Supporting information

Self-assembly of Gd^{3+}-bound keplerate polyanions into nanoparticles as the route for synthesis of positive MRI contrast agents. Impact of the structure on the magnetic relaxivity

Julia Elistratova[a]*, Bulat Akhmadeev,[b] Vladimir Korenev,[c] Maxim Sokolov,[c] Irek Nizameev[a], Aidar Gubaidullin,[a] Alexandra Voloshina,[a] Asiya Mustafina[a]

[a] Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center of RAS,

Arbuzov str., 8, 420088, Kazan, Russia

[b] Kazan (Volga region) Federal University, Kremlyovskaya str., 18, 420008, Kazan, Russia

[c] – Nikolaev Institute of Inorganic Chemistry, 3 Acad. Lavrentiev Prosp., Novosibirsk, Russia

*Corresponding author: 969_969@bk.ru

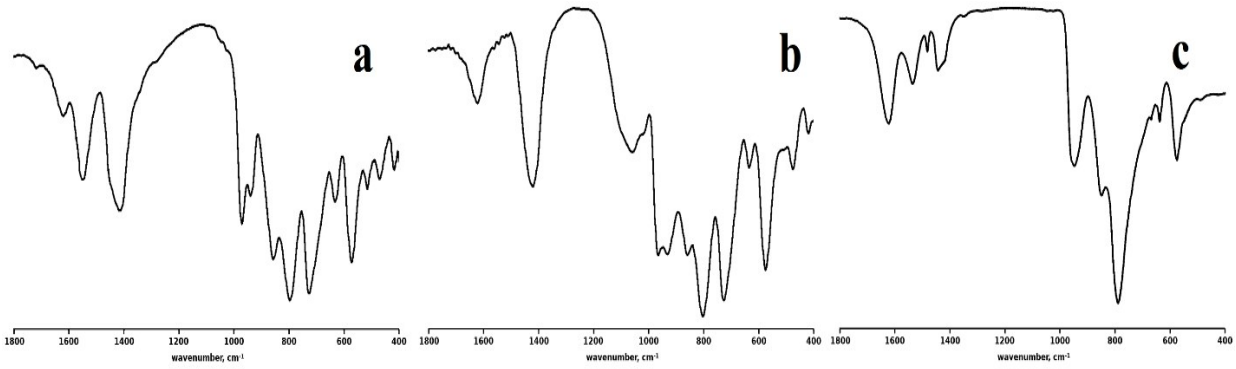
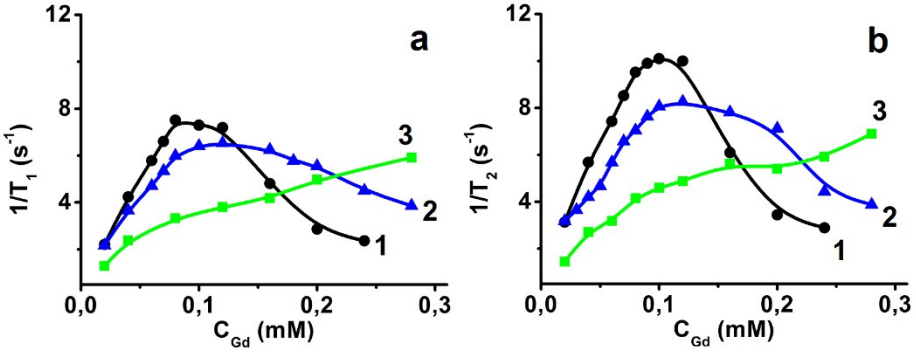


Fig. S.1 The IR-spectra of synthezised keplerate: a – Kp(OAc), b – Kp(PO_4), c – Kp(S).



