

Supporting Information

Templated assembly of μ_5 -CO₃²⁻ decanuclear praseodymium and neodymium clusters through spontaneous fixation of atmospheric carbon dioxide

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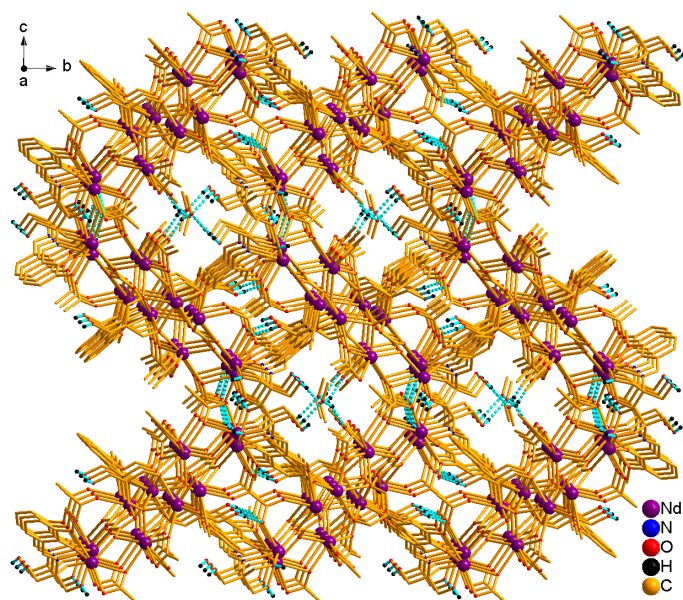


Fig. S1 Three-dimensional frameworks in the crystal structure of 1.

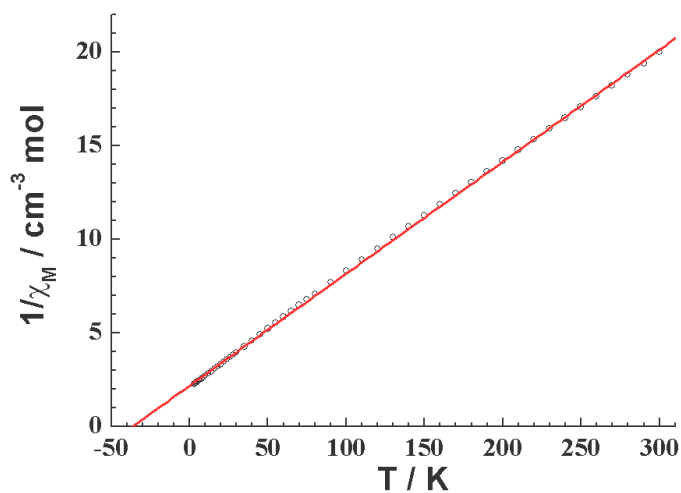


Fig S2. Plot of $1/\chi_M$ vs. T for **1**. The solid line is the best-fit to a Curie-Weiss law

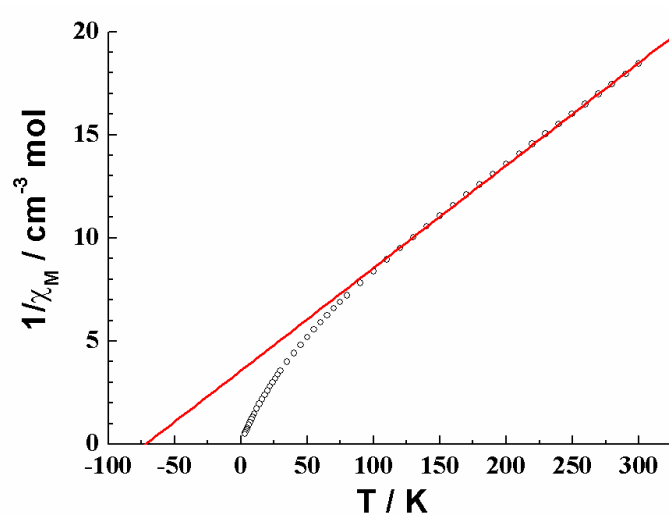


Fig S3. Plot of $1/\chi_M$ vs. T for **2**. The solid line is the best-fit to a Curie-Weiss law

