Supplementary Information

Pure and Mixed {Nd/Yb} Carborane-based Metal-Organic Frameworks integrating Slow Magnetic Relaxation, Magnetocaloric Effect and NIR emission

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S1. Summary of Nd(III) compounds with SMM and/or NIR behaviour

Table S1. Review of Nd(III) compounds across dimensions showing SMM behaviour; in italic font, *ab initio*-calculated values. Temperature dependence of the relaxation rate: $\tau^{-1}(T) = \tau_{QT}^{-1} + A \cdot T + C \cdot T^n + \tau_0^{-1} \exp(-U/k_B T)$.

Compound		g_x*	g_y*	g_z*	H (kOe)	U_{eff}/k_B (K)	τ_0 (s)	C ($s^{-1}K^{-n}$)	n	τ_{QT}^{-1} (s^{-1})	A ($s^{-1}K^{-1}$)	Ref.
0D Nd Single-Ion Magnets (SIMs)												
$[Nd^{III}(Tp)_3]$					0.1	4.1	4.2×10^{-5}					1
$Na_9[Nd^{III}(W_5O_{18})_2]$					1	73.9	3.55×10^{-10}					2
$[Nd^{III}(NO_3)_3$(1,10-diaza-18-crown-6)]					1	73(2)	1.4×10^{-10}					3
$[Nd(ntfa)_3$(5,50 -Me_2bipy)]					1.5	44.64	1.0×10^{-9}	186	3.0			4
$[Nd(ntfa)_3$(4,40 -Mt_2bipy)]					1.5	27.36	8.7×10^{-8}	59	2.3			4
$[Nd(ntfa)_3$(phen)]					1.5	25.92	2.2×10^{-7}	135	2.4			4
$[Nd^{III}(NO_3)_3$(18-crown-6)]					1	33.4(5)	1.6×10^{-9}					3
$[Nd^{III}(^tBuPO(NH^iPr)_2)_2(H_2O)_5]I_3 \cdot H_2O$					2	39.21	8.98×10^{-6}					5
					0	24.69	5.03×10^{-6}					
$[Li(dme)_3][Nd^{III}(COT'')_2]$					1	21	5.5×10^{-5}					6
$[Nd^{III}(TTA)_3(MeOH)_2] \cdot 0.5$Azo-py					1	19.7	3.7×10^{-7}					7
0D Nd_2 dimeric systems												
$[Nd_2$(2-FBz)4-$(NO_3)_2(phen)_2]$					1.5	13.67	7.4×10^{-6}	0.02	9		265.21	8
$[\{LNd(H_2O)_2\}_2(C_2O_4)] \cdot 64H_2O$					0.5	6.78	5.48×10^{-12}					9
$[Nd_2(L)_4(H_2O)_6](L)_2(H_2O)_{14}$					1.2	6.2	2.2×10^{-5}					10
$[Nd_2(\mu_2$-9-AC$)_4$(9-AC$)_2$(bpy$)_2]$					2	12	7.5×10^{-6}	1.03	6		823.60	11
1D coordination polymers												
$\{[Nd(L)_3(H_2O)] \cdot DMF\}_n$					2			464	2.43			12
$\{[Nd(pzdo)(H_2O)_4][Co(CN)_6]\} \cdot 0.5(pzdo) \cdot 4H_2O$					1	52 (2)	4.5×10^{-8}	0.09	5.6	2.2		13
$[Nd(NO_3)\{Zn(L)(SCN)\}_2]$					1	38.5	2.07×10^{-7}					14
$[Nd_2(CNCH_2COO)_6(H_2O)_4] \cdot 2H_2O$					1.5	26.6	1.75×10^{-7}					15
$\{[Nd(\mu_2$-$L_1)_3(H_2O)_2] \cdot MeCN\}_n$		1.021	2.012	3.514	2	27	4.1×10^{-7}					16
$[Nd(\mu_2$-L2)(L2)$(CH_3COO)(H_2O)_2]_n$		0.622	1.730	4.122	3.5	29	3.1×10^{-7}					16
$[Nd(\mu_2$-$L_1)_3(H_2O)_2] \cdot H_2O$					2.0	28	7.29×10^{-7}			0.014		17
$[Nd(\mu_2$-$L_2)_2(CH_3COO)(H_2O)_2]_n$					2.0	19.7	3.43×10^{-6}			0.0026		17
$\{Nd(\alpha$-fur$)_3(H_2O)_2\}$	Exp.				1.2	174.24	1.04×10^{-13}	1.41×10^2	3.7	3.5×10^2	1.9×10^3	18
	Ab initio	0.52	1.03	4.41		180						
$\{Nd_{0.065}La_{0.935}L(H_2O)_2\}_n$	Exp.				1.2	87.84	3.63×10^{-11}	2.89×10^{-3}	9.9	7.82	0.247	18
	Ab initio	1.35	1.98	3.88		84.67						
2D MOFs												
$\{[Nd^{III}_4(H_2O)_{17}L][M^{IV}(CN)_8]_3\}$ M=Mo					1.5			312	2.997		$5.51(7) \times 10^{-6}$	19
M=W					1.5			241	2.604		$2.00(18) \times 10^{-7}$	
3D MOFs												
$[Nd^{III}(H_2O)_3][M^I(CN)_2]_3$ M=Ag		2.51	2.57	2.7	2	18.8						20
M=Au		2.51	2.57	2.7	2	25.6						
$\{[Nd_2L(H_2O)_4] \cdot 6H_2O\}_n$					2 / 1	—	—	35.4 /42.2×10^{-3}	9		169 /148	21
$[Nd^{III}L)_2(H_2O)]$-$[Cu_2^I(CN)_5] \cdot 5H_2O$		0.24	1.44	4.80	1.75			0.09	7		5.7	22

