Supporting Information for:

Lanthanide Near Infrared Imaging in Living cells with Yb^{3+} Nano Metal Organic Frameworks

Alexandra Foucault-Collet[a], Kristy A. Gogick[b], Kiley A. White[b], Sandrine Villette[a], Agnès Pallier[a], Guillaume Collet[a], Claudine Kieda[a], Tao Li[b], Steven J. Geib[b], Nathaniel L. Rosi[b*], Stéphane Petoud[a,b*]

[a]Centre de Biophysique Moléculaire, CNRS, rue Charles Sadron, 45071 Orléans, France

[b]Department of Chemistry, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh, Pennsylvania 15260

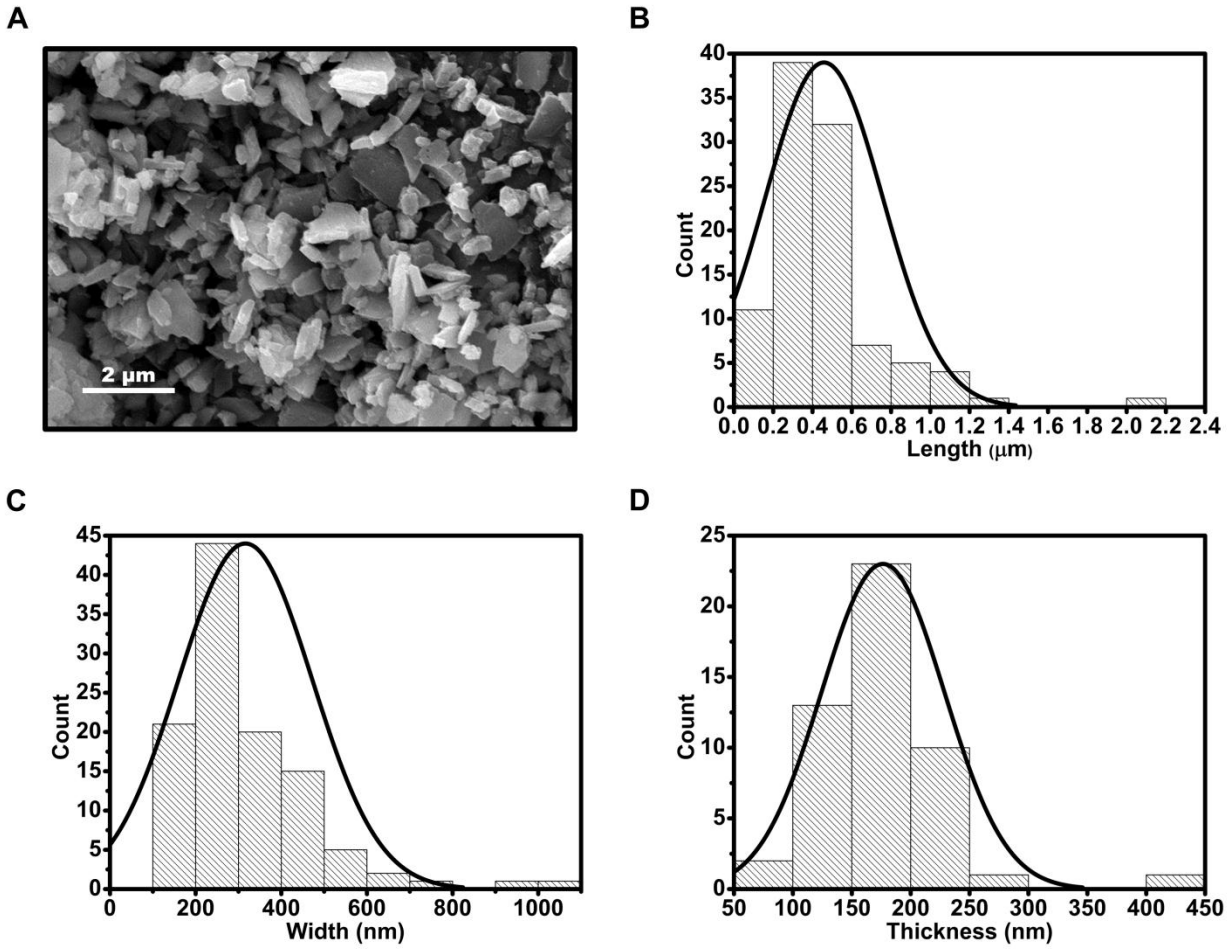

Fig. S1. Size characterization of nano-Yb-PVDC-3. Representative SEM image (A) and histograms of length (B), width (C), and thickness (D) measurements.

