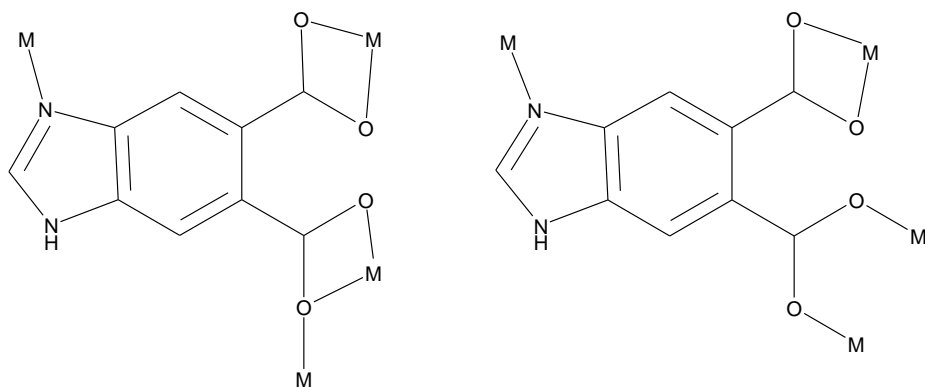


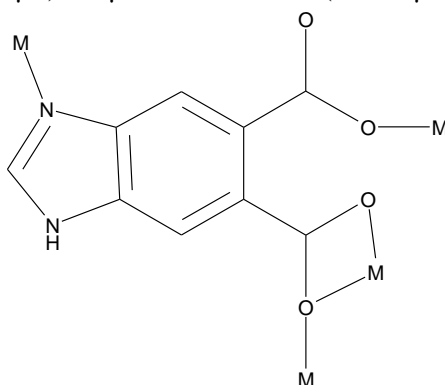
Hydrothermal synthesis, crystal structure and properties of Ni(II)-4f complexes based on 1*H*-benzimidazole-5,6- dicarboxylic acid

Ya-Guang Sun, Gang Xiong, Mei-Yan Guo, Fu Ding, Shu-Ju Wang, Philippe F. Smet,
Dirk Poelman, En-Jun Gao, Francis Verpoort



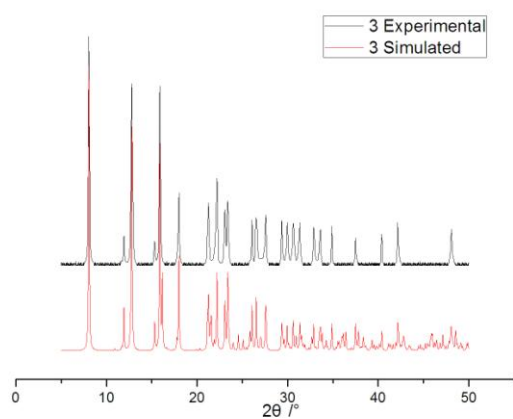
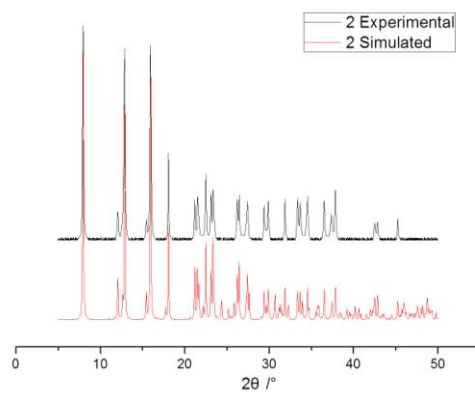
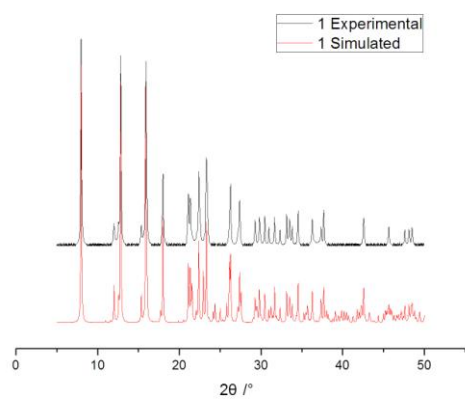
Model 1: (κ¹-κ¹-μ¹)-(κ¹-κ²-μ²)-κ¹-μ⁴

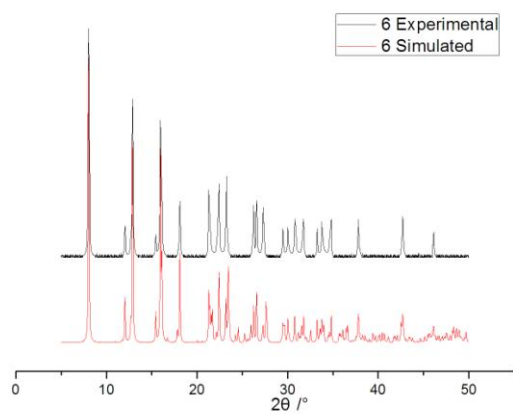
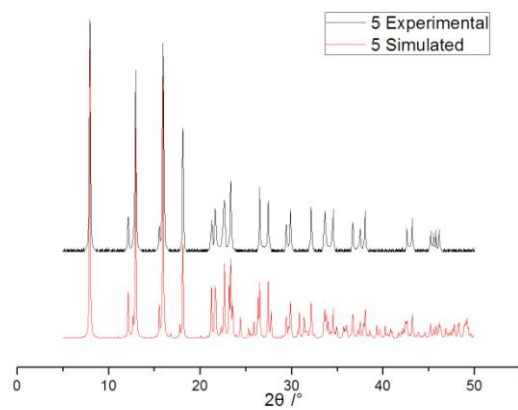
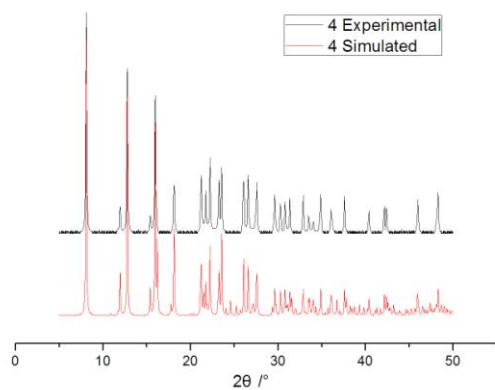
Model 2: (κ¹-κ¹-μ¹)-(κ¹-κ¹-μ²)-κ¹-μ⁴



Model 3: (κ¹-μ¹)-(κ¹-κ²-μ²)-κ¹-μ⁴

Scheme 1. Schematic representation of the observed coordination modes of Hbidc²⁻ in complex **1**, **8** and **9**.