Table S2. Review of Nd(III) compounds showing photophysical properties in solid state at 298 K.

Compound	λ_{em} (nm)	τ_{obs} (μs)	Q_{Ln}^{Ln} (*)	Ref.
0 D				
[Nd(L1)(NO$_3$)$_3$]	865	0.27	3.38×10^{-2} (0.8ms)	[23]
Nd(TFI)$_3$(H$_2$O)$_2$	1060	2.62	0.011 (0.27 ms)	[24]
Nd(TFI)$_3$(bpy)	1060	9.95	0.040 (0.27 ms)	[24]
Nd(TFI)$_3$(Phen)	1060	11.3	0.046 (0.27 ms)	[24]
[(PPh$_3$)$_2$Pt(μ-pdo)Nd(tta)$_3$]	1055	0.95	4×10^{-3} (0.25 ms)	[25]
[Nd(tta)$_3$(BPTZ)]	1055	1.25	3×10^{-3} (0.25 ms)	[26]
Nd(DBM)$_3$(phen)	1060	0.7	8.6×10^{-2} (0.25 ms)	[27]
[Nd(tnm)$_3$(DMSO)$_2$]	1060	11	0.012 (0.917 ms)	[28]
Nd(hfpyr)$_3$(H$_2$O)	1069	2.8	0.0104 (0.27 ms)	[29]
Nd(hfpyr)$_3$(bath)	1069	6.16	0.0228 (0.27 ms)	[29]
complex a	1060	0.783	-	[30]
complex b	1060	1.08	-	[30]
Nd(5,6-DTFI)$_3$(H$_2$O)(CH$_3$OH)	1060	1.89	0.007 (0.27 ms)	[31]
Nd(5,6-DTFI)$_3$(phen)	1060	7.95	0.029 (0.27 ms)	[31]
1 D CP				
[Nd(tfbdc)$_{0.5}$(bta)$_2$(CH$_3$OH)$_2$]·CH$_3$OH	900, 1065, 1345	11.35	0.042 (0.27 ms)	[32]
2 D MOF				
{[Nd(DSPT)(ox)$_{0.5}$]·H$_2$O}$_n$	900, 1073, 1354	-	-	[33]
[Nd$_2$(NDC)$_6$(DMF)$_4$]$_n$	888, 1064, 1345	4.14	0.0166 (0.25 ms)	[34]
[Nd$_2$(Cptpy)$_2$(Glu)$_2$(H$_2$O)$_2$]$_n$ · 5n(H$_2$O)	900, 1060, 1335	-	-	[35]
3 D MOF				
[Nd(HL)]	1063	τ_1 = 0.058 ms, τ_2 = 0.33ms (**).	-	[36]
[Nd(BPTC)(H$_2$O)$_2$]·H$_3$O·DMF	1062	τ_1 = 6.332 μs, τ_2 = 6.330 μs	-	[37]
{[Nd(Oaobtc)(H$_2$O)$_4$]·Hbipy·H$_2$O}$_n$	1065	0.392	0.0207 (0.27 ms)	[38]
[Nd(BPTC)(H$_2$O)$_2$]·H$_3$O·DMF	894, 1062, 1330	τ_1 = 6.332 ± 0.815 μs, τ_2 = 6.330 ± 0.076 μs	-	[39]
{[ZnLnCl(pydc)$_2$(H$_2$O)$_6$]·3H$_2$O}$_n$	883–916, 1053, 1327 nm	-	-	[40]
{[Nd$_2$L$_2$]·2NH$_2$(CH$_3$)$_2$·3H$_2$O}	1060	*6.03*	0.012 (0.5 ms)	[41]

