

Supplementary Information

Synthesis, DNA binding profile and DNA cleavage pathway of divalent metal complexes

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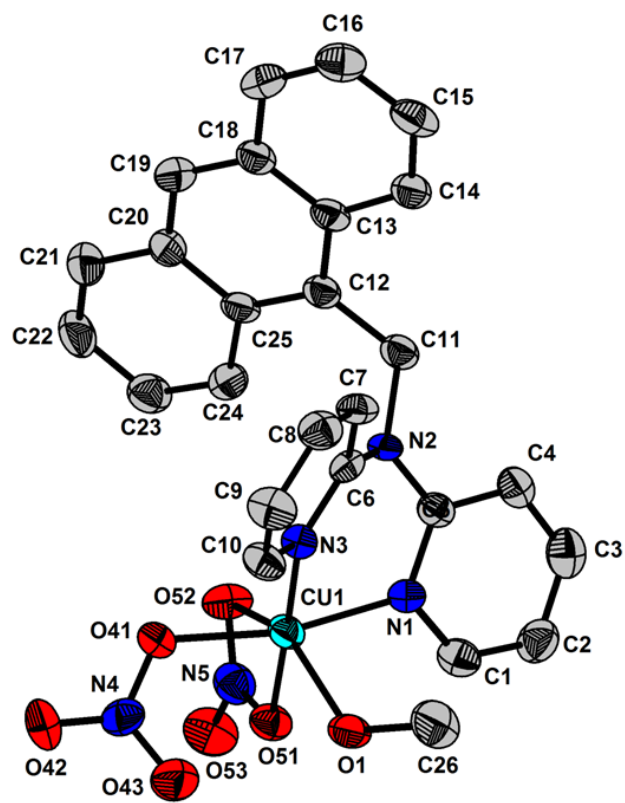


Fig. S1. Crystal structure of complex **2**. All hydrogen atoms were omitted for clarity.

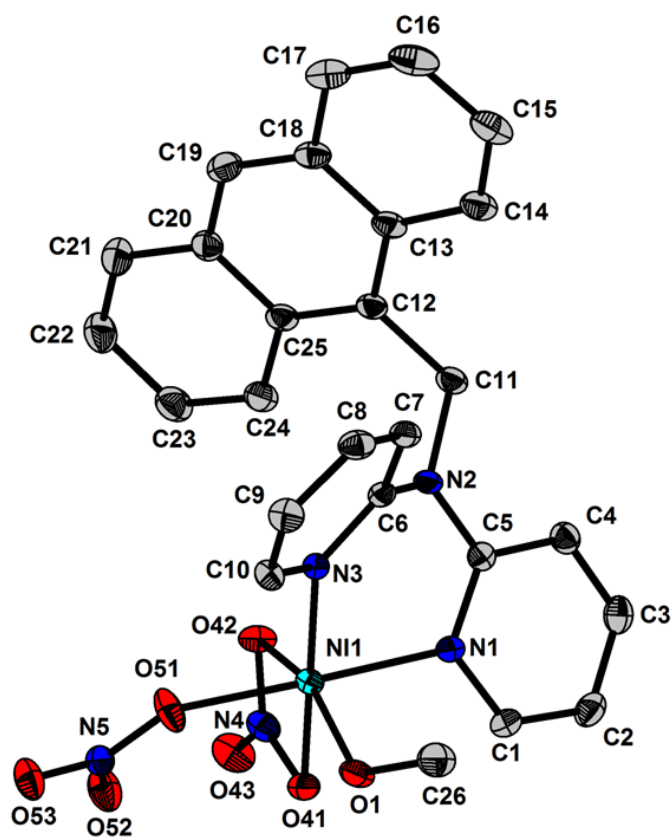


Fig. S2. Crystal structure of complex **3**. All hydrogen atoms were omitted for clarity.

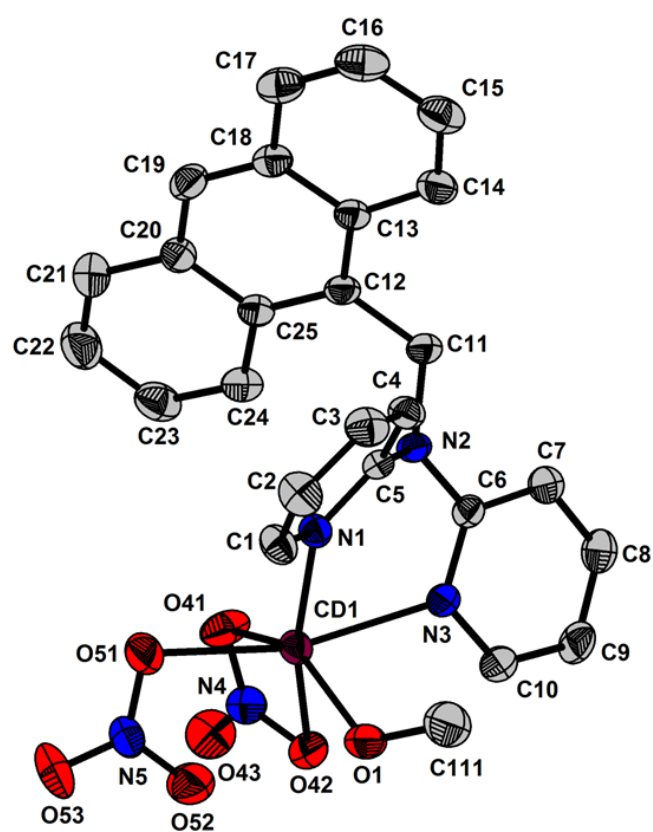


Fig. S3. Crystal structure of complex **5**. All hydrogen atoms were omitted for clarity.

