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Synthesis, antimicrobial activity and application in polymers of praseodymium complexes based on pyridine nitrogen oxide

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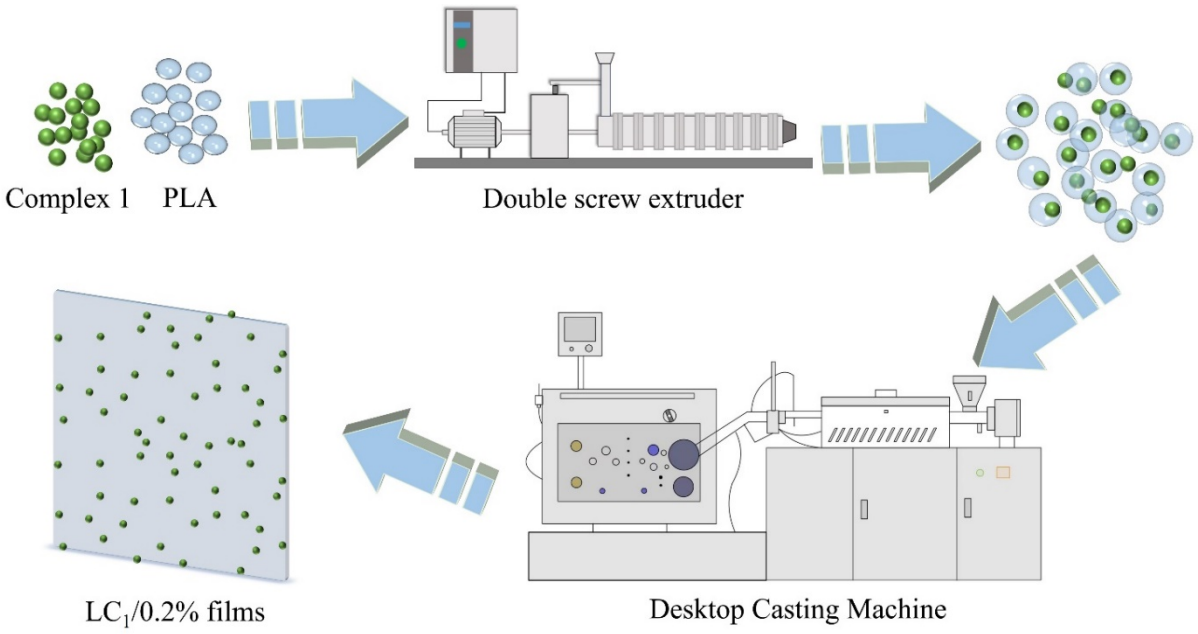

Fig. S1. Schematic illustration of the preparation of antibacterial plastic films.

Table S1 Crystallographic data for the complexes **1** and **2**.

	Complex 1	**Complex 2**
Formula	$C_{30}H_{40}N_6O_{14}Pr_2S_6$	$C_{30}H_{32}N_6O_{12}Pr_2S_4$
Formulaweithgt	1182.86	1078.701
Crystal system	Triclinic	triclinic
Volume	1080.09	942.614
Wavelength	0.71073	0.71073
Space group	$P\bar{1}$	P1
a, nm	0.84728(5)	0.65405(4)
b, nm	0.97873(5)	1.09927(6)
c, nm	1.37277(8)	1.44650(8)
α, deg	92.265(2)	68.977(2)
β, deg	107.891(2)	81.458(2)
γ, deg	92.928(2)	76.809(2)
Z	1	1
$\rho_{calc}g/cm^3$	1.819	1.900
μ/mm^{-1}	2.586	2.843
Goodness-of-fifit on F^2	1.078	1.068
Final R indices [I＞2σ(I)]	R_1=0.0371, wR_2=0.0939	R_1=0.0321, wR_2=0.0627
Final R indexes [all data]	R_1=0.0371, wR_2=0.0939	R_1=0.0439, wR_2=0.0704