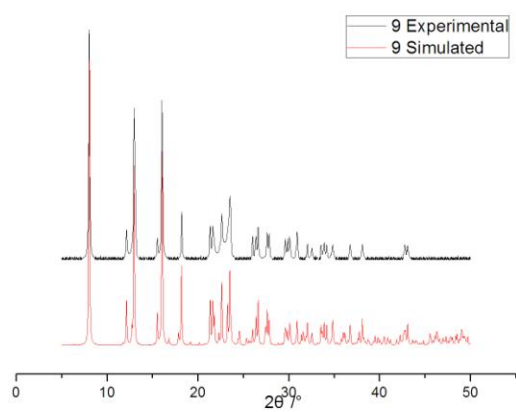
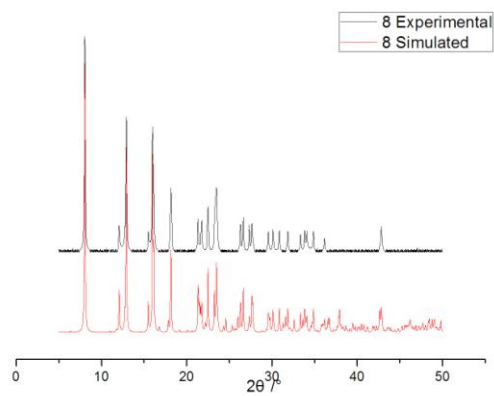
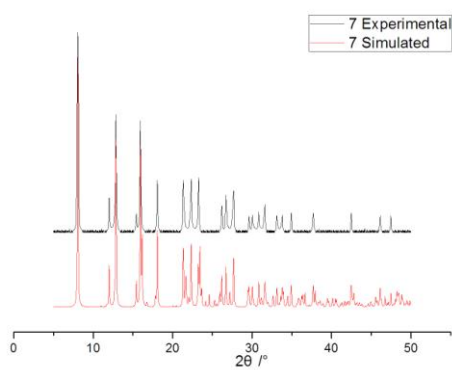


Fig. S1 The simulated and experimental PXR D patterns of **1-9**

Table S1. Selected Bond Lengths (Å) and Angle (°) for Compounds **1-9**

1			
O(5)-Pr(1)#1	2.515(7)	Pr(1)-O(3)#2	2.390(8)
O(4)-Pr(1)#1	2.665(7)	Pr(1)-O(7)#2	2.433(7)
C(9)-Pr(1)#1	2.979(11)	Pr(1)-O(13)	2.453(7)
O(7)-Pr(1)#2	2.433(7)	Pr(1)-O(5)#3	2.515(7)
N(1)-Ni(2)	2.083(10)	Pr(1)-O(4)#3	2.665(7)
O(12)-Pr(1)	2.551(8)	Pr(1)-C(9)#3	2.979(11)
O(9)-Ni(2)	2.074(14)	Pr(1)-Pr(1)#2	4.1112(14)
O(1)-Pr(1)	2.443(7)	Ni(2)-O(10)#4	2.054(9)
O(3)-Pr(1)#2	2.390(8)	Ni(2)-O(10)	2.054(9)
O(3)-Pr(1)	2.830(7)	Ni(2)-O(11)	2.059(13)
O(2)-Pr(1)	2.467(7)	Ni(2)-N(1)#4	2.083(10)
Pr(1)#2-O(3)-Pr(1)	103.6(3)	O(2)-Pr(1)-O(4)#3	125.6(2)
O(3)#2-Pr(1)-O(7)#2	81.2(2)	O(5)#3-Pr(1)-O(4)#3	49.9(2)
O(3)#2-Pr(1)-O(1)	79.3(3)	O(12)-Pr(1)-O(4)#3	103.3(2)
O(7)#2-Pr(1)-O(1)	132.2(3)	O(3)#2-Pr(1)-O(3)	76.4(3)
O(3)#2-Pr(1)-O(13)	81.1(3)	O(7)#2-Pr(1)-O(3)	65.3(2)
O(7)#2-Pr(1)-O(13)	78.0(3)	O(1)-Pr(1)-O(3)	67.9(2)
O(1)-Pr(1)-O(13)	139.7(3)	O(13)-Pr(1)-O(3)	139.2(2)
O(3)#2-Pr(1)-O(2)	124.9(3)	O(2)-Pr(1)-O(3)	48.8(2)
O(7)#2-Pr(1)-O(2)	80.9(3)	O(5)#3-Pr(1)-O(3)	121.2(2)
O(1)-Pr(1)-O(2)	75.7(3)	O(12)-Pr(1)-O(3)	109.9(2)
O(13)-Pr(1)-O(2)	143.1(3)	O(4)#3-Pr(1)-O(3)	137.6(2)
O(3)#2-Pr(1)-O(5)#3	136.0(2)	O(10)#4-Ni(2)-O(10)	174.7(5)
O(7)#2-Pr(1)-O(5)#3	142.3(3)	O(10)#4-Ni(2)-O(11)	87.3(3)
O(1)-Pr(1)-O(5)#3	73.0(3)	O(10)-Ni(2)-O(11)	87.3(3)
O(13)-Pr(1)-O(5)#3	98.6(3)	O(10)#4-Ni(2)-O(9)	92.7(3)
O(2)-Pr(1)-O(5)#3	80.4(3)	O(10)-Ni(2)-O(9)	92.7(3)
O(3)#2-Pr(1)-O(12)	148.6(2)	O(11)-Ni(2)-O(9)	180.000(10)
O(7)#2-Pr(1)-O(12)	74.6(2)	O(10)#4-Ni(2)-N(1)#4	93.0(3)
O(1)-Pr(1)-O(12)	132.0(3)	O(10)-Ni(2)-N(1)#4	86.9(3)
O(13)-Pr(1)-O(12)	74.7(3)	O(11)-Ni(2)-N(1)#4	89.2(3)
O(2)-Pr(1)-O(12)	70.7(3)	O(9)-Ni(2)-N(1)#4	90.8(3)
O(5)#3-Pr(1)-O(12)	68.4(2)	O(10)#4-Ni(2)-N(1)	86.9(3)
O(3)#2-Pr(1)-O(4)#3	88.9(2)	O(10)-Ni(2)-N(1)	93.0(3)
O(7)#2-Pr(1)-O(4)#3	151.8(3)	O(11)-Ni(2)-N(1)	89.2(3)
O(1)-Pr(1)-O(4)#3	70.3(3)	O(9)-Ni(2)-N(1)	90.8(3)
O(13)-Pr(1)-O(4)#3	74.4(2)	N(1)#4-Ni(2)-N(1)	178.5(6)
2			
O(7)-Sm(1)#1	2.394(5)	Sm(1)-O(13)	2.510(5)
O(12)-Sm(1)	2.397(5)	Sm(1)-O(1)#3	2.636(6)
O(9)-Ni(2)	2.059(6)	Sm(1)-O(4)	2.839(5)