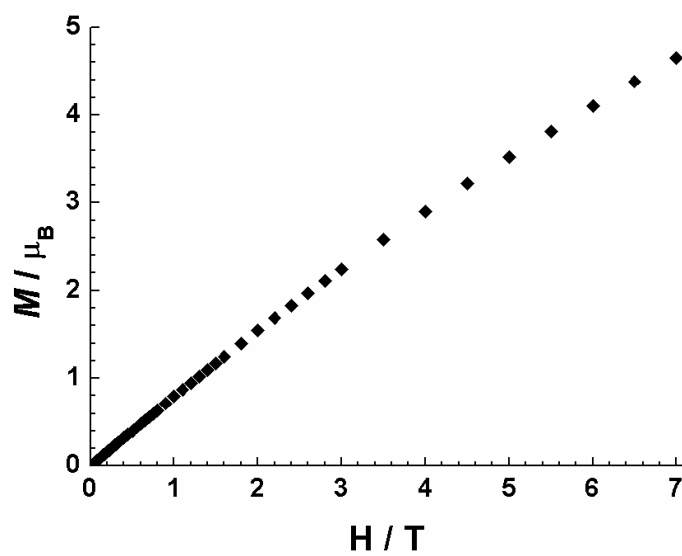


Fig. S4 M vs H plot of the complex **1** at 1.9 K

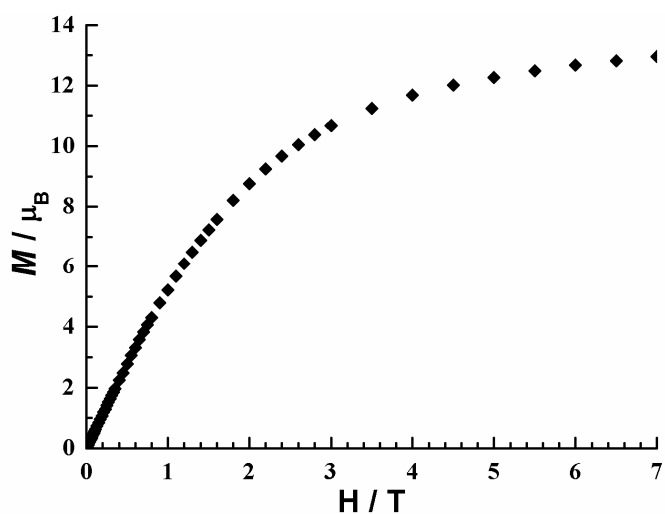


Fig. S5 M vs H plot of the complex 2 at 1.9 K

Table S1 Selected bond lengths (Å) and angles (°) for **1^a**

Pr(1)-O(1)	2.382(10)	Pr(3)-O(15)	2.684(8)
Pr(1)-O(11)	2.431(9)	Pr(3)-O(7)	2.731(9)
Pr(1)-O(28)	2.467(7)	Pr(3)-O(25)	2.733(9)
Pr(1)-O(15)	2.494(9)	Pr(3)-C(29)	2.963(14)
Pr(1)-O(4)	2.504(8)	Pr(3)-C(38)	2.990(14)
Pr(1)-O(14)	2.534(10)	Pr(4)-O(22)	2.441(11)
Pr(1)-O(13)	2.545(9)	Pr(4)-O(10)	2.447(8)
Pr(1)-N(1)	2.606(11)	Pr(4)-O(8)	2.450(7)
Pr(1)-O(3)	2.640(9)	Pr(4)-O(29)	2.554(8)
Pr(2)-O(21)	2.374(11)	Pr(4)-O(18)	2.570(8)
Pr(2)-O(13)	2.406(11)	Pr(4)-O(32)#1	2.583(12)
Pr(2)-O(1)	2.468(8)	Pr(4)-O(31)#1	2.587(9)
Pr(2)-O(29)	2.470(8)	Pr(4)-O(26)	2.619(10)
Pr(2)-O(20)	2.499(11)	Pr(4)-O(27)	2.629(14)
Pr(2)-O(17)	2.559(9)	Pr(4)-O(30)	2.933(8)
Pr(2)-O(18)	2.571(10)	Pr(5)-O(31)	2.446(8)
Pr(2)-O(19)	2.606(11)	Pr(5)-O(6)	2.456(8)
Pr(2)-O(2)	2.683(10)	Pr(5)-O(25)	2.458(9)
Pr(3)-O(12)	2.419(9)	Pr(5)-O(30)	2.501(8)
Pr(3)-O(6)	2.425(8)	Pr(5)-O(8)	2.508(7)
Pr(3)-O(23)	2.506(10)	Pr(5)-O(10)	2.533(7)
Pr(3)-O(24)	2.507(10)	Pr(5)-N(2)	2.547(11)
Pr(3)-O(16)	2.518(10)	Pr(5)-O(10)#1	2.552(7)
Pr(3)-O(28)	2.528(8)	Pr(5)-O(8)#1	2.582(8)
Pr(3)-O(30)	2.646(8)		
O(1)-Pr(1)-O(11)	79.3(3)	O(10)-Pr(4)-O(8)	60.1(2)

