Supporting Information for Langmuir

Biocompatible Nanoparticles of Coordination Polymer $KGd(H_2O)_2[Fe(CN)_6]\cdot H_2O$ with Extremely High T_1-Weighted Relaxivity: Towards Stable Cellular MR Probes Containing Two Coordinated Water Molecules on the Gd(III) Center

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Summary of structure determination for $KGd(H_2O)_2[Fe(CN)_6]\cdot H_2O$

R-Values

Rexp : 1.26 Rwp : 1.87 Rp : 1.41 GOF : 1.48

Rexp`: 8.39  Rwp`: 12.40 Rp` : 19.27 DW : 0.96

Background

Chebyschev polynomial, No. Coefficients 12

Instrument

Powder Diffractometer	Bruker D8 Advance
Detector	PSD: LynxEye
Exposition	1sec
Radiation	CuKα, λ=1.54178 Å

Goniometer radius (mm)	217.5
Linear PSD 2Th angular range (°)	3
FDS angle (°)	0.5
Beam spill, sample length (mm)	15
Intensity corrected	
Simple axial model (mm)	5.1(2)

Corrections

Zero error	0.024
Specimen displacement	-0.055(2)
LP Factor	90
Absorption (1/cm)	26.9(7)
Sample Thickness (mm)	0.2
Intensity correction applied	

Structure 1

Phase name	K[GdFe(CN)6].3H2O
R-Bragg	1.27%
Spacegroup	Pnma
Scale	0.0002102(6)
Cell Mass	1825.21
Cell Volume (Å^3)	1244.63(7)
Wt% - Rietveld	100.000
Crystallite Size Lorentzian (nm)	465(19)
Strain Lorentzian	0.125
Crystal Linear Absorption Coeff. (1/cm)	465.19(3)
Crystal Density (g/cm^3)	2.43513(13)
Preferred Orientation (Dir 1 : 0 1 0)	1.23(3)
(Dir 2 : 1 0 0)	0.843(14)
Fraction of Dir 1	0.45(7)
Lattice parameters	

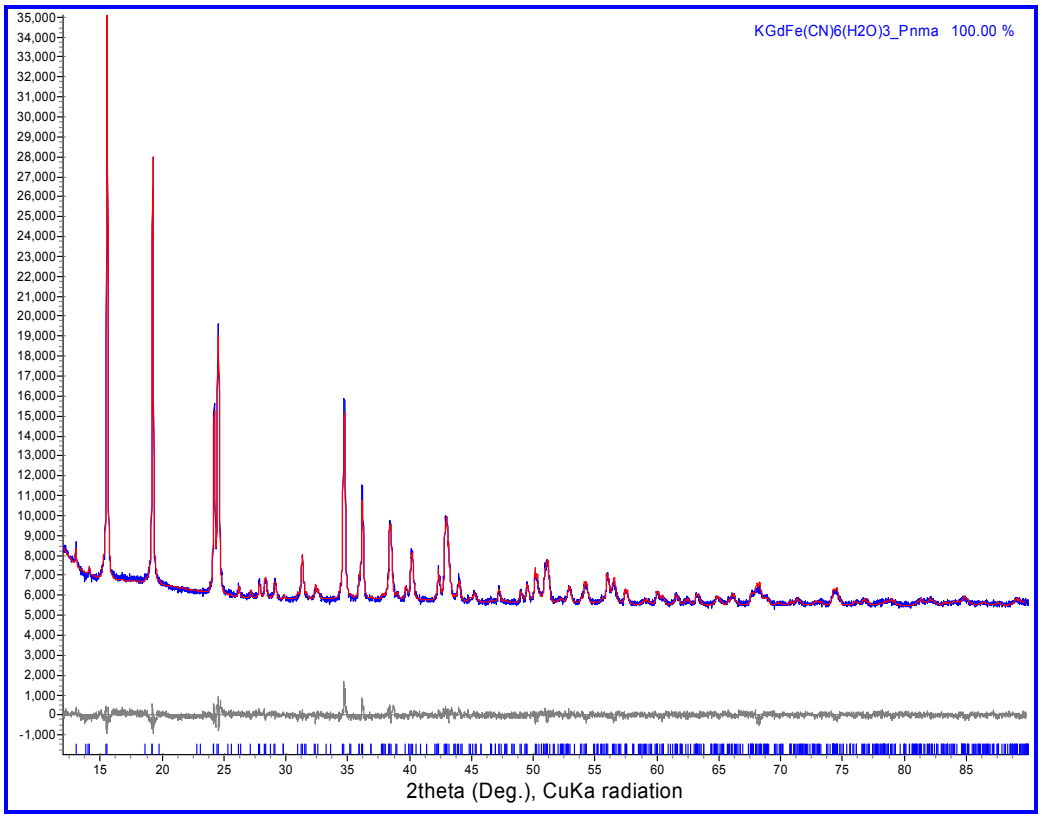
a (Å)	12.6098(4)
b (Å)	13.6161(4)
c (Å)	7.2490(3)

