New organometallic framework coordination polymer {(NMe_2H_2)[Sm(TDA)(HCOO)]}: synthesis, structure and effect of isomorphic substitution of samarium with Gd^{3+} and Tb^{3+} ions on luminescent properties

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Supporting information

Table S1. Selected crystal data and parameters for structure refinement of the Sm-TDA and Gd-TDA

Chemical formula	$[(CH_3)_2NH_2]^+[Sm(C_4N_3O_4)(HCOO)]^- \cdot 0.5H_2O$ (**Sm-TDA**)	$[(CH_3)_2NH_2]^+[Gd(C_4N_3O_4)(HCOO)]^- \cdot 0.5H_2O$ (Gd-TDA)
M_r	404.54	411.44
Temperature, K	100(2)	120(2)
Crystal system	Orthorhombic	
Space group	*Pna2₁*	
a, Å	12.8521(5)	12.8145(9)
b, Å	10.0035(5)	9.9105(6)
c, Å	8.9281(7)	8.8666(6)
α (= β = γ), °	90	
V, Å^3	1147.85(12)	1126.04(13)
Z	4	
ϱ_{calc}, g/cm^3	2.341	2.427
μ (Mo$K\alpha$), mm^{-1}	5.149	5.924
F(000)	776	784
θ_{min} - θ_{max}, °	2.58 – 30.00	2.60 – 30.50
No. of measured reflections	9670	10981
No. of unique reflections (R_{int})	3309 (R_{int} = 0.0283)	3060 (R_{int} = 0.0569)
No. of parameters	196	193
GoF	1.235	1.132
R_1 (I>2σ(I))	0.0303	0.0460
ωR_2 (all reflections)	0.0616	0.0852
$\Delta\varrho_{max}/\Delta\varrho_{min}$, e/Å^3	1.91/-2.645	2.29/-2.44

Table S2. Sm^{3+} luminescence fitting parameters for Sm_xGd_{1-x}-TDA

		Value	Standard Error	Reduced Chi-Sqr	Adj. R-Square
Sm100	y0	9.80E-04	3.53E-05	1.43E-07	0.99998
	A1	0.76118	9.43E-04		
	t1	3.85709	0.0063		
	A2	0.01974	9.71E-04		
	t2	17.41743	0.62067		
Sm90Gd10	y0	0.01041	5.33E-04	8.77E-06	0.99935
	A1	0.61145	0.01268		
	t1	3.6055	0.07618		
	A2	0.12063	0.01292		
	t2	13.56254	0.99967		
Sm80Gd20	y0	0.00329	1.12E-04	6.30E-07	0.99993
	A1	0.77906	9.56E-04		
	t1	4.8335	0.01089		
	A2	0.02501	8.59E-04		
	t2	34.75123	1.36292		
Sm70Gd30	y0	0.00406	2.48E-04	5.75E-06	0.99936
	A1	0.6951	0.00574		
	t1	4.92712	0.05251		
	A2	0.06959	0.00593		
	t2	21.70083	1.35538		
Sm60Gd40	y0	0.00241	1.16E-04	7.18E-07	0.99994
	A1	0.78901	0.0015		
	t1	6.34083	0.01748		
	A2	0.0443	0.00152		
	t2	31.93394	0.97294		
Sm50Gd50	y0	0.00114	5.96E-05	1.60E-07	0.99999
	A1	0.81526	9.44E-04		
	t1	7.87333	0.01092		
	A2	0.0674	9.70E-04		
	t2	33.27221	0.37929		
Sm40Gd60	y0	0.00241	2.04E-04	1.80E-06	0.99991
	A1	0.72117	0.00378		
	t1	8.56416	0.04838		
	A2	0.16548	0.00389		
	t2	33.08668	0.57253		
Sm30Gd70	y0	0.00176	1.50E-04	4.90E-07	0.99998
	A1	0.68538	0.00224		
	t1	11.06936	0.03519		
	A2	0.24306	0.00227		
	t2	41.04383	0.29758		
Sm20Gd80	y0	0.00432	2.80E-04	1.60E-06	0.99995
	A1	0.46825	0.00394		
	t1	11.16875	0.09253		
	A2	0.45829	0.00397		
	t2	42.02734	0.29074		
Sm90Gd10	y0	0.00272	2.89E-04	8.05E-07	0.99998