Table S1. Bond lengths [Å] and angles [°] for **1**.

Co(1)-O(51)	2.060(2)
Co(1)-O(1)	2.072(2)
Co(1)-N(3)	2.076(2)
Co(1)-N(1)	2.119(2)
Co(1)-O(41)	2.174(2)
Co(1)-O(42)	2.185(2)
N(1)-C(5)	1.351(3)
N(1)-C(1)	1.359(4)
N(2)-C(5)	1.400(3)
N(2)-C(6)	1.416(3)
N(2)-C(11)	1.492(3)
N(3)-C(6)	1.341(3)
N(3)-C(10)	1.349(4)
N(4)-O(43)	1.226(3)
N(4)-O(42)	1.263(3)
N(4)-O(41)	1.282(3)
N(5)-O(53)	1.215(3)
N(5)-O(52)	1.228(3)
N(5)-O(51)	1.260(3)
O(1)-C(111)	1.440(4)
O(1)-H(10)	0.87(3)
C(1)-C(2)	1.361(4)
C(1)-H(1)	0.9300
C(2)-C(3)	1.373(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.373(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.399(4)
C(4)-H(4)	0.9300
C(6)-C(7)	1.379(4)
C(7)-C(8)	1.371(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.379(4)

C(8)-H(8)	0.9300
C(9)-C(10)	1.355(4)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.517(4)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.405(4)
C(12)-C(25)	1.416(4)
C(13)-C(14)	1.425(4)
C(13)-C(18)	1.439(5)
C(14)-C(15)	1.357(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.411(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.333(6)
C(16)-H(16)	0.9300
C(17)-C(18)	1.435(5)
C(17)-H(17)	0.9300
C(18)-C(19)	1.383(5)
C(19)-C(20)	1.380(5)
C(19)-H(19)	0.9300
C(20)-C(21)	1.427(5)
C(20)-C(25)	1.434(4)
C(21)-C(22)	1.331(5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.425(6)
C(22)-H(22)	0.9300
C(23)-C(24)	1.355(4)
C(23)-H(23)	0.9300
C(24)-C(25)	1.417(4)
C(24)-H(24)	0.9300
C(111)-H(11C)	0.9600
C(111)-H(11D)	0.9600
C(111)-H(11E)	0.9600

O(51)-Co(1)-O(1)	90.76(10)
O(51)-Co(1)-N(3)	90.65(9)
O(1)-Co(1)-N(3)	91.81(9)
O(51)-Co(1)-N(1)	175.49(9)
O(1)-Co(1)-N(1)	88.82(10)
N(3)-Co(1)-N(1)	84.88(9)
O(51)-Co(1)-O(41)	92.94(9)
O(1)-Co(1)-O(41)	93.96(9)
N(3)-Co(1)-O(41)	173.16(9)
N(1)-Co(1)-O(41)	91.57(9)
O(51)-Co(1)-O(42)	94.46(9)
O(1)-Co(1)-O(42)	152.89(9)
N(3)-Co(1)-O(42)	114.66(8)
N(1)-Co(1)-O(42)	87.94(10)
O(41)-Co(1)-O(42)	59.25(8)
C(5)-N(1)-C(1)	117.8(3)
C(5)-N(1)-Co(1)	123.01(18)
C(1)-N(1)-Co(1)	117.1(2)
C(5)-N(2)-C(6)	121.8(2)
C(5)-N(2)-C(11)	116.6(2)
C(6)-N(2)-C(11)	117.8(2)
C(6)-N(3)-C(10)	117.5(2)
C(6)-N(3)-Co(1)	123.68(18)
C(10)-N(3)-Co(1)	116.38(18)
O(43)-N(4)-O(42)	122.8(3)
O(43)-N(4)-O(41)	121.5(3)
O(42)-N(4)-O(41)	115.7(3)
N(4)-O(41)-Co(1)	92.13(16)
N(4)-O(42)-Co(1)	92.16(18)
O(53)-N(5)-O(52)	120.0(3)
O(53)-N(5)-O(51)	120.1(3)
O(52)-N(5)-O(51)	119.9(3)
N(5)-O(51)-Co(1)	132.8(2)
C(111)-O(1)-Co(1)	130.06(19)

C(111)-O(1)-H(1O)	111(2)
Co(1)-O(1)-H(1O)	118(2)
N(1)-C(1)-C(2)	123.9(3)
N(1)-C(1)-H(1)	118.0
C(2)-C(1)-H(1)	118.0
C(1)-C(2)-C(3)	117.8(3)
C(1)-C(2)-H(2)	121.1
C(3)-C(2)-H(2)	121.1
C(2)-C(3)-C(4)	120.3(3)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	119.3(3)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
N(1)-C(5)-C(4)	120.7(3)
N(1)-C(5)-N(2)	117.2(2)
C(4)-C(5)-N(2)	122.1(3)
N(3)-C(6)-C(7)	121.6(3)
N(3)-C(6)-N(2)	118.1(2)
C(7)-C(6)-N(2)	120.3(2)
C(8)-C(7)-C(6)	119.7(3)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(7)-C(8)-C(9)	119.2(3)
C(7)-C(8)-H(8)	120.4
C(9)-C(8)-H(8)	120.4
C(10)-C(9)-C(8)	118.0(3)
C(10)-C(9)-H(9)	121.0
C(8)-C(9)-H(9)	121.0
N(3)-C(10)-C(9)	124.0(3)
N(3)-C(10)-H(10)	118.0
C(9)-C(10)-H(10)	118.0
N(2)-C(11)-C(12)	114.1(2)
N(2)-C(11)-H(11A)	108.7
C(12)-C(11)-H(11A)	108.7

