

Table 1. Selected bond distances for **Ia** and **Ib**

| Compound Ia | | Compound Ib | |
|--------------------|--------------|--------------------|--------------|
| Bond | Distance (Å) | Bond | Distance (Å) |
| Cd(1)-O(1) | 2.226(3) | Cd(1)-O(1) | 2.328(2) |
| Cd(1)-O(2) | 2.378(3) | Cd(1)-O(2) | 2.429(2) |
| Cd(1)-O(3) | 2.400(3) | Cd(1)-O(3)#1 | 2.213(2) |
| Cd(1)-O(4) | 2.445(3) | O(3)-Cd(1)#2 | 2.213(2) |
| Cd(1)-N(1) | 2.319(3) | Cd(1)-O(5) | 2.320(2) |
| Cd(1)-N(2) | 2.365(3) | Cd(1)-N(1) | 2.374(3) |
| O(1)-C(18) | 1.267(4) | Cd(1)-N(2) | 2.329(2) |
| O(3)-C(11) | 1.265(4) | O(1)-C(11) | 1.256(4) |
| O(4)-C(11) | 1.233(4) | O(3)-C(18) | 1.258(4) |
| O(5)-C(18) | 1.239(4) | O(2)-C(11) | 1.263(4) |
| N(1)-C(1) | 1.338(5) | O(4)-C(18) | 1.245(5) |
| N(1)-C(5) | 1.344(5) | N(1)-C(1) | 1.335(4) |
| N(2)-C(10) | 1.343(5) | N(1)-C(5) | 1.355(4) |
| N(2)-C(6) | 1.359(4) | N(2)-C(6) | 1.343(4) |
| | | N(2)-C(10) | 1.349(4) |

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

Table 2. Selected bond angles for **Ia** and **Ib**

| Compound Ia | | Compound Ib | |
|--------------------|------------|--------------------|-----------|
| Bond | Amplitude | Bond | Amplitude |
| O(1)-Cd(1)-O(2) | 93.52(10) | O(1)-Cd(1)-O(2) | 55.27(7) |
| O(1)-Cd(1)-O(3) | 115.51(10) | O(3)#1-Cd(1)-O(1) | 152.30(8) |
| O(1)-Cd(1)-O(4) | 165.32(10) | O(3)#1-Cd(1)-O(2) | 98.50(8) |
| O(2)-Cd(1)-O(3) | 85.06(10) | O(5)-Cd(1)-O(1) | 95.94(8) |
| O(2)-Cd(1)-O(4) | 76.43(9) | O(5)-Cd(1)-O(2) | 117.93(8) |
| O(3)-Cd(1)-O(4) | 53.72(9) | O(3)#1-Cd(1)-O(5) | 88.93(8) |
| O(1)-Cd(1)-N(1) | 110.85(11) | O(1)-Cd(1)-N(1) | 100.13(8) |
| O(1)-Cd(1)-N(2) | 97.48(10) | O(1)-Cd(1)-N(2) | 91.20(8) |
| N(1)-Cd(1)-O(2) | 150.92(10) | N(1)-Cd(1)-O(2) | 88.48(9) |
| N(2)-Cd(1)-O(2) | 90.98(10) | N(2)-Cd(1)-O(2) | 136.81(8) |
| N(1)-Cd(1)-O(3) | 97.76(10) | O(3)#1-Cd(1)-N(1) | 86.51(9) |
| N(1)-Cd(1)-O(4) | 82.00(9) | O(3)#1-Cd(1)-N(2) | 116.19(8) |
| N(2)-Cd(1)-O(3) | 146.94(9) | O(5)-Cd(1)-N(1) | 153.59(8) |
| N(2)-Cd(1)-O(4) | 93.42(9) | O(5)-Cd(1)-N(2) | 89.03(8) |
| N(1)-Cd(1)-N(2) | 70.91(10) | N(2)-Cd(1)-N(1) | 69.91(8) |
| O(5)-C(18)-O(1) | 123.7(3) | O(1)-C(11)-O(2) | 122.5(3) |
| O(4)-C(11)-O(3) | 122.5(4) | | |