O(1)-Sm(1)#2	2.636(6)	Sm(1)-Sm(1)#1	4.0760(12)
O(2)-Sm(1)#2	2.472(5)	Ni(2)-O(11)	2.058(8)
Sm(1)-O(4)#1	2.336(5)	Ni(2)-O(9)#4	2.059(6)
Sm(1)-O(5)	2.387(5)	Ni(2)-N(1)#4	2.070(7)
Sm(1)-O(7)#1	2.394(5)	Ni(2)-N(1)	2.070(7)
Sm(1)-O(3)	2.417(5)	Ni(2)-O(10)	2.080(9)
Sm(1)-O(2)#3	2.472(5)	O(4)-Sm(1)#1	2.336(5)
S(1)-O(7)-Sm(1)#1	141.2(3)	O(13)-Sm(1)-O(1)#3	103.96(18)
O(4)#1-Sm(1)-O(5)	81.40(17)	O(4)#1-Sm(1)-O(4)	76.50(17)
O(4)#1-Sm(1)-O(7)#1	79.80(18)	O(5)-Sm(1)-O(4)	65.01(16)
O(5)-Sm(1)-O(7)#1	131.73(18)	O(7)#1-Sm(1)-O(4)	67.49(17)
O(4)#1-Sm(1)-O(12)	80.73(18)	O(12)-Sm(1)-O(4)	139.33(19)
O(5)-Sm(1)-O(12)	78.67(19)	O(3)-Sm(1)-O(4)	48.96(16)
O(7)#1-Sm(1)-O(12)	139.96(19)	O(2)#3-Sm(1)-O(4)	121.57(15)
O(4)#1-Sm(1)-O(3)	125.22(17)	O(13)-Sm(1)-O(4)	110.67(17)
O(5)-Sm(1)-O(3)	80.06(17)	O(1)#3-Sm(1)-O(4)	137.10(15)
O(7)#1-Sm(1)-O(3)	75.52(19)	O(11)-Ni(2)-O(9)	87.27(16)
O(12)-Sm(1)-O(3)	143.04(18)	O(11)-Ni(2)-O(9)#4	87.27(16)
O(4)#1-Sm(1)-O(2)#3	135.86(18)	O(9)-Ni(2)-O(9)#4	174.5(3)
O(5)-Sm(1)-O(2)#3	142.12(17)	O(11)-Ni(2)-N(1)#4	89.39(18)
O(7)#1-Sm(1)-O(2)#3	73.20(18)	O(9)-Ni(2)-N(1)#4	87.1(2)
O(12)-Sm(1)-O(2)#3	98.18(19)	O(9)#4-Ni(2)-N(1)#4	92.9(2)
O(3)-Sm(1)-O(2)#3	80.86(17)	O(11)-Ni(2)-N(1)	89.39(18)
O(4)#1-Sm(1)-O(13)	147.59(18)	O(9)-Ni(2)-N(1)	92.9(2)
O(5)-Sm(1)-O(13)	74.17(18)	O(9)#4-Ni(2)-N(1)	87.1(2)
O(7)#1-Sm(1)-O(13)	132.54(19)	N(1)#4-Ni(2)-N(1)	178.8(4)
O(12)-Sm(1)-O(13)	73.91(19)	O(11)-Ni(2)-O(10)	180.000(1)
O(3)-Sm(1)-O(13)	71.37(18)	O(9)-Ni(2)-O(10)	92.73(16)
O(2)#3-Sm(1)-O(13)	68.81(18)	O(9)#4-Ni(2)-O(10)	92.73(16)
O(4)#1-Sm(1)-O(1)#3	87.73(17)	N(1)#4-Ni(2)-O(10)	90.61(18)
O(5)-Sm(1)-O(1)#3	151.89(17)	N(1)-Ni(2)-O(10)	90.61(18)
O(7)#1-Sm(1)-O(1)#3	70.58(17)	S(1)-O(5)-Sm(1)	137.8(3)
O(12)-Sm(1)-O(1)#3	74.02(19)	Sm(1)#1-O(4)-Sm(1)	103.50(17)
O(3)-Sm(1)-O(1)#3	126.65(17)	O(2)#3-Sm(1)-O(1)#3	50.71(16)
3			
Eu(1)-O(1)	2.304(2)	Eu(2)-O(24)	2.430(2)
Eu(1)-O(13)	2.382(2)	Eu(2)-O(23)	2.456(2)
Eu(1)-O(8)	2.426(2)	Eu(2)-O(4)#1	2.457(2)
Eu(1)-O(22)	2.426(2)	Eu(2)-O(3)#1	2.498(2)
Eu(1)-O(9)	2.429(2)	Eu(2)-O(1)	2.857(2)
Eu(1)-O(5)	2.453(2)	Ni(3)-O(19)	2.022(3)
Eu(1)-O(21)	2.478(2)	Ni(3)-O(17)	2.061(3)
Eu(1)-O(6)	2.641(2)	Ni(3)-O(18)	2.070(3)