Site	Np	x	y	z	Atom	Occ	Beq
Gd	4	0.16014	0.25000	-0.00846	Gd	1	1.121
Fe	4	0.50000	0.50000	0.00000	Fe	1	1.287
C1	8	0.38070	0.41230	-0.01010	C	1	1.816
N1	8	0.30880	0.36020	-0.00970	N	1	2.763
C2	8	0.41770	0.58710	0.14510	C	1	1.816
N2	8	0.36540	0.64070	0.23130	N	1	2.606
C3	8	0.54850	0.43280	0.21400	C	1	1.737
N3	8	0.57820	0.38840	0.34270	N	1	2.763
O1	4	0.22440	0.25000	0.32570	O	1	2.763
O2	4	-0.04090	0.25000	-0.09200	O	1	3
O3	8	0.16650	0.59000	0.01080	O	0.5	4.422
K	8	0.16770	0.57910	-0.04510	K	0.5	4.185

Gd:0	N1:1	0	-1	0	2.40112
	N1:0	0	0	0	2.40112
	N2:7	-1	-1	0	2.42436
	N2:6	-1	0	0	2.42436
	N3:3	0	-1	-1	2.46226
	N3:2	0	0	-1	2.46226
	O1:0	0	0	0	2.55421
	O2:0	0	0	0	2.60647
Fe:0	C2:5	-1	-1	0	1.89469
	C2:0	0	0	0	1.89469

	C3:0	0	0	0	1.90203
	C3:5	-1	-1	0	1.90203
	C1:5	-1	-1	0	1.92208
	C1:0	0	0	0	1.92208
C1:0	N1:0	0	0	0	1.15120
	Fe:0	0	0	0	1.92208
N1:0	C1:0	0	0	0	1.15120
	Gd:0	0	0	0	2.40112
C2:0	N2:0	0	0	0	1.16534
	Fe:0	0	0	0	1.89469
N2:0	C2:0	0	0	0	1.16534
	Gd:3	-1	-1	-1	2.42436
C3:0	N3:0	0	0	0	1.17309
	Fe:0	0	0	0	1.90203
N3:0	C3:0	0	0	0	1.17309
	Gd:1	-1	0	-1	2.46226
O1:0	Gd:0	0	0	0	2.55421
	K:6	-1	0	-1	2.85365
	K:7	-1	-1	-1	2.85365
O2:0	Gd:0	0	0	0	2.60647
	K:4	0	0	0	2.99319

	K:5	0	-1	0	2.99319
O3:0	K:0	0	0	0	0.43181
K:0	O3:0	0	0	0	0.43181
	O1:3	-1	-1	0	2.85365
	O2:2	0	-1	0	2.99319
	N3:2	0	0	-1	3.18883