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O(1)-Pr(1)-O(28)	77.6(3)	O(22)-Pr(4)-O(29)	78.2(3)
O(11)-Pr(1)-O(28)	78.3(3)	O(10)-Pr(4)-O(29)	112.4(2)
O(1)-Pr(1)-O(15)	142.2(3)	O(8)-Pr(4)-O(29)	86.5(2)
O(11)-Pr(1)-O(15)	75.1(3)	O(22)-Pr(4)-O(18)	72.0(3)
O(28)-Pr(1)-O(15)	70.4(3)	O(10)-Pr(4)-O(18)	154.7(3)
O(1)-Pr(1)-O(4)	132.6(3)	O(8)-Pr(4)-O(18)	141.2(3)
O(11)-Pr(1)-O(4)	95.5(3)	O(29)-Pr(4)-O(18)	65.8(3)
O(28)-Pr(1)-O(4)	148.0(3)	O(22)-Pr(4)-O(32)#1	70.8(5)
O(15)-Pr(1)-O(4)	77.7(3)	O(10)-Pr(4)-O(32)#1	112.0(4)
O(1)-Pr(1)-O(14)	119.3(3)	O(8)-Pr(4)-O(32)#1	114.8(4)
O(11)-Pr(1)-O(14)	152.9(3)	O(29)-Pr(4)-O(32)#1	135.6(4)
O(28)-Pr(1)-O(14)	86.4(3)	O(18)-Pr(4)-O(32)#1	74.7(3)
O(15)-Pr(1)-O(14)	78.8(3)	O(22)-Pr(4)-O(31)#1	81.0(4)
O(4)-Pr(1)-O(14)	85.7(3)	O(10)-Pr(4)-O(31)#1	70.6(3)
O(1)-Pr(1)-O(13)	68.4(3)	O(8)-Pr(4)-O(31)#1	71.1(3)
O(11)-Pr(1)-O(13)	140.5(3)	O(29)-Pr(4)-O(31)#1	152.5(3)
O(28)-Pr(1)-O(13)	73.1(3)	O(18)-Pr(4)-O(31)#1	123.6(3)
O(15)-Pr(1)-O(13)	118.3(3)	O(32)#1-Pr(4)-O(31)#1	49.6(3)
O(4)-Pr(1)-O(13)	123.0(3)	O(22)-Pr(4)-O(26)	144.3(3)
O(14)-Pr(1)-O(13)	50.9(3)	O(10)-Pr(4)-O(26)	79.6(3)
O(1)-Pr(1)-N(1)	67.9(3)	O(8)-Pr(4)-O(26)	124.8(3)
O(11)-Pr(1)-N(1)	75.4(3)	O(29)-Pr(4)-O(26)	75.1(3)
O(28)-Pr(1)-N(1)	139.7(3)	O(18)-Pr(4)-O(26)	75.6(3)
O(15)-Pr(1)-N(1)	129.3(3)	O(32)#1-Pr(4)-O(26)	114.5(4)
O(4)-Pr(1)-N(1)	65.2(3)	O(31)#1-Pr(4)-O(26)	130.8(3)
O(14)-Pr(1)-N(1)	128.3(3)	O(22)-Pr(4)-O(27)	133.2(4)
O(13)-Pr(1)-N(1)	110.8(3)	O(10)-Pr(4)-O(27)	83.4(3)
O(1)-Pr(1)-O(3)	82.2(3)	O(8)-Pr(4)-O(27)	142.2(3)
O(11)-Pr(1)-O(3)	133.6(3)	O(29)-Pr(4)-O(27)	118.8(3)
O(28)-Pr(1)-O(3)	137.6(3)	O(18)-Pr(4)-O(27)	76.7(4)
O(15)-Pr(1)-O(3)	135.4(3)	O(32)#1-Pr(4)-O(27)	68.0(5)
O(4)-Pr(1)-O(3)	67.7(3)	O(31)#1-Pr(4)-O(27)	88.7(4)
O(14)-Pr(1)-O(3)	71.7(3)	O(26)-Pr(4)-O(27)	48.9(3)
O(13)-Pr(1)-O(3)	64.9(3)	O(22)-Pr(4)-O(30)	114.2(3)
N(1)-Pr(1)-O(3)	58.3(3)	O(10)-Pr(4)-O(30)	65.7(2)
O(21)-Pr(2)-O(13)	148.6(4)	O(8)-Pr(4)-O(30)	68.5(2)
O(21)-Pr(2)-O(1)	132.7(3)	O(29)-Pr(4)-O(30)	47.0(2)
O(13)-Pr(2)-O(1)	69.3(3)	O(18)-Pr(4)-O(30)	105.4(2)
O(21)-Pr(2)-O(29)	83.0(3)	O(32)#1-Pr(4)-O(30)	174.9(5)
O(13)-Pr(2)-O(29)	75.8(3)	O(31)#1-Pr(4)-O(30)	130.9(2)
O(1)-Pr(2)-O(29)	86.4(3)	O(26)-Pr(4)-O(30)	60.9(3)
O(21)-Pr(2)-O(20)	87.5(4)	O(27)-Pr(4)-O(30)	107.0(3)
O(13)-Pr(2)-O(20)	121.9(4)	O(31)-Pr(5)-O(6)	79.9(3)

