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Linear Chain and Mononuclear Tri-Spin Compounds Based on the Lanthanide-Nitronyl Nitroxide Radicals: Structural Design and Magnetic Properties

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Table S1. Selected bond lengths (Å) and angles (deg) for **1**

Ce(1)-O(1)	2.454(4)	Ce (1)-O(7)	2.431(2)
Ce (1)-O(6)	2.460(5)	Ce (1)-O(8)	2.458(2)
Ce (1)-O(4)	2.463(2)	O(1)-N(1)	1.285(3)
Ce (1)-O(9)	2.456(4)	O(2)-N(2)	1.291(3)
Ce (1)-O(5)	2.420(3)	O(2)-Ce(1)#2	2.498(4)
O(7)- Ce (1)-O(5)	139.86(8)	O(7)- Ce (1)-O(1)	86.42(14)
O(5)- Ce (1)-O(1)	104.92(14)	O(7)- Ce (1)-O(6)	69.47(16)
O(6)- Ce (1)-O(5)	77.38(14)	O(1)- Ce (1)-O(6)	140.56(15)
O(7)- Ce (1)-O(9)	144.96(17)	O(5)- Ce (1)-O(9)	76.46(17)
O(1)- Ce (1)-O(9)	79.87(15)	O(6)- Ce (1)-O(9)	136.76(15)
O(7)- Ce (1)-O(4)	78.09(16)	O(5)- Ce (1)-O(4)	69.11(17)
O(4)- Ce (1)-O(1)	70.93(18)	O(4)- Ce (1)-O(6)	73.76(18)
O(9)- Ce (1)-O(4)	125.86(16)	O(7)- Ce (1)-O(8)	76.74(15)
O(8)- Ce (1)-O(5)	143.89(15)	O(8)- Ce (1)-O(1)	79.68(16)
O(6)- Ce (1)-O(8)	121.64(16)	O(9)- Ce (1)-O(8)	69.19(15)
O(8)- Ce (1)-O(4)	142.14(16)	N(1)-O(1)- Ce (1)	141.1(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x, y-1/2,-z+1/2 #2 -x, y+1/2,-z+1/2

Table S2. Selected bond lengths (Å) and angles (deg) for **2**

Pr(1)-O(1)	2.477(5)	Pr(1)-O(7)	2.403(6)
Pr(1)-O(2)	2.441(5)	Pr(1)-O(8)	2.454(6)
Pr(1)-O(4)	2.453(5)	O(1)-N(1)	1.275(7)
Pr(1)-O(9)	2.409(5)	O(2)-N(2)	1.277(7)
Pr(1)-O(5)	2.456(5)	Pr(1)-O(6)	2.469(6)
O(7)- Pr (1)-O(9)	139.6(2)	O(7)- Pr (1)-O(6)	70.2(2)
O(9)- Pr (1)-O(6)	77.9(2)	O(7)- Pr (1)-O(4)	75.7(2)
O(6)- Pr (1)-O(4)	125.96(19)	O(4)- Pr (1)-O(9)	144.70(18)
O(8)- Pr (1)-O(6)	74.2(2)	O(5)- Pr (1)-O(6)	141.2(2)
O(7)- Pr (1)-O(8)	77.5(2)	O(7)- Pr (1)-O(1)	86.5(2)
O(8)- Pr (1)-O(9)	70.27(18)	O(9)- Pr (1)-O(1)	104.89(18)
O(4)- Pr (1)-O(8)	136.24(19)	O(4)- Pr (1)-O(1)	73.24(18)
O(5)- Pr (1)-O(7)	143.59(19)	O(1)- Pr (1)-O(8)	71.22(19)
O(9)- Pr (1)-O(5)	76.06(17)	O(5)- Pr (1)-O(1)	73.47(18)
O(6)- Pr (1)-O(1)	141.7(2)	O(4)- Pr (1)-O(5)	69.61(17)
O(8)- Pr (1)-O(5)	121.69(19)	N(1)-O(1)-Pr(1)	141.9(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x, y-1/2,-z+1/2 #2 -x, y+1/2,-z+1/2