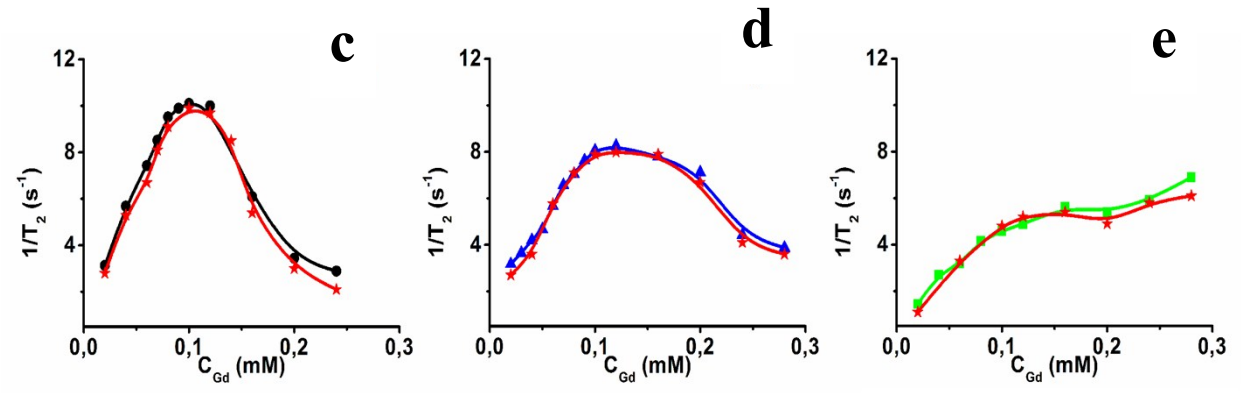


Fig. S.2 $1/(T_1)$ (a) and $1/(T_2)$ (b) vs Gd concentration measured at 25°C and 20 Hz for F-127 stabilized colloids (0.32 mM F-127, 0.007 mM Kp) : 1 – $Gd_x(\mathbf{1})_y$, 2 - $Gd_x(\mathbf{2})_y$, 3 - $Gd_x(\mathbf{3})_y$. Reproducibility of the $1/T_1$ vs Gd concentration profiles is illustrated by c-e: $Gd_x(\mathbf{1})_y$ (c), $Gd_x(\mathbf{2})_y$ (d), $Gd_x(\mathbf{1})_y$ $Gd_x(\mathbf{3})_y$ (e).