N(2)-C(11)-H(11B)	108.7
C(12)-C(11)-H(11B)	108.7
H(11A)-C(11)-H(11B)	107.6
C(13)-C(12)-C(25)	120.8(3)
C(13)-C(12)-C(11)	121.0(3)
C(25)-C(12)-C(11)	118.1(3)
C(12)-C(13)-C(14)	124.9(3)
C(12)-C(13)-C(18)	118.9(3)
C(14)-C(13)-C(18)	116.2(3)
C(15)-C(14)-C(13)	122.3(4)
C(15)-C(14)-H(14)	118.9
C(13)-C(14)-H(14)	118.9
C(14)-C(15)-C(16)	120.7(4)
C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(17)-C(16)-C(15)	120.0(4)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	121.6(4)
C(16)-C(17)-H(17)	119.2
C(18)-C(17)-H(17)	119.2
C(19)-C(18)-C(17)	121.1(3)
C(19)-C(18)-C(13)	119.6(3)
C(17)-C(18)-C(13)	119.2(3)
C(20)-C(19)-C(18)	122.0(3)
C(20)-C(19)-H(19)	119.0
C(18)-C(19)-H(19)	119.0
C(19)-C(20)-C(21)	121.2(3)
C(19)-C(20)-C(25)	119.9(3)
C(21)-C(20)-C(25)	118.9(3)
C(22)-C(21)-C(20)	121.8(4)
C(22)-C(21)-H(21)	119.1
C(20)-C(21)-H(21)	119.1
C(21)-C(22)-C(23)	119.9(4)
C(21)-C(22)-H(22)	120.1

C(23)-C(22)-H(22)	120.1
C(24)-C(23)-C(22)	120.3(4)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(23)-C(24)-C(25)	121.9(3)
C(23)-C(24)-H(24)	119.0
C(25)-C(24)-H(24)	119.0
C(12)-C(25)-C(24)	124.0(3)
C(12)-C(25)-C(20)	118.8(3)
C(24)-C(25)-C(20)	117.2(3)
O(1)-C(111)-H(11C)	109.5
O(1)-C(111)-H(11D)	109.5
H(11C)-C(111)-H(11D)	109.5
O(1)-C(111)-H(11E)	109.5
H(11C)-C(111)-H(11E)	109.5
H(11D)-C(111)-H(11E)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S2. Bond lengths [Å] and angles [°] for **2**.

Cu(1)-N(3)	1.963(4)
Cu(1)-O(41)	1.984(3)
Cu(1)-N(1)	1.989(4)
Cu(1)-O(51)	1.999(3)
Cu(1)-O(1)	2.306(3)
O(1)-C(26)	1.408(5)
O(1)-H(1O)	0.930(2)
N(1)-C(1)	1.337(6)
N(1)-C(5)	1.360(5)
N(2)-C(5)	1.391(6)
N(2)-C(6)	1.411(6)
N(2)-C(11)	1.490(5)
N(3)-C(6)	1.343(5)
N(3)-C(10)	1.351(6)
N(4)-O(42)	1.208(5)
N(4)-O(43)	1.229(5)
N(4)-O(41)	1.292(5)
N(5)-O(52)	1.229(5)
N(5)-O(53)	1.230(5)
N(5)-O(51)	1.308(5)
C(1)-C(2)	1.356(7)
C(1)-H(1)	0.9500
C(2)-C(3)	1.382(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.372(7)
C(3)-H(3)	0.9500
C(4)-C(5)	1.404(6)
C(4)-H(4)	0.9500
C(6)-C(7)	1.397(6)
C(7)-C(8)	1.365(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.387(6)
C(8)-H(8)	0.9500

C(9)-C(10)	1.362(6)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(12)	1.497(6)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(25)	1.423(6)
C(12)-C(13)	1.423(6)
C(13)-C(18)	1.423(6)
C(13)-C(14)	1.441(6)
C(14)-C(15)	1.352(6)
C(14)-H(14)	0.9500
C(15)-C(16)	1.395(7)
C(15)-H(15)	0.9500
C(16)-C(17)	1.351(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.421(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.408(6)
C(19)-C(20)	1.389(6)
C(19)-H(19)	0.9500
C(20)-C(25)	1.422(6)
C(20)-C(21)	1.438(6)
C(21)-C(22)	1.348(7)
C(21)-H(21)	0.9500
C(22)-C(23)	1.411(7)
C(22)-H(22)	0.9500
C(23)-C(24)	1.364(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.432(6)
C(24)-H(24)	0.9500
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800