Eu(1)-O(7)	2.661(3)	Ni(3)-N(3)#2	2.072(3)
Eu(2)-O(14)	2.358(2)	Ni(3)-N(1)	2.074(3)
Eu(2)-O(6)	2.371(3)	Ni(3)-O(20)	2.096(3)
Eu(2)-O(2)	2.391(2)	O(3)-Eu(2)#3	2.498(2)
Eu(2)-O(10)	2.401(2)	O(4)-Eu(2)#3	2.457(2)
O(1)-Eu(1)-O(13)	78.44(9)	O(2)-Eu(2)-O(24)	81.45(8)
O(1)-Eu(1)-O(8)	136.37(9)	O(10)-Eu(2)-O(24)	77.34(8)
O(13)-Eu(1)-O(8)	139.71(8)	O(14)-Eu(2)-O(23)	133.49(9)
O(1)-Eu(1)-O(22)	79.99(8)	O(6)-Eu(2)-O(23)	75.25(8)
O(13)-Eu(1)-O(22)	76.70(9)	O(2)-Eu(2)-O(23)	146.49(9)
O(8)-Eu(1)-O(22)	88.92(8)	O(10)-Eu(2)-O(23)	71.89(8)
O(1)-Eu(1)-O(9)	84.11(8)	O(24)-Eu(2)-O(23)	73.75(9)
O(13)-Eu(1)-O(9)	137.53(8)	O(14)-Eu(2)-O(4)#1	74.26(8)
O(8)-Eu(1)-O(9)	76.20(8)	O(6)-Eu(2)-O(4)#1	95.53(8)
O(22)-Eu(1)-O(9)	137.65(9)	O(2)-Eu(2)-O(4)#1	125.73(8)
O(1)-Eu(1)-O(5)	128.66(8)	O(10)-Eu(2)-O(4)#1	148.29(8)
O(13)-Eu(1)-O(5)	86.89(8)	O(24)-Eu(2)-O(4)#1	89.32(8)
O(8)-Eu(1)-O(5)	82.88(8)	O(23)-Eu(2)-O(4)#1	76.81(8)
O(22)-Eu(1)-O(5)	143.53(9)	O(14)-Eu(2)-O(3)#1	72.59(8)
O(9)-Eu(1)-O(5)	74.42(9)	O(6)-Eu(2)-O(3)#1	137.83(9)
O(1)-Eu(1)-O(21)	139.21(8)	O(2)-Eu(2)-O(3)#1	74.46(8)
O(13)-Eu(1)-O(21)	68.56(8)	O(10)-Eu(2)-O(3)#1	140.46(8)
O(8)-Eu(1)-O(21)	71.16(8)	O(24)-Eu(2)-O(3)#1	68.78(8)
O(22)-Eu(1)-O(21)	69.83(8)	O(23)-Eu(2)-O(3)#1	115.31(8)
O(9)-Eu(1)-O(21)	136.62(8)	O(4)#1-Eu(2)-O(3)#1	52.66(8)
O(5)-Eu(1)-O(21)	73.89(8)	O(14)-Eu(2)-O(1)	71.64(8)
O(1)-Eu(1)-O(6)	77.90(8)	O(6)-Eu(2)-O(1)	72.60(8)
O(13)-Eu(1)-O(6)	70.43(8)	O(2)-Eu(2)-O(1)	48.76(8)
O(8)-Eu(1)-O(6)	126.96(7)	O(10)-Eu(2)-O(1)	63.28(7)
O(22)-Eu(1)-O(6)	143.30(8)	O(24)-Eu(2)-O(1)	118.45(8)
O(9)-Eu(1)-O(6)	68.17(8)	O(23)-Eu(2)-O(1)	127.53(8)
O(5)-Eu(1)-O(6)	50.92(8)	O(4)#1-Eu(2)-O(1)	145.86(8)
O(21)-Eu(1)-O(6)	111.05(8)	O(3)#1-Eu(2)-O(1)	116.46(7)
O(1)-Eu(1)-O(7)	85.46(8)	C(23)#1-Eu(2)-O(1)	135.10(8)
O(13)-Eu(1)-O(7)	146.25(8)	O(19)-Ni(3)-O(17)	173.72(11)
O(8)-Eu(1)-O(7)	51.17(8)	O(19)-Ni(3)-O(18)	85.88(10)
O(22)-Eu(1)-O(7)	71.36(8)	O(17)-Ni(3)-O(18)	87.84(10)
O(9)-Eu(1)-O(7)	68.44(8)	O(19)-Ni(3)-N(3)#2	87.42(11)
O(5)-Eu(1)-O(7)	125.74(8)	O(17)-Ni(3)-N(3)#2	92.48(11)
O(21)-Eu(1)-O(7)	109.00(8)	O(18)-Ni(3)-N(3)#2	86.51(10)
O(6)-Eu(1)-O(7)	134.72(8)	O(19)-Ni(3)-N(1)	92.02(11)
O(14)-Eu(2)-O(6)	72.23(8)	O(17)-Ni(3)-N(1)	87.93(11)
O(14)-Eu(2)-O(2)	79.68(9)	O(18)-Ni(3)-N(1)	92.04(10)

O(6)-Eu(2)-O(2)	120.45(8)	N(3)#2-Ni(3)-N(1)	178.47(13)
O(14)-Eu(2)-O(10)	132.81(8)	O(19)-Ni(3)-O(20)	96.71(10)
O(6)-Eu(2)-O(10)	81.48(9)	O(17)-Ni(3)-O(20)	89.57(10)
O(2)-Eu(2)-O(10)	81.05(8)	O(18)-Ni(3)-O(20)	175.44(9)
O(14)-Eu(2)-O(24)	140.27(8)	N(3)#2-Ni(3)-O(20)	89.85(10)
O(6)-Eu(2)-O(24)	146.59(8)	N(1)-Ni(3)-O(20)	91.62(10)
4			
O(13)-Gd(1)	2.403(4)	Gd(1)-O(2)	2.548(3)
O(4)-Gd(1)#1	2.400(3)	Gd(1)-O(3)#5	2.765(3)
O(3)-Gd(1)#2	2.316(3)	N(1)-Ni(1)	2.066(3)
O(3)-Gd(1)#1	2.765(3)	O(7)-Gd(1)#4	2.361(3)
Gd(1)-O(3)#3	2.316(3)	Ni(1)-O(10)#6	2.044(3)
Gd(1)-O(7)#4	2.361(3)	Ni(1)-O(10)	2.044(3)
Gd(1)-O(5)	2.366(3)	Ni(1)-O(9)	2.058(4)
Gd(1)-O(4)#5	2.400(3)	Ni(1)-N(1)#6	2.066(3)
Gd(1)-O(12)	2.441(3)	Ni(1)-O(11)	2.084(5)
Gd(1)-O(1)	2.452(3)		
Gd(1)#2-O(3)-Gd(1)#1	104.90(10)	O(13)-Gd(1)-O(2)	72.28(14)
O(3)#3-Gd(1)-O(7)#4	78.26(13)	O(12)-Gd(1)-O(2)	99.59(11)
O(3)#3-Gd(1)-O(5)	80.42(10)	O(1)-Gd(1)-O(2)	51.14(10)
O(7)#4-Gd(1)-O(5)	134.49(13)	O(3)#3-Gd(1)-O(3)#5	75.10(10)
O(3)#3-Gd(1)-O(4)#5	124.59(11)	O(7)#4-Gd(1)-O(3)#5	69.26(11)
O(7)#4-Gd(1)-O(4)#5	76.95(15)	O(5)-Gd(1)-O(3)#5	66.58(12)
O(5)-Gd(1)-O(4)#5	83.04(12)	O(4)#5-Gd(1)-O(3)#5	49.86(10)
O(3)#3-Gd(1)-O(13)	79.00(16)	O(13)-Gd(1)-O(3)#5	137.43(16)
O(7)#4-Gd(1)-O(13)	136.53(14)	O(12)-Gd(1)-O(3)#5	114.75(10)
O(5)-Gd(1)-O(13)	76.28(16)	O(1)-Gd(1)-O(3)#5	121.57(11)
O(4)#5-Gd(1)-O(13)	145.50(14)	O(2)-Gd(1)-O(3)#5	139.67(11)
O(3)#3-Gd(1)-O(12)	143.75(11)	O(10)#6-Ni(1)-O(10)	174.00(18)
O(7)#4-Gd(1)-O(12)	137.92(12)	O(10)#6-Ni(1)-O(9)	87.00(9)
O(5)-Gd(1)-O(12)	73.24(11)	O(10)-Ni(1)-O(9)	87.00(9)
O(4)#5-Gd(1)-O(12)	76.82(12)	O(10)#6-Ni(1)-N(1)	92.42(12)
O(13)-Gd(1)-O(12)	70.96(14)	O(10)-Ni(1)-N(1)	87.51(12)
O(3)#3-Gd(1)-O(1)	137.49(10)	O(9)-Ni(1)-N(1)	89.31(9)
O(7)#4-Gd(1)-O(1)	73.69(12)	O(10)#6-Ni(1)-N(1)#6	87.51(12)
O(5)-Gd(1)-O(1)	141.34(11)	O(10)-Ni(1)-N(1)#6	92.42(12)
O(4)#5-Gd(1)-O(1)	79.08(11)	O(9)-Ni(1)-N(1)#6	89.31(9)
O(13)-Gd(1)-O(1)	100.32(17)	N(1)-Ni(1)-N(1)#6	178.63(19)
O(12)-Gd(1)-O(1)	69.45(11)	O(10)#6-Ni(1)-O(11)	93.00(9)
O(3)#3-Gd(1)-O(2)	89.86(10)	O(10)-Ni(1)-O(11)	93.00(9)
O(7)#4-Gd(1)-O(2)	71.13(12)	O(9)-Ni(1)-O(11)	180.000(1)
O(5)-Gd(1)-O(2)	148.33(14)	N(1)-Ni(1)-O(11)	90.69(9)
O(4)#5-Gd(1)-O(2)	126.19(10)	N(1)#6-Ni(1)-O(11)	90.69(9)