	A1	0.3292	0.00494		
	t1	15.29796	0.16643		
	A2	0.62657	0.0049		
	t2	47.50363	0.26211		
Sm08Gd92	y0	0.00679	6.19E-04	8.81E-06	0.99976
	A1	0.23515	0.00456		
	t1	8.03598	0.23395		
	A2	0.6507	0.00442		
	t2	44.5726	0.34073		
Sm06Gd94	y0	0.00938	5.53E-04	9.60E-06	0.99976
	A1	0.18441	0.00341		
	t1	5.49536	0.19087		
	A2	0.7225	0.00291		
	t2	42.67809	0.23131		
Sm04Gd96	y0	0.00536	4.63E-04	3.54E-06	0.99993
	A1	0.14384	0.00372		
	t1	9.89864	0.32534		
	A2	0.79546	0.00366		
	t2	47.34877	0.22836		
Sm02Gd98	y0	0.06057	0.00113	3.32E-05	0.9974
	A1	0.39989	0.00545		
	t1	4.12159	0.11395		
	A2	0.31707	0.0035		
	t2	48.00162	0.94742		

Table S3. Tb^{3+} luminescence fitting parameters for Sm_xTb_{1-x}-TDA

		Value	Standard Error	Reduced Chi-Sqr	Adj. R-Square
Sm90Tb10	y0	0.1324	0.1878	0.75923	0.99016
	A1	-2.02E+07	--		
	t1	0.02315	8.50E+15		
	A2	106.07984	5.1217		
	t2	7.75162	0.25497		
Sm80Tb20	y0	-0.34332	0.13882	0.39717	0.9994
	A1	2.62E+12	3.84E+13		
	t1	0.34217	0.19144		
	A2	344.34815	6.54948		
	t2	7.41737	0.07835		
Sm70Tb30	y0	-0.34269	0.09244	0.16989	0.99885
	A1	8.70E+09	1.26E+11		
	t1	0.41801	0.28294		
	A2	158.59406	4.21378		
	t2	7.58036	0.1128		
Sm60Tb40	y0	-0.23662	0.09777	0.16356	0.99936
	A1	1814.41753	3423.844		
	t1	0.54296	0.56264		
	A2	214.98878	10.58073		
	t2	7.31989	0.15076		
Sm50Tb50	y0	-0.57201	0.17955	0.631	0.99873
	A1	1.01E+08	6.42E+08		
	t1	0.55664	0.2223		
	A2	289.15008	8.86876		
	t2	7.56383	0.12621		
Sm40Tb60	y0	-0.11624	0.01952	0.00682	0.99972
	A1	3662.87351	2821.111		
	t1	0.67100	0.149		
	A2	64.36181	1.69518		
	t2	7.36749	0.08721		
Sm30Tb70	y0	-0.36427	0.12423	0.33198	0.9992
	A1	7.77E+12	2.13E+14		
	t1	0.32236	0.31683		
	A2	290.33067	6.45823		
	t2	7.17237	0.0861		
Sm20Tb80	y0	-0.47851	0.17938	0.65873	0.99885
	A1	3.75E+06	2.28E+07		
	t1	0.68625	0.3237		
	A2	335.98149	11.29084		
	t2	7.19245	0.12184		
Sm90Tb10	y0	0.03792	0.02464	0.00815	0.99996
	A1	481.91706	129.1183		
	t1	2.08193	0.16224		
	A2	168.46724	2.86231		