Table S2 Bond Lengths for Complex **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pr1	S3	2.9399(8)	O1	N1	1.343(3)
Pr1	S2	3.0009(8)	N2	C10	1.366(4)
Pr1	S1	2.9247(8)	N2	C6	1.353(4)
Pr1	O3	2.382(2)	C12	C13	1.370(5)
Pr1	O4	2.479(2)	N1	C5	1.366(4)
Pr1	O2	2.490(2)	N1	C1	1.352(4)
Pr1	$O2^{1}$	2.535(2)	C14	C15	1.368(5)
Pr1	O1	2.364(2)	C14	C13	1.397(5)
S3	C11	1.728(3)	C10	C9	1.412(5)
S2	C10	1.728(4)	C8	C9	1.366(7)
S1	C5	1.709(3)	C8	C7	1.383(7)
O3	N3	1.353(3)	C6	C7	1.375(5)
O2	N2	1.354(3)	C5	C4	1.419(4)
N3	C11	1.342(4)	C1	C2	1.372(5)
N3	C15	1.362(4)	C4	C3	1.366(6)
C11	C12	1.418(4)	C2	C3	1.400(6)

Table S3 Angles for Complex **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S3	Pr1	S2	79.42(2)	N2	O2	Pr1[1]	122.64(16)
S1	Pr1	S3	76.32(2)	N2	O2	Pr1	114.43(16)
S1	Pr1	S2	91.46(3)	O3	N3	C15	116.2(3)
O3	Pr1	S3	65.45(5)	C11	N3	O3	120.0(2)
O3	Pr1	S2	144.40(5)	C11	N3	C15	123.8(3)
O3	Pr1	S1	85.94(6)	N3	C11	S3	120.6(2)
O3	Pr1	O4	71.73(8)	N3	C11	C12	116.5(3)
O3	Pr1	O2	137.83(7)	C12	C11	S3	122.9(3)
O3	Pr1	O2[1]	82.31(7)	N1	O1	Pr1	132.44(18)
O4	Pr1	S3	136.24(6)	O2	N2	C10	118.7(3)
O4	Pr1	S2	140.97(6)	C6	N2	O2	117.5(3)
O4	Pr1	S1	109.82(6)	C6	N2	C10	123.7(3)
O4	Pr1	O2[1]	81.07(7)	C13	C12	C11	120.8(3)
O4	Pr1	O2	79.00(7)	O1	N1	C5	119.8(3)
O2	Pr1	S3	129.42(5)	O1	N1	C1	116.5(3)
O2[1]	Pr1	S3	84.73(5)	C1	N1	C5	123.6(3)
O2	Pr1	S2	63.00(5)	C15	C14	C13	118.4(3)
O2[1]	Pr1	S2	89.17(5)	N3	C15	C14	120.3(3)
O2[1]	Pr1	S1	160.58(5)	N2	C10	S2	120.0(2)
O2	Pr1	S1	133.23(5)	N2	C10	C9	115.4(3)
O2	Pr1	O2[1]	63.39(8)	C9	C10	S2	124.6(3)
O1	Pr1	S3	138.04(6)	C12	C13	C14	120.2(3)
O1	Pr1	S2	85.34(6)	C9	C8	C7	119.6(3)
O1	Pr1	S1	65.17(6)	C8	C9	C10	121.9(4)
O1	Pr1	O3	124.65(8)	N2	C6	C7	119.7(4)
O1	Pr1	O4	75.37(8)	C6	C7	C8	119.2(4)
O1	Pr1	O2	73.78(7)	N1	C5	S1	119.2(2)
O1	Pr1	O2[1]	134.19(7)	N1	C5	C4	115.7(3)
C11	S3	Pr1	100.48(11)	C4	C5	S1	125.1(3)
C10	S2	Pr1	93.25(11)	N1	C1	C2	120.6(3)
C5	S1	Pr1	101.82(11)	C3	C4	C5	121.7(3)
N3	O3	Pr1	131.53(17)	C1	C2	C3	118.5(3)
Pr1	O2	Pr1[1]	116.61(8)	C4	C3	C2	119.9(3)