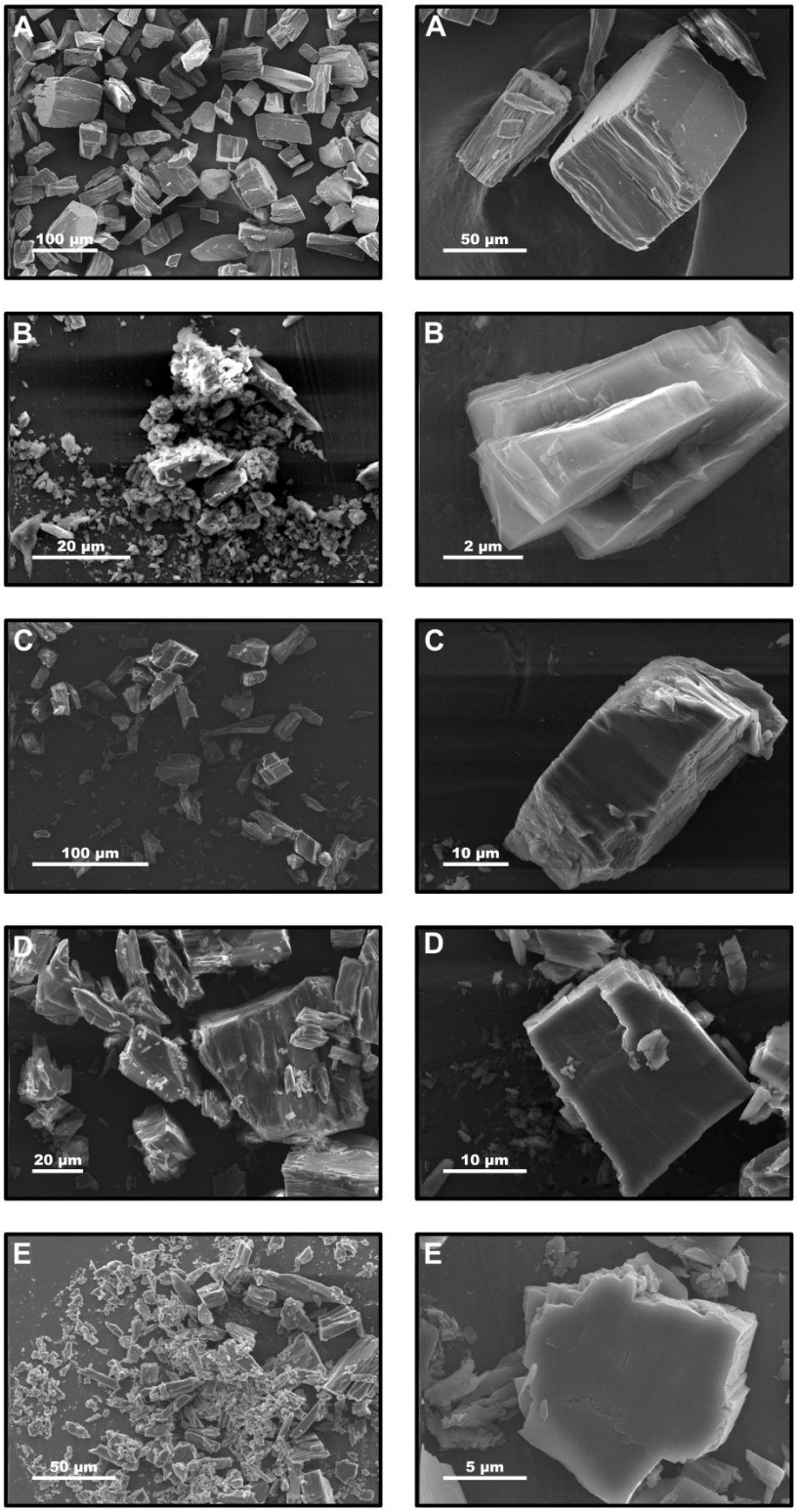

Fig. S2. SEM images of Yb-PVDC-3 (A) soaked in water for 1 week (B), 2 weeks (C), 3 weeks (D), and 4 weeks (E).

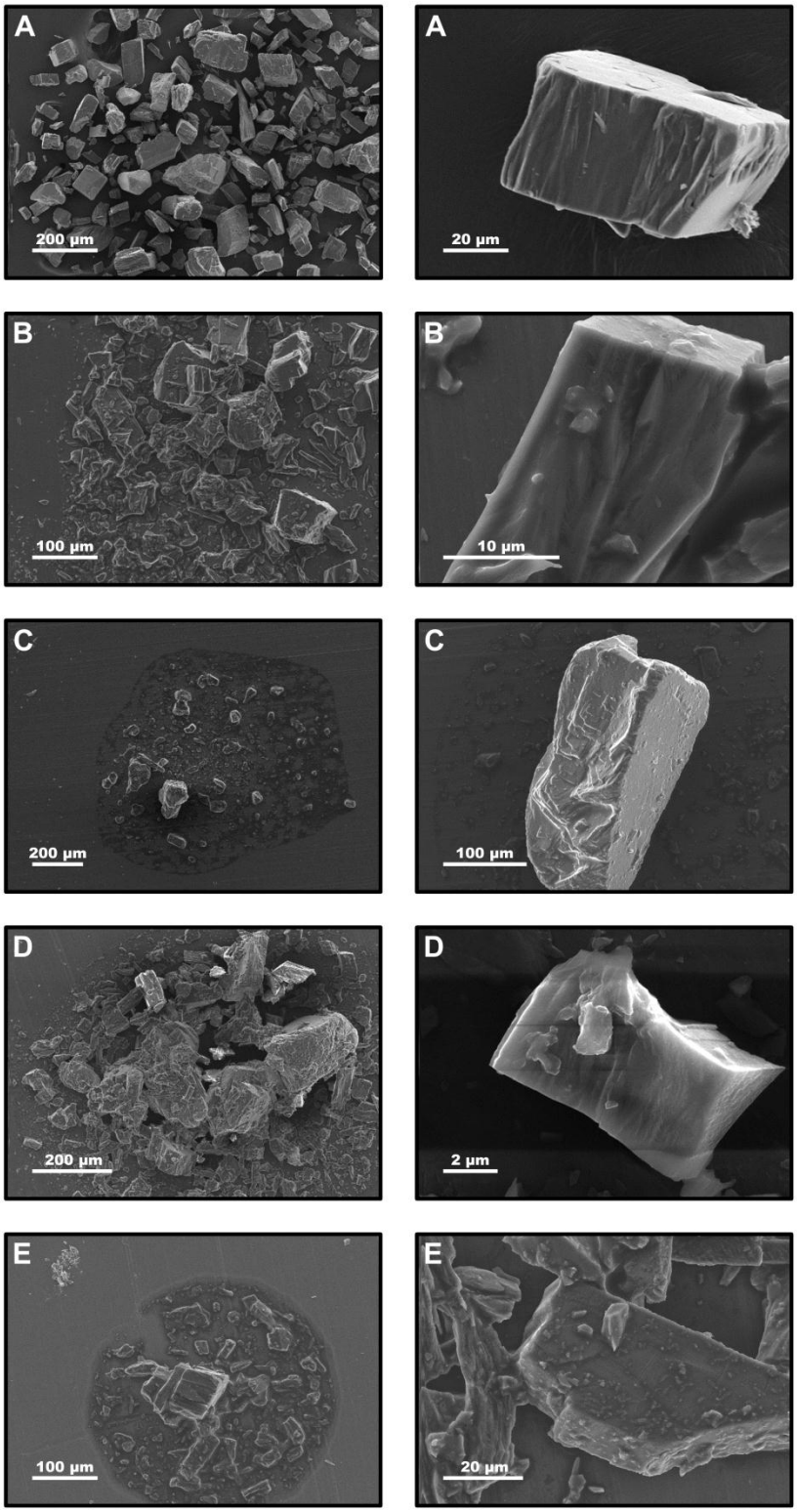

Fig. S3. SEM images of Yb-PVDC-3 (A) soaked in 0.1 M HEPES buffer (pH 7.3) for 1 week (B), 2 weeks (C), 3 weeks (D), and 4 weeks (E).

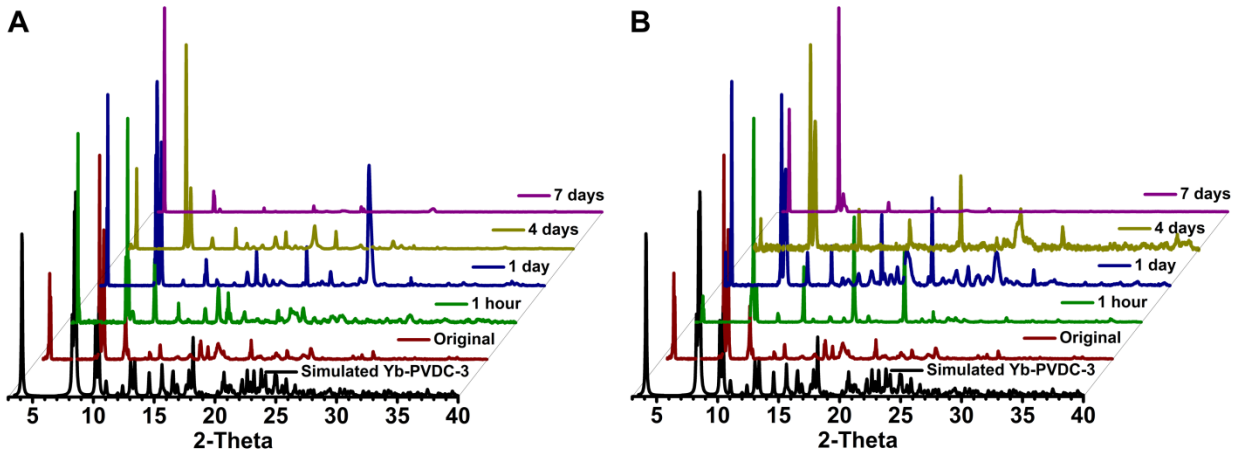

Fig. S4. Powder X-ray diffraction patterns over a period of seven days for Yb-PVDC-3 soaked in water (A) or 0.1 M HEPES buffer (pH 7.3) (B).

