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# Mixed-metal-organic frameworks (M'MOFs) from 1D to 3D based on the "organic" connectivity with the inorganic connectivity: Syntheses, structures and magnetic properties

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**Table S1** Crystal data and structure refinement details for **1-10.**

| Compound | **1** | **2** | **3** | **4** | **5** |
|---|---|---|---|---|---|
| Empirical formula | $C_{12}H_{24}Ca_2CoN_6O_{24}$ | $C_{12}H_{24}$ $Sr_2CoN_4O_{18}Cl_2$ | $C_{12}H_{24}Ba_2CoN_4O_{18}Cl_2$ | $C_{12}H_{24}Ca_2NiN_6O_{24}$ | $C_{12}H_{24}Sr_2NiN_4O_{18}Cl_2$ |
| Formula weight | 775.46 | 817.42 | 916.86 | 775.24 | 817.20 |
| Crystal system | Triclinic | Triclinic | Triclinic | Triclinic | Triclinic |
| space group | *P*-1 | *P*-1 | *P*-1 | *P*-1 | *P*-1 |
| a (Å) | 6.6762(9) | 6.5863(9) | 6.6953(4) | 6.6503(9) | 6.6133(15) |
| b (Å) | 7.9864(11) | 7.6421(11) | 7.6428(5) | 7.9533(11) | 7.6512(17) |
| c (Å) | 13.7450(19) | 13.809(2) | 14.0935(8) | 13.656(2) | 13.778(3) |
| α (°) | 78.535(2) | 96.335(2) | 96.5830(10) | 78.411(2) | 96.312(4) |
| β (°) | 84.941(2) | 94.647(2) | 95.1290(10) | 84.660(2) | 95.186(3) |
| γ (°) | 76.907(2) | 97.679(2) | 96.1710(10) | 77.080(2) | 97.792(4) |
| V (Å$^3$) | 698.86(17) | 681.37(17) | 708.48(7) | 688.77(17) | 682.6(3) |
| Z | 1 | 1 | 1 | 1 | 1 |
| F000 | 397.0 | 405.0 | 441.0 | 398.0 | 406.0 |
| Goodness-of-fit on F^2 | 1.000 | 1.082 | 1.004 | 1.003 | 1.008 |
| R indices (all data) | $R_1$ =0.0787<br>$wR_2$ =0.1378 | $R_1$ = 0.0585<br>$wR_2$ = 0.0911 | $R_1$ = 0.0197<br>$wR_2$ = 0.0472 | $R_1$ = 0.0429<br>$wR_2$ = 0.1015 | $R_1$ = 0.0473<br>$wR_2$ = 0.0882 |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.0563<br>$wR_2$ = 0.1378 | $R_1$ = 0.0439<br>$wR_2$ = 0.0852 | $R_1$ = 0.0190<br>$wR_2$ = 0.0468 | $R_1$ = 0.0373<br>$wR_2$ = 0.0971 | $R_1$ = 0.0365<br>$wR_2$ = 0.0820 |