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O(1)-Pr(2)-O(20)	79.6(3)	O(31)-Pr(5)-O(25)	83.7(3)
O(29)-Pr(2)-O(20)	150.2(3)	O(6)-Pr(5)-O(25)	69.1(3)
O(21)-Pr(2)-O(17)	77.7(4)	O(31)-Pr(5)-O(30)	144.1(3)
O(13)-Pr(2)-O(17)	91.5(3)	O(6)-Pr(5)-O(30)	66.6(3)
O(1)-Pr(2)-O(17)	145.6(3)	O(25)-Pr(5)-O(30)	73.1(3)
O(29)-Pr(2)-O(17)	117.3(3)	O(31)-Pr(5)-O(8)	135.9(3)
O(20)-Pr(2)-O(17)	87.8(3)	O(6)-Pr(5)-O(8)	119.7(3)
O(21)-Pr(2)-O(18)	76.0(4)	O(25)-Pr(5)-O(8)	138.9(3)
O(13)-Pr(2)-O(18)	74.4(3)	O(30)-Pr(5)-O(8)	75.2(2)
O(1)-Pr(2)-O(18)	139.3(3)	O(31)-Pr(5)-O(10)	135.1(3)
O(29)-Pr(2)-O(18)	67.0(3)	O(6)-Pr(5)-O(10)	136.3(2)
O(20)-Pr(2)-O(18)	137.3(3)	O(25)-Pr(5)-O(10)	87.3(3)
O(17)-Pr(2)-O(18)	50.6(3)	O(30)-Pr(5)-O(10)	71.7(2)
O(21)-Pr(2)-O(19)	132.7(4)	O(8)-Pr(5)-O(10)	58.2(2)
O(13)-Pr(2)-O(19)	71.0(4)	O(31)-Pr(5)-N(2)	85.4(4)
O(1)-Pr(2)-O(19)	70.1(3)	O(6)-Pr(5)-N(2)	69.3(3)
O(29)-Pr(2)-O(19)	144.3(4)	O(25)-Pr(5)-N(2)	138.2(3)
O(20)-Pr(2)-O(19)	52.5(4)	O(30)-Pr(5)-N(2)	93.9(3)
O(17)-Pr(2)-O(19)	76.8(3)	O(8)-Pr(5)-N(2)	68.8(3)
O(18)-Pr(2)-O(19)	114.6(4)	O(10)-Pr(5)-N(2)	127.0(3)
O(21)-Pr(2)-O(2)	72.3(3)	O(31)-Pr(5)-O(10)#1	71.2(3)
O(13)-Pr(2)-O(2)	122.8(3)	O(6)-Pr(5)-O(10)#1	128.0(3)
O(1)-Pr(2)-O(2)	60.4(3)	O(25)-Pr(5)-O(10)#1	144.2(3)
O(29)-Pr(2)-O(2)	75.4(3)	O(30)-Pr(5)-O(10)#1	140.4(3)
O(20)-Pr(2)-O(2)	74.8(3)	O(8)-Pr(5)-O(10)#1	65.9(2)
O(17)-Pr(2)-O(2)	145.7(4)	O(10)-Pr(5)-O(10)#1	92.8(2)
O(18)-Pr(2)-O(2)	133.1(3)	N(2)-Pr(5)-O(10)#1	66.2(3)
O(19)-Pr(2)-O(2)	112.3(4)	O(31)-Pr(5)-O(8)#1	71.2(3)
O(12)-Pr(3)-O(6)	80.0(3)	O(6)-Pr(5)-O(8)#1	146.7(3)
O(12)-Pr(3)-O(23)	139.2(3)	O(25)-Pr(5)-O(8)#1	91.2(3)
O(6)-Pr(3)-O(23)	126.7(3)	O(30)-Pr(5)-O(8)#1	134.6(3)
O(12)-Pr(3)-O(24)	134.0(4)	O(8)-Pr(5)-O(8)#1	92.9(2)
O(6)-Pr(3)-O(24)	93.0(3)	O(10)-Pr(5)-O(8)#1	65.1(2)
O(23)-Pr(3)-O(24)	80.2(4)	N(2)-Pr(5)-O(8)#1	122.8(3)
O(12)-Pr(3)-O(16)	78.2(4)	O(10)#1-Pr(5)-O(8)#1	57.0(2)
O(6)-Pr(3)-O(16)	134.9(3)	O(31)-Pr(5)-Pr(5)#1	106.1(2)
O(23)-Pr(3)-O(16)	94.6(4)	O(6)-Pr(5)-Pr(5)#1	165.9(2)
O(24)-Pr(3)-O(16)	75.3(3)	O(25)-Pr(5)-Pr(5)#1	123.7(2)
O(12)-Pr(3)-O(28)	69.3(3)	O(30)-Pr(5)-Pr(5)#1	109.50(18)
O(6)-Pr(3)-O(28)	94.0(3)	O(8)-Pr(5)-Pr(5)#1	47.33(17)
O(23)-Pr(3)-O(28)	77.7(3)	O(10)-Pr(5)-Pr(5)#1	46.63(17)
O(24)-Pr(3)-O(28)	156.6(3)	N(2)-Pr(5)-Pr(5)#1	98.1(2)
O(16)-Pr(3)-O(28)	114.0(3)	O(10)#1-Pr(5)-Pr(5)#1	46.16(17)