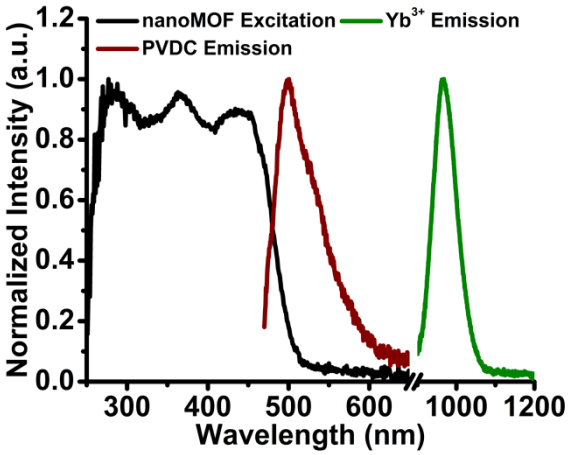

Fig. S5. Spectroscopic characterization of nano-Yb-PVDC-3 in water. Nano-Yb-PVDC-3 excitation spectrum (black, λ_{em} = 980 nm), and emission spectra for both the ligand (red) and lanthanide (green) obtained by exciting nano-Yb-PVDC-3 at 355 nm.

Table S1. Determination of Cellular Uptake by ICP

Sample	Concentration of nano-Yb-PVDC-3 in Cell Media (μg/mL)	Theoretical Concentration of Yb^{3+} in Cell Media (μg/mL)	Concentration of Yb^{3+} in $1x10^6$ cells (μg/mL)
HeLa Cells	0	0	0.000±0.002
	20	4.06	0.113±0.003
	30	6.09	0.213±0.003
	40	8.12	0.270±0.003
NIH 3T3 Cells	0	0	0.000±0.002
	20	4.06	0.466±0.010
	30	6.09	0.996±0.020
	40	8.12	1.130±0.003

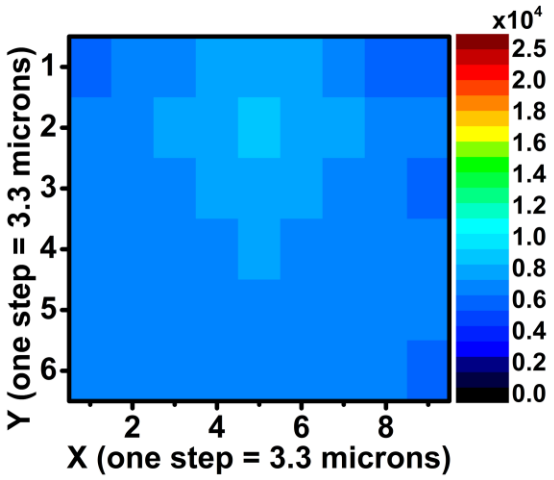

Fig. S6. Fluorescence intensity map of untreated NIH 3T3 cells by spectral microscopy in the visible region showing autofluorescence contribution.

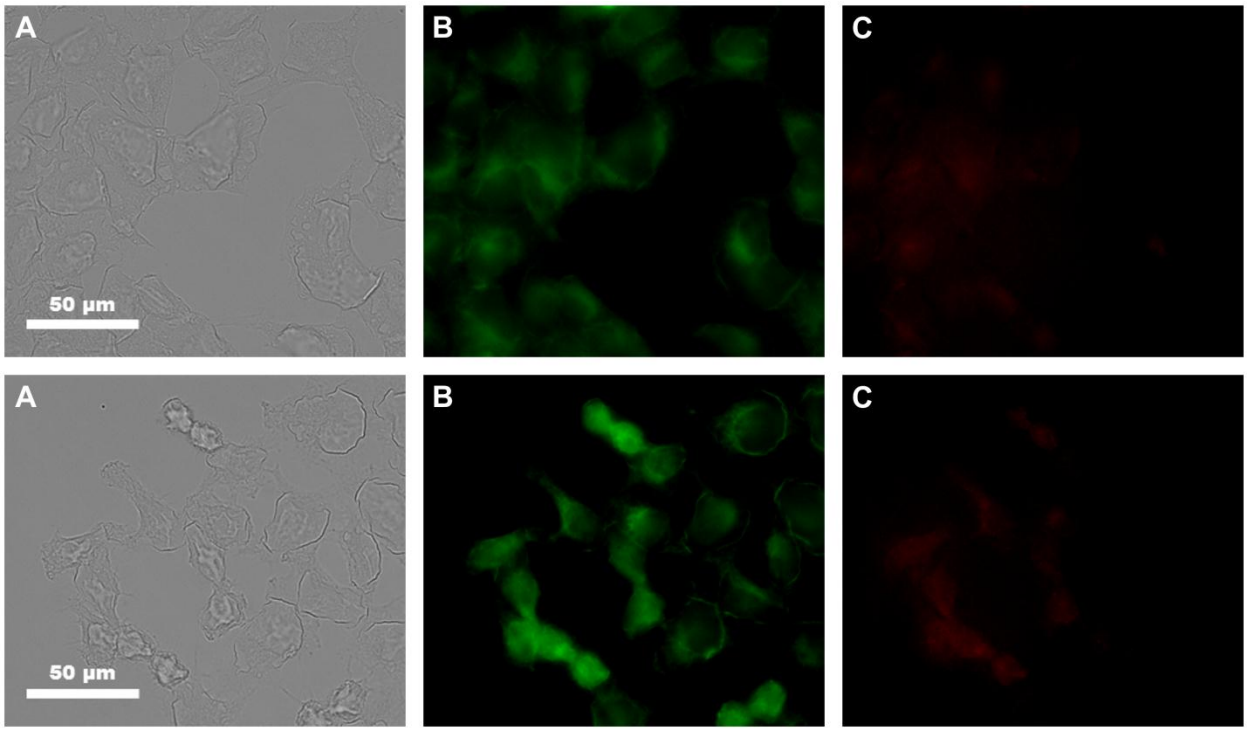

Fig. S7. Visible and NIR microscopy of untreatred NIH 3T3 (upper) and HeLa cells (lower) showing cell autofluorescence in the visible and NIR. (A) Brightfield, (B) visible, and (C) NIR.