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

Table 2. Selected bond distances and bond angles for **II**

| Bond distances | | Bond angles | |
|----------------|--------------|--------------------|------------|
| Bond | Distance (Å) | Bond | Amplitude |
| Cd(1)-O(1) | 2.531(3) | O(2)-Cd(1)-O(1) | 53.34(9) |
| Cd(1)-O(2) | 2.304(2) | O(3)-Cd(1)-O(1) | 97.79(11) |
| Cd(1)-O(3) | 2.190(2) | O(3)-Cd(1)-O(2) | 132.03(9) |
| Cd(1)-O(5) | 2.349(2) | O(5)-Cd(1)-O(1) | 130.29(10) |
| Cd(1)-N(1) | 2.355(3) | O(2)-Cd(1)-O(5) | 89.72(9) |
| Cd(1)-N(2) | 2.391(3) | O(3)-Cd(1)-O(5) | 83.07(9) |
| Cd(2)-O(11) | 2.407(2) | N(1)-Cd(1)-O(1) | 79.46(10) |
| Cd(2)-O(11)#1 | 2.538(2) | N(2)-Cd(1)-O(1) | 143.57(11) |
| Cd(2)-O(12) | 2.403(2) | O(2)-Cd(1)-N(1) | 114.99(9) |
| Cd(2)-O(13) | 2.177(2) | O(2)-Cd(1)-N(2) | 123.14(9) |
| Cd(2)-N(3) | 2.350(3) | O(3)-Cd(1)-N(1) | 91.26(9) |
| Cd(2)-N(4) | 2.342(3) | O(3)-Cd(1)-N(2) | 102.82(10) |
| O(1)-C(51) | 1.226(4) | O(5)-Cd(1)-N(1) | 150.16(10) |
| O(2)-C(51) | 1.271(4) | O(5)-Cd(1)-N(2) | 82.25(9) |
| O(3)-C(41) | 1.268(4) | N(1)-Cd(1)-N(2) | 70.45(9) |
| O(4)-C(41) | 1.243(4) | O(11)-Cd(2)-(11)#1 | 74.05(10) |
| O(11)-C(48) | 1.260(4) | O(12)-Cd(2)-O(11) | 54.34(8) |
| O(12)-C(48) | 1.261(4) | O(12)-Cd(2)-(11)#1 | 113.45(9) |
| O(13)-C(58) | 1.267(4) | O(13)-Cd(2)-O(11) | 120.72(10) |
| O(14)-C(58) | 1.227(4) | O(13)-Cd(2)-(11)#1 | 85.45(9) |
| N(1)-C(1) | 1.326(4) | O(13)-Cd(2)-O(12) | 87.66(9) |
| N(1)-C(12) | 1.357(4) | N(3)-Cd(2)-O(11) | 84.07(9) |
| N(2)-C(10) | 1.330(4) | N(3)-Cd(2)-O(11)#1 | 129.82(9) |
| N(2)-C(11) | 1.365(4) | N(4)-Cd(2)-O(11) | 116.29(9) |
| N(3)-C(21) | 1.329(4) | N(4)-Cd(2)-O(11)#1 | 78.76(9) |
| N(3)-C(32) | 1.365(4) | N(3)-Cd(2)-O(12) | 86.58(9) |
| N(4)-C(30) | 1.326(5) | N(4)-Cd(2)-O(12) | 157.43(9) |
| N(4)-C(31) | 1.359(4) | N(4)-Cd(2)-N(3) | 71.45(10) |
| | | O(1)-C(51)-O(2) | 121.6(3) |
| | | O(4)-C(41)-O(3) | 126.5(3) |
| | | O(11)-C(48)-O(12) | 121.2(3) |
| | | O(14)-C(58)-O(13) | 123.3(3) |

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

Table 3. Selected bond distances for **III**, **IV** and **V**

| III | | IV | | V | |
|------------|--------------|---------------|--------------|--------------|--------------|
| Bond | Distance (Å) | Bond | Distance (Å) | Bond | Distance (Å) |
| Zn(1)-O(1) | 2.392(2) | Cd(1)-O(1) | 2.238(2) | Cd(1)-O(1) | 2.340(3) |
| Zn(1)-O(2) | 2.124(2) | Cd(1)-O(1)#1 | 2.238(2) | Cd(1)-O(2) | 2.591(3) |
| Zn(1)-O(3) | 1.996(2) | Cd(1)-O(2) | 2.679(2) | O(2)-Cd(1)#1 | 2.374(3) |
| Zn(1)-O(5) | 2.124(2) | Cd(1)-O(2) #1 | 2.679(2) | Cd(1)-O(2)#1 | 2.374(3) |
| Zn(1)-N(1) | 2.143(2) | Cd(1)-O(2)#2 | 2.381(2) | Cd(1)-O(3) | 2.348(3) |
| Zn(1)-N(2) | 2.158(2) | Cd(1)-O(2)#3 | 2.381(2) | Cd(1)-O(4) | 2.430(3) |
| O(1)-C(21) | 1.245(4) | Cd(1)-O(100) | 2.246(4) | Cd(1)-N(1) | 2.340(3) |
| O(2)-C(21) | 1.267(3) | O(1)-C(1) | 1.249(4) | Cd(1)-N(2) | 2.406(3) |
| O(3)-C(28) | 1.271(3) | O(2)-C(1) | 1.271(4) | O(1)-C(21) | 1.251(5) |
| N(2)-C(10) | 1.330(4) | | | N(1)-C(1) | 1.322(5) |
| N(2)-C(11) | 1.357(4) | | | N(1)-C(12) | 1.359(5) |
| | | | | N(2)-C(10) | 1.329(5) |
| | | | | N(2)-C(11) | 1.356(5) |