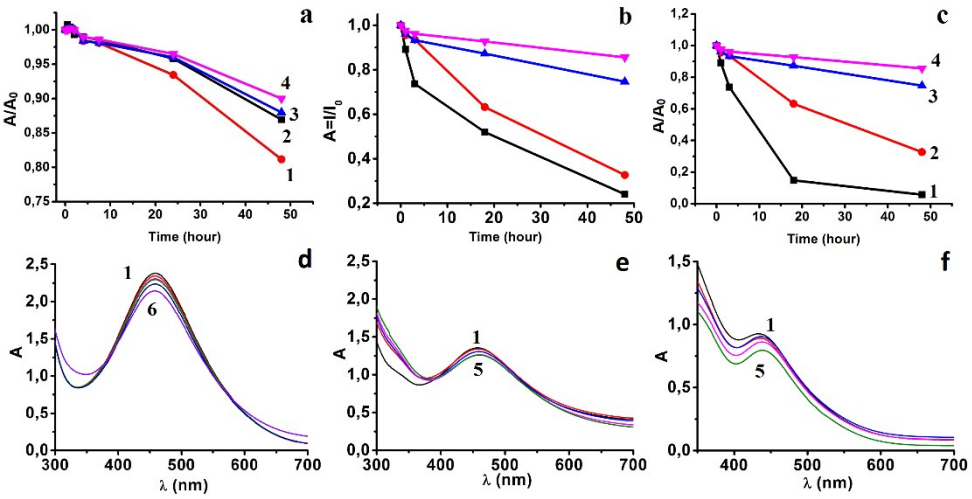


Fig. S.3 Destruction of $Gd_x(Kp)_y$ monitored by using A/A_0 values for F-127-stabilized system (1 – 0.08 mM F-127, 2 – 0.16 mM F-127, 3 – 0.24 mM F-127, 4 – 0.32 mM F-127): a – 0.007 mM Kp(OAc), 0.08 mM Gd^{3+}; 0.007 mM Kp(PO4), 0.1 mM Gd^{3+}; c - 0.007 mM Kp(S), 0.04 mM Gd^{3+}. 1-5(6) the UV-Vis spectra of the aqueous colloids $Gd_x(Kp)_y$ monitored within 50 hours: d – 0.007 mM Kp(OAc), 0.08 mM Gd^{3+}, 0.32 mM F-127; e - 0.007 mM Kp(PO4), 0.1 mM Gd^{3+}, 0.32 mM F-127; f - 0.007 mM Kp(S), 0.04 mM Gd^{3+}, 0.32 mM F-127.

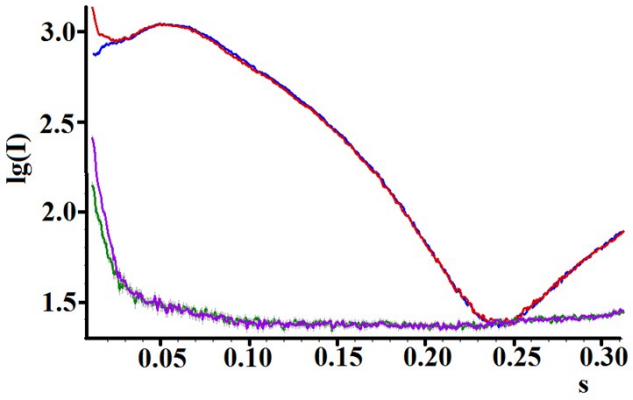


Fig. S. 4 SAXS diffraction intensity profiles at 23 °C (in logarithmic scale, Log(I) vs s) for 1mM keplerat solution (blue curve) in water, with addition acetic acid (red curve), water in capillary (green curve) and acetic acid solution in water (violet curve). Scattering vector s = 4πSinθ/λ, $Å^{-1}$; λ = 1.5418Å is the X-ray wavelength.

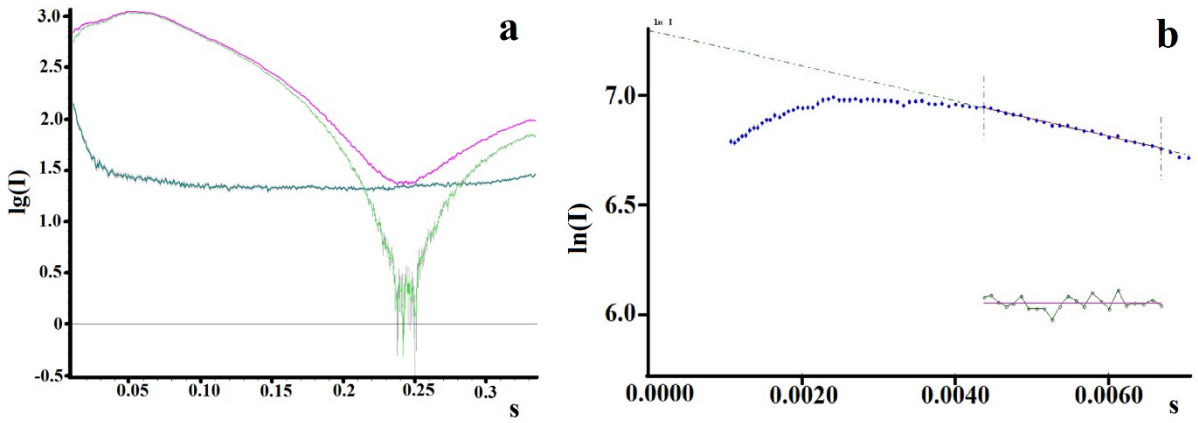


Fig. S. 5 (a) SAXS diffraction intensity profiles at 23 °C (in logarithmic scale, Log(I) vs s) for 1mM keplerat solution in water after background substraction. Scattering vector s = 4πSinθ/λ, $Å^{-1}$; λ = 1.5418Å is the X-ray wavelength.