Firgure S1. Rietveld refinement plot of $KGd(H_2O)_2[Fe(CN)_6]\cdot H_2O$ with the difference between observed and calculated patterns shown at the bottom and the reflection positions shown as the vertical lines

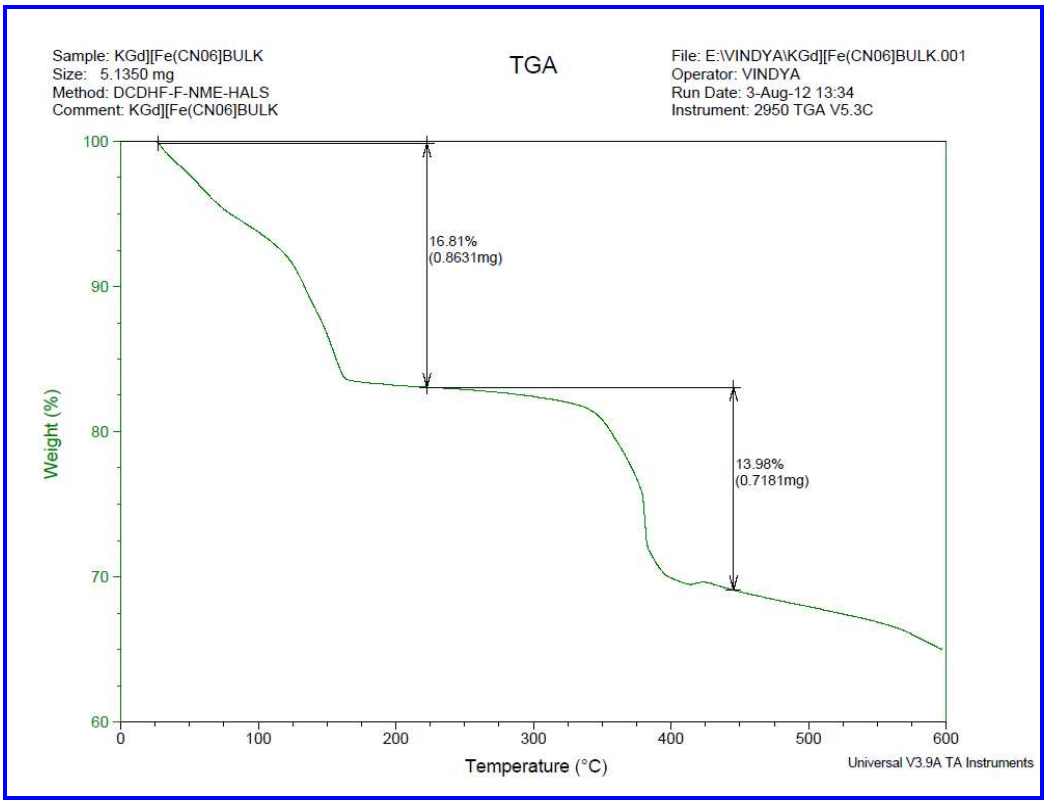