Symmetry transformations used to generate equivalent atoms: #1 $x, -y+1/2, -z+1$ #2 $-x+2, y+1/2, z$
 #3 $-x+2, -y, -z+1$ for **IV** and #1 $-x, -y+2, -z+1$ for **V**

Table 7 Selected bond angles for **III**, **IV** and **V**

| III | | IV | | V | |
|-----------------|-----------|---------------------|------------|-------------------|------------|
| Bond | Amplitude | Bond | Amplitude | Bond | Amplitude |
| O(2)-Zn(1)-O(1) | 57.81(7) | O(1)-Cd(1)-O(1)#1 | 163.50(13) | O(1)-Cd(1)-O(2) | 52.73(10) |
| O(3)-Zn(1)-O(1) | 160.36(8) | O(1)-Cd(1)-O(100) | 98.25(6) | O(1)-Cd(1)-O(2)#1 | 124.05(11) |
| O(5)-Zn(1)-O(1) | 83.43(8) | O(1)#1-Cd(1)-O(100) | 98.25(6) | O(1)-Cd(1)-O(3) | 113.98(12) |
| O(3)-Zn(1)-O(2) | 105.23(8) | O(1)#1-Cd(1)-O(2)#2 | 96.30(9) | O(1)-Cd(1)-O(4) | 84.24(11) |
| O(5)-Zn(1)-O(2) | 94.59(8) | O(1)-Cd(1)-O(2)#2 | 84.50(9) | O(2)#1-Cd(1)-O(2) | 78.22(10) |
| O(3)-Zn(1)-O(5) | 88.65(8) | O(100)-Cd(1)-O(2)#2 | 87.22(5) | O(3)-Cd(1)-O(2) | 89.07(10) |
| N(1)-Zn(1)-O(1) | 95.38(8) | O(1)-Cd(1)-O(2)#3 | 96.30(9) | O(3)-Cd(1)-O(2)#1 | 87.00(11) |
| N(2)-Zn(1)-O(1) | 86.70(8) | O(1)#1-Cd(1)-O(2)#3 | 84.50(9) | O(4)-Cd(1)-O(2) | 106.76(10) |
| O(2)-Zn(1)-N(1) | 151.68(8) | O(100)-Cd(1)-O(2)#3 | 87.22(5) | O(2)#1-Cd(1)-O(4) | 140.81(10) |
| O(3)-Zn(1)-N(1) | 102.69(9) | O(2)#2-Cd(1)-O(2)#3 | 174.45(11) | O(3)-Cd(1)-O(4) | 54.86(10) |
| O(3)-Zn(1)-N(2) | 104.59(9) | O(1)-C(1)-O(2) | 121.4(3) | O(1)-Cd(1)-N(1) | 87.36(11) |
| O(5)-Zn(1)-N(2) | 163.74(9) | | | N(1)-Cd(1)-O(2)#1 | 80.92(11) |
| O(4)-C(28)-O(3) | 125.2(3) | | | N(2)-Cd(1)-O(2) | 173.07(10) |
| O(1)-C(21)-O(2) | 121.8(3) | | | N(1)-Cd(1)-O(2) | 105.42(11) |
| | | | | O(2)#1-Cd(1)-N(2) | 95.58(11) |
| | | | | N(1)-Cd(1)-O(3) | 158.65(12) |
| | | | | O(3)-Cd(1)-N(2) | 93.70(11) |
| | | | | N(1)-Cd(1)-O(4) | 131.47(11) |
| | | | | N(2)-Cd(1)-O(4) | 79.98(11) |
| | | | | N(1)-Cd(1)-N(2) | 70.24(12) |
| | | | | O(1)-C(21)-O(2) | 122.2(4) |
| | | | | O(4)-C(31)-O(3) | 122.1(4) |

Symmetry transformations used to generate equivalent atoms: #1 $x, -y+1/2, -z+1$ #2 $-x+2, y+1/2, z$
 #3 $-x+2, -y, -z+1$ for **IV** and #1 $-x, -y+2, -z+1$ for **V**