	t2	7.92291	0.054		
Sm08Tb92	y0	-0.10212	0.0386	0.03573	0.9997
	A1	7.93E+11	1.26E+13		
	t1	2.04088	0.20611		
	A2	141.76163	1.69561		
	t2	8.09928	0.05348		
Sm06Tb94	y0	0.07544	0.09276	0.44074	0.99914
	A1	4246.93205	5.27E+08		
	t1	2.51358	--		
	A2	349.70135	3.65767		
	t2	8.28745	0.05122		
Sm04Tb96	y0	0.11311	0.03236	0.03083	0.99994
	A1	177.37358	23.74793		
	t1	3.37104	0.30187		
	A2	224.64578	5.52201		
	t2	9.89412	0.08839		
Sm02Tb98	y0	0.17476	0.0311	0.0198	0.99995
	A1	95.15387	2.16904		
	t1	9.64323	0.23446		
	A2	82.14667	2.86458		
	t2	23.46238	0.32499		

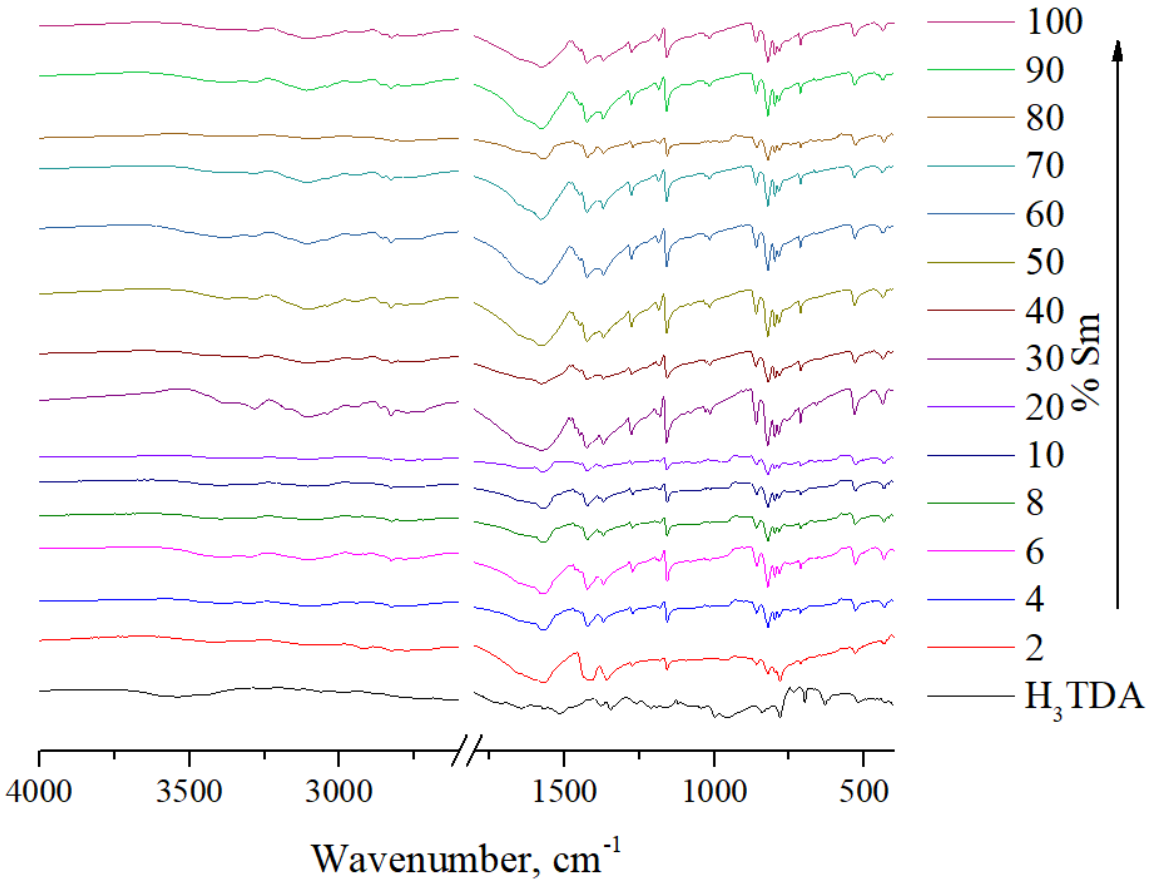

Figure S1. IR spectra of complexes Sm_xGd_{1-x}-TDA and free H_3TDA ligand

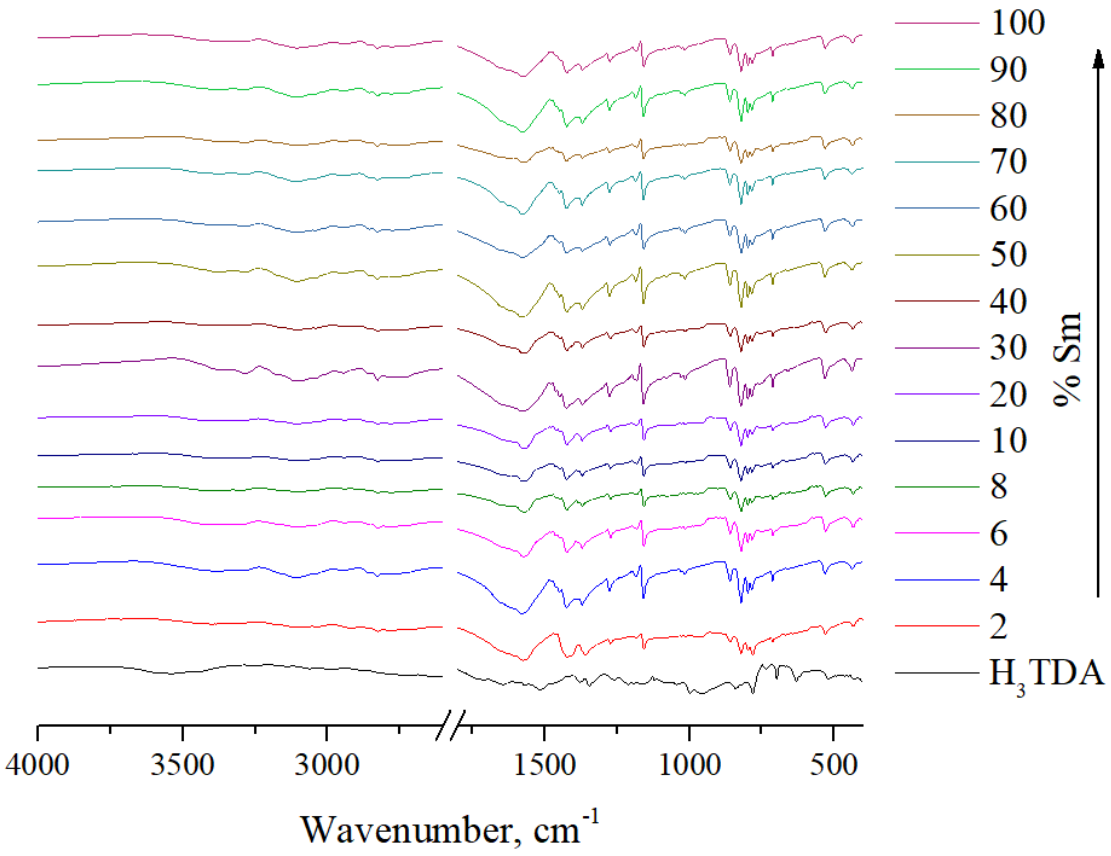

Figure S2. IR spectra of complexes Sm_xTb_{1-x}-TDA and free H_3TDA ligand

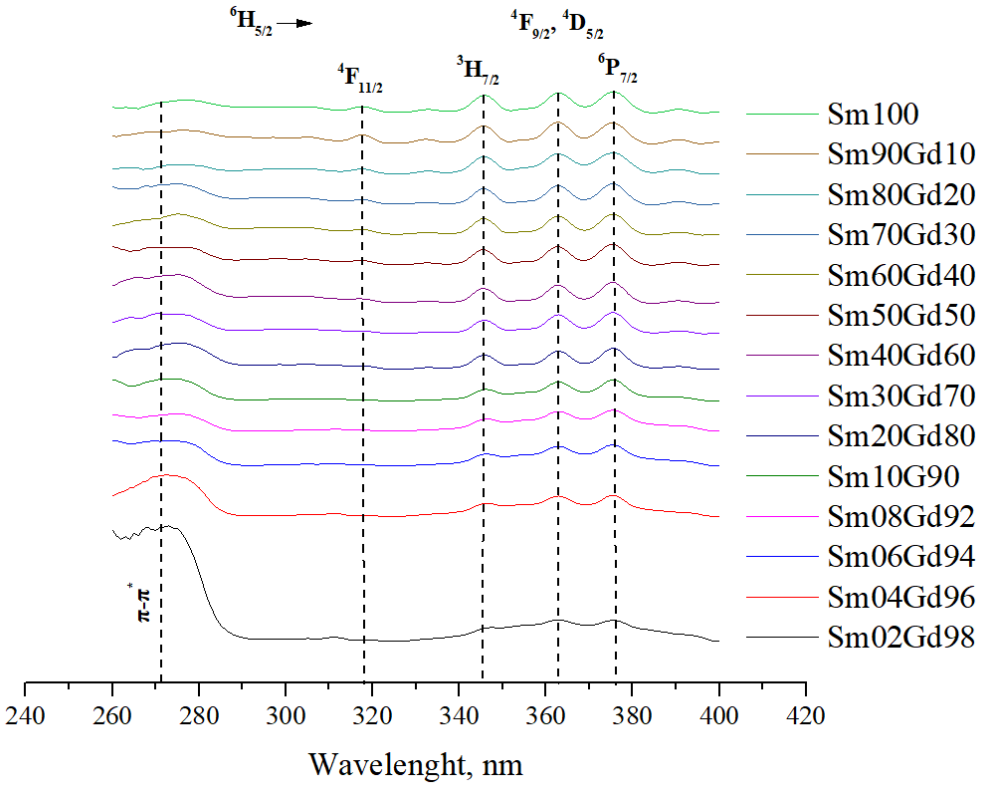

Figure S3. Excitation spectra of Sm_xGd_{1-x}-TDA complexes (λ_{em} 648 nm).