* Quantum yield determined in the original paper as Q_{Ln}^{Ln} = τ_{obs}/ τ_{rad} (the τ_{rad} value assumed for Nd(III), given in parenthesis); (**) Lifetime decay was fit with a biexponential function, $I = I_0 + A_1 \exp(-t/\tau_1) + A_2 \exp(-t/\tau_2)$.

S2. Summary of Yb(III) compounds with SMM and/or NIR behaviour

Table S3. Review of Yb(III) compounds across dimensions showing SMM behaviour; in italic, *ab initio*-calculated values. Temperature dependence of the relaxation rate: $\tau^{-1}(T) = \tau_{QT}^{-1} + A \cdot T + C \cdot T^{n} + \tau_0^{-1} \exp(-U/k_B T)$.

Compound	g_x*	g_y*	g_z*	H (kOe)	U_{eff}/k_B /Δ_{lum} (K)	τ_0 (s)	C ($s^{-1}K^{-n}$)	n	τ_{QT}^{-1} (s^{-1})	A ($s^{-1}K^{-1}$)	Ref.
0D SIMs											
$[Yb(H_3L^1)_2]Cl_3$ $5CH_3OH{\cdot}2H_2O$	3.76	2.71	0.722	0.4				2.37			42
$[Yb(tta)_3(L^2)]{\cdot}2CH_2Cl_2$	5.96	0.73	0.33	1	6	1.9×10^{-5}					43
$[N(C_2H_5)4]_3[Yb(dipic)_3].nH_2O$					*187*						44
$Na[YbDOTA\ (H_2O)]{\cdot}4H_2O$				1	39	4×10^{-7}					45
$[Yb(QR1)_2](NO_3){\cdot}CH_3OH{\cdot}0.5H_2O$				1	5.4	1.0×10^{-5}					46
$[Yb(QR1)(tta)_2]{\cdot}CH_3OH$				1	16.1	1.8×10^{-7}					46
[Yb(trensal)]				2	(54.7) / 667.6		0.15	6.2		258	47
$[Yb(acac)_2(Q)(Phen)]$				1.5	(26.4) / 722.3	(4.8×10^{-6})	0.055	6.5	21.4		48
K5 $[Yb(\alpha\text{-}SiW_{11}O_{39})(C_20H_{22}Br_2N_2O_4)]{\cdot}14H_2O$				1	21.29						49
$[Yb(PyrCOO)\ (acac)_2(H_2O)_2]$				2	54	7.4×10^{-8}	0.013	7		1.1 $\times 10^{-12}$ (n_{dir}=4)	50
0D Yb_2 dimeric systems											
$[Yb_2(L^3)_2(acac)_2(H_2O)]{\cdot}2CH_2Cl_2$				1.6	24.5	6.8×10^{-7}					51
$[Yb(tta)_2(L^4)(L^5)]_2{\cdot}1.4CH_2Cl_2$				2	20.1/ 23	1.7×10^{-6}					52