N(3)-Cu(1)-O(41)	89.79(15)
N(3)-Cu(1)-N(1)	87.59(15)
O(41)-Cu(1)-N(1)	165.65(14)
N(3)-Cu(1)-O(51)	178.80(14)
O(41)-Cu(1)-O(51)	89.33(14)
N(1)-Cu(1)-O(51)	93.05(14)
N(3)-Cu(1)-O(1)	86.48(13)
O(41)-Cu(1)-O(1)	103.53(13)
N(1)-Cu(1)-O(1)	90.39(14)
O(51)-Cu(1)-O(1)	94.53(12)
C(26)-O(1)-Cu(1)	126.3(3)
C(26)-O(1)-H(1O)	111(3)
Cu(1)-O(1)-H(1O)	118(3)
C(1)-N(1)-C(5)	117.8(4)
C(1)-N(1)-Cu(1)	118.9(3)
C(5)-N(1)-Cu(1)	123.1(3)
C(5)-N(2)-C(6)	121.3(3)
C(5)-N(2)-C(11)	116.2(4)
C(6)-N(2)-C(11)	119.0(4)
C(6)-N(3)-C(10)	117.8(4)
C(6)-N(3)-Cu(1)	124.9(3)
C(10)-N(3)-Cu(1)	117.0(3)
O(42)-N(4)-O(43)	122.1(4)
O(42)-N(4)-O(41)	120.1(4)
O(43)-N(4)-O(41)	117.7(4)
O(52)-N(5)-O(53)	124.5(4)
O(52)-N(5)-O(51)	118.1(4)
O(53)-N(5)-O(51)	117.4(4)
N(4)-O(41)-Cu(1)	119.0(3)
N(5)-O(51)-Cu(1)	109.1(3)
N(1)-C(1)-C(2)	125.2(5)
N(1)-C(1)-H(1)	117.4
C(2)-C(1)-H(1)	117.4
C(1)-C(2)-C(3)	117.2(5)
C(1)-C(2)-H(2)	121.4

C(3)-C(2)-H(2)	121.4
C(4)-C(3)-C(2)	120.0(5)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	119.6(5)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
N(1)-C(5)-N(2)	117.9(4)
N(1)-C(5)-C(4)	120.1(5)
N(2)-C(5)-C(4)	122.0(4)
N(3)-C(6)-C(7)	121.0(4)
N(3)-C(6)-N(2)	117.5(4)
C(7)-C(6)-N(2)	121.5(4)
C(8)-C(7)-C(6)	119.7(4)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(7)-C(8)-C(9)	119.7(5)
C(7)-C(8)-H(8)	120.2
C(9)-C(8)-H(8)	120.2
C(10)-C(9)-C(8)	117.6(5)
C(10)-C(9)-H(9)	121.2
C(8)-C(9)-H(9)	121.2
N(3)-C(10)-C(9)	124.1(4)
N(3)-C(10)-H(10)	117.9
C(9)-C(10)-H(10)	117.9
N(2)-C(11)-C(12)	114.6(4)
N(2)-C(11)-H(11A)	108.6
C(12)-C(11)-H(11A)	108.6
N(2)-C(11)-H(11B)	108.6
C(12)-C(11)-H(11B)	108.6
H(11A)-C(11)-H(11B)	107.6
C(25)-C(12)-C(13)	119.7(4)
C(25)-C(12)-C(11)	118.7(4)
C(13)-C(12)-C(11)	121.4(4)
C(18)-C(13)-C(12)	119.7(4)

C(18)-C(13)-C(14)	116.3(4)
C(12)-C(13)-C(14)	124.0(4)
C(15)-C(14)-C(13)	121.3(5)
C(15)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
C(14)-C(15)-C(16)	121.8(5)
C(14)-C(15)-H(15)	119.1
C(16)-C(15)-H(15)	119.1
C(17)-C(16)-C(15)	119.4(5)
C(17)-C(16)-H(16)	120.3
C(15)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	121.4(5)
C(16)-C(17)-H(17)	119.3
C(18)-C(17)-H(17)	119.3
C(19)-C(18)-C(17)	120.3(5)
C(19)-C(18)-C(13)	119.8(4)
C(17)-C(18)-C(13)	119.9(4)
C(20)-C(19)-C(18)	120.7(5)
C(20)-C(19)-H(19)	119.6
C(18)-C(19)-H(19)	119.6
C(19)-C(20)-C(25)	120.7(4)
C(19)-C(20)-C(21)	120.5(5)
C(25)-C(20)-C(21)	118.8(4)
C(22)-C(21)-C(20)	121.4(5)
C(22)-C(21)-H(21)	119.3
C(20)-C(21)-H(21)	119.3
C(21)-C(22)-C(23)	120.1(5)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	120.6(5)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	121.3(5)
C(23)-C(24)-H(24)	119.4
C(25)-C(24)-H(24)	119.4

C(20)-C(25)-C(12)	119.3(4)
C(20)-C(25)-C(24)	117.8(4)
C(12)-C(25)-C(24)	122.9(4)
O(1)-C(26)-H(26A)	109.5
O(1)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(1)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **3**.

Ni(1)-N(3)	2.0229(17)
Ni(1)-O(1)	2.0537(16)
Ni(1)-N(1)	2.0543(18)
Ni(1)-O(51)	2.0659(17)
Ni(1)-O(41)	2.1005(15)
Ni(1)-O(42)	2.1462(16)
N(1)-C(1)	1.348(3)
N(1)-C(5)	1.353(3)
N(2)-C(5)	1.395(3)
N(2)-C(6)	1.414(3)
N(2)-C(11)	1.492(3)
N(3)-C(6)	1.349(3)
N(3)-C(10)	1.357(3)
N(4)-O(43)	1.221(2)
N(4)-O(42)	1.268(2)
N(4)-O(41)	1.292(2)
N(5)-O(52)	1.228(2)
N(5)-O(53)	1.235(2)
N(5)-O(51)	1.277(2)
O(1)-C(26)	1.431(3)
O(1)-H(10)	0.929(2)
C(1)-C(2)	1.373(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.382(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.372(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.399(3)
C(4)-H(4)	0.9500
C(6)-C(7)	1.389(3)
C(7)-C(8)	1.376(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.380(3)