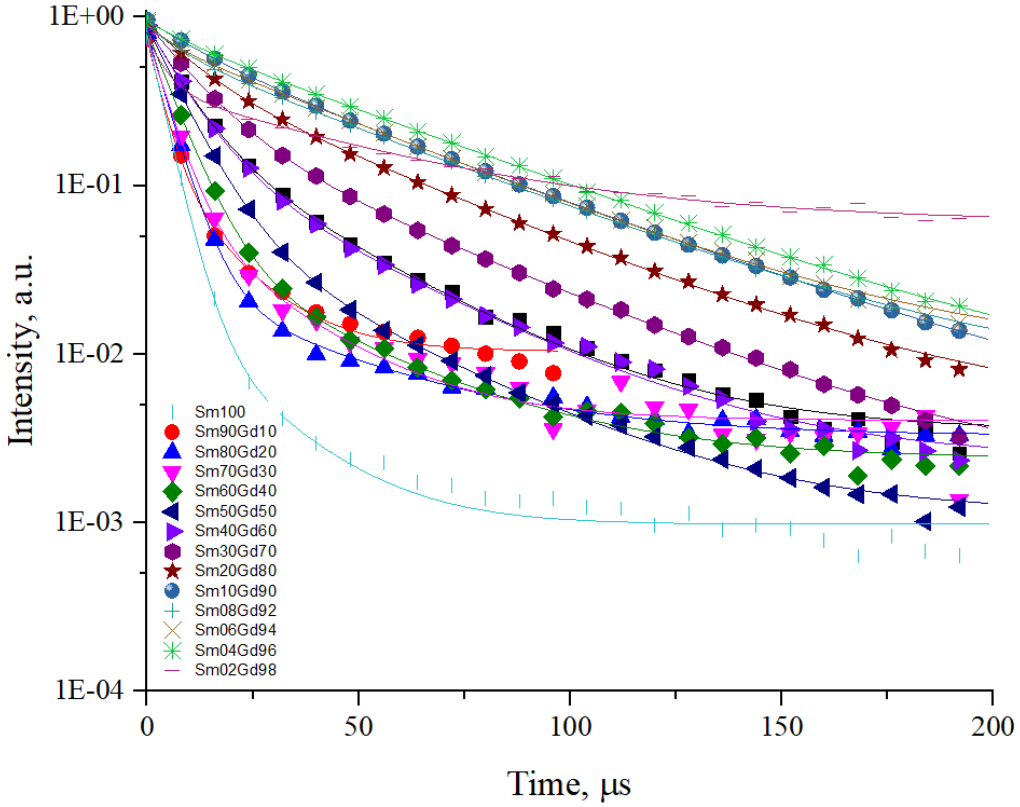

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Figure S4. Sm^{3+} decay curves for Sm_xGd_{1-x}-TDA; λ_{EX}=280 nm, λ_{EM}=648 nm.