Figure S2. The TGA curve of bulk $KGd(H_2O)_2[Fe(CN)_6]\cdot H_2O$ sample

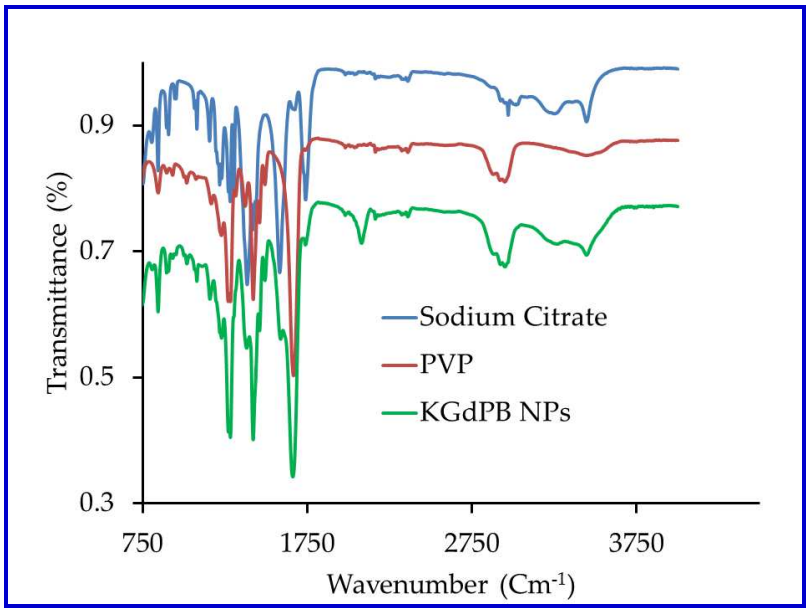
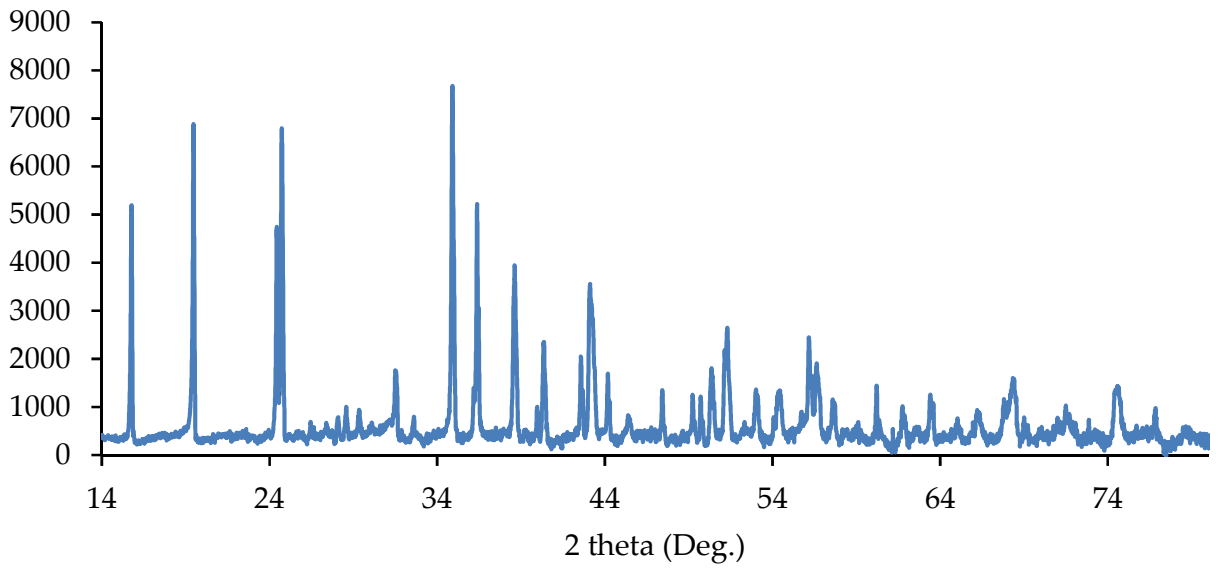


Figure S3. FT-IR spectra of sodium citrate, PVP and PVP-C-KGdFeCN NPs.