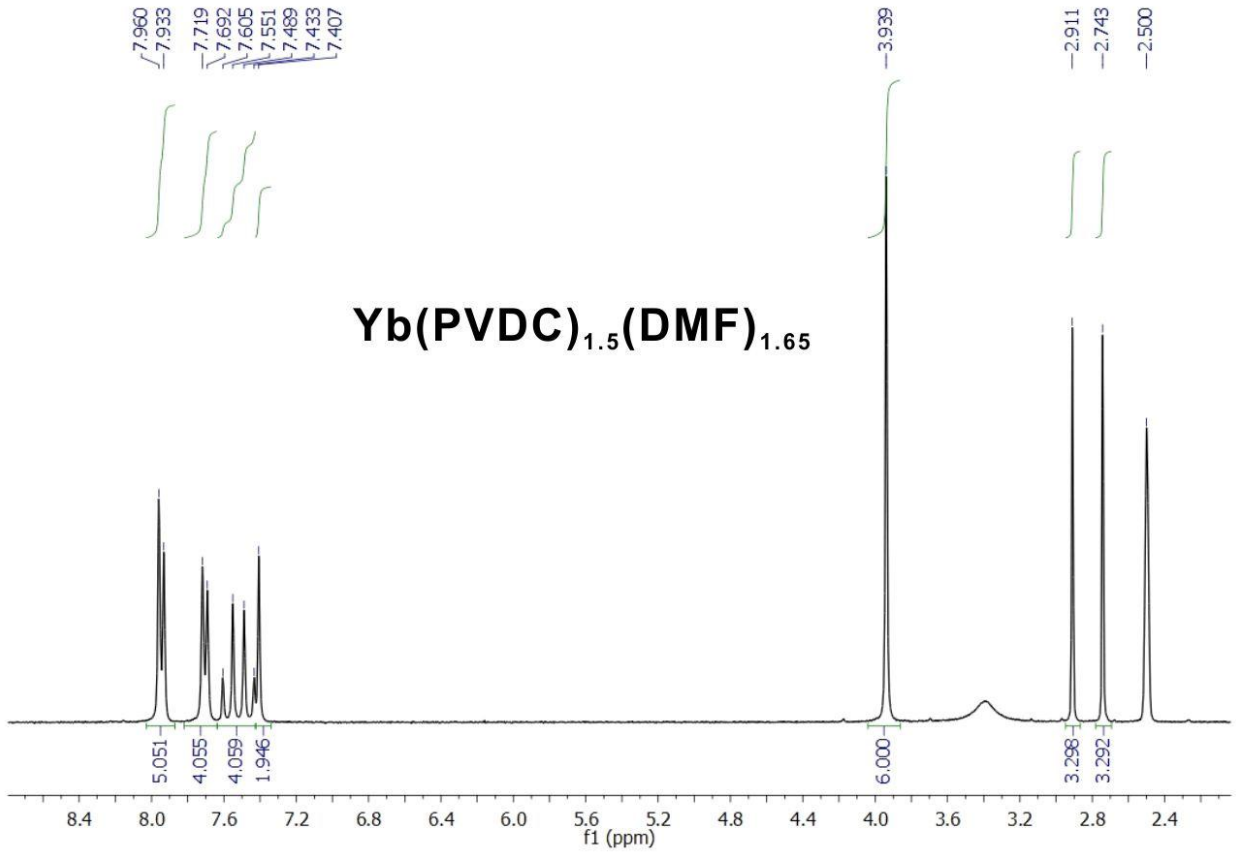

Fig. S8. ^{1}H NMR of digested Yb-PVDC-3.

Approximately 5 mg of as-synthesized Yb-PVDC-3 was first dried under argon flow and then dissolved in 0.65 mL d_6-DMSO and 3 µL concentrate DCl mixture. Proton nuclear magnetic resonance spectra (^{1}H-NMR) were collected on Bruker Avance 300 MHz spectrometers. Chemical shifts are in parts per million using the residual solvent peak as the reference value. The value used for proton spectra is 2.5 ppm for d_6-DMSO. The integration for the six methyl hydrogen atoms in PVDC was set as 6.

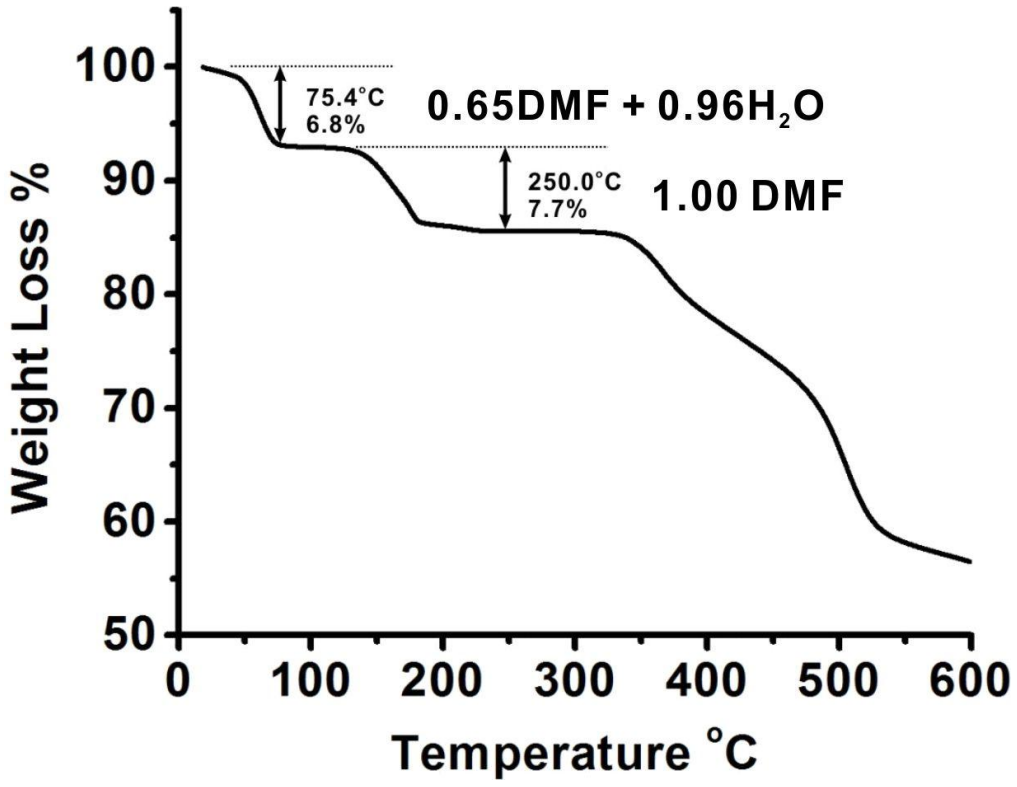

Fig. S9. Thermogravimetric analysis (TGA) of Yb-PVDC-3.

Thermogravimetric analysis (TGA) was conducted on a TGA Q500 thermal analysis system. Prior to analysis, as-synthesized Yb-PVDC-3 was dried under argon flow (UHP) to remove excess solvent. Approximately 10 mg of sample were loaded into a platinum pan and heated under a constant N_2 (UHP) flow from room temperature to 600 °C at a rate of 1 °C/min.

Single Crystal X-ray Diffraction Study for Yb-PVDC3

An X-ray crystal structure was determined for $C_{42}H_{41}NO_{12}Yb$, Yb-PVDC-3, using a single crystal on a Bruker Smart Apex CCD diffractometer with graphite-monochromated MoK_α (λ= 0.71073 Å) radiation. The parameters used during the collection of diffraction data are summarized in Table S1. The crystal was mounted in a glass loop with Paratone® N oil and placed in a cold N_2 stream (203 K) for data collection.

Unit-cell parameters and lack of systematic absences indicated Yb-PVDC-3 crystallized in triclinic space groups P 1 or P-1; centrosymmetric P-1 was chosen based on E-values and the successful solution and refinement of the structure. Unit-cell dimensions were derived from the least-squares fit of the angular settings of 1373 reflections. Data were corrected for absorption using the Bruker program SADABS[1]. The structure was solved via direct methods, which located Yb and most of the remaining non-hydrogen atoms. Yb was found to be disordered over at least two sites. The two Yb sites are occupied at 56% and 44%. Remaining non-hydrogen atoms were gradually found from several subsequent different Fourier syntheses. All non-hydrogen atoms were refined anisotropically excepting O6, O11, C24, C27, O12, N, C40, C41, C42, O10, C39A, C39B, and O13. A total of 47 restraints were applied to optimize the bond lengths, bond angles, and atomic displacement parameters. Idealized atom positions were calculated for all hydrogen atoms (*d*-(Cmethyl-H) = 0.97 Å, *d*-(Cphenyl-H) = 0.94 Å), *U* = 1.2 *Uiso* of attached carbon). The coordinated DMF seen in other Ln-PVDC isomorphs could not be resolved in this structure, probably because of overlap with the disordered Yb sites.

