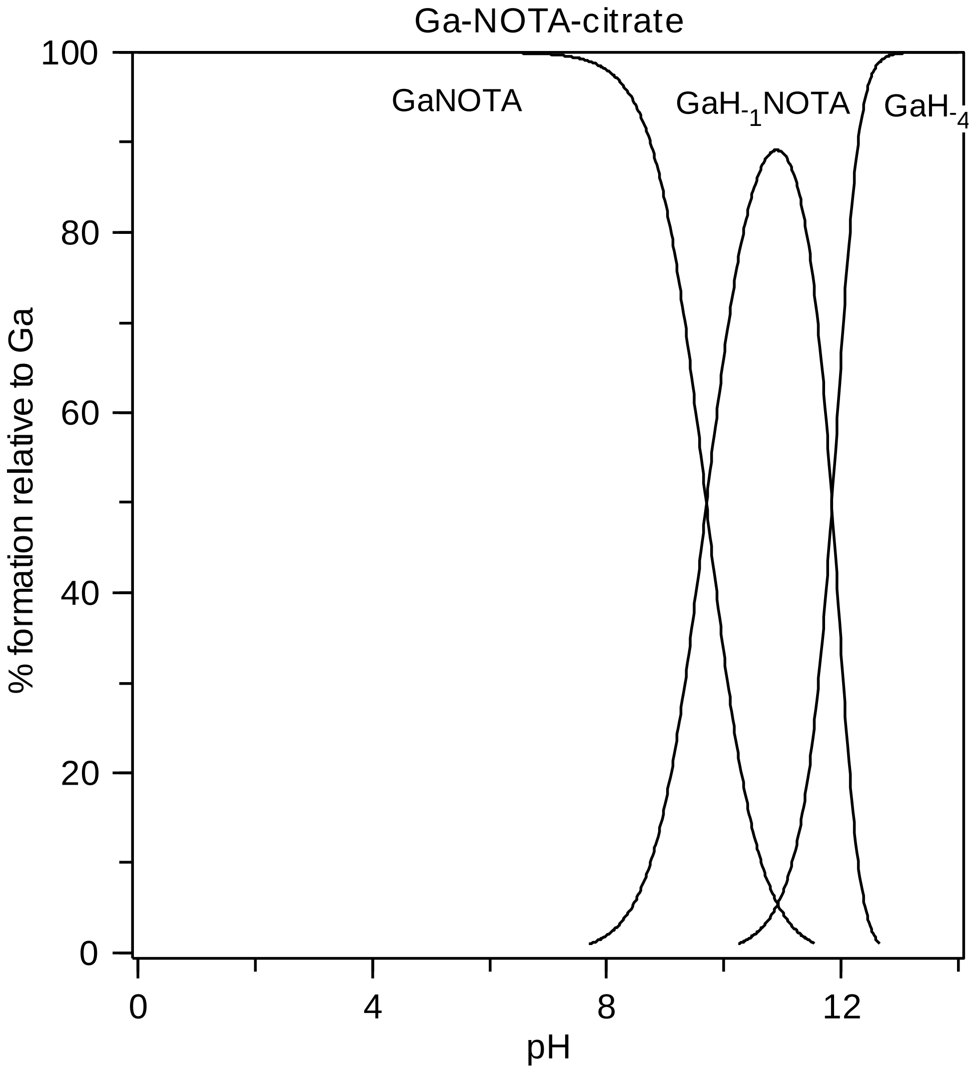

Figure S7a. Representative series of pseudo-first-order rate constants, k_{obs}, as a function of NOTA concentration. c_{Ga} = 4 mM, $c_{citrate}$= 9.8 mM. The curves represent the fit to the data points as explained in the text.

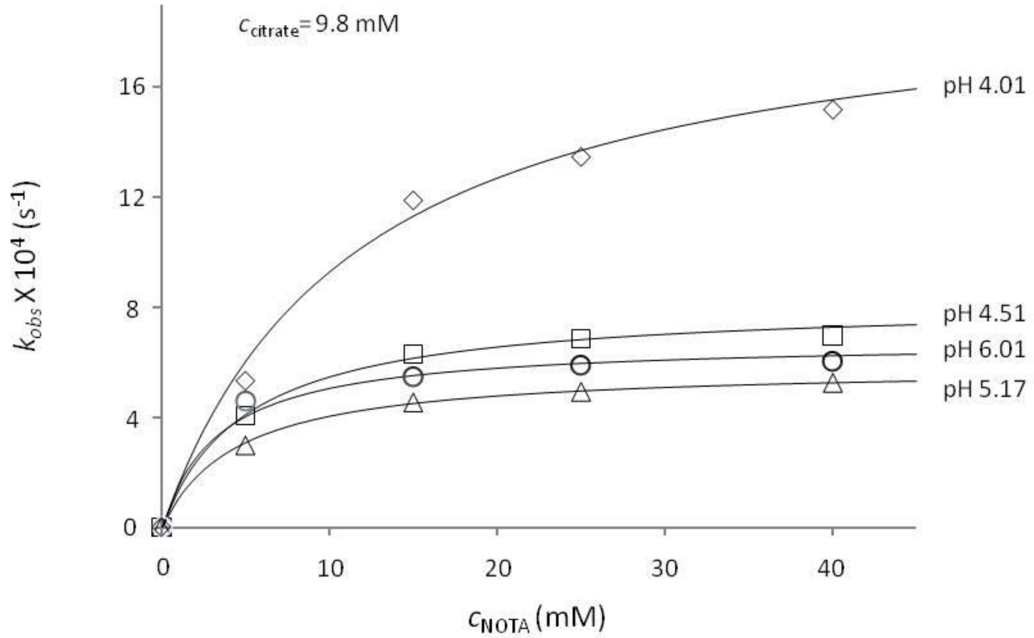

Figure S7b. Representative series of pseudo-first-order rate constants, k_{obs}, as a function of NOTA concentration. c_{Ga} = 4 mM, $c_{citrate}$= 19.0 mM. The curves represent the fit to the data points as explained in the text.