$[Yb_2(L^{11})3(CH_3OH)]{\cdot}3CH_3CN$				3	14.54	1.6×10^{-6}					53
$[Yb_2(L^{11})(L^{12})(L^{13})(CH_3OH)(H_2O)_2](ClO_4)_2$				3	2.02	3.7×10^{-5}					53
$Yb_2(L^{11})(OAc)_4(CH_3OH)_2]{\cdot}2CH_3OH$				3	9.50	4.8×10^{-6}					53
$[Yb_2(HMBA)_2(MBA)_2(DMF)_2(H_2O)_2]{\cdot}6H_2O$				0.6	(25.9)	(5.2×10^{-7})	0.8	5.9	6.5×10^{-4}		54
$[Yb_2(HL)_4(NO_3)_6]$				3	4.0	5.93×10^{-5}					55
$[Yb_2(2\text{-}FBz)_6(phen)_2]$				2	5.33	2.2×10^{-5}	0.09	9			56
$[Yb(dnbz)(acac)_2(H_2O)(EtOH)]_2$				2	26	2.2×10^{-7}					57
1D coordination polymers (CP)				3							
$[Yb(\mu^3\text{-}OH)(na)(PyrCOO)]_n$				3	14.1	2.13					58
$[Yb(acac)_2(BcrCOO)(H_2O)]_n$				2	36	1.5×10^{-7}					59
$\{[Yb_2(L^{11})(OAc)_4{\cdot}3H_2O\}_n$				3	1.7	1.0×10^{-5}					53
$[Yb(acac)_2(Q)]_n$				1.5	(40) / 456.4	(7×10^{-8})	0.56	6	195		48
$[NH_4][Yb(HMBA)_4]$				2.5	20	9.5×10^{-8}					54
$\{[Yb(L)(H_2O)_3(DMF)]{\cdot}(HL){\cdot}(H_2O)\}_n$				1	28	3.3×10^{-7}					60
				1.6	14.8	1.24×10^{-7}	288.4	3.16			61
$\{[Yb(3\text{-}pyr)_3(H_2O)_2][Co(CN)_6]\}_n$				1	45	2.6×10^{-7}					62
3D MOF											
$[Yb^{III}L)_2(H_2O)]\text{-}[Cu_2^{I}(CN)_5]{\cdot}5H_2O$	0.06	0.07	7.58	1			1.7	5		116	22

*In parenthesis, *U* in compounds where Orbach processes was shown not to be involved, but was given for comparative purposes only. H_3L^1=tris(((2-hydroxy-3-methoxybenzyl)amino)ethyl)-amine; L^2=4,5-ethylendioxy-4',5'-bis(2-pyridyl-N-oxidemethylthio)tetrathiafulvalene; L^4=4,5-bis(thiomethyl)-40-carboxylictetrathiafulvalene; L^5 = 4,5-bis(thiomethyl)-40-ortho-pyridyl-N-oxide-carbamoyl-tetrathiafulvalene.

Table S4. Review of Yb(III) compounds showing photophysical properties in solid state at 298 K.