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O(12)-Pr(3)-O(30)	103.5(3)	O(8)#1-Pr(5)-Pr(5)#1	45.58(17)
O(6)-Pr(3)-O(30)	64.7(3)	O(31)-Pr(5)-Pr(4)#1	41.3(2)
O(23)-Pr(3)-O(30)	70.5(3)	O(6)-Pr(5)-Pr(4)#1	119.94(19)
O(24)-Pr(3)-O(30)	114.4(3)	O(25)-Pr(5)-Pr(4)#1	106.5(2)
O(16)-Pr(3)-O(30)	159.4(3)	O(30)-Pr(5)-Pr(4)#1	173.10(19)
O(28)-Pr(3)-O(30)	50.2(2)	O(8)-Pr(5)-Pr(4)#1	101.97(17)
O(12)-Pr(3)-O(15)	72.9(3)	O(10)-Pr(5)-Pr(4)#1	101.45(17)
O(6)-Pr(3)-O(15)	150.8(3)	N(2)-Pr(5)-Pr(4)#1	90.9(2)
O(23)-Pr(3)-O(15)	72.3(3)	O(10)#1-Pr(5)-Pr(4)#1	38.49(17)
O(24)-Pr(3)-O(15)	113.7(3)	O(8)#1-Pr(5)-Pr(4)#1	38.69(17)
O(16)-Pr(3)-O(15)	49.4(3)	Pr(5)#1-Pr(5)-Pr(4)#1	64.77(2)
O(28)-Pr(3)-O(15)	66.4(3)	Pr(1)-O(1)-Pr(2)	111.5(4)
O(30)-Pr(3)-O(15)	110.9(3)	Pr(3)-O(6)-Pr(5)	105.6(3)
O(12)-Pr(3)-O(7)	65.1(3)	Pr(4)-O(8)-Pr(5)	105.9(3)
O(6)-Pr(3)-O(7)	59.6(3)	Pr(4)-O(8)-Pr(5)#1	100.1(3)
O(23)-Pr(3)-O(7)	152.1(4)	Pr(5)-O(8)-Pr(5)#1	87.1(2)
O(24)-Pr(3)-O(7)	72.1(4)	Pr(4)-O(10)-Pr(5)	105.2(3)
O(16)-Pr(3)-O(7)	75.4(3)	Pr(4)-O(10)-Pr(5)#1	101.0(3)
O(28)-Pr(3)-O(7)	130.2(3)	Pr(5)-O(10)-Pr(5)#1	87.2(2)
O(30)-Pr(3)-O(7)	124.2(3)	Pr(2)-O(13)-Pr(1)	108.2(4)
O(15)-Pr(3)-O(7)	115.8(3)	Pr(1)-O(15)-Pr(3)	108.0(3)
O(12)-Pr(3)-O(25)	144.7(3)	Pr(4)-O(18)-Pr(2)	109.4(3)
O(6)-Pr(3)-O(25)	65.0(3)	Pr(5)-O(25)-Pr(3)	96.9(3)
O(23)-Pr(3)-O(25)	71.7(3)	Pr(1)-O(28)-Pr(3)	114.1(3)
O(24)-Pr(3)-O(25)	48.6(3)	Pr(2)-O(29)-Pr(4)	113.2(3)
O(16)-Pr(3)-O(25)	123.4(3)	Pr(5)-O(30)-Pr(3)	98.1(3)
O(28)-Pr(3)-O(25)	115.8(3)	Pr(5)-O(30)-Pr(4)	93.1(2)
O(30)-Pr(3)-O(25)	66.6(3)	Pr(3)-O(30)-Pr(4)	160.8(3)
O(15)-Pr(3)-O(25)	142.2(3)	Pr(5)-O(31)-Pr(4)#1	100.1(3)
O(7)-Pr(3)-O(25)	91.8(3)	O(28)-C(42)-O(30)	118.4(10)
O(22)-Pr(4)-O(10)	133.2(3)	O(28)-C(42)-O(29)	123.0(10)
O(22)-Pr(4)-O(8)	76.1(3)	O(30)-C(42)-O(29)	118.6(10)

^a Symmetry operation: #1 -x+1,-y,-z+2

Table S2 Selected bond lengths (Å) and angles (°) for **2^a**

Nd(1)-O(1)	2.382(5)	Nd(3)-O(15)	2.659(5)
Nd(1)-O(11)	2.423(5)	Nd(3)-O(7)	2.721(5)
Nd(1)-O(29)	2.452(5)	Nd(3)-O(25)	2.741(5)
Nd(1)-O(15)	2.472(5)	Nd(4)-O(22)	2.420(6)
Nd(1)-O(4)	2.496(5)	Nd(4)-O(9)	2.445(5)
Nd(1)-O(14)	2.524(6)	Nd(4)-O(10)	2.450(5)
Nd(1)-O(13)	2.530(5)	Nd(4)-O(28)	2.532(5)
Nd(1)-N(1)	2.609(6)	Nd(4)-O(18)	2.549(5)