| **6** | **7** | **8** | **9** | **10** |
|---|---|---|---|---|
| $C_{12}H_{24}NiBa_2N_4O_{18}Cl_2$ | $C_{12}H_{20}Ca_2CuN_6O_{22}$ | $C_{12}H_{24}Cl_2Sr_2CuN_4O_{18}$ | $C_{12}H_{24}Sr_2CuN_6O_{24}$ | $C_{12}H_{10}Ba_2CuN_4$ $O_{11}Cl$ |
| 916.64 | 744.04 | 822.03 | 875.15 | 759.91 |
| Triclinic | Triclinic | Triclinic | Monoclinic | Monoclinic |
| *P*-1 | *P*-1 | *P*-1 | $P2_1$/n | *C*2/c |
| 6.6818(9) | 7.7073(7) | 6.5961(5) | 14.3621(13) | 18.685(8) |
| 7.6135(10) | 8.5422(8) | 7.7866(6) | 6.9800(6) | 11.722(5) |
| 14.034(2) | 10.0834(9) | 13.4353(11) | 15.7788(15) | 9.244(4) |
| 96.685(2) | 94.5500(10) | 83.4050(10) | 90.00 | 90 |
| 95.671(2) | 105.3350(10) | 80.9610(10) | 114.1210(10) | 91.771(6) |
| 95.868(2) | 95.4270(10) | 81.5450(10) | 90.00 | 90 |
| 700.93(17) | 633.58(10) | 671.10(9) | 1443.7(2) | 2023.8(14) |
| 1 | 1 | 1 | 2 | 4 |
| 442.0 | 379.0 | 407.0 | 870.0 | 1424.0 |
| 1.057 | 1.019 | 1.075 | 1.011 | 1.437 |
| $R_1$ = 0.0353<br>$wR_2$ = 0.0642 | $R_1$ =0.0401<br>$wR_2$ = 0.0895 | $R_1$ = 0.0341<br>$wR_2$ = 0.0701 | $R_1$ = 0.0408<br>$wR_2$ = 0.0819 | *R1* = 0.0693<br>*wR2* = 0.2256 |
| $R_1$ = 0.0318<br>$wR_2$ = 0.0621 | $R_1$ = 0.0356<br>$wR_2$ = 0.0863 | $R_1$ = 0.0287<br>$wR_2$ = 0.0727 | $R_1$ = 0.0299<br>$wR_2$ = 0.0761 | *R1* = 0.0676<br>*wR2* = 0.2223 |

[a] $R = \Sigma|F_0|-|F_C|/\Sigma|F_0|$, $wR_2 = [\Sigma[w(F_0^2-F_C^2)^2]/\Sigma[(F_0^2)^2]]^{1/2}$

**Table S2** Selected bond lengths/Å and bond angles/° in **1-10.**

| Compound **1** | | | |
|---|---|---|---|
| Co(1)-O(1) | 2.066(4) | O(18)-Ca(1)-O(5)#2 | 161.08(15) |
| Co(1)-O(1)#1 | 2.066(4) | O(18)-Ca(1)-O(13) | 90.17(16) |
| Co(1)-N(1)#1 | 2.103(4) | O(5)#2-Ca(1)-O(13) | 97.07(16) |
| Co(1)-N(1) | 2.103(4) | O(18)-Ca(1)-O(11) | 92.40(16) |
| Co(1)-O(7) | 2.113(4) | O(5)#2-Ca(1)-O(11) | 87.02(15) |
| Co(1)-O(7)#1 | 2.113(4) | O(13)-Ca(1)-O(11) | 159.16(17) |
| Ca(1)-O(18) | 2.361(4) | O(18)-Ca(1)-O(5) | 128.98(15) |
| Ca(1)-O(5)#2 | 2.364(4) | O(5)#2-Ca(1)-O(5) | 69.42(14) |
| Ca(1)-O(13) | 2.379(4) | O(13)-Ca(1)-O(5) | 83.75(14) |
| Ca(1)-O(11) | 2.466(5) | O(11)-Ca(1)-O(5) | 78.57(16) |
| Ca(1)-O(5) | 2.479(4) | O(18)-Ca(1)-O(20) | 78.67(14) |
| Ca(1)-O(20) | 2.484(4) | O(5)#2-Ca(1)-O(20) | 82.96(13) |
| Ca(1)-O(10) | 2.511(4) | O(13)-Ca(1)-O(20) | 126.10(14) |
| Ca(1)-O(6) | 2.600(4) | O(11)-Ca(1)-O(20) | 74.62(15) |
| O(5)-Ca(1)#2 | 2.364(4) | O(5)-Ca(1)-O(20) | 142.22(14) |
| O(1)-Co(1)-O(1)#1 | 180 | O(18)-Ca(1)-O(10) | 80.98(16) |
| O(1)-Co(1)-N(1)#1 | 100.85(15) | O(5)#2-Ca(1)-O(10) | 83.96(14) |
| O(1)#1-Co(1)-N(1)#1 | 79.15(15) | O(13)-Ca(1)-O(10) | 75.45(14) |
| O(1)-Co(1)-N(1) | 79.15(15) | O(11)-Ca(1)-O(10) | 125.37(16) |
| O(1)#1-Co(1)-N(1) | 100.85(15) | O(5)-Ca(1)-O(10) | 143.82(14) |
| N(1)#1-Co(1)-N(1) | 180 | O(20)-Ca(1)-O(10) | 50.83(13) |
| O(1)-Co(1)-O(7) | 90.76(15) | O(18)-Ca(1)-O(6) | 77.63(14) |
| O(1)#1-Co(1)-O(7) | 89.24(15) | O(5)#2-Ca(1)-O(6) | 120.81(12) |
| N(1)#1-Co(1)-O(7) | 89.11(16) | O(13)-Ca(1)-O(6) | 79.60(14) |
| N(1)-Co(1)-O(7) | 90.89(16) | O(11)-Ca(1)-O(6) | 80.76(15) |
| O(1)-Co(1)-O(7)#1 | 89.24(15) | O(5)-Ca(1)-O(6) | 51.41(11) |
| O(1)#1-Co(1)-O(7)#1 | 90.76(15) | O(20)-Ca(1)-O(6) | 144.80(14) |
| N(1)#1-Co(1)-O(7)#1 | 90.89(16) | O(10)-Ca(1)-O(6) | 146.88(14) |
| N(1)-Co(1)-O(7)#1 | 89.11(16) | Ca(2)#2-O(1)-Ca(1) | 110.58(14) |
| O(7)-Co(1)-O(7)#1 | 180 | | |