C(8)-H(8)	0.9500
C(9)-C(10)	1.360(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(12)	1.520(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.409(3)
C(12)-C(25)	1.414(3)
C(13)-C(14)	1.433(3)
C(13)-C(18)	1.439(3)
C(14)-C(15)	1.352(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.423(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.351(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.426(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.387(3)
C(19)-C(20)	1.388(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.422(3)
C(20)-C(25)	1.436(3)
C(21)-C(22)	1.346(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.417(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.356(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.430(3)
C(24)-H(24)	0.9500
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800

N(3)-Ni(1)-O(1)	90.84(7)
N(3)-Ni(1)-N(1)	87.10(7)
O(1)-Ni(1)-N(1)	90.98(7)
N(3)-Ni(1)-O(51)	89.56(7)
O(1)-Ni(1)-O(51)	87.25(7)
N(1)-Ni(1)-O(51)	176.20(7)
N(3)-Ni(1)-O(41)	171.92(7)
O(1)-Ni(1)-O(41)	96.74(6)
N(1)-Ni(1)-O(41)	89.97(7)
O(51)-Ni(1)-O(41)	93.58(7)
N(3)-Ni(1)-O(42)	111.40(7)
O(1)-Ni(1)-O(42)	157.72(6)
N(1)-Ni(1)-O(42)	91.44(7)
O(51)-Ni(1)-O(42)	91.47(7)
O(41)-Ni(1)-O(42)	61.12(6)
C(1)-N(1)-C(5)	118.52(19)
C(1)-N(1)-Ni(1)	117.19(15)
C(5)-N(1)-Ni(1)	122.56(14)
C(5)-N(2)-C(6)	121.89(17)
C(5)-N(2)-C(11)	116.52(17)
C(6)-N(2)-C(11)	117.71(17)
C(6)-N(3)-C(10)	117.57(18)
C(6)-N(3)-Ni(1)	122.86(15)
C(10)-N(3)-Ni(1)	117.32(13)
O(43)-N(4)-O(42)	123.6(2)
O(43)-N(4)-O(41)	121.39(18)
O(42)-N(4)-O(41)	115.02(17)
O(52)-N(5)-O(53)	121.73(19)
O(52)-N(5)-O(51)	119.90(19)
O(53)-N(5)-O(51)	118.37(19)
C(26)-O(1)-Ni(1)	128.27(14)
C(26)-O(1)-H(10)	110.4(15)
Ni(1)-O(1)-H(10)	118.3(15)
N(4)-O(41)-Ni(1)	92.37(11)

N(4)-O(42)-Ni(1)	90.96(12)
N(5)-O(51)-Ni(1)	132.72(15)
N(1)-C(1)-C(2)	123.5(2)
N(1)-C(1)-H(1)	118.2
C(2)-C(1)-H(1)	118.2
C(1)-C(2)-C(3)	117.8(2)
C(1)-C(2)-H(2)	121.1
C(3)-C(2)-H(2)	121.1
C(4)-C(3)-C(2)	119.9(2)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	119.6(2)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
N(1)-C(5)-N(2)	117.40(19)
N(1)-C(5)-C(4)	120.4(2)
N(2)-C(5)-C(4)	122.22(19)
N(3)-C(6)-C(7)	121.5(2)
N(3)-C(6)-N(2)	118.29(18)
C(7)-C(6)-N(2)	120.24(19)
C(8)-C(7)-C(6)	119.6(2)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(7)-C(8)-C(9)	119.1(2)
C(7)-C(8)-H(8)	120.4
C(9)-C(8)-H(8)	120.4
C(10)-C(9)-C(8)	118.6(2)
C(10)-C(9)-H(9)	120.7
C(8)-C(9)-H(9)	120.7
N(3)-C(10)-C(9)	123.5(2)
N(3)-C(10)-H(10)	118.2
C(9)-C(10)-H(10)	118.2
N(2)-C(11)-C(12)	114.43(18)
N(2)-C(11)-H(11A)	108.7
C(12)-C(11)-H(11A)	108.7

N(2)-C(11)-H(11B)	108.7
C(12)-C(11)-H(11B)	108.7
H(11A)-C(11)-H(11B)	107.6
C(13)-C(12)-C(25)	120.7(2)
C(13)-C(12)-C(11)	120.86(19)
C(25)-C(12)-C(11)	118.30(19)
C(12)-C(13)-C(14)	124.8(2)
C(12)-C(13)-C(18)	119.0(2)
C(14)-C(13)-C(18)	116.2(2)
C(15)-C(14)-C(13)	122.7(3)
C(15)-C(14)-H(14)	118.6
C(13)-C(14)-H(14)	118.6
C(14)-C(15)-C(16)	120.3(2)
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-H(15)	119.8
C(17)-C(16)-C(15)	119.6(2)
C(17)-C(16)-H(16)	120.2
C(15)-C(16)-H(16)	120.2
C(16)-C(17)-C(18)	121.7(3)
C(16)-C(17)-H(17)	119.1
C(18)-C(17)-H(17)	119.1
C(19)-C(18)-C(17)	121.0(2)
C(19)-C(18)-C(13)	119.6(2)
C(17)-C(18)-C(13)	119.4(2)
C(18)-C(19)-C(20)	122.2(2)
C(18)-C(19)-H(19)	118.9
C(20)-C(19)-H(19)	118.9
C(19)-C(20)-C(21)	121.9(2)
C(19)-C(20)-C(25)	119.2(2)
C(21)-C(20)-C(25)	118.9(2)
C(22)-C(21)-C(20)	121.9(2)
C(22)-C(21)-H(21)	119.0
C(20)-C(21)-H(21)	119.0
C(21)-C(22)-C(23)	119.6(2)
C(21)-C(22)-H(22)	120.2