Table S3. Selected bond lengths (Å) and angles (deg) for **3**

Ce(1)-O(1)	2.4060(19)	Ce(1)-O(8)	2.4822(19)
Ce(1)-O(11)	2.4421(18)	Ce(1)-O(12)	2.4875(19)
Ce(1)-O(4)	2.4504(19)	O(1)-N(1)	1.308(3)
Ce(1)-O(9)	2.4526(18)	O(2)-N(2)	1.272(3)
Ce(1)-O(7)	2.4534(18)	O(4)-N(3)	1.295(3)
Ce(1)-O(10)	2.4802(18)	O(5)-N(4)	1.274(3)
O(1)-Ce(1)-O(11)	107.40(7)	O(1)-Ce(1)-O(8)	75.76(6)
O(1)-Ce(1)-O(4)	141.41(6)	O(11)-Ce(1)-O(8)	147.82(6)
O(11)-Ce(1)-O(4)	88.83(6)	O(4)-Ce(1)-O(8)	72.61(6)
O(1)-Ce(1)-O(9)	87.13(7)	O(9)-Ce(1)-O(8)	75.61(6)
O(11)-Ce(1)-O(9)	135.82(6)	O(7)-Ce(1)-O(8)	70.39(6)
O(4)-Ce(1)-O(9)	105.54(6)	O(10)-Ce(1)-O(8)	121.78(6)
O(1)-Ce(1)-O(7)	71.40(6)	O(1)-Ce(1)-O(12)	74.96(6)
O(11)-Ce(1)-O(7)	80.21(6)	O(11)-Ce(1)-O(12)	70.27(6)
O(4)-Ce(1)-O(7)	77.52(6)	O(4)-Ce(1)-O(12)	143.34(6)
O(9)-Ce(1)-O(7)	143.19(6)	O(9)-Ce(1)-O(12)	74.03(6)
O(1)-Ce(1)-O(10)	144.20(6)	O(7)-Ce(1)-O(12)	125.26(6)
O(11)-Ce(1)-O(10)	74.86(6)	O(10)-Ce(1)-O(12)	72.42(7)
O(4)-Ce(1)-O(10)	73.19(6)	O(8)-Ce(1)-O(12)	138.39(6)
O(9)-Ce(1)-O(10)	70.14(6)	N(1)-O(1)-Ce(1)	138.41(14)
O(7)-Ce(1)-O(10)	141.53(6)	N(3)-O(4)-Ce(1)	137.17(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x, y-1/2,-z+1/2 #2 -x, y+1/2,-z+1/2

Table S4. Selected bond lengths (Å) and angles (deg) for **4**

N(1)-O(3)	1.306(9)	O(7)-Pr(1)	2.479(6)
N(2)-O(4)	1.276(11)	O(8)-Pr(1)	2.410(6)
N(3)-O(1)	1.307(8)	O(9)-Pr(1)	2.457(6)
N(4)-O(2)	1.287(10)	O(10)-Pr(1)	2.451(6)
O(1)-Pr(1)	2.420(6)	O(11)-Pr(1)	2.432(6)
O(3)-Pr(1)	2.420(6)	O(12)-Pr(1)	2.479(6)
O(8)-Pr(1)-O(1)	97.6(2)	O(8)-Pr(1)-O(7)	69.48(18)
O(8)-Pr(1)-O(3)	86.0(2)	O(1)-Pr(1)-O(7)	72.3(2)
O(1)-Pr(1)-O(3)	142.7(2)	O(3)-Pr(1)-O(7)	141.3(2)
O(8)-Pr(1)-O(11)	142.8(2)	O(11)-Pr(1)-O(7)	79.3(2)
O(1)-Pr(1)-O(11)	91.4(2)	O(10)-Pr(1)-O(7)	135.7(19)
O(3)-Pr(1)-O(11)	108.0(2)	O(9)-Pr(1)-O(7)	127.4(2)
O(8)-Pr(1)-O(10)	146.0(2)	O(8)-Pr(1)-O(12)	82.0(2)
O(1)-Pr(1)-O(10)	76.2(2)	O(1)-Pr(1)-O(12)	143.4(2)
O(3)-Pr(1)-O(10)	80.4(2)	O(3)-Pr(1)-O(12)	73.8(2)
O(11)-Pr(1)-O(10)	71.1(2)	O(11)-Pr(1)-O(12)	69.9(2)
O(8)-Pr(1)-O(9)	76.7(2)	O(10)-Pr(1)-O(12)	122.9(2)
O(1)-Pr(1)-O(9)	73.8(2)	O(9)-Pr(1)-O(12)	139.7(2)
O(3)-Pr(1)-O(9)	71.0(2)	O(7)-Pr(1)-O(12)	73.5(2)
O(11)-Pr(1)-O(9)	140.2(2)	N(3)-O(1)-Pr(1)	144.2(5)
O(10)-Pr(1)-O(9)	69.4(2)	N(1)-O(3)-Pr(1)	142.6(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x, y-1/2,-z+1/2 #2 -x, y+1/2,-z+1/2