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Nd(1)-O(3)	2.625(5)	Nd(4)-O(31)#1	2.553(5)
Nd(2)-O(21)	2.357(6)	Nd(4)-O(26)	2.563(7)
Nd(2)-O(13)	2.396(6)	Nd(4)-O(32)#1	2.580(6)
Nd(2)-O(1)	2.449(5)	Nd(4)-O(27)	2.610(5)
Nd(2)-O(28)	2.459(5)	Nd(4)-O(30)	2.945(5)
Nd(2)-O(19)	2.467(6)	Nd(4)-Nd(5)#1	3.8297(5)
Nd(2)-O(18)	2.551(6)	Nd(5)-O(31)	2.421(5)
Nd(2)-O(17)	2.554(5)	Nd(5)-O(25)	2.432(5)
Nd(2)-O(20)	2.583(6)	Nd(5)-O(6)	2.436(5)
Nd(2)-O(2)	2.679(5)	Nd(5)-O(9)	2.476(5)
Nd(2)-C(31)	2.938(8)	Nd(5)-O(30)	2.483(5)
Nd(3)-O(12)	2.407(5)	Nd(5)-O(10)#1	2.520(4)
Nd(3)-O(6)	2.412(5)	Nd(5)-O(10)	2.527(5)
Nd(3)-O(23)	2.485(5)	Nd(5)-N(2)	2.538(6)
Nd(3)-O(24)	2.490(5)	Nd(5)-O(9)#1	2.572(5)
Nd(3)-O(16)	2.499(5)	Nd(5)-Nd(5)#1	3.4714(7)
Nd(3)-O(29)	2.505(5)	Nd(5)-Nd(4)#1	3.8297(5)
Nd(3)-O(30)	2.609(5)		
O(1)-Nd(1)-O(11)	79.14(18)	O(10)-Nd(4)-O(18)	153.87(17)
O(1)-Nd(1)-O(29)	77.32(17)	O(28)-Nd(4)-O(18)	65.90(16)
O(11)-Nd(1)-O(29)	78.51(17)	O(22)-Nd(4)-O(31)#1	81.75(19)
O(1)-Nd(1)-O(15)	141.50(17)	O(9)-Nd(4)-O(31)#1	71.35(16)
O(11)-Nd(1)-O(15)	75.15(17)	O(10)-Nd(4)-O(31)#1	70.08(16)
O(29)-Nd(1)-O(15)	69.87(16)	O(28)-Nd(4)-O(31)#1	152.77(17)
O(1)-Nd(1)-O(4)	133.89(17)	O(18)-Nd(4)-O(31)#1	124.69(16)
O(11)-Nd(1)-O(4)	95.56(17)	O(22)-Nd(4)-O(26)	132.9(2)
O(29)-Nd(1)-O(4)	147.07(17)	O(9)-Nd(4)-O(26)	142.47(19)
O(15)-Nd(1)-O(4)	77.27(16)	O(10)-Nd(4)-O(26)	83.74(19)
O(1)-Nd(1)-O(14)	120.18(18)	O(28)-Nd(4)-O(26)	119.01(18)
O(11)-Nd(1)-O(14)	152.75(18)	O(18)-Nd(4)-O(26)	76.0(2)
O(29)-Nd(1)-O(14)	86.93(17)	O(31)#1-Nd(4)-O(26)	88.17(19)
O(15)-Nd(1)-O(14)	78.25(18)	O(22)-Nd(4)-O(32)#1	69.9(2)
O(4)-Nd(1)-O(14)	84.21(18)	O(9)-Nd(4)-O(32)#1	114.79(19)
O(1)-Nd(1)-O(13)	68.78(18)	O(10)-Nd(4)-O(32)#1	112.96(19)
O(11)-Nd(1)-O(13)	140.75(18)	O(28)-Nd(4)-O(32)#1	135.09(19)
O(29)-Nd(1)-O(13)	73.02(16)	O(18)-Nd(4)-O(32)#1	74.81(18)
O(15)-Nd(1)-O(13)	117.76(17)	O(31)#1-Nd(4)-O(32)#1	50.29(17)
O(4)-Nd(1)-O(13)	122.87(17)	O(26)-Nd(4)-O(32)#1	68.4(2)
O(14)-Nd(1)-O(13)	51.45(18)	O(22)-Nd(4)-O(27)	144.43(18)
O(1)-Nd(1)-N(1)	68.23(19)	O(9)-Nd(4)-O(27)	123.80(16)
O(11)-Nd(1)-N(1)	74.69(18)	O(10)-Nd(4)-O(27)	79.00(16)
O(29)-Nd(1)-N(1)	139.46(19)	O(28)-Nd(4)-O(27)	74.79(16)