Table S4 Torsion Angles for Complex **1**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Pr1	S3	C11	N3	8.9(3)	C11	N3	C15	C14	0.6(5)
Pr1	S3	C11	C12	-170.3(2)	C11	C12	C13	C14	0.8(5)
Pr1	S2	C10	N2	28.8(3)	O1	N1	C5	S1	-1.7(4)
Pr1	S2	C10	C9	-148.6(3)	O1	N1	C5	C4	179.5(3)
Pr1	S1	C5	N1	-6.3(3)	O1	N1	C1	C2	-179.7(3)
Pr1	S1	C5	C4	172.4(3)	N2	C10	C9	C8	-4.6(5)
Pr1	O3	N3	C11	-13.7(4)	N2	C6	C7	C8	0.0(5)
Pr1	O3	N3	C15	165.1(2)	N1	C5	C4	C3	-0.5(5)
Pr1[1]	O2	N2	C10	97.7(3)	N1	C1	C2	C3	0.7(6)
Pr1	O2	N2	C10	-53.4(3)	C15	N3	C11	S3	-179.1(2)
Pr1	O2	N2	C6	124.4(2)	C15	N3	C11	C12	0.2(4)
Pr1[1]	O2	N2	C6	-84.6(3)	C15	C14	C13	C12	0.0(5)
Pr1	O1	N1	C5	13.7(4)	C10	N2	C6	C7	-5.5(5)
Pr1	O1	N1	C1	-167.6(2)	C13	C14	C15	N3	-0.7(5)
S3	C11	C12	C13	178.4(3)	C9	C8	C7	C6	2.8(6)
S2	C10	C9	C8	173.0(3)	C6	N2	C10	S2	-170.0(2)
S1	C5	C4	C3	-179.2(3)	C6	N2	C10	C9	7.6(5)
O3	N3	C11	S3	-0.4(4)	C7	C8	C9	C10	-0.4(6)
O3	N3	C11	C12	178.8(3)	C5	N1	C1	C2	-1.1(5)
O3	N3	C15	C14	-178.1(3)	C5	C4	C3	C2	0.2(6)
O2	N2	C10	S2	7.6(4)	C1	N1	C5	S1	179.7(3)
O2	N2	C10	C9	-174.8(3)	C1	N1	C5	C4	0.9(5)
O2	N2	C6	C7	176.8(3)	C1	C2	C3	C4	-0.3(6)
N3	C11	C12	C13	-0.9(5)					

Table S5 Bond Lengths for Complex **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pr1	S1	2.94847(15)	N3	C11	1.3905(4)
Pr1	S2	2.87964(15)	N3	C15	1.3906(5)
Pr1	O1	2.4360(3)	N4	C16	1.3867(4)
Pr1	O1W	2.5461(4)	N4	C20	1.3191(7)
Pr1	O2	2.4770(4)	N5	C21	1.3808(5)
Pr1	O2W	2.4808(2)	N5	C25	1.3040(4)
Pr1	O3'	2.4510(3)	N6	C26	1.3915(4)
Pr1	O3	2.4055(3)	N6	C30	1.3913(4)
Pr2	S3	2.92877(15)	C1	C2	1.4543(6)
Pr2	S4	2.92127(15)	C2	C3	1.2550(5)
Pr2	O3W	2.5249(2)	C3	C4	1.5541(6)
Pr2	O4	2.4227(4)	C4	C5	1.3223(6)
Pr2	O4W	2.5703(4)	C6	C7	1.4101(10)
Pr2	O5	2.3994(3)	C7	C8	1.3233(8)
Pr2	O6	2.5000(3)	C8	C9	1.4407(5)
Pr2	O6'	2.6688(3)	C9	C10	1.3523(10)
S1	C1	1.6795(4)	C11	C12	1.3900(5)
S2	C6	1.7579(6)	C12	C13	1.3903(5)
S3	C16	1.6178(6)	C13	C14	1.3904(4)
S4	C21	1.7089(4)	C14	C15	1.3901(5)
O1	N1	1.3720(4)	C16	C17	1.4183(10)
O2	N2	1.2871(7)	C17	C18	1.3956(7)
O3'	C11	1.3520(5)	C18	C19	1.2988(5)
O3	N3	1.3527(4)	C19	C20	1.3826(10)
O4	N4	1.4040(7)	C21	C22	1.3759(6)
O5	N5	1.3151(4)	C22	C23	1.4703(5)
O6	N6	1.2965(4)	C23	C24	1.2020(5)
O6'	C26	1.3820(4)	C24	C25	1.3891(6)
N1	C1	1.3487(5)	C26	C27	1.3918(5)
N1	C5	1.4268(4)	C27	C28	1.3914(5)
N2	C6	1.3677(5)	C28	C29	1.3913(4)
N2	C10	1.3896(7)	C29	C30	1.3912(5)