All computer programs used in the data collection and refinements are contained in the Bruker program packages SMART (vers. 5.625), SAINT (vers. 6.22)[1], and SHELXTL (vers. 6.10)[2].

References

1. APEX II software suite, Bruker-AXS, 2006.

2. Sheldrick GM (2008) A short history of SHELX. *Acta Crystallogr A* 64(1):112-122.

Table S2. Crystal data and structure refinement for Yb-PVDC-3

Identification code	Yb-PVDC-3	
Empirical formula	C42 H41 N O12 Yb	
Formula weight	924.80	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.811(2) Å	α= 77.152(5)°
	b = 10.951(3) Å	β= 87.703(5)°
	c = 21.944(5) Å	γ = 78.251(6)°
Volume	2021.1(9) $Å^3$	
Z	2	
Density (calculated)	1.520 Mg/m^3	
Absorption coefficient	2.377 mm^{-1}	
F(000)	932	
Crystal size	0.30 x 0.13 x 0.08 mm^3	
Theta range for data collection	1.90 to 23.33°	
Index ranges	-9<=h<=9, -12<=k<=12, -24<=l<=24	
Reflections collected	13440	
Independent reflections	5809 [R(int) = 0.0628]	
Completeness to theta = 23.33°	99.5 %	
Absorption correction	Multi-Scan (SADABS)	
Max. and min. transmission	0.8326 and 0.5358	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5809 / 47 / 469	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.1240, wR2 = 0.2941	
R indices (all data)	R1 = 0.1946, wR2 = 0.3318	
Largest diff. peak and hole	2.609 and -1.103 e.$Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Yb-PVDC-3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Yb	2868(2)	4658(4)	4952(1)	85(1)
Yb'	2770(3)	3647(6)	4893(1)	95(2)
O(1)	1350(19)	3760(20)	5765(6)	147(7)
C(1)	80(30)	4220(30)	5975(8)	96(8)
C(2)	-150(30)	3710(20)	6692(8)	79(6)
O(2)	-880(20)	5071(18)	5680(6)	114(6)
O(3)	-5318(12)	2141(10)	9236(4)	61(3)
C(3)	-1370(20)	4356(18)	6963(7)	73(5)
O(4)	-862(12)	1061(10)	11080(4)	61(3)
C(4)	-1650(20)	3916(14)	7592(6)	62(5)
C(5)	-762(18)	2814(13)	7925(6)	48(4)
O(5)	-6970(30)	-3110(30)	14275(7)	267(18)
C(6)	480(20)	2199(17)	7628(7)	73(5)
O(6)	-4643(15)	-2821(12)	14550(6)	92(4)
C(7)	790(20)	2640(20)	7018(8)	82(6)
O(7)	5710(30)	4594(18)	4345(9)	229(11)
C(8)	-1050(20)	2284(14)	8595(7)	61(4)
O(8)	3980(20)	3600(20)	4070(8)	199(10)
C(9)	-2431(18)	2474(13)	8855(6)	51(4)
C(10)	-2732(18)	2043(13)	9521(6)	46(4)
C(11)	-4247(18)	1875(13)	9702(6)	50(4)
O(11)	1960(30)	2110(20)	4938(12)	203(9)
C(12)	-4569(16)	1460(13)	10342(6)	46(3)
C(13)	-3446(18)	1186(12)	10788(6)	47(4)
C(14)	-1932(18)	1357(13)	10603(7)	54(4)
C(15)	-1640(18)	1761(12)	9970(6)	50(4)
C(16)	-3743(18)	692(14)	11455(7)	57(4)
C(17)	-4962(17)	157(13)	11678(7)	58(4)
C(18)	-5236(19)	-399(15)	12333(6)	57(4)
C(19)	-6380(20)	-1092(16)	12468(7)	74(5)
C(20)	-6590(20)	-1747(17)	13074(7)	74(5)
C(21)	-5680(20)	-1751(18)	13545(6)	73(5)
C(22)	-4530(20)	-1033(18)	13417(7)	77(5)
C(23)	-4350(20)	-368(16)	12819(7)	68(5)
C(24)	-5810(20)	-2590(20)	14204(9)	120(8)
C(25)	-6867(16)	2003(15)	9390(7)	62(4)
C(26)	685(18)	1206(16)	10907(7)	64(4)

C(27)	5030(30)	4160(30)	3970(12)	153(10)
C(28)	5770(20)	4130(20)	3316(9)	97(7)
C(29)	6700(20)	4880(20)	3109(8)	151(12)
C(30)	7390(20)	5000(20)	2535(9)	116(9)
C(31)	7062(19)	4330(18)	2145(7)	68(5)
C(32)	6140(20)	3484(18)	2356(8)	79(5)
C(33)	5470(20)	3400(20)	2932(9)	86(6)
C(34)	7770(20)	4369(18)	1507(8)	87(6)
C(35)	8800(30)	4747(15)	1254(8)	106(9)
C(36)	9370(20)	4828(14)	592(7)	62(5)
C(37)	10960(20)	4787(14)	515(7)	61(4)
C(38)	8419(18)	5052(14)	92(8)	59(4)
O(12)	-830(50)	670(40)	3050(20)	302(17)
N	870(30)	1960(30)	2892(15)	170(10)
C(40)	1290(70)	1690(60)	3560(30)	300(30)
C(41)	1750(40)	2580(30)	2295(16)	172(12)
C(42)	0(50)	1240(40)	2660(20)	198(15)
O(10)	1820(50)	6190(30)	5220(20)	410(30)
C(39A)	13630(40)	4620(30)	884(18)	70(13)
O(9)	12000(17)	4626(14)	995(6)	48(6)
C(39B)	13780(70)	4390(50)	740(30)	57(18)
O(13)	6900(40)	5070(30)	-76(15)	81(13)

Table S4. Bond lengths [Å] and angles [°] for Yb-PVDC-3

Yb-Yb'	1.163(3)
Yb-O(10)	1.95(3)
Yb-O(2)#1	2.209(16)
Yb-O(1)	2.345(13)
Yb-O(6)#2	2.360(13)
Yb-O(7)#3	2.40(3)
Yb-O(8)	2.54(2)
Yb-O(5)#4	2.59(3)
Yb-O(7)	2.78(2)
Yb-C(27)	2.89(2)
Yb-O(11)	3.06(2)
Yb-Yb#3	4.001(6)
Yb'-O(11)	1.94(2)
Yb'-O(6)#2	2.024(14)
Yb'-O(8)	2.064(16)
Yb'-O(2)#1	2.181(19)
Yb'-O(1)	2.257(13)
Yb'-C(27)	2.83(2)
Yb'-O(10)	2.98(3)
Yb'-O(7)	3.08(2)
O(1)-C(1)	1.24(3)
C(1)-O(2)	1.21(3)
C(1)-C(2)	1.57(2)
C(2)-C(3)	1.35(3)
C(2)-C(7)	1.36(3)
O(2)-Yb'#1	2.181(19)
O(2)-Yb#1	2.209(16)
O(3)-C(11)	1.361(17)
O(3)-C(25)	1.423(17)
C(3)-C(4)	1.389(19)
C(3)-H(3A)	0.9400
O(4)-C(14)	1.376(18)
O(4)-C(26)	1.431(17)
C(4)-C(5)	1.37(2)
C(4)-H(4A)	0.9400
C(5)-C(6)	1.38(2)
C(5)-C(8)	1.487(19)
O(5)-C(24)	1.254(16)
O(5)-Yb#5	2.59(3)