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O(15)-Nd(1)-N(1)	129.28(17)	O(18)-Nd(4)-O(27)	75.35(17)
O(4)-Nd(1)-N(1)	66.24(19)	O(31)#1-Nd(4)-O(27)	130.39(17)
O(14)-Nd(1)-N(1)	128.57(19)	O(26)-Nd(4)-O(27)	49.87(18)
O(13)-Nd(1)-N(1)	111.47(18)	O(32)#1-Nd(4)-O(27)	115.9(2)
O(1)-Nd(1)-O(3)	82.41(18)	O(22)-Nd(4)-O(30)	114.05(18)
O(11)-Nd(1)-O(3)	133.72(17)	O(9)-Nd(4)-O(30)	67.89(14)
O(29)-Nd(1)-O(3)	137.26(16)	O(10)-Nd(4)-O(30)	65.32(14)
O(15)-Nd(1)-O(3)	135.81(18)	O(28)-Nd(4)-O(30)	46.96(14)
O(4)-Nd(1)-O(3)	68.48(17)	O(18)-Nd(4)-O(30)	105.11(14)
O(14)-Nd(1)-O(3)	71.45(18)	O(31)#1-Nd(4)-O(30)	130.15(14)
O(13)-Nd(1)-O(3)	64.61(16)	O(26)-Nd(4)-O(30)	107.53(18)
N(1)-Nd(1)-O(3)	59.06(18)	O(32)#1-Nd(4)-O(30)	175.9(2)
O(21)-Nd(2)-O(13)	148.72(19)	O(27)-Nd(4)-O(30)	60.39(15)
O(21)-Nd(2)-O(1)	132.6(2)	O(22)-Nd(4)-Nd(5)#1	95.78(13)
O(13)-Nd(2)-O(1)	69.92(17)	O(9)-Nd(4)-Nd(5)#1	41.49(11)
O(13)-Nd(2)-O(28)	76.27(16)	O(10)-Nd(4)-Nd(5)#1	40.28(10)
O(1)-Nd(2)-O(28)	86.72(16)	O(28)-Nd(4)-Nd(5)#1	126.01(11)
O(21)-Nd(2)-O(19)	86.8(2)	O(18)-Nd(4)-Nd(5)#1	162.27(12)
O(13)-Nd(2)-O(19)	122.21(19)	O(31)#1-Nd(4)-Nd(5)#1	38.41(11)
O(1)-Nd(2)-O(19)	79.40(18)	O(26)-Nd(4)-Nd(5)#1	104.24(15)
O(28)-Nd(2)-O(19)	149.93(18)	O(32)#1-Nd(4)-Nd(5)#1	88.69(13)
O(21)-Nd(2)-O(18)	76.0(2)	O(27)-Nd(4)-Nd(5)#1	118.78(12)
O(13)-Nd(2)-O(18)	74.33(17)	O(30)-Nd(4)-Nd(5)#1	91.82(9)
O(1)-Nd(2)-O(18)	139.69(17)	O(31)-Nd(5)-O(25)	83.39(18)
O(28)-Nd(2)-O(18)	66.94(16)	O(31)-Nd(5)-O(6)	79.65(16)
O(19)-Nd(2)-O(18)	137.27(18)	O(25)-Nd(5)-O(6)	69.33(17)
O(21)-Nd(2)-O(17)	77.4(2)	O(31)-Nd(5)-O(9)	136.10(17)
O(13)-Nd(2)-O(17)	91.47(19)	O(25)-Nd(5)-O(9)	138.94(16)
O(1)-Nd(2)-O(17)	145.58(18)	O(6)-Nd(5)-O(9)	120.02(16)
O(28)-Nd(2)-O(17)	117.62(17)	O(31)-Nd(5)-O(30)	143.72(16)
O(19)-Nd(2)-O(17)	87.41(19)	O(25)-Nd(5)-O(30)	73.05(16)
O(18)-Nd(2)-O(17)	50.99(17)	O(6)-Nd(5)-O(30)	66.50(16)
O(21)-Nd(2)-O(20)	131.8(2)	O(9)-Nd(5)-O(30)	75.56(15)
O(13)-Nd(2)-O(20)	71.33(19)	O(31)-Nd(5)-O(10)#1	71.09(16)
O(1)-Nd(2)-O(20)	70.38(18)	O(25)-Nd(5)-O(10)#1	143.46(16)
O(28)-Nd(2)-O(20)	145.09(18)	O(6)-Nd(5)-O(10)#1	128.01(15)
O(19)-Nd(2)-O(20)	52.3(2)	O(9)-Nd(5)-O(10)#1	66.14(15)
O(18)-Nd(2)-O(20)	114.79(19)	O(30)-Nd(5)-O(10)#1	141.07(15)
O(17)-Nd(2)-O(20)	76.36(18)	O(31)-Nd(5)-O(10)	134.76(16)
O(21)-Nd(2)-O(2)	72.27(19)	O(25)-Nd(5)-O(10)	86.59(16)
O(13)-Nd(2)-O(2)	123.21(17)	O(6)-Nd(5)-O(10)	136.29(15)
O(1)-Nd(2)-O(2)	60.34(17)	O(9)-Nd(5)-O(10)	58.62(15)
O(28)-Nd(2)-O(2)	75.33(17)	O(30)-Nd(5)-O(10)	71.89(15)