Table S6 Bond Angles for Complex **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S2	Pr1	S1	92.837(2)	N4	O4	Pr2	130.950(15)
O1	Pr1	S1	65.473(6)	N5	O5	Pr2	131.99(2)
O1	Pr1	S2	135.293(9)	N6	O6	Pr2	116.748(16)
O1W	Pr1	S1	87.682(6)	C26	O6'	Pr2	105.974(19)
O1W	Pr1	S2	141.116(4)	C1	N1	O1	122.17(3)
O1W	Pr1	O1	79.486(10)	C5	N1	O1	110.74(3)
O2	Pr1	S1	96.660(6)	C5	N1	C1	126.99(4)
O2	Pr1	S2	64.753(6)	C6	N2	O2	123.39(4)
O2	Pr1	O1	78.871(11)	C10	N2	O2	118.70(3)
O2	Pr1	O1W	153.745(7)	C10	N2	C6	117.29(5)
O2W	Pr1	S1	72.020(6)	C11	N3	O3	117.17(3)
O2W	Pr1	S2	69.608(9)	C15	N3	O3	119.70(2)
O2W	Pr1	O1	130.051(9)	C15	N3	C11	123.08(3)
O2W	Pr1	O1W	73.681(10)	C16	N4	O4	115.46(4)
O2W	Pr1	O2	132.279(11)	C20	N4	O4	116.71(3)
O3'	Pr1	S1	138.697(6)	C20	N4	C16	127.17(6)
O3'	Pr1	S2	121.085(9)	C21	N5	O5	118.59(3)
O3'	Pr1	O1	73.546(8)	C25	N5	O5	123.91(3)
O3'	Pr1	O1W	79.902(10)	C25	N5	C21	117.29(4)
O3'	Pr1	O2	79.854(11)	C26	N6	O6	121.50(3)
O3'	Pr1	O2W	138.482(9)	C30	N6	O6	112.03(2)
O3	Pr1	S1	151.057(6)	C30	N6	C26	126.46(3)
O3	Pr1	S2	83.693(9)	N1	C1	S1	120.35(3)
O3	Pr1	O1	133.865(9)	C2	C1	S1	123.76(3)
O3	Pr1	O1W	77.660(11)	C2	C1	N1	115.82(3)
O3	Pr1	O2	107.553(10)	C3	C2	C1	123.15(4)
O3	Pr1	O2W	79.903(7)	C4	C3	C2	117.63(4)
O3	Pr1	O3'	63.344(7)	C5	C4	C3	122.41(3)
S4	Pr2	S3	92.625(2)	C4	C5	N1	113.77(3)
O3W	Pr2	S3	69.270(9)	N2	C6	S2	115.75(5)
O3W	Pr2	S4	72.174(6)	C7	C6	S2	125.15(3)
O4	Pr2	S3	65.450(7)	C7	C6	N2	118.85(5)
O4	Pr2	S4	94.623(6)	C8	C7	C6	125.79(4)
O4	Pr2	O3W	132.025(11)	C9	C8	C7	113.55(6)
O4W	Pr2	S3	139.008(4)	C10	C9	C8	122.14(5)
O4W	Pr2	S4	87.381(6)	C9	C10	N2	121.65(3)
O4W	Pr2	O3W	71.811(10)	N3	C11	O3'	113.62(3)
O4W	Pr2	O4	155.436(8)	C12	C11	O3'	129.35(3)

Table S6 Bond Angles for Complex **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O5	Pr2	S3	135.102(9)	C12	C11	N3	116.86(3)
O5	Pr2	S4	65.219(6)	C13	C12	C11	123.13(3)
O5	Pr2	O3W	130.086(9)	C14	C13	C12	116.80(3)
O5	Pr2	O4	77.441(11)	C15	C14	C13	123.15(4)
O5	Pr2	O4W	81.264(10)	C14	C15	N3	116.83(3)
O6	Pr2	S3	121.019(9)	N4	C16	S3	124.83(5)
O6	Pr2	S4	138.913(6)	C17	C16	S3	122.45(3)
O6	Pr2	O3W	138.480(9)	C17	C16	N4	112.42(5)
O6	Pr2	O4	80.809(11)	C18	C17	C16	116.42(4)
O6	Pr2	O4W	81.675(10)	C19	C18	C17	129.53(7)
O6	Pr2	O5	73.993(8)	C20	C19	C18	113.04(5)
O6'	Pr2	S3	86.089(8)	C19	C20	N4	120.79(4)
O6'	Pr2	S4	144.132(5)	N5	C21	S4	120.75(3)
O6'	Pr2	O3W	73.918(7)	C22	C21	S4	123.37(3)
O6'	Pr2	O4	116.925(10)	C22	C21	N5	115.74(3)
O6'	Pr2	O4W	71.140(10)	C23	C22	C21	119.53(3)
O6'	Pr2	O5	134.950(10)	C24	C23	C22	123.72(4)
O6'	Pr2	O6	67.447(7)	C25	C24	C23	114.00(3)
C1	S1	Pr1	101.779(15)	C24	C25	N5	129.09(4)
C6	S2	Pr1	104.521(18)	N6	C26	O6'	125.36(3)
C16	S3	Pr2	102.27(2)	C27	C26	O6'	120.78(3)
C21	S4	Pr2	100.750(15)	C27	C26	N6	113.51(3)
N1	O1	Pr1	126.79(2)	C28	C27	C26	126.42(3)
N2	O2	Pr1	129.922(16)	C29	C28	C27	113.57(3)
C11	O3'	Pr1	122.989(17)	C30	C29	C28	126.37(3)
N3	O3	Pr1	122.786(15)	C29	C30	N6	113.55(3)