C(23)-C(22)-H(22)	120.2
C(24)-C(23)-C(22)	120.8(2)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(23)-C(24)-C(25)	121.6(2)
C(23)-C(24)-H(24)	119.2
C(25)-C(24)-H(24)	119.2
C(12)-C(25)-C(24)	123.5(2)
C(12)-C(25)-C(20)	119.3(2)
C(24)-C(25)-C(20)	117.1(2)
O(1)-C(26)-H(26A)	109.5
O(1)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(1)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond lengths [Å] and angles [°] for **4**.

Zn(1)-O(41)	1.965(3)
Zn(1)-O(51)	2.031(3)
Zn(1)-N(1)	2.037(3)
Zn(1)-N(3)	2.038(3)
Zn(1)-O(52)	2.484(4)
N(1)-C(5)	1.349(4)
N(1)-C(1)	1.354(5)
N(2)-C(5)	1.417(5)
N(2)-C(6)	1.422(5)
N(2)-C(11)	1.493(5)
N(3)-C(6)	1.351(4)
N(3)-C(10)	1.354(5)
N(4)-O(42)	1.205(5)
N(4)-O(43)	1.215(5)
N(4)-O(41)	1.272(5)
N(5)-O(53)	1.211(5)
N(5)-O(52)	1.244(5)
N(5)-O(51)	1.280(4)
C(1)-C(2)	1.369(5)
C(1)-H(1)	0.9300
C(2)-C(3)	1.365(6)
C(2)-H(2)	0.9300
C(3)-C(4)	1.376(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.392(5)
C(4)-H(4)	0.9300
C(6)-C(7)	1.390(5)
C(7)-C(8)	1.378(6)
C(7)-H(7)	0.9300
C(8)-C(9)	1.386(6)
C(8)-H(8)	0.9300
C(9)-C(10)	1.373(5)
C(9)-H(9)	0.9300

C(10)-H(10)	0.9300
C(11)-C(12)	1.524(6)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.402(5)
C(12)-C(25)	1.417(6)
C(13)-C(14)	1.420(6)
C(13)-C(18)	1.450(6)
C(14)-C(15)	1.372(6)
C(14)-H(14)	0.9300
C(15)-C(16)	1.414(7)
C(15)-H(15)	0.9300
C(16)-C(17)	1.321(8)
C(16)-H(16)	0.9300
C(17)-C(18)	1.434(7)
C(17)-H(17)	0.9300
C(18)-C(19)	1.399(6)
C(19)-C(20)	1.375(7)
C(19)-H(19)	0.9300
C(20)-C(21)	1.433(6)
C(20)-C(25)	1.435(6)
C(21)-C(22)	1.334(8)
C(21)-H(21)	0.9300
C(22)-C(23)	1.386(9)
C(22)-H(22)	0.9300
C(23)-C(24)	1.362(7)
C(23)-H(23)	0.9300
C(24)-C(25)	1.444(6)
C(24)-H(24)	0.9300
O(41)-Zn(1)-O(51)	116.71(12)
O(41)-Zn(1)-N(1)	118.75(13)
O(51)-Zn(1)-N(1)	97.31(11)
O(41)-Zn(1)-N(3)	105.79(12)
O(51)-Zn(1)-N(3)	125.25(11)

N(1)-Zn(1)-N(3)	90.52(12)
O(41)-Zn(1)-O(52)	87.39(14)
O(51)-Zn(1)-O(52)	55.47(11)
N(1)-Zn(1)-O(52)	150.14(13)
N(3)-Zn(1)-O(52)	96.11(12)
C(5)-N(1)-C(1)	118.4(3)
C(5)-N(1)-Zn(1)	120.9(2)
C(1)-N(1)-Zn(1)	120.7(2)
C(5)-N(2)-C(6)	120.4(3)
C(5)-N(2)-C(11)	113.3(3)
C(6)-N(2)-C(11)	119.4(3)
C(6)-N(3)-C(10)	119.1(3)
C(6)-N(3)-Zn(1)	120.1(2)
C(10)-N(3)-Zn(1)	120.7(3)
O(42)-N(4)-O(43)	123.7(5)
O(42)-N(4)-O(41)	116.9(4)
O(43)-N(4)-O(41)	119.4(4)
N(4)-O(41)-Zn(1)	112.9(3)
O(53)-N(5)-O(52)	123.8(4)
O(53)-N(5)-O(51)	120.2(4)
O(52)-N(5)-O(51)	115.9(4)
N(5)-O(51)-Zn(1)	104.2(3)
N(5)-O(52)-Zn(1)	83.6(2)
N(1)-C(1)-C(2)	123.2(4)
N(1)-C(1)-H(1)	118.4
C(2)-C(1)-H(1)	118.4
C(3)-C(2)-C(1)	118.2(4)
C(3)-C(2)-H(2)	120.9
C(1)-C(2)-H(2)	120.9
C(2)-C(3)-C(4)	120.2(4)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	119.3(4)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3