Compound	λ_{em} (nm)	τ_{obs} (μs)	Q_{Ln}^{Ln} (∗)	Ref.
0D SIMs				
[Yb(L1)(NO$_3$)$_3$]	978	9.7	0.0049 (2 ms)	[23]
Yb(TFI)$_3$(H$_2$O)$_2$	975	10.85	0.032 (0.34 ms)	[24]
[Yb(tta)$_3$(H$_2$O)$_2$]	975	0.85	-	[24]
Yb(TFI)$_3$(bpy)	975	19.92	0.044 (0.45 ms)	[24]
[(PPh$_3$)$_2$Pt(μ-pdo)Yb(tta)$_3$]	980	11.0	5.3×10^{-3} (2 ms)	[25]
[{Yb(tta)$_3$}$_2$(μ-BPTZ)]	980	14.1	7×10^{-3} (2 ms)	[26]
[Yb(tnm)$_3$(DMSO)$_2$]	980	18	0.042 (0.53 ms)	[28]
[Yb(tnm)$_3$(d6-DMSO)$_2$]	980	35	0.061 (0.53 ms)	[28]
Yb(5,6-DTFI)$_3$(H$_2$O)$_2$	980	2.85	0.0065 (0.44 ms)	[31]
Yb(5,6-DTFI)3(phen)	980	9.12	0.017 (0.55 ms)	[31]
Yb(hfpyr)$_3$(H$_2$O)	979	6.88	0.0034 (2 ms)	[29]
Yb(hfpyr)$_3$(bath)	979	13.45	0.0067 (2 ms)	[29]
Yb(pctrop)$_3$(DMF)$_2$	980	14	-	[63]
Yb(pctrop)$_3$(DMF-d$_7$)$_2$	980	180	-	[63]
1D CP				
[Yb(tfbdc)$_{0.5}$(bta)$_2$(CH$_3$OH)]	972, 1024	7.94	0.004 (2 ms)	[32]
2D MOFs				
{[Yb(DSPT)(*p*BDC)$_{0.5}$(H$_2$O)$_2$]·5H$_2$O}$_n$	983	-	-	[33]
{[Yb(DSPT)(ox)$_{0.5}$]·H$_2$O}$_n$	983			
[Yb$_2$(NDC)$_6$(DMF)$_4$]$_n$	977	9.24	0.0046 (2 ms)	[34]
3D MOFs				
{[Yb(Oaobtc)(H$_2$O)$_4$]·Hbipy·H$_2$O}$_n$	983	0.761	0.0128	[38]

(∗) Quantum yield determined in the original paper as Q_{Ln}^{Ln} = τ_{obs}/ τ_{rad} (the τ_{rad} value assumed for Yb(III) is given in parenthesis).

S3. Summary of mixed Nd(III)/Yb(III) compounds with SMM and/or NIR behaviour

Table S5. Review of mixed Nd/Yb compounds showing photophysical properties in solid state at 298 K.

Compound	λ_{em} (nm)	τ_{obs} (μs)	ϕ_{ET}	Ref.
0 D				
YbNdYb	976 1065	9.3 0.24	0.87 (*)	64 64
3D CPs				
$Nd_xYb_{1-x}(BTC)(H_2O)_6$, x=1, 0.943, 0.953, 0.890 $Nd_xYb_{1-x}(BTC)$, x=0.017, 0	975 1058		(**)	65

* The efficiency of the Nd−Yb energy transfer was calculated as: $\phi_{ET} = 1 - \tau_{DA}/\tau_D$, where τ_{DA} and τ_D are the donor lifetimes with and without acceptor.
** Complete calculation of ET

Table S6. Review of mixed Nd/Yb compounds across dimensions showing SMM behaviour; in italic font, ab initio-calculated values. Temperature dependence of the relaxation rate: $\tau^{-1}(T) = \tau_{QT}^{-1} + A\cdot T + C\cdot T^n + \tau_0^{-1} \exp(-U/k_B T)$.

Compound	g_x*	g_y*	g_z*	H (kOe)	U_{eff}/k_B (K)	τ_0 (s)	C ($s^{-1}K^{-n}$)	n	τ_{QT}^{-1} (s^{-1})	A ($s^{-1}\cdot kOe^{-4}\cdot K^{-1}$)	Ref.
3D MOFs											
$[Nd_x^{III}Yb_{1-x}^{III}L)_2(H_2O)]$-$[Cu_2^I(CN)_5]\cdot 5H_2O$											22
x=1	0.24	1.44	4.80	1.75			0.09	7		5.7	
x=0.75				2			0.1	7		2.1	
x=0.5				1			2.6	5		36	
x=0.25				1			2.8	5		35	