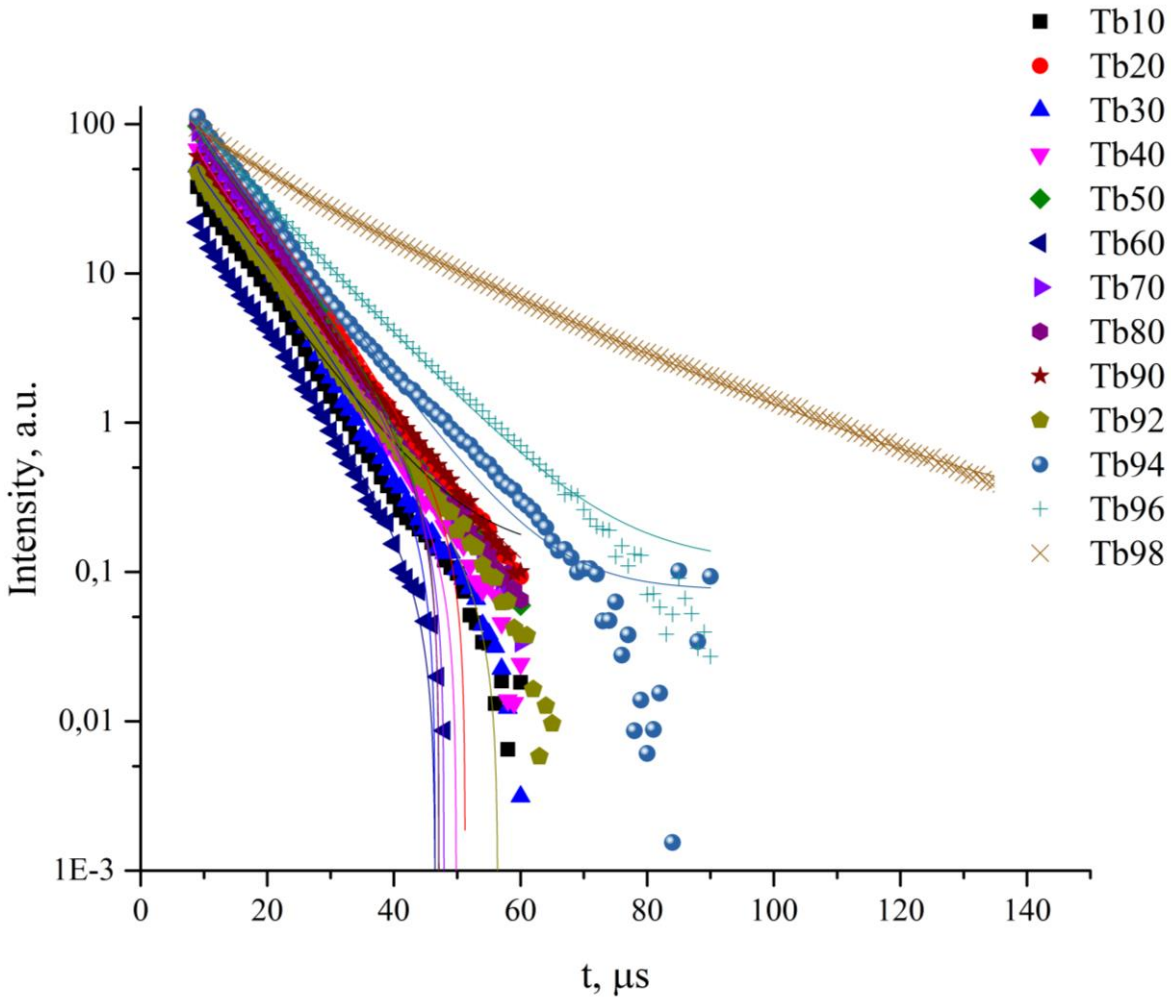

Figure S5. Tb^{3+} decay curves for Sm_xTb_{1-x}-TDA; λ_{EX}=280 nm, λ_{EM}=545 nm.