N(1)-C(5)-C(4)	120.7(4)
N(1)-C(5)-N(2)	117.3(3)
C(4)-C(5)-N(2)	122.0(4)
N(3)-C(6)-C(7)	120.3(4)
N(3)-C(6)-N(2)	118.1(3)
C(7)-C(6)-N(2)	121.5(4)
C(8)-C(7)-C(6)	119.8(4)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(7)-C(8)-C(9)	119.9(4)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	117.7(4)
C(10)-C(9)-H(9)	121.1
C(8)-C(9)-H(9)	121.1
N(3)-C(10)-C(9)	123.0(4)
N(3)-C(10)-H(10)	118.5
C(9)-C(10)-H(10)	118.5
N(2)-C(11)-C(12)	115.2(3)
N(2)-C(11)-H(11A)	108.5
C(12)-C(11)-H(11A)	108.5
N(2)-C(11)-H(11B)	108.5
C(12)-C(11)-H(11B)	108.5
H(11A)-C(11)-H(11B)	107.5
C(13)-C(12)-C(25)	120.5(4)
C(13)-C(12)-C(11)	120.4(4)
C(25)-C(12)-C(11)	118.8(4)
C(12)-C(13)-C(14)	123.4(4)
C(12)-C(13)-C(18)	119.1(4)
C(14)-C(13)-C(18)	117.5(4)
C(15)-C(14)-C(13)	120.6(5)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(14)-C(15)-C(16)	121.1(5)
C(14)-C(15)-H(15)	119.5

C(16)-C(15)-H(15)	119.5
C(17)-C(16)-C(15)	120.4(5)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	121.7(5)
C(16)-C(17)-H(17)	119.1
C(18)-C(17)-H(17)	119.1
C(19)-C(18)-C(17)	122.0(5)
C(19)-C(18)-C(13)	119.4(4)
C(17)-C(18)-C(13)	118.6(5)
C(20)-C(19)-C(18)	121.5(4)
C(20)-C(19)-H(19)	119.3
C(18)-C(19)-H(19)	119.3
C(19)-C(20)-C(21)	120.2(5)
C(19)-C(20)-C(25)	120.1(4)
C(21)-C(20)-C(25)	119.7(5)
C(22)-C(21)-C(20)	120.9(6)
C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(21)-C(22)-C(23)	120.7(6)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(24)-C(23)-C(22)	121.6(6)
C(24)-C(23)-H(23)	119.2
C(22)-C(23)-H(23)	119.2
C(23)-C(24)-C(25)	120.8(5)
C(23)-C(24)-H(24)	119.6
C(25)-C(24)-H(24)	119.6
C(12)-C(25)-C(20)	119.3(4)
C(12)-C(25)-C(24)	124.6(4)
C(20)-C(25)-C(24)	116.1(4)

Symmetry transformations used to generate equivalent atoms:

Table S5. Bond lengths [Å] and angles [°] for **5**.

Cd(1)-N(1)	2.2749(18)
Cd(1)-N(3)	2.318(2)
Cd(1)-O(1)	2.3199(19)
Cd(1)-O(41)	2.3576(19)
Cd(1)-O(51)	2.373(2)
Cd(1)-O(42)	2.4953(19)
Cd(1)-O(52)	2.506(2)
N(1)-C(5)	1.339(3)
N(1)-C(1)	1.345(3)
N(2)-C(6)	1.397(3)
N(2)-C(5)	1.421(3)
N(2)-C(11)	1.490(3)
N(3)-C(6)	1.338(3)
N(3)-C(10)	1.353(3)
N(4)-O(43)	1.222(3)
N(4)-O(41)	1.253(3)
N(4)-O(42)	1.267(3)
N(5)-O(53)	1.212(3)
N(5)-O(51)	1.241(3)
N(5)-O(52)	1.245(3)
O(1)-C(111)	1.409(3)
O(1)-H(10)	0.860(2)
C(1)-C(2)	1.357(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.381(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.372(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.386(3)
C(4)-H(4)	0.9300
C(6)-C(7)	1.388(3)
C(7)-C(8)	1.372(4)
C(7)-H(7)	0.9300

C(8)-C(9)	1.368(4)
C(8)-H(8)	0.9300
C(9)-C(10)	1.359(4)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.513(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.404(3)
C(12)-C(25)	1.415(3)
C(13)-C(14)	1.434(3)
C(13)-C(18)	1.439(3)
C(14)-C(15)	1.351(4)
C(14)-H(14)	0.9300
C(15)-C(16)	1.406(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.348(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.426(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.377(4)
C(19)-C(20)	1.388(4)
C(19)-H(19)	0.9300
C(20)-C(21)	1.420(4)
C(20)-C(25)	1.424(3)
C(21)-C(22)	1.336(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.412(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.355(4)
C(23)-H(23)	0.9300
C(24)-C(25)	1.425(3)
C(24)-H(24)	0.9300
C(111)-H(11C)	0.9600
C(111)-H(11D)	0.9600