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O(19)-Nd(2)-O(2)	74.62(19)	O(10)#1-Nd(5)-O(10)	93.09(14)
O(18)-Nd(2)-O(2)	132.86(16)	O(31)-Nd(5)-N(2)	85.88(19)
O(17)-Nd(2)-O(2)	145.32(19)	O(25)-Nd(5)-N(2)	138.54(18)
O(20)-Nd(2)-O(2)	112.34(19)	O(6)-Nd(5)-N(2)	69.37(18)
O(12)-Nd(3)-O(6)	80.32(17)	O(9)-Nd(5)-N(2)	68.73(18)
O(12)-Nd(3)-O(23)	140.34(18)	O(30)-Nd(5)-N(2)	93.75(17)
O(6)-Nd(3)-O(23)	126.21(16)	O(10)#1-Nd(5)-N(2)	66.59(17)
O(12)-Nd(3)-O(24)	133.96(19)	O(10)-Nd(5)-N(2)	127.28(17)
O(6)-Nd(3)-O(24)	93.24(18)	O(31)-Nd(5)-O(9)#1	71.38(16)
O(23)-Nd(3)-O(24)	78.8(2)	O(25)-Nd(5)-O(9)#1	90.18(16)
O(12)-Nd(3)-O(16)	78.1(2)	O(6)-Nd(5)-O(9)#1	146.31(16)
O(6)-Nd(3)-O(16)	134.20(18)	O(9)-Nd(5)-O(9)#1	93.13(14)
O(23)-Nd(3)-O(16)	95.0(2)	O(30)-Nd(5)-O(9)#1	134.17(15)
O(24)-Nd(3)-O(16)	74.40(18)	O(10)#1-Nd(5)-O(9)#1	57.48(14)
O(12)-Nd(3)-O(29)	69.48(17)	O(10)-Nd(5)-O(9)#1	64.64(14)
O(6)-Nd(3)-O(29)	94.71(17)	N(2)-Nd(5)-O(9)#1	123.70(17)
O(23)-Nd(3)-O(29)	78.54(18)	O(31)-Nd(5)-Nd(5)#1	106.10(12)
O(24)-Nd(3)-O(29)	156.33(18)	O(25)-Nd(5)-Nd(5)#1	122.69(12)
O(16)-Nd(3)-O(29)	114.32(17)	O(6)-Nd(5)-Nd(5)#1	166.73(12)
O(12)-Nd(3)-O(30)	103.74(17)	O(9)-Nd(5)-Nd(5)#1	47.72(11)
O(6)-Nd(3)-O(30)	64.86(16)	O(30)-Nd(5)-Nd(5)#1	109.79(11)
O(23)-Nd(3)-O(30)	70.69(16)	O(10)#1-Nd(5)-Nd(5)#1	46.62(10)
O(24)-Nd(3)-O(30)	114.55(16)	O(10)-Nd(5)-Nd(5)#1	46.47(10)
O(16)-Nd(3)-O(30)	160.13(17)	N(2)-Nd(5)-Nd(5)#1	98.77(13)
O(29)-Nd(3)-O(30)	50.55(15)	O(9)#1-Nd(5)-Nd(5)#1	45.40(10)
O(12)-Nd(3)-O(15)	73.21(17)	O(31)-Nd(5)-Nd(4)#1	40.92(12)
O(6)-Nd(3)-O(15)	151.38(16)	O(25)-Nd(5)-Nd(4)#1	105.39(12)
O(23)-Nd(3)-O(15)	72.73(16)	O(6)-Nd(5)-Nd(4)#1	119.50(11)
O(24)-Nd(3)-O(15)	112.90(17)	O(9)-Nd(5)-Nd(4)#1	102.62(10)
O(16)-Nd(3)-O(15)	50.19(17)	O(30)-Nd(5)-Nd(4)#1	173.17(11)
O(29)-Nd(3)-O(15)	66.10(16)	O(10)#1-Nd(5)-Nd(4)#1	38.94(10)
O(30)-Nd(3)-O(15)	110.86(15)	O(10)-Nd(5)-Nd(4)#1	101.48(10)
O(12)-Nd(3)-O(7)	65.52(18)	N(2)-Nd(5)-Nd(4)#1	91.67(13)
O(6)-Nd(3)-O(7)	59.91(16)	O(9)#1-Nd(5)-Nd(4)#1	39.02(10)
O(23)-Nd(3)-O(7)	150.48(18)	Nd(5)#1-Nd(5)-Nd(4)#1	65.175(12)
O(24)-Nd(3)-O(7)	71.86(19)	Nd(1)-O(1)-Nd(2)	111.0(2)
O(16)-Nd(3)-O(7)	74.39(18)	Nd(3)-O(6)-Nd(5)	105.70(18)
O(29)-Nd(3)-O(7)	130.98(17)	Nd(4)-O(9)-Nd(5)	106.56(17)
O(30)-Nd(3)-O(7)	124.71(15)	Nd(4)-O(9)-Nd(5)#1	99.49(16)
O(15)-Nd(3)-O(7)	115.97(16)	Nd(5)-O(9)-Nd(5)#1	86.87(14)
O(12)-Nd(3)-O(25)	144.68(17)	Nd(4)-O(10)-Nd(5)#1	100.78(16)
O(6)-Nd(3)-O(25)	64.64(16)	Nd(4)-O(10)-Nd(5)	104.81(16)
O(23)-Nd(3)-O(25)	70.84(17)	Nd(5)#1-O(10)-Nd(5)	86.91(14)

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O(24)-Nd(3)-O(25)	49.20(16)	Nd(2)-O(13)-Nd(1)	107.9(2)
O(16)-Nd(3)-O(25)	123.20(17)	Nd(1)-O(15)-Nd(3)	108.49(18)
O(29)-Nd(3)-O(25)	115.80(15)	Nd(4)-O(18)-Nd(2)	109.57(19)
O(30)-Nd(3)-O(25)	66.26(15)	Nd(5)-O(25)-Nd(3)	96.48(17)
O(15)-Nd(3)-O(25)	142.00(16)	Nd(2)-O(28)-Nd(4)	113.17(18)
O(7)-Nd(3)-O(25)	91.66(16)	Nd(1)-O(29)-Nd(3)	114.30(19)
O(22)-Nd(4)-O(9)	76.21(17)	Nd(5)-O(30)-Nd(3)	98.72(16)
O(22)-Nd(4)-O(10)	133.31(17)	C(42)-O(30)-Nd(4)	84.0(4)
O(9)-Nd(4)-O(10)	60.05(15)	Nd(5)-O(30)-Nd(4)	92.81(14)
O(22)-Nd(4)-O(28)	78.19(18)	Nd(3)-O(30)-Nd(4)	160.9(2)
O(9)-Nd(4)-O(28)	86.03(15)	Nd(5)-O(31)-Nd(4)#1	100.67(18)
O(10)-Nd(4)-O(28)	111.89(15)	O(29)-C(42)-O(30)	117.5(6)
O(22)-Nd(4)-O(18)	72.71(19)	O(29)-C(42)-O(28)	123.1(6)
O(9)-Nd(4)-O(18)	141.48(17)	O(30)-C(42)-O(28)	119.4(6)

^a Symmetry operation: #1 -x+2,-y,-z+2