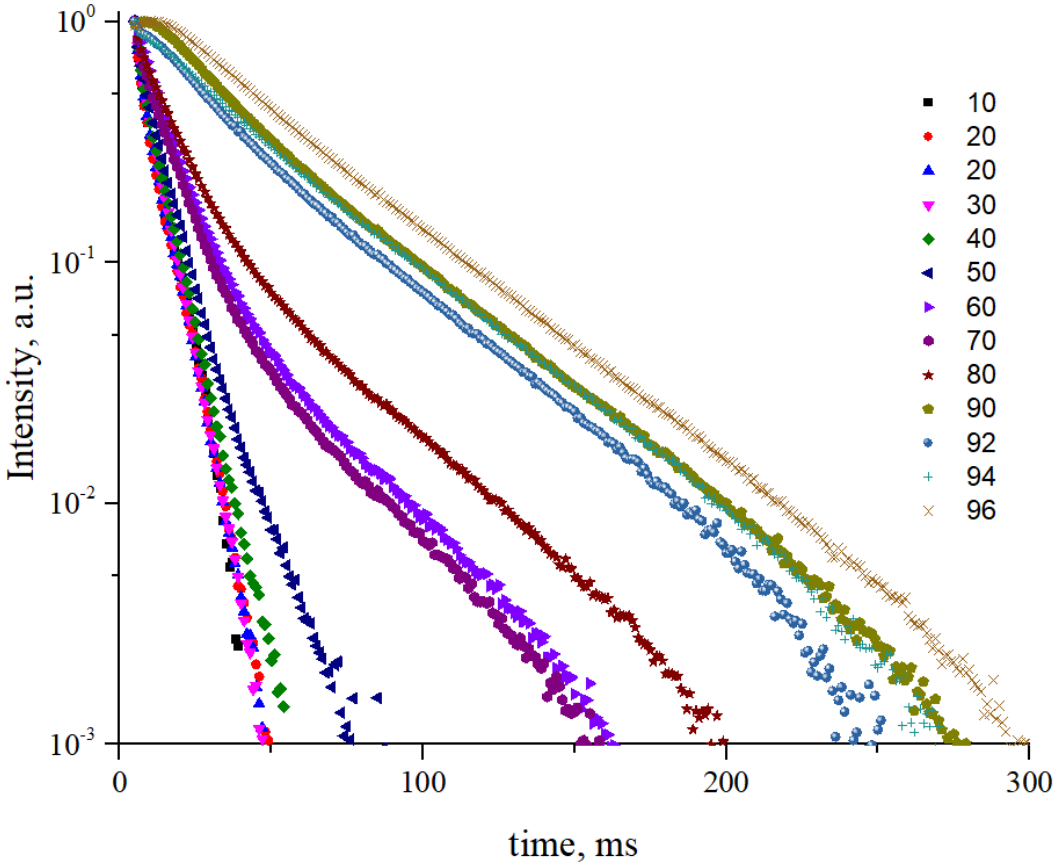

Figure S6. Sm^{3+} decay curves for Sm_xTb_{1-x}-TDA; λ_{EX}=280 nm, λ_{EM}=648 nm.