C(6)-C(7)	1.36(2)
C(6)-H(6A)	0.9400
O(6)-C(24)	1.254(15)
O(6)-Yb'#2	2.024(13)
O(6)-Yb#2	2.360(13)
C(7)-H(7A)	0.9400
O(7)-C(27)	1.264(18)
O(7)-Yb#3	2.40(3)
C(8)-C(9)	1.32(2)
C(8)-H(8A)	0.9400
O(8)-C(27)	1.195(18)
C(9)-C(10)	1.462(17)
C(9)-H(9A)	0.9400
C(10)-C(15)	1.346(19)
C(10)-C(11)	1.41(2)
C(11)-C(12)	1.413(18)
C(12)-C(13)	1.361(19)
C(12)-H(12A)	0.9400
C(13)-C(14)	1.42(2)
C(13)-C(16)	1.475(18)
C(14)-C(15)	1.392(18)
C(15)-H(15A)	0.9400
C(16)-C(17)	1.35(2)
C(16)-H(16A)	0.9400
C(17)-C(18)	1.462(19)
C(17)-H(17A)	0.9400
C(18)-C(23)	1.36(2)
C(18)-C(19)	1.36(2)
C(19)-C(20)	1.39(2)
C(19)-H(19A)	0.9400
C(20)-C(21)	1.34(2)
C(20)-H(20A)	0.9400
C(21)-C(22)	1.39(2)
C(21)-C(24)	1.544(17)
C(22)-C(23)	1.37(2)
C(22)-H(22A)	0.9400
C(23)-H(23A)	0.9400
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(25)-H(25C)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700

C(27)-C(28)	1.556(19)
C(28)-C(29)	1.27(3)
C(28)-C(33)	1.35(3)
C(29)-C(30)	1.37(3)
C(29)-H(29A)	0.9400
C(30)-C(31)	1.32(2)
C(30)-H(30A)	0.9400
C(31)-C(32)	1.35(2)
C(31)-C(34)	1.50(2)
C(32)-C(33)	1.37(2)
C(32)-H(32A)	0.9400
C(33)-H(33A)	0.9400
C(34)-C(35)	1.15(3)
C(34)-H(34A)	0.9400
C(35)-C(36)	1.51(2)
C(35)-H(35A)	0.9400
C(36)-C(38)	1.36(2)
C(36)-C(37)	1.40(2)
C(37)-O(9)	1.38(2)
C(37)-C(38)#6	1.41(2)
C(38)-O(13)	1.39(4)
C(38)-C(37)#6	1.41(2)
O(12)-C(42)	1.25(5)
N-C(42)	1.39(4)
N-C(40)	1.48(6)
N-C(41)	1.58(4)
C(39A)-O(9)	1.45(4)
C(39B)-O(13)#6	1.53(6)
O(13)-C(39B)#6	1.53(6)

Yb'-Yb-O(10)	145.6(15)
Yb'-Yb-O(2)#1	73.3(5)
O(10)-Yb-O(2)#1	87.8(16)
Yb'-Yb-O(1)	71.2(5)
O(10)-Yb-O(1)	79.7(16)
O(2)#1-Yb-O(1)	87.6(5)
Yb'-Yb-O(6)#2	59.0(4)
O(10)-Yb-O(6)#2	132.7(15)
O(2)#1-Yb-O(6)#2	132.3(6)
O(1)-Yb-O(6)#2	78.7(6)
Yb'-Yb-O(7)#3	133.6(5)
O(10)-Yb-O(7)#3	63.7(15)
O(2)#1-Yb-O(7)#3	151.1(8)

O(1)-Yb-O(7)#3	92.1(6)
O(6)#2-Yb-O(7)#3	75.6(6)
Yb'-Yb-O(8)	53.4(6)
O(10)-Yb-O(8)	148.9(16)
O(2)#1-Yb-O(8)	75.4(6)
O(1)-Yb-O(8)	124.5(8)
O(6)#2-Yb-O(8)	75.6(5)
O(7)#3-Yb-O(8)	126.6(7)
Yb'-Yb-O(5)#4	139.8(5)
O(10)-Yb-O(5)#4	60.2(16)
O(2)#1-Yb-O(5)#4	80.8(5)
O(1)-Yb-O(5)#4	138.5(8)
O(6)#2-Yb-O(5)#4	136.4(6)
O(7)#3-Yb-O(5)#4	80.4(5)
O(8)-Yb-O(5)#4	90.9(8)
Yb'-Yb-O(7)	93.6(5)
O(10)-Yb-O(7)	120.5(16)
O(2)#1-Yb-O(7)	113.9(7)
O(1)-Yb-O(7)	149.5(6)
O(6)#2-Yb-O(7)	70.8(5)
O(7)#3-Yb-O(7)	79.2(7)
O(8)-Yb-O(7)	49.0(6)
O(5)#4-Yb-O(7)	69.3(7)
Yb'-Yb-C(27)	75.4(6)
O(10)-Yb-C(27)	134.7(17)
O(2)#1-Yb-C(27)	91.1(7)
O(1)-Yb-C(27)	145.5(8)
O(6)#2-Yb-C(27)	76.9(7)
O(7)#3-Yb-C(27)	104.9(7)
O(8)-Yb-C(27)	24.4(5)
O(5)#4-Yb-C(27)	74.9(9)
O(7)-Yb-C(27)	25.7(4)
Yb'-Yb-O(11)	12.1(5)
O(10)-Yb-O(11)	133.6(16)
O(2)#1-Yb-O(11)	68.6(7)
O(1)-Yb-O(11)	60.7(7)
O(6)#2-Yb-O(11)	64.9(6)
O(7)#3-Yb-O(11)	135.0(6)
O(8)-Yb-O(11)	63.9(7)
O(5)#4-Yb-O(11)	144.0(6)
O(7)-Yb-O(11)	105.7(7)
C(27)-Yb-O(11)	86.8(7)
Yb'-Yb-Yb#3	117.3(2)