S4. Chemical and Structural Characterization

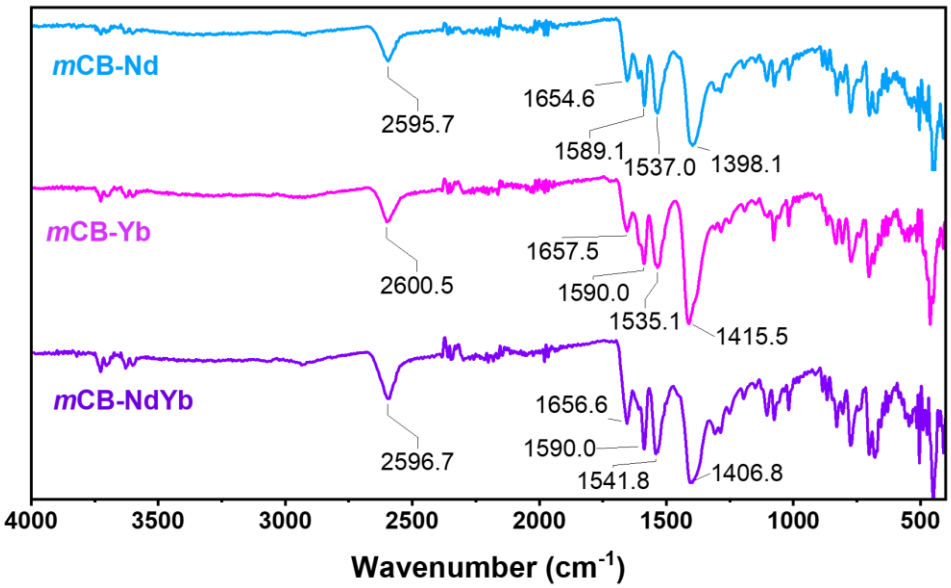

Figure S1. FTIR spectra for ***m*CB-Nd**, ***m*CB-Yb** and ***m*CB-NdYb**.

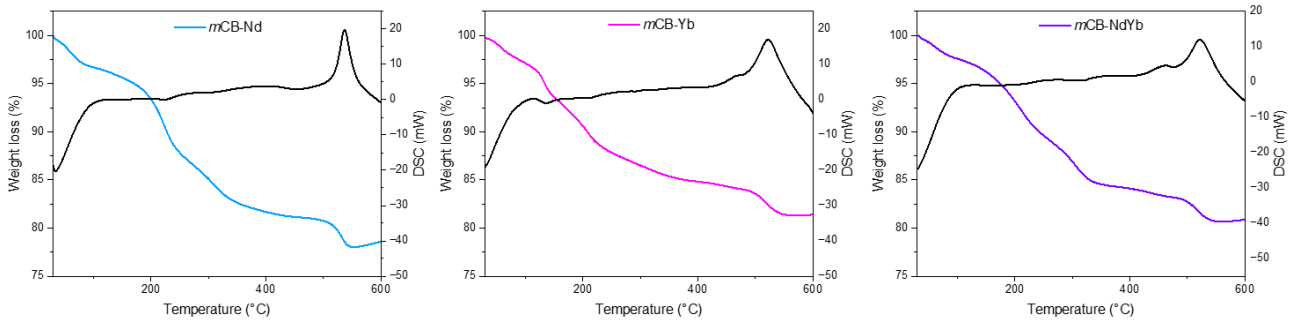

Figure S2. TGA results for ***m*CB-Nd**, ***m*CB-Yb** and ***m*CB-NdYb**.