Table S7 Torsion Angles for Complex **2**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Pr1	S1	C1	N1	8.51(3)	O3'	C11	N3	C15	-178.76(5)
Pr1	S1	C1	C2	-168.44(4)	O3'	C11	C12	C13	174.94(7)
Pr1	O1	N1	C1	-20.66(5)	O3	N3	C11	C12	174.51(6)
Pr1	O1	N1	C5	162.82(5)	O3	N3	C15	C14	-174.66(6)
Pr1	O2	N2	C6	16.32(4)	O4	N4	C16	C17	175.86(4)
Pr1	O2	N2	C10	-172.98(3)	O4	N4	C20	C19	-176.98(3)
Pr1	O3'	C11	N3	3.21(4)	O5	N5	C21	C22	176.40(6)
Pr1	O3'	C11	C12	-171.89(5)	O5	N5	C25	C24	-176.15(6)
Pr1	O3	N3	C11	-1.25(5)	O6	N6	C26	O6'	-8.04(6)
Pr1	O3	N3	C15	176.36(4)	O6	N6	C26	C27	178.77(6)
Pr2	S3	C16	N4	11.69(2)	O6	N6	C30	C29	179.14(5)
Pr2	S3	C16	C17	-175.09(3)	O6'	C26	N6	C30	171.49(6)
Pr2	O4	N4	C16	1.44(3)	O6'	C26	C27	C28	-172.19(6)
Pr2	O4	N4	C20	172.75(3)	N1	C1	C2	C3	1.24(8)
Pr2	O5	N5	C21	15.94(5)	N1	C5	C4	C3	-5.32(8)
Pr2	O5	N5	C25	-158.62(5)	N2	C6	C7	C8	-7.95(6)
Pr2	O6	N6	C26	-8.16(5)	N2	C10	C9	C8	6.14(5)
Pr2	O6	N6	C30	172.24(4)	N3	C11	C12	C13	-0.03(8)
Pr2	O6'	C26	N6	17.33(4)	N3	C15	C14	C13	0.46(8)
Pr2	O6'	C26	C27	-169.95(4)	N4	C16	C17	C18	-4.88(5)
S1	C1	N1	O1	4.41(7)	N4	C20	C19	C18	6.82(5)
S1	C1	N1	C5	-179.66(5)	N5	C21	C22	C23	5.60(8)
S1	C1	C2	C3	178.33(6)	N5	C25	C24	C23	-5.20(9)
S2	C6	N2	O2	-6.12(4)	N6	C26	C27	C28	1.35(8)
S2	C6	N2	C10	-176.95(3)	N6	C30	C29	C28	3.36(8)
S2	C6	C7	C8	177.94(4)	C1	C2	C3	C4	-2.11(9)
S3	C16	N4	O4	-10.33(5)	C2	C3	C4	C5	4.54(9)
S3	C16	N4	C20	179.43(4)	C6	C7	C8	C9	5.60(6)
S3	C16	C17	C18	-178.87(4)	C7	C8	C9	C10	-4.64(5)
S4	C21	N5	O5	0.62(7)	C11	C12	C13	C14	3.00(8)
S4	C21	N5	C25	175.54(5)	C12	C13	C14	C15	-3.22(8)
S4	C21	C22	C23	-178.76(6)	C16	C17	C18	C19	6.92(6)
O1	N1	C1	C2	-178.40(6)	C17	C18	C19	C20	-7.47(6)
O1	N1	C5	C4	-179.07(5)	C21	C22	C23	C24	-1.95(9)
O2	N2	C6	C7	179.22(4)	C22	C23	C24	C25	1.17(9)
O2	N2	C10	C9	-179.20(4)	C26	C27	C28	C29	1.06(9)
O3'	C11	N3	O3	-1.24(7)	C27	C28	C29	C30	-3.64(8)