C(111)-H(11E)	0.9600
N(1)-Cd(1)-N(3)	79.94(7)
N(1)-Cd(1)-O(1)	86.06(7)
N(3)-Cd(1)-O(1)	86.08(7)
N(1)-Cd(1)-O(41)	123.86(7)
N(3)-Cd(1)-O(41)	98.96(8)
O(1)-Cd(1)-O(41)	150.07(7)
N(1)-Cd(1)-O(51)	84.14(7)
N(3)-Cd(1)-O(51)	163.43(7)
O(1)-Cd(1)-O(51)	97.44(8)
O(41)-Cd(1)-O(51)	86.09(8)
N(1)-Cd(1)-O(42)	163.80(7)
N(3)-Cd(1)-O(42)	85.15(7)
O(1)-Cd(1)-O(42)	99.27(7)
O(41)-Cd(1)-O(42)	52.33(6)
O(51)-Cd(1)-O(42)	110.08(7)
N(1)-Cd(1)-O(52)	126.54(7)
N(3)-Cd(1)-O(52)	144.91(7)
O(1)-Cd(1)-O(52)	74.85(8)
O(41)-Cd(1)-O(52)	84.90(8)
O(51)-Cd(1)-O(52)	50.89(7)
O(42)-Cd(1)-O(52)	69.64(7)
C(5)-N(1)-C(1)	118.1(2)
C(5)-N(1)-Cd(1)	123.51(15)
C(1)-N(1)-Cd(1)	116.03(15)
C(6)-N(2)-C(5)	122.26(17)
C(6)-N(2)-C(11)	116.99(18)
C(5)-N(2)-C(11)	116.55(17)
C(6)-N(3)-C(10)	118.4(2)
C(6)-N(3)-Cd(1)	123.06(14)
C(10)-N(3)-Cd(1)	116.82(16)
O(43)-N(4)-O(41)	121.9(2)
O(43)-N(4)-O(42)	121.5(2)
O(41)-N(4)-O(42)	116.6(2)

N(4)-O(41)-Cd(1)	98.04(14)
N(4)-O(42)-Cd(1)	91.10(14)
O(53)-N(5)-O(51)	122.1(2)
O(53)-N(5)-O(52)	122.6(2)
O(51)-N(5)-O(52)	115.3(2)
N(5)-O(51)-Cd(1)	100.26(15)
N(5)-O(52)-Cd(1)	93.58(15)
C(111)-O(1)-Cd(1)	127.77(17)
C(111)-O(1)-H(1O)	111(2)
Cd(1)-O(1)-H(1O)	120(2)
N(1)-C(1)-C(2)	123.9(2)
N(1)-C(1)-H(1)	118.1
C(2)-C(1)-H(1)	118.1
C(1)-C(2)-C(3)	118.0(2)
C(1)-C(2)-H(2)	121.0
C(3)-C(2)-H(2)	121.0
C(4)-C(3)-C(2)	119.0(2)
C(4)-C(3)-H(3)	120.5
C(2)-C(3)-H(3)	120.5
C(3)-C(4)-C(5)	119.9(2)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
N(1)-C(5)-C(4)	120.9(2)
N(1)-C(5)-N(2)	118.03(19)
C(4)-C(5)-N(2)	121.0(2)
N(3)-C(6)-C(7)	120.7(2)
N(3)-C(6)-N(2)	117.74(19)
C(7)-C(6)-N(2)	121.6(2)
C(8)-C(7)-C(6)	119.2(2)
C(8)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
C(9)-C(8)-C(7)	120.4(2)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	117.5(2)

C(10)-C(9)-H(9)	121.3
C(8)-C(9)-H(9)	121.3
N(3)-C(10)-C(9)	123.7(2)
N(3)-C(10)-H(10)	118.2
C(9)-C(10)-H(10)	118.2
N(2)-C(11)-C(12)	113.05(18)
N(2)-C(11)-H(11A)	109.0
C(12)-C(11)-H(11A)	109.0
N(2)-C(11)-H(11B)	109.0
C(12)-C(11)-H(11B)	109.0
H(11A)-C(11)-H(11B)	107.8
C(13)-C(12)-C(25)	120.6(2)
C(13)-C(12)-C(11)	120.9(2)
C(25)-C(12)-C(11)	118.4(2)
C(12)-C(13)-C(14)	124.9(2)
C(12)-C(13)-C(18)	118.7(2)
C(14)-C(13)-C(18)	116.3(2)
C(15)-C(14)-C(13)	121.7(3)
C(15)-C(14)-H(14)	119.2
C(13)-C(14)-H(14)	119.2
C(14)-C(15)-C(16)	121.4(3)
C(14)-C(15)-H(15)	119.3
C(16)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	119.8(3)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	121.2(3)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(19)-C(18)-C(17)	120.6(2)
C(19)-C(18)-C(13)	119.8(2)
C(17)-C(18)-C(13)	119.6(2)
C(18)-C(19)-C(20)	122.1(2)
C(18)-C(19)-H(19)	119.0
C(20)-C(19)-H(19)	119.0

C(19)-C(20)-C(21)	121.2(2)
C(19)-C(20)-C(25)	119.3(2)
C(21)-C(20)-C(25)	119.5(2)
C(22)-C(21)-C(20)	121.2(3)
C(22)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4
C(21)-C(22)-C(23)	120.2(3)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	120.7(3)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(23)-C(24)-C(25)	121.2(3)
C(23)-C(24)-H(24)	119.4
C(25)-C(24)-H(24)	119.4
C(12)-C(25)-C(20)	119.4(2)
C(12)-C(25)-C(24)	123.4(2)
C(20)-C(25)-C(24)	117.2(2)
O(1)-C(111)-H(11C)	109.5
O(1)-C(111)-H(11D)	109.5
H(11C)-C(111)-H(11D)	109.5
O(1)-C(111)-H(11E)	109.5
H(11C)-C(111)-H(11E)	109.5
H(11D)-C(111)-H(11E)	109.5

Symmetry transformations used to generate equivalent atoms: