

Supporting Information

The effect of pyridinecarboxylate chelating groups on the stability and electronic relaxation of gadolinium complexes

Nicholas Chatterton, Christelle Gateau, Marinella Mazzanti*, Jacques Pécaut, Alain Borel, André Merbach, Lothar Helm

Table S1: X-band ($\sim 9.44 \times 10^9$ Hz) and Q-band ($\sim 3.4 \times 10^{10}$ Hz) peak-to-peak width ΔH_{pp} and central field B_c as a function of temperature for aqueous $[\text{Gd}(\text{bpeda})]\text{K}$. The values were obtained by fitting one single Lorentzian derivative.

T / K	ΔH_{pp} / G	B_c / G	EPR Frequency / Hz
274.2	1234.0	3378.0	9.4434E+09
280.5	1137.4	3433.2	9.4427E+09
288.9	1059.8	3424.6	9.4384E+09
297.4	965.0	3457.0	9.4400E+09
297.4	947.6	3464.7	9.4399E+09
307.9	896.4	3475.7	9.4384E+09
316.9	854.5	3467.8	9.4397E+09
327.8	825.6	3441.4	9.4391E+09
339.7	825.5	3439.4	9.4388E+09
296.9	886.4	3470.9	9.4383E+09
297.5	90.1	12254.9	3.3980E+10
274.6	98.3	12252.9	3.3968E+10
278.6	94.2	12257.3	3.3984E+10
283.9	90.7	12256.1	3.3981E+10
289.6	89.7	12255.1	3.3978E+10
293.9	89.5	12253.7	3.3974E+10
304.6	91.5	12259.9	3.3990E+10
310.8	95.2	12256.6	3.3979E+10
319.6	101.8	12260.8	3.3978E+10
329.5	113.8	12256.2	3.3972E+10

Table S2: X-band ($\sim 9.44 \times 10^9$ Hz) and Q-band ($\sim 3.4 \times 10^{10}$ Hz) peak-to-peak width ΔH_{pp} and central field B_c as a function of temperature for the sharp component of the aqueous $[\text{Gd}(\text{bpeda})]\text{K}$ spectrum, obtained by fitting two Lorentzian derivatives.

T / K	ΔH_{pp} / G	B_c / G	EPR Frequency / Hz
274.2	574.4	2885.3	9.4434E+09
280.5	601.2	2923.5	9.4427E+09
288.9	694.0	2958.0	9.4384E+09
297.4	774.5	3007.5	9.4400E+09
297.4	606.4	2960.0	9.4399E+09

307.9	542.3	2939.7	9.4384E+09
327.8	520.2	2922.5	9.4391E+09
309.9	556.4	2943.7	9.4383E+09
297.5	84.4	12252.5	3.3980E+10
274.6	94.9	12251.8	3.3968E+10
278.6	89.9	12251.8	3.3984E+10
283.9	86.6	12255.0	3.3981E+10
289.6	84.5	12253.9	3.3978E+10
293.9	83.5	12252.5	3.3974E+10
304.6	83.8	12258.3	3.3990E+10
310.8	85.5	12254.7	3.3979E+10
319.6	88.2	12258.8	3.3978E+10
329.5	93.9	12253.9	3.3972E+10

Table S3: X-band ($\sim 9.44 \times 10^9$ Hz) and Q-band ($\sim 3.4 \times 10^{10}$ Hz) peak-to-peak width ΔH_{pp} and central field B_c as a function of temperature for the broad component of the aqueous [Gd(bpeda)]K spectrum, obtained by fitting two Lorentzian derivatives.

T / K	ΔH_{pp} / G	B_c / G	EPR Frequency / Hz
274.2	1146.2	3419.2	9.4434E+09
280.5	820.0	3451.2	9.4427E+09
288.9	771.4	3526.1	9.4384E+09
297.4	721.1	3526.4	9.4400E+09
297.4	790.3	3516.7	9.4399E+09
307.9	812.1	3499.3	9.4384E+09
327.8	773.0	3453.3	9.4391E+09
309.9	800.2	3495.3	9.4383E+09
297.5	856.6	12100.3	3.3980E+10
274.6	1076.8	12103.0	3.3968E+10
278.6	887.7	12138.2	3.3984E+10
283.9	855.4	12133.7	3.3981E+10
289.6	720.1	12156.9	3.3978E+10
293.9	672.2	12170.4	3.3974E+10
304.6	582.9	12179.2	3.3990E+10
310.8	569.9	12186.0	3.3979E+10
319.6	490.3	12205.9	3.3978E+10
329.5	482.6	12210.6	3.3972E+10