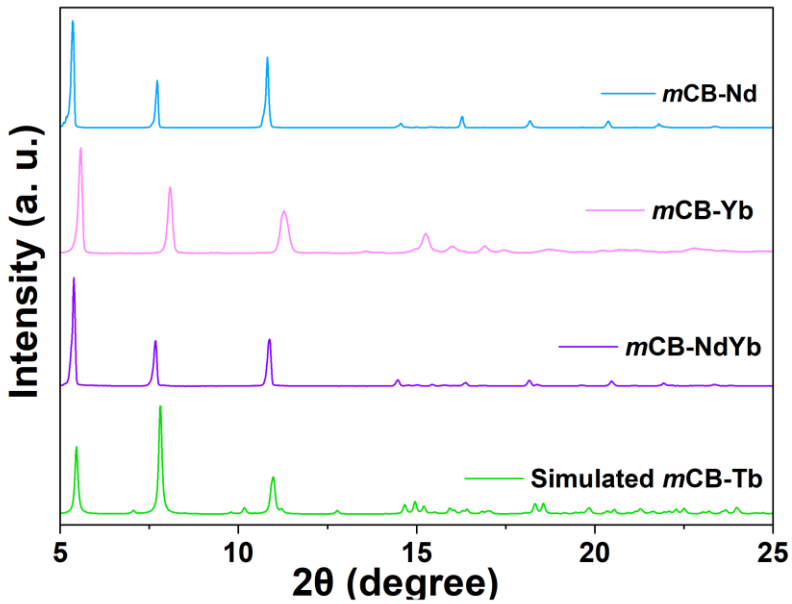

Figure S3. Comparison between PXRD for ***m*CB-Nd**, ***m*CB-Yb** and ***m*CB-NdYb** with calculated from SCXRD measured for ***m*CB-Tb**.[66,67]

S5. Additional magnetic data

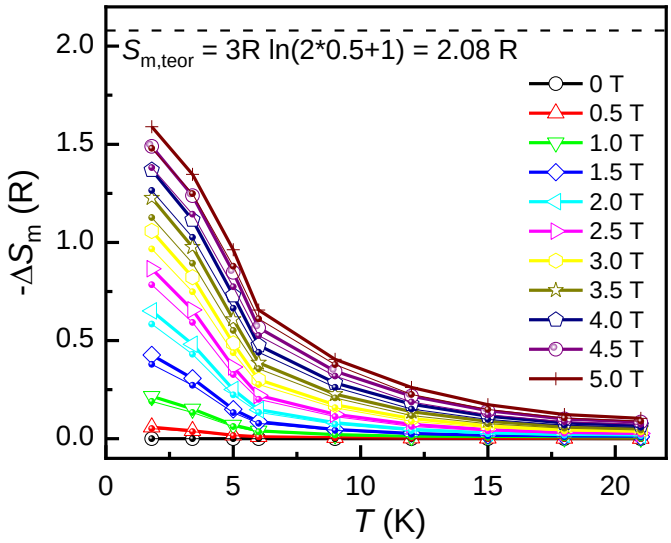

Figure S4. Magnetic entropy change, $-\Delta S_m(T)$, for different field variations (ΔB = 0–5 T) in the mixed MOF ***m*CB–NdYb** (open symbols), compared with the calculated linear combination, $-\Delta S_m(T)$ = (%Nd)·ΔS_m(Nd) + (%Yb)·ΔS_m(Yb), based on the magnetic entropy change plots obtained for the individual ***m*CB-Nd** and ***m*CB-Yb** compounds (bold symbols).

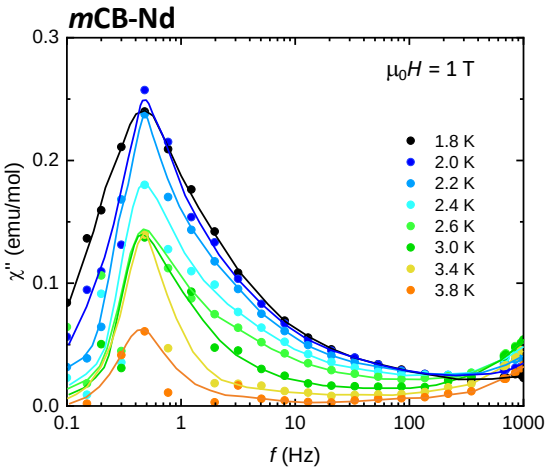

Figure S5. Out-of-phase component of the ac susceptibility as a function of the frequency, $\chi''(f)$, at 1 T and different temperatures for ***m*CB-Nd**.