O(10)-Yb-Yb#3	95.0(15)
O(2)#1-Yb-Yb#3	143.8(3)
O(1)-Yb-Yb#3	128.4(4)
O(6)#2-Yb-Yb#3	67.8(3)
O(7)#3-Yb-Yb#3	43.1(5)
O(8)-Yb-Yb#3	84.3(5)
O(5)#4-Yb-Yb#3	69.7(5)
O(7)-Yb-Yb#3	36.1(6)
C(27)-Yb-Yb#3	61.8(5)
O(11)-Yb-Yb#3	127.8(5)
Yb-Yb'-O(11)	160.7(8)
Yb-Yb'-O(6)#2	91.4(4)
O(11)-Yb'-O(6)#2	96.9(8)
Yb-Yb'-O(8)	99.8(8)
O(11)-Yb'-O(8)	96.8(11)
O(6)#2-Yb'-O(8)	94.6(6)
Yb-Yb'-O(2)#1	76.0(5)
O(11)-Yb'-O(2)#1	95.4(8)
O(6)#2-Yb'-O(2)#1	167.4(6)
O(8)-Yb'-O(2)#1	86.6(6)
Yb-Yb'-O(1)	79.6(6)
O(11)-Yb'-O(1)	83.4(9)
O(6)#2-Yb'-O(1)	88.1(6)
O(8)-Yb'-O(1)	177.2(7)
O(2)#1-Yb'-O(1)	90.6(6)
Yb-Yb'-C(27)	81.1(6)
O(11)-Yb'-C(27)	116.9(10)
O(6)#2-Yb'-C(27)	83.6(7)
O(8)-Yb'-C(27)	21.9(7)
O(2)#1-Yb'-C(27)	93.3(7)
O(1)-Yb'-C(27)	158.8(8)
Yb-Yb'-O(10)	21.6(10)
O(11)-Yb'-O(10)	139.2(13)
O(6)#2-Yb'-O(10)	102.5(11)
O(8)-Yb'-O(10)	116.7(13)
O(2)#1-Yb'-O(10)	66.0(11)
O(1)-Yb'-O(10)	62.0(11)
C(27)-Yb'-O(10)	100.8(12)
Yb-Yb'-O(7)	64.2(4)
O(11)-Yb'-O(7)	135.0(9)
O(6)#2-Yb'-O(7)	68.4(6)
O(8)-Yb'-O(7)	45.9(7)
O(2)#1-Yb'-O(7)	104.4(6)

O(1)-Yb'-O(7)	135.2(7)
C(27)-Yb'-O(7)	24.2(4)
O(10)-Yb'-O(7)	85.7(11)
C(1)-O(1)-Yb'	145.3(15)
C(1)-O(1)-Yb	131.0(17)
Yb'-O(1)-Yb	29.20(18)
O(2)-C(1)-O(1)	124.6(17)
O(2)-C(1)-C(2)	120(2)
O(1)-C(1)-C(2)	115(2)
C(3)-C(2)-C(7)	121.9(16)
C(3)-C(2)-C(1)	117(2)
C(7)-C(2)-C(1)	121(2)
C(1)-O(2)-Yb'#1	170.3(16)
C(1)-O(2)-Yb#1	139.6(16)
Yb'#1-O(2)-Yb#1	30.7(2)
C(11)-O(3)-C(25)	119.2(11)
C(2)-C(3)-C(4)	118.9(18)
C(2)-C(3)-H(3A)	120.6
C(4)-C(3)-H(3A)	120.6
C(14)-O(4)-C(26)	116.7(11)
C(5)-C(4)-C(3)	120.4(15)
C(5)-C(4)-H(4A)	119.8
C(3)-C(4)-H(4A)	119.8
C(4)-C(5)-C(6)	118.3(13)
C(4)-C(5)-C(8)	122.5(13)
C(6)-C(5)-C(8)	119.2(14)
C(24)-O(5)-Yb#5	127.1(19)
C(7)-C(6)-C(5)	121.5(18)
C(7)-C(6)-H(6A)	119.2
C(5)-C(6)-H(6A)	119.2
C(24)-O(6)-Yb'#2	165.9(15)
C(24)-O(6)-Yb#2	136.3(14)
Yb'#2-O(6)-Yb#2	29.5(2)
C(6)-C(7)-C(2)	118.9(17)
C(6)-C(7)-H(7A)	120.6
C(2)-C(7)-H(7A)	120.6
C(27)-O(7)-Yb#3	177(2)
C(27)-O(7)-Yb	81.8(17)
Yb#3-O(7)-Yb	100.8(7)
C(27)-O(7)-Yb'	66.5(14)
Yb#3-O(7)-Yb'	115.4(6)
Yb-O(7)-Yb'	22.11(18)
C(9)-C(8)-C(5)	123.2(15)

C(9)-C(8)-H(8A)	118.4
C(5)-C(8)-H(8A)	118.4
C(27)-O(8)-Yb'	118(2)
C(27)-O(8)-Yb	95(2)
Yb'-O(8)-Yb	26.9(3)
C(8)-C(9)-C(10)	124.5(14)
C(8)-C(9)-H(9A)	117.8
C(10)-C(9)-H(9A)	117.8
C(15)-C(10)-C(11)	118.0(12)
C(15)-C(10)-C(9)	123.8(14)
C(11)-C(10)-C(9)	118.2(13)
O(3)-C(11)-C(12)	124.1(13)
O(3)-C(11)-C(10)	116.6(11)
C(12)-C(11)-C(10)	119.3(14)
Yb'-O(11)-Yb	7.2(3)
C(13)-C(12)-C(11)	121.7(13)
C(13)-C(12)-H(12A)	119.2
C(11)-C(12)-H(12A)	119.2
C(12)-C(13)-C(14)	118.7(12)
C(12)-C(13)-C(16)	122.4(14)
C(14)-C(13)-C(16)	118.9(14)
O(4)-C(14)-C(15)	126.0(14)
O(4)-C(14)-C(13)	115.3(12)
C(15)-C(14)-C(13)	118.6(15)
C(10)-C(15)-C(14)	123.7(14)
C(10)-C(15)-H(15A)	118.2
C(14)-C(15)-H(15A)	118.2
C(17)-C(16)-C(13)	125.2(15)
C(17)-C(16)-H(16A)	117.4
C(13)-C(16)-H(16A)	117.4
C(16)-C(17)-C(18)	126.1(16)
C(16)-C(17)-H(17A)	117
C(18)-C(17)-H(17A)	117
C(23)-C(18)-C(19)	116.8(14)
C(23)-C(18)-C(17)	124.6(15)
C(19)-C(18)-C(17)	118.4(14)
C(18)-C(19)-C(20)	121.1(16)
C(18)-C(19)-H(19A)	119.5
C(20)-C(19)-H(19A)	119.5
C(21)-C(20)-C(19)	121.7(16)
C(21)-C(20)-H(20A)	119.2
C(19)-C(20)-H(20A)	119.2
C(20)-C(21)-C(22)	117.8(13)

C(20)-C(21)-C(24)	121.6(15)
C(22)-C(21)-C(24)	120.5(15)
C(23)-C(22)-C(21)	119.8(16)
C(23)-C(22)-H(22A)	120.1
C(21)-C(22)-H(22A)	120.1
C(18)-C(23)-C(22)	122.8(16)
C(18)-C(23)-H(23A)	118.6
C(22)-C(23)-H(23A)	118.6
O(6)-C(24)-O(5)	128.7(19)
O(6)-C(24)-C(21)	115.7(16)
O(5)-C(24)-C(21)	114.4(16)
O(3)-C(25)-H(25A)	109.5
O(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(3)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(4)-C(26)-H(26A)	109.5
O(4)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
O(8)-C(27)-O(7)	129(3)
O(8)-C(27)-C(28)	113(2)
O(7)-C(27)-C(28)	118(2)
O(8)-C(27)-Yb'	40.2(15)
O(7)-C(27)-Yb'	89.3(15)
C(28)-C(27)-Yb'	153.1(18)
O(8)-C(27)-Yb	61.1(17)
O(7)-C(27)-Yb	72.5(15)
C(28)-C(27)-Yb	162.7(18)
Yb'-C(27)-Yb	23.5(2)
C(29)-C(28)-C(33)	116.3(17)
C(29)-C(28)-C(27)	119(2)
C(33)-C(28)-C(27)	125(2)
C(28)-C(29)-C(30)	125(2)
C(28)-C(29)-H(29A)	117.3
C(30)-C(29)-H(29A)	117.3
C(31)-C(30)-C(29)	119.2(19)
C(31)-C(30)-H(30A)	120.4
C(29)-C(30)-H(30A)	120.4
C(30)-C(31)-C(32)	117.4(16)