5			
O(3)-Tb(1)#1	2.290(8)	Tb(1)-O(12)	2.473(8)
O(3)-Tb(1)#2	2.885(8)	Tb(1)-O(2)	2.628(9)
O(4)-Tb(1)#2	2.372(8)	Tb(1)-O(3)#5	2.885(8)
Tb(1)-O(3)#3	2.290(8)	Ni(2)-O(10)	2.060(15)
Tb(1)-O(13)	2.344(8)	Ni(2)-O(9)#6	2.060(10)
Tb(1)-O(5)	2.346(8)	Ni(2)-O(9)	2.060(10)
Tb(1)-O(7)#4	2.355(8)	Ni(2)-N(1)	2.068(11)
Tb(1)-O(4)#5	2.372(8)	Ni(2)-N(1)#6	2.068(11)
Tb(1)-O(1)	2.428(9)	Ni(2)-O(11)	2.073(15)
O(7)-Tb(1)#4	2.355(8)		
Tb(1)#1-O(3)-Tb(1)#2	103.4(3)	O(4)#5-Tb(1)-O(2)	127.5(3)
O(3)#3-Tb(1)-O(13)	81.0(3)	O(1)-Tb(1)-O(2)	51.0(3)
O(3)#3-Tb(1)-O(5)	81.3(3)	O(12)-Tb(1)-O(2)	104.7(3)
O(13)-Tb(1)-O(5)	79.8(3)	O(3)#3-Tb(1)-O(3)#5	76.6(3)
O(3)#3-Tb(1)-O(7)#4	80.5(3)	O(13)-Tb(1)-O(3)#5	140.0(3)
O(13)-Tb(1)-O(7)#4	140.6(3)	O(5)-Tb(1)-O(3)#5	64.5(3)
O(5)-Tb(1)-O(7)#4	130.7(3)	O(7)#4-Tb(1)-O(3)#5	66.8(3)
O(3)#3-Tb(1)-O(4)#5	125.0(3)	O(4)#5-Tb(1)-O(3)#5	48.6(3)
O(13)-Tb(1)-O(4)#5	142.8(3)	O(1)-Tb(1)-O(3)#5	121.8(3)
O(5)-Tb(1)-O(4)#5	78.9(3)	O(12)-Tb(1)-O(3)#5	111.0(3)
O(7)#4-Tb(1)-O(4)#5	75.0(3)	O(2)-Tb(1)-O(3)#5	136.2(3)
O(3)#3-Tb(1)-O(1)	135.7(3)	O(10)-Ni(2)-O(9)#6	87.4(3)
O(13)-Tb(1)-O(1)	97.4(3)	O(10)-Ni(2)-O(9)	87.4(3)
O(5)-Tb(1)-O(1)	142.5(3)	O(9)#6-Ni(2)-O(9)	174.8(6)
O(7)#4-Tb(1)-O(1)	73.1(3)	O(10)-Ni(2)-N(1)	89.6(3)
O(4)#5-Tb(1)-O(1)	81.8(3)	O(9)#6-Ni(2)-N(1)	93.3(4)
O(3)#3-Tb(1)-O(12)	147.5(3)	O(9)-Ni(2)-N(1)	86.7(4)
O(13)-Tb(1)-O(12)	73.6(3)	O(10)-Ni(2)-N(1)#6	89.6(3)
O(5)-Tb(1)-O(12)	74.6(3)	O(9)#6-Ni(2)-N(1)#6	86.7(4)
O(7)#4-Tb(1)-O(12)	131.9(3)	O(9)-Ni(2)-N(1)#6	93.3(4)
O(4)#5-Tb(1)-O(12)	71.5(3)	N(1)-Ni(2)-N(1)#6	179.1(6)
O(1)-Tb(1)-O(12)	68.8(3)	O(10)-Ni(2)-O(11)	180.000(1)
O(3)#3-Tb(1)-O(2)	86.9(3)	O(9)#6-Ni(2)-O(11)	92.6(3)
O(13)-Tb(1)-O(2)	74.0(3)	O(9)-Ni(2)-O(11)	92.6(3)
O(5)-Tb(1)-O(2)	152.7(3)	N(1)-Ni(2)-O(11)	90.4(3)
O(7)#4-Tb(1)-O(2)	70.5(3)	N(1)#6-Ni(2)-O(11)	90.4(3)
6			
O(7)-Dy(1)#1	2.336(8)	Dy(1)-O(7)#1	2.336(8)
O(13')-Dy(1)	2.33(2)	Dy(1)-O(3)	2.365(9)
O(13)-Dy(1)	2.42(2)	Dy(1)-O(2)#3	2.428(8)
O(12)-Dy(1)	2.426(9)	Dy(1)-O(1)#3	2.578(9)
O(11)-Ni(2)	2.067(16)	N(1)-Ni(2)	2.082(9)

O(9)-Ni(2)	2.073(17)	Ni(2)-O(10)#4	2.042(8)
O(5)-Dy(1)	2.335(9)	Ni(2)-O(10)	2.042(8)
O(4)-Dy(1)#1	2.283(9)	Ni(2)-N(1)#4	2.082(9)
O(4)-Dy(1)	2.844(10)	O(1)-Dy(1)#2	2.578(9)
Dy(1)-O(4)#1	2.283(9)	O(2)-Dy(1)#2	2.428(8)
Dy(1)#1-O(4)-Dy(1)	104.6(3)	O(5)-Dy(1)-O(1)#3	71.1(3)
O(4)#1-Dy(1)-O(13')	72.1(7)	O(7)#1-Dy(1)-O(1)#3	149.3(4)
O(4)#1-Dy(1)-O(5)	78.1(4)	O(3)-Dy(1)-O(1)#3	127.4(3)
O(13')-Dy(1)-O(5)	137.5(6)	O(13)-Dy(1)-O(1)#3	67.2(5)
O(4)#1-Dy(1)-O(7)#1	80.6(3)	O(12)-Dy(1)-O(1)#3	100.4(3)
O(13')-Dy(1)-O(7)#1	70.9(6)	O(2)#3-Dy(1)-O(1)#3	51.2(3)
O(5)-Dy(1)-O(7)#1	133.1(3)	O(4)#1-Dy(1)-O(4)	75.4(3)
O(4)#1-Dy(1)-O(3)	124.2(3)	O(13')-Dy(1)-O(4)	128.8(7)
O(13')-Dy(1)-O(3)	145.4(6)	O(5)-Dy(1)-O(4)	68.8(3)
O(5)-Dy(1)-O(3)	76.9(4)	O(7)#1-Dy(1)-O(4)	65.5(3)
O(7)#1-Dy(1)-O(3)	81.5(3)	O(3)-Dy(1)-O(4)	49.2(3)
O(4)#1-Dy(1)-O(13)	85.5(6)	O(13)-Dy(1)-O(4)	145.4(4)
O(13')-Dy(1)-O(13)	17.2(7)	O(12)-Dy(1)-O(4)	114.0(3)
O(5)-Dy(1)-O(13)	135.3(6)	O(2)#3-Dy(1)-O(4)	121.4(3)
O(7)#1-Dy(1)-O(13)	83.3(5)	O(1)#3-Dy(1)-O(4)	139.1(3)
O(3)-Dy(1)-O(13)	143.3(6)	O(10)#4-Ni(2)-O(10)	173.9(6)
O(4)#1-Dy(1)-O(12)	145.8(3)	O(10)#4-Ni(2)-O(11)	87.0(3)
O(13')-Dy(1)-O(12)	77.6(7)	O(10)-Ni(2)-O(11)	87.0(3)
O(5)-Dy(1)-O(12)	136.0(3)	O(10)#4-Ni(2)-O(9)	93.0(3)
O(7)#1-Dy(1)-O(12)	74.8(3)	O(10)-Ni(2)-O(9)	93.0(3)
O(3)-Dy(1)-O(12)	75.3(4)	O(11)-Ni(2)-O(9)	180.000(9)
O(13)-Dy(1)-O(12)	68.5(6)	O(10)#4-Ni(2)-N(1)	87.0(3)
O(4)#1-Dy(1)-O(2)#3	136.4(3)	O(10)-Ni(2)-N(1)	92.9(3)
O(13')-Dy(1)-O(2)#3	109.4(7)	O(11)-Ni(2)-N(1)	89.6(3)
O(5)-Dy(1)-O(2)#3	73.2(3)	O(9)-Ni(2)-N(1)	90.4(3)
O(7)#1-Dy(1)-O(2)#3	142.5(3)	O(10)#4-Ni(2)-N(1)#4	92.9(3)
O(3)-Dy(1)-O(2)#3	80.2(3)	O(10)-Ni(2)-N(1)#4	87.0(3)
O(13)-Dy(1)-O(2)#3	92.3(5)	O(11)-Ni(2)-N(1)#4	89.6(3)
O(12)-Dy(1)-O(2)#3	68.9(3)	O(9)-Ni(2)-N(1)#4	90.4(3)
O(4)#1-Dy(1)-O(1)#3	88.7(3)	N(1)-Ni(2)-N(1)#4	179.2(6)
O(13')-Dy(1)-O(1)#3	78.4(6)		
7			
Ho(1)-O(4)#1	2.263(4)	Ni(1)-O(13)	2.044(8)
Ho(1)-O(5)	2.319(5)	Ni(1)-O(12)	2.048(6)
Ho(1)-O(6)#2	2.328(5)	Ni(1)-O(12)#4	2.048(6)
Ho(1)-O(3)#3	2.350(5)	Ni(1)-N(2)	2.066(6)
Ho(1)-O(9)	2.368(6)	Ni(1)-N(2)#4	2.066(6)
Ho(1)-O(10)	2.428(5)	Ni(1)-O(11)	2.088(8)

Ho(1)-O(1)	2.431(5)	O(3)-Ho(1)#5	2.350(5)
Ho(1)-O(2)	2.537(6)	O(4)-Ho(1)#6	2.263(4)
Ho(1)-O(4)#3	2.854(5)	O(4)-Ho(1)#5	2.854(5)
O(4)#1-Ho(1)-O(5)	78.29(18)	O(10)-Ho(1)-O(2)	99.6(2)
O(4)#1-Ho(1)-O(6)#2	80.90(17)	O(1)-Ho(1)-O(2)	51.96(17)
O(5)-Ho(1)-O(6)#2	133.08(18)	O(4)#1-Ho(1)-O(4)#3	75.35(17)
O(4)#1-Ho(1)-O(3)#3	123.98(18)	O(5)-Ho(1)-O(4)#3	68.71(17)
O(5)-Ho(1)-O(3)#3	77.1(2)	O(6)#2-Ho(1)-O(4)#3	65.50(16)
O(6)#2-Ho(1)-O(3)#3	80.72(18)	O(3)#3-Ho(1)-O(4)#3	48.89(15)
O(4)#1-Ho(1)-O(9)	78.7(2)	O(9)-Ho(1)-O(4)#3	136.9(2)
O(5)-Ho(1)-O(9)	137.5(2)	O(10)-Ho(1)-O(4)#3	114.73(17)
O(6)#2-Ho(1)-O(9)	76.9(2)	O(1)-Ho(1)-O(4)#3	120.74(16)
O(3)#3-Ho(1)-O(9)	144.8(2)	O(2)-Ho(1)-O(4)#3	139.18(18)
O(4)#1-Ho(1)-O(10)	145.38(18)	O(13)-Ni(1)-O(12)	87.43(16)
O(5)-Ho(1)-O(10)	136.26(18)	O(13)-Ni(1)-O(12)#4	87.43(16)
O(6)#2-Ho(1)-O(10)	74.78(18)	O(12)-Ni(1)-O(12)#4	174.9(3)
O(3)#3-Ho(1)-O(10)	76.11(19)	O(13)-Ni(1)-N(2)	89.63(18)
O(9)-Ho(1)-O(10)	72.1(2)	O(12)-Ni(1)-N(2)	92.3(2)
O(4)#1-Ho(1)-O(1)	137.19(18)	O(12)#4-Ni(1)-N(2)	87.6(2)
O(5)-Ho(1)-O(1)	73.23(17)	O(13)-Ni(1)-N(2)#4	89.63(18)
O(6)#2-Ho(1)-O(1)	141.50(18)	O(12)-Ni(1)-N(2)#4	87.6(2)
O(3)#3-Ho(1)-O(1)	79.76(18)	O(12)#4-Ni(1)-N(2)#4	92.3(2)
O(9)-Ho(1)-O(1)	101.7(2)	N(2)-Ni(1)-N(2)#4	179.3(4)
O(10)-Ho(1)-O(1)	68.47(19)	O(13)-Ni(1)-O(11)	180.000(3)
O(4)#1-Ho(1)-O(2)	89.00(18)	O(12)-Ni(1)-O(11)	92.57(16)
O(5)-Ho(1)-O(2)	71.3(2)	O(12)#4-Ni(1)-O(11)	92.57(16)
O(6)#2-Ho(1)-O(2)	149.58(19)	N(2)-Ni(1)-O(11)	90.37(18)
O(3)#3-Ho(1)-O(2)	127.72(18)	N(2)#4-Ni(1)-O(11)	90.37(19)
O(9)-Ho(1)-O(2)	73.0(2)		
8			
Er(1)-O(15)	2.290(3)	Er(2)-O(11)	2.346(3)
Er(1)-O(10)	2.294(3)	Er(2)-O(12)#1	2.370(3)
Er(1)-O(2)	2.311(3)	Er(2)-O(9)	2.426(3)
Er(1)-O(19)	2.338(3)	Er(2)-O(10)	2.687(3)
Er(1)-O(6)	2.357(3)	Er(2)-O(13)#1	2.793(3)
Er(1)-O(7)	2.367(3)	Ni(1)-O(25)	2.012(3)
Er(1)-O(4)	2.394(3)	Ni(1)-O(24)	2.071(4)
Er(1)-O(5)	2.454(3)	Ni(1)-N(4)#2	2.072(4)
Er(2)-O(3)	2.232(3)	Ni(1)-N(1)	2.077(4)
Er(2)-O(14)	2.303(3)	Ni(1)-O(23)	2.086(3)
Er(2)-O(18)	2.345(3)	Ni(1)-O(22)	2.097(4)
Er(2)-O(8)	2.345(3)		
O(15)-Er(1)-O(10)	72.48(12)	O(8)-Er(2)-O(12)#1	87.36(12)

O(15)-Er(1)-O(2)	79.60(12)	O(11)-Er(2)-O(12)#1	85.44(12)
O(10)-Er(1)-O(2)	116.88(12)	O(3)-Er(2)-O(9)	144.51(12)
O(15)-Er(1)-O(19)	130.77(12)	O(14)-Er(2)-O(9)	74.46(12)
O(10)-Er(1)-O(19)	80.04(12)	O(18)-Er(2)-O(9)	132.17(12)
O(2)-Er(1)-O(19)	77.57(12)	O(8)-Er(2)-O(9)	72.09(12)
O(15)-Er(1)-O(6)	140.77(12)	O(11)-Er(2)-O(9)	70.76(12)
O(10)-Er(1)-O(6)	146.34(11)	O(12)#1-Er(2)-O(9)	70.09(11)
O(2)-Er(1)-O(6)	82.30(12)	O(3)-Er(2)-O(10)	79.80(12)
O(19)-Er(1)-O(6)	77.56(12)	O(14)-Er(2)-O(10)	69.21(10)
O(15)-Er(1)-O(7)	133.63(13)	O(18)-Er(2)-O(10)	67.71(11)
O(10)-Er(1)-O(7)	75.69(12)	O(8)-Er(2)-O(10)	145.42(11)
O(2)-Er(1)-O(7)	145.95(12)	O(11)-Er(2)-O(10)	51.20(11)
O(19)-Er(1)-O(7)	73.68(12)	O(12)#1-Er(2)-O(10)	126.94(11)
O(6)-Er(1)-O(7)	74.09(13)	O(9)-Er(2)-O(10)	112.21(11)
O(15)-Er(1)-O(4)	74.77(12)	O(3)-Er(2)-O(13)#1	81.37(11)
O(10)-Er(1)-O(4)	97.11(12)	O(14)-Er(2)-O(13)#1	146.51(11)
O(2)-Er(1)-O(4)	128.24(12)	O(18)-Er(2)-O(13)#1	68.10(11)
O(19)-Er(1)-O(4)	150.04(11)	O(8)-Er(2)-O(13)#1	69.74(11)
O(6)-Er(1)-O(4)	90.10(12)	O(11)-Er(2)-O(13)#1	127.97(11)
O(7)-Er(1)-O(4)	76.72(12)	O(12)#1-Er(2)-O(13)#1	49.56(11)
O(15)-Er(1)-O(5)	72.64(12)	O(9)-Er(2)-O(13)#1	107.76(11)
O(10)-Er(1)-O(5)	139.32(11)	O(10)-Er(2)-O(13)#1	133.49(10)
O(2)-Er(1)-O(5)	76.15(12)	O(25)-Ni(1)-O(24)	85.69(13)
O(19)-Er(1)-O(5)	139.89(11)	O(25)-Ni(1)-N(4)#2	92.78(14)
O(6)-Er(1)-O(5)	69.35(11)	O(24)-Ni(1)-N(4)#2	92.46(15)
O(7)-Er(1)-O(5)	116.20(12)	O(25)-Ni(1)-N(1)	86.75(15)
O(4)-Er(1)-O(5)	53.59(11)	O(24)-Ni(1)-N(1)	87.03(15)
O(3)-Er(2)-O(14)	79.72(12)	N(4)#2-Ni(1)-N(1)	179.33(17)
O(3)-Er(2)-O(18)	83.27(12)	O(25)-Ni(1)-O(23)	173.39(15)
O(14)-Er(2)-O(18)	135.75(11)	O(24)-Ni(1)-O(23)	87.70(13)
O(3)-Er(2)-O(8)	79.80(12)	N(4)#2-Ni(1)-O(23)	87.16(14)
O(14)-Er(2)-O(8)	79.86(12)	N(1)-Ni(1)-O(23)	93.26(14)
O(18)-Er(2)-O(8)	136.35(11)	O(25)-Ni(1)-O(22)	95.86(13)
O(3)-Er(2)-O(11)	130.90(12)	O(24)-Ni(1)-O(22)	176.84(13)
O(14)-Er(2)-O(11)	84.94(12)	N(4)#2-Ni(1)-O(22)	90.22(15)
O(18)-Er(2)-O(11)	76.08(12)	N(1)-Ni(1)-O(22)	90.30(15)
O(8)-Er(2)-O(11)	142.41(12)	O(23)-Ni(1)-O(22)	90.76(13)
O(3)-Er(2)-O(12)#1	130.54(12)	Er(1)-O(10)-Er(2)	109.46(12)
O(14)-Er(2)-O(12)#1	144.49(12)	O(18)-Er(2)-O(12)#1	73.87(12)
9			
Yb(1)-O(13)	2.272(3)	Yb(2)-O(24)	2.324(3)
Yb(1)-O(5)	2.281(3)	Yb(2)-O(7)#1	2.348(3)
Yb(1)-O(3)	2.283(3)	Yb(2)-O(25)	2.400(3)

Yb(1)-O(14)	2.320(3)	Yb(2)-O(5)	2.682(3)
Yb(1)-O(22)	2.329(3)	Yb(2)-O(8)#1	2.913(3)
Yb(1)-O(23)	2.348(3)	Yb(2)-C(18)#1	3.008(4)
Yb(1)-O(1)	2.363(3)	Ni(3)-O(20)	2.018(3)
Yb(1)-O(2)	2.439(3)	Ni(3)-N(3)#2	2.065(3)
Yb(2)-O(4)	2.207(3)	Ni(3)-O(19)	2.072(4)
Yb(2)-O(12)	2.274(3)	Ni(3)-N(1)	2.073(3)
Yb(2)-O(6)	2.318(3)	Ni(3)-O(21)	2.094(4)
Yb(2)-O(15)	2.321(3)	Ni(3)-O(18)	2.114(3)
O(13)-Yb(1)-O(5)	72.17(10)	O(6)-Yb(2)-O(7)#1	87.89(10)
O(13)-Yb(1)-O(3)	79.37(11)	O(15)-Yb(2)-O(7)#1	72.88(10)
O(5)-Yb(1)-O(3)	114.26(10)	O(24)-Yb(2)-O(7)#1	84.85(10)
O(13)-Yb(1)-O(14)	130.07(11)	O(4)-Yb(2)-O(25)	145.19(11)
O(5)-Yb(1)-O(14)	79.32(10)	O(12)-Yb(2)-O(25)	76.39(10)
O(3)-Yb(1)-O(14)	76.19(11)	O(6)-Yb(2)-O(25)	70.25(11)
O(13)-Yb(1)-O(22)	141.34(10)	O(15)-Yb(2)-O(25)	131.16(10)
O(5)-Yb(1)-O(22)	146.16(10)	O(24)-Yb(2)-O(25)	71.91(11)
O(3)-Yb(1)-O(22)	83.93(11)	O(7)#1-Yb(2)-O(25)	71.15(10)
O(14)-Yb(1)-O(22)	77.84(10)	O(4)-Yb(2)-O(5)	81.23(10)
O(13)-Yb(1)-O(23)	133.21(11)	O(12)-Yb(2)-O(5)	69.39(10)
O(5)-Yb(1)-O(23)	75.38(10)	O(6)-Yb(2)-O(5)	51.33(9)
O(3)-Yb(1)-O(23)	145.84(11)	O(15)-Yb(2)-O(5)	67.44(10)
O(14)-Yb(1)-O(23)	73.64(10)	O(24)-Yb(2)-O(5)	147.24(10)
O(22)-Yb(1)-O(23)	74.43(11)	O(7)#1-Yb(2)-O(5)	127.82(10)
O(13)-Yb(1)-O(1)	75.64(11)	O(25)-Yb(2)-O(5)	112.85(10)
O(5)-Yb(1)-O(1)	98.78(10)	O(4)-Yb(2)-O(8)#1	78.59(9)
O(3)-Yb(1)-O(1)	129.46(10)	O(12)-Yb(2)-O(8)#1	145.58(10)
O(14)-Yb(1)-O(1)	150.16(10)	O(6)-Yb(2)-O(8)#1	129.01(9)
O(22)-Yb(1)-O(1)	89.06(10)	O(15)-Yb(2)-O(8)#1	67.57(10)
O(23)-Yb(1)-O(1)	77.06(10)	O(24)-Yb(2)-O(8)#1	68.85(10)
O(13)-Yb(1)-O(2)	72.47(10)	O(7)#1-Yb(2)-O(8)#1	48.15(9)
O(5)-Yb(1)-O(2)	139.90(10)	O(25)-Yb(2)-O(8)#1	108.30(9)
O(3)-Yb(1)-O(2)	76.70(10)	O(5)-Yb(2)-O(8)#1	132.25(9)
O(14)-Yb(1)-O(2)	139.48(9)	O(20)-Ni(3)-N(3)#2	92.85(12)
O(22)-Yb(1)-O(2)	69.84(10)	O(20)-Ni(3)-O(19)	85.62(12)
O(23)-Yb(1)-O(2)	118.18(10)	N(3)#2-Ni(3)-O(19)	92.69(13)
O(1)-Yb(1)-O(2)	54.14(9)	O(20)-Ni(3)-N(1)	87.14(12)
O(4)-Yb(2)-O(12)	79.80(10)	N(3)#2-Ni(3)-N(1)	179.82(19)
O(4)-Yb(2)-O(6)	132.48(11)	O(19)-Ni(3)-N(1)	87.48(13)
O(12)-Yb(2)-O(6)	85.14(11)	O(20)-Ni(3)-O(21)	95.76(12)
O(4)-Yb(2)-O(15)	83.42(11)	N(3)#2-Ni(3)-O(21)	90.22(13)
O(12)-Yb(2)-O(15)	135.47(10)	O(19)-Ni(3)-O(21)	176.71(10)
O(6)-Yb(2)-O(15)	76.53(11)	N(1)-Ni(3)-O(21)	89.61(13)

O(4)-Yb(2)-O(24)	79.69(11)	O(20)-Ni(3)-O(18)	173.18(15)
O(12)-Yb(2)-O(24)	81.16(11)	N(3)#2-Ni(3)-O(18)	86.80(12)
O(6)-Yb(2)-O(24)	141.80(10)	O(19)-Ni(3)-O(18)	87.59(12)
O(15)-Yb(2)-O(24)	135.50(11)	N(1)-Ni(3)-O(18)	93.23(12)
O(4)-Yb(2)-O(7)#1	126.48(10)	O(21)-Ni(3)-O(18)	91.05(12)
O(12)-Yb(2)-O(7)#1	147.26(10)		