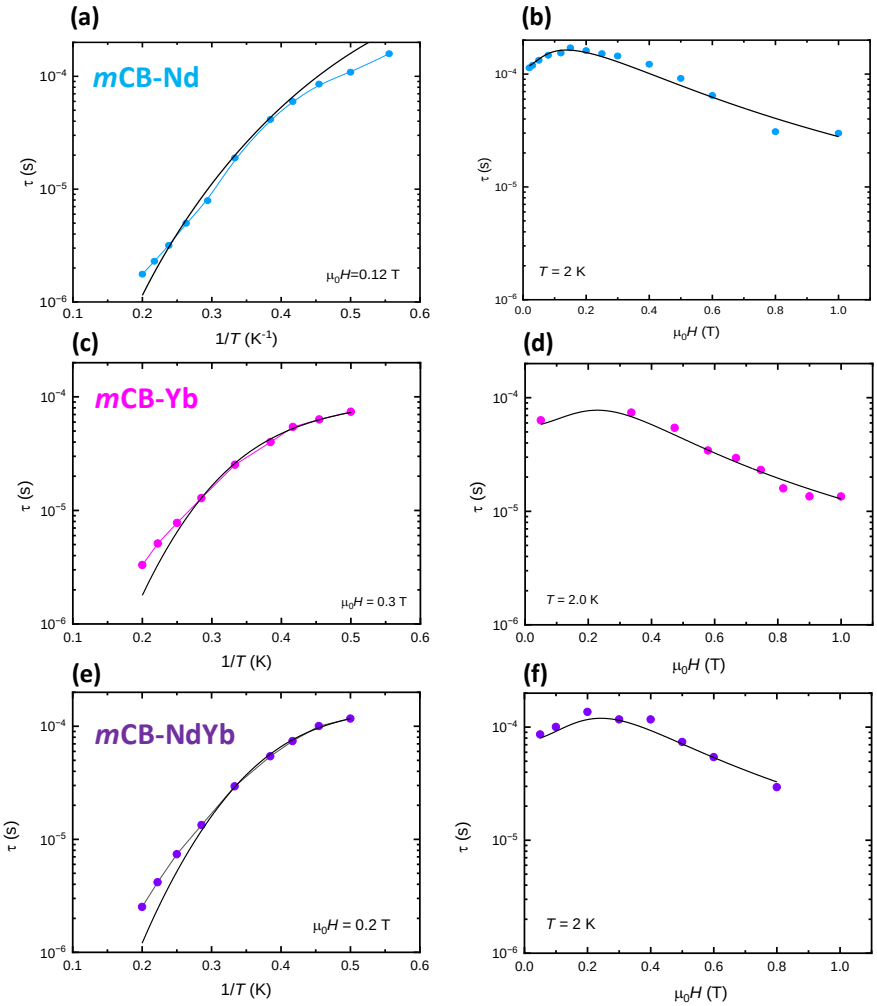

Figure S6. Fit of the high-frequency process relaxation time data, $\tau_{HF}(1/T)$ (left) and $\tau_{HF}(H)$ (right), to the texpression: $\tau_{HF}^{-1} = \frac{B_1}{1+B_2H^2} + D_2H^2T + CT^n$ (i.e. Eq. 1 without the Orbach term and $D_1 = 0$) for ***m*CB-Nd**, ***m*CB-Yb** and ***m*CB-NdYb** with fitting parameters summarized in Table S7.

MOF	**Dependence**	**B_1** **(s^{-1})**	**B_2** **(T^{-2})**	**D_2** **($s^{-1}K^{-1}T^{-2}$)**	**C** **($s^{-1}K^{-n}$)**	**n**
***m*CB-Nd**	$\tau_{HF}^{-1}(H,1/T)$	3965	0.24 x 10^2	155 x 10^2	98	5.6
***m*CB-Yb**	$\tau_{HF}^{-1}(H,1/T)$	15950	0.24x 10^2	376 x 10^2	27	6.2
***m*CB-NdYb**	$\tau_{HF}^{-1}(H,1/T)$	11418	0.32 x 10^2	220 x 10^2	17.2	6.7

Table 7. Parameters obtained from the simultaneous fit $\tau_{HF}(1/T)$ and $\tau_{HF}(H)$ using Eq. [1] without the Orbach term and $D_1 = 0$: $\tau_{HF}^{-1} = \frac{B_1}{1+B_2H^2} + D_2H^2T + CT^n$.

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