C(30)-C(31)-C(34)	123.9(18)
C(32)-C(31)-C(34)	118.6(18)
C(31)-C(32)-C(33)	121.3(18)
C(31)-C(32)-H(32A)	119.4
C(33)-C(32)-H(32A)	119.4
C(28)-C(33)-C(32)	120.3(18)
C(28)-C(33)-H(33A)	119.8
C(32)-C(33)-H(33A)	119.8
C(35)-C(34)-C(31)	135(2)
C(35)-C(34)-H(34A)	112.4
C(31)-C(34)-H(34A)	112.4
C(34)-C(35)-C(36)	132(3)
C(34)-C(35)-H(35A)	114.1
C(36)-C(35)-H(35A)	114.1
C(38)-C(36)-C(37)	121.1(14)
C(38)-C(36)-C(35)	123.4(18)
C(37)-C(36)-C(35)	115.2(18)
O(9)-C(37)-C(36)	124.8(15)
O(9)-C(37)-C(38)#6	116.1(17)
C(36)-C(37)-C(38)#6	119.1(15)
C(36)-C(38)-O(13)	143(2)
C(36)-C(38)-C(37)#6	119.8(15)
O(13)-C(38)-C(37)#6	97.0(19)
C(42)-N-C(40)	122(4)
C(42)-N-C(41)	103(3)
C(40)-N-C(41)	130(4)
O(12)-C(42)-N	115(4)
Yb-O(10)-Yb'	12.7(5)
C(37)-O(9)-C(39A)	122.2(19)
C(38)-O(13)-C(39B)#6	125(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1	#2 -x,-y,-z+2	#3 -x+1,-y+1,-z+1
#4 x+1,y+1,z-1	#5 x-1,y-1,z+1	#6 -x+2,-y+1,-z

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Yb-PVDC-3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Yb	88(1)	125(3)	43(1)	-15(1)	41(1)	-37(1)
Yb'	107(2)	146(4)	36(1)	-6(1)	38(1)	-59(2)
O(1)	110(11)	280(20)	51(8)	-15(10)	48(8)	-75(13)
C(1)	105(17)	190(20)	23(9)	-10(12)	23(11)	-114(18)
C(2)	93(14)	125(17)	44(10)	-30(11)	39(11)	-73(14)
O(2)	125(13)	198(17)	26(6)	13(8)	7(7)	-88(12)
O(3)	63(7)	84(8)	33(5)	-9(5)	-2(5)	-9(6)
C(3)	106(14)	94(13)	28(8)	-8(8)	3(9)	-50(12)
O(4)	61(7)	92(8)	30(5)	-8(5)	5(5)	-24(6)
C(4)	101(13)	35(9)	42(8)	-4(7)	30(9)	-5(9)
C(5)	74(10)	42(9)	35(7)	-18(7)	19(8)	-21(8)
O(5)	220(20)	570(50)	54(9)	47(16)	-2(11)	-300(30)
C(6)	82(12)	84(12)	53(10)	-12(9)	23(9)	-24(10)
C(7)	67(12)	141(19)	46(10)	-31(12)	27(9)	-29(13)
O(7)	370(20)	123(13)	146(15)	31(12)	167(17)	-40(16)
C(8)	80(12)	56(10)	39(8)	-6(7)	9(8)	-2(9)
O(8)	107(12)	300(20)	106(12)	59(13)	54(10)	28(14)
C(9)	64(10)	44(9)	30(7)	10(6)	8(7)	-1(8)
C(10)	65(10)	40(8)	26(7)	-1(6)	1(7)	2(8)
C(11)	75(11)	41(9)	30(8)	-8(6)	17(8)	-6(8)
C(12)	45(8)	50(9)	40(8)	-8(7)	2(7)	-5(7)
C(13)	68(10)	32(8)	36(8)	-5(6)	15(8)	-4(7)
C(14)	72(11)	36(8)	48(9)	-6(7)	21(8)	-6(8)
C(15)	61(9)	33(8)	42(8)	7(6)	19(8)	4(7)
C(16)	62(10)	57(10)	44(8)	-4(7)	9(8)	-5(8)
C(17)	53(9)	52(10)	49(9)	13(7)	15(7)	5(8)
C(18)	67(10)	77(11)	28(8)	-13(7)	6(8)	-17(9)
C(19)	90(13)	85(13)	54(10)	-5(9)	9(9)	-49(11)
C(20)	96(13)	90(13)	43(9)	0(9)	25(9)	-55(11)
C(21)	93(13)	121(15)	18(7)	-18(8)	17(8)	-50(12)
C(22)	90(13)	119(15)	34(8)	-13(9)	19(8)	-57(12)
C(23)	73(11)	95(13)	45(9)	-18(9)	25(9)	-40(10)
C(25)	43(9)	71(11)	62(10)	-13(8)	-4(8)	11(8)
C(26)	63(11)	71(11)	57(10)	-16(8)	-6(8)	-8(9)
C(28)	112(16)	96(16)	61(12)	14(12)	56(12)	-12(13)
C(29)	270(30)	190(30)	43(11)	-49(14)	66(17)	-140(30)
C(30)	170(20)	150(20)	62(13)	-26(13)	36(14)	-114(19)

C(31)	63(11)	96(14)	38(9)	0(9)	0(8)	-19(10)
C(32)	95(14)	81(13)	61(11)	-15(10)	10(11)	-20(12)
C(33)	87(14)	99(15)	60(12)	19(11)	19(11)	-37(12)
C(34)	93(14)	89(14)	51(10)	7(9)	44(10)	18(11)
C(35)	170(20)	42(10)	58(11)	29(8)	58(13)	43(12)
C(36)	80(12)	49(10)	44(9)	-4(7)	24(9)	4(9)
C(37)	98(14)	41(9)	45(9)	-18(7)	-6(10)	-7(9)
C(38)	56(10)	35(9)	80(12)	-11(8)	-4(9)	5(8)
O(9)	55(10)	65(11)	29(9)	-25(7)	8(7)	-11(8)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Yb-PVDC-3

	x	y	z	U(eq)
H(3A)	-2005	5092	6729	87
H(4A)	-2463	4379	7791	74
H(6A)	1124	1459	7855	87
H(7A)	1636	2213	6822	99
H(8A)	-204	1791	8845	74
H(9A)	-3279	2916	8595	61
H(12A)	-5583	1371	10463	55
H(15A)	-623	1842	9849	60
H(16A)	-3028	754	11747	68
H(17A)	-5704	141	11385	70
H(19A)	-7026	-1128	12145	89
H(20A)	-7406	-2199	13154	89
H(22A)	-3872	-1003	13738	92
H(23A)	-3584	131	12742	82
H(25A)	-7484	2216	9011	93
H(25B)	-7303	2573	9662	93
H(25C)	-6870	1127	9604	93
H(26A)	1332	975	11279	96
H(26B)	678	2088	10701	96
H(26C)	1093	654	10624	96
H(29A)	6939	5384	3373	181
H(30A)	8082	5562	2419	140
H(32A)	5958	2940	2102	95
H(33A)	4790	2833	3063	103
H(34A)	7242	3994	1257	105
H(35A)	9396	5065	1505	127