Firgure S4. XRD Patterns of PVP-C-KGd$(H_2O)_2[Fe(CN)_6]\cdot H_2O$

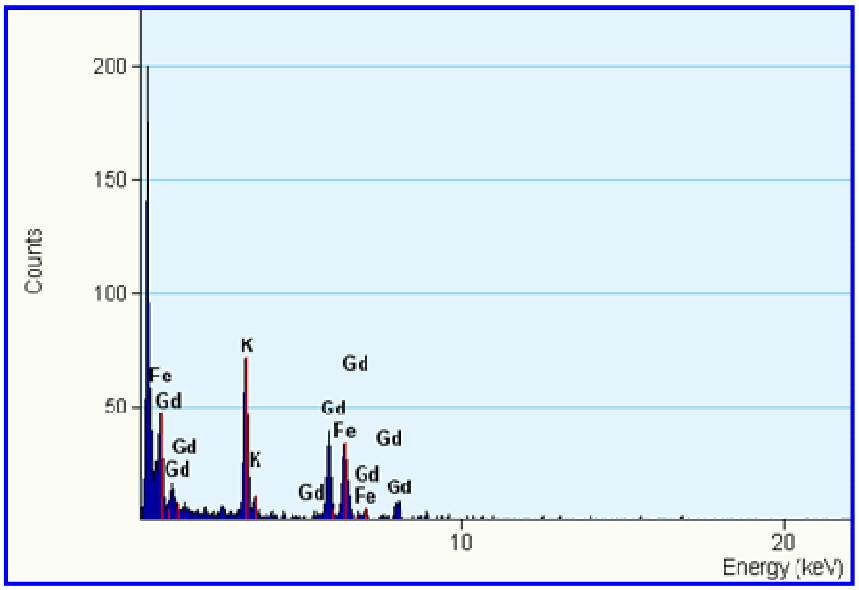


Figure S5. EDX spectrum on a typical PVP-coated nanoparticle

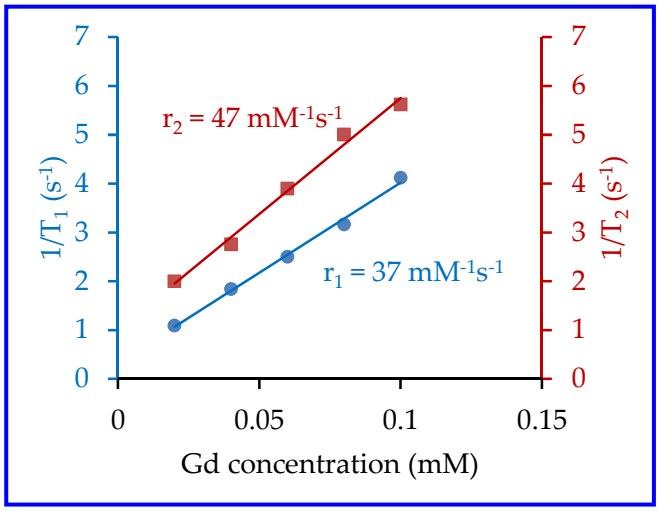


Figure S6. Plots of $1/T_i$ (i=1,2) versus Gd^{3+}-concentration at the magnetic field strength of 1.4 T for PVP-coated NPs.

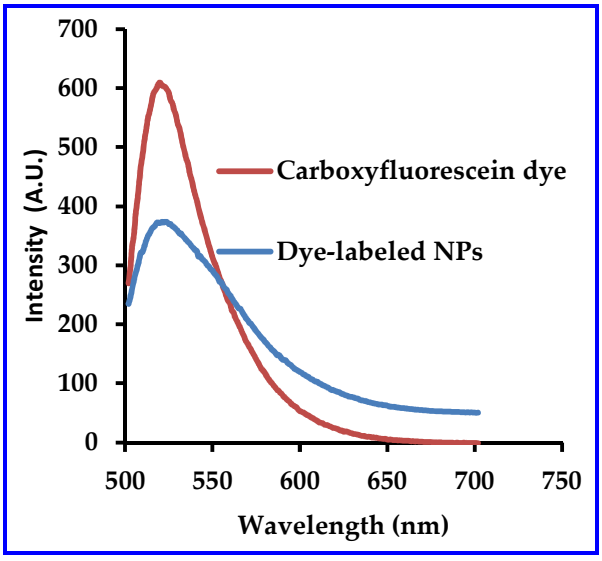


Figure S7. Fluorescence spectra of carboxyfluorescein dye and dye labeled nanoparticles.