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

| Compound **2** | | | |
|---|---|---|---|
| Sr(1)-O(4)#1 | 2.590(4) | O(2)-Sr(1)-O(3)#2 | 137.99(12) |
| Sr(1)-O(6) | 2.596(4) | O(7)-Sr(1)-O(3)#2 | 141.85(12) |
| Sr(1)-O(2) | 2.601(3) | O(8)-Sr(1)-O(3)#2 | 95.09(11) |
| Sr(1)-O(7) | 2.611(4) | O(9)-Sr(1)-O(3)#2 | 74.93(11) |
| Sr(1)-O(8) | 2.637(3) | O(4)#1-Sr(1)-O(4)#2 | 63.66(13) |
| Sr(1)-O(9) | 2.645(3) | O(6)-Sr(1)-O(4)#2 | 122.84(13) |
| Sr(1)-O(3)#2 | 2.726(4) | O(2)-Sr(1)-O(4)#2 | 138.15(12) |
| Sr(1)-O(4)#2 | 2.749(4) | O(7)-Sr(1)-O(4)#2 | 137.96(13) |
| Sr(1)-O(8)#2 | 2.824(4) | O(8)-Sr(1)-O(4)#2 | 68.44(11) |
| Co(1)-O(1)#3 | 2.075(3) | O(9)-Sr(1)-O(4)#2 | 79.07(11) |
| Co(1)-O(1) | 2.075(3) | O(3)#2-Sr(1)-O(4)#2 | 47.41(11) |
| Co(1)-O(5)#3 | 2.089(4) | O(4)#1-Sr(1)-O(8)#2 | 141.28(11) |

| | | | |
|---|---|---|---|
| Co(1)-O(5) | 2.089(4) | O(6)-Sr(1)-O(8)#2 | 67.79(12) |
| Co(1)-N(1)#3 | 2.120(4) | O(2)-Sr(1)-O(8)#2 | 77.31(11) |
| Co(1)-N(1) | 2.120(4) | O(7)-Sr(1)-O(8)#2 | 134.94(13) |
| O(3)-Sr(1)#2 | 2.726(4) | O(8)-Sr(1)-O(8)#2 | 68.09(13) |
| O(4)-Sr(1)#4 | 2.590(4) | O(9)-Sr(1)-O(8)#2 | 129.71(11) |
| O(4)-Sr(1)#2 | 2.749(4) | O(3)#2-Sr(1)-O(8)#2 | 60.75(11) |
| O(8)-Sr(1)#2 | 2.824(4) | O(4)#2-Sr(1)-O(8)#2 | 87.02(11) |
| O(4)#1-Sr(1)-O(6) | 149.13(12) | O(1)#3-Co(1)-O(1) | 180 |
| O(4)#1-Sr(1)-O(2) | 107.19(12) | O(1)#3-Co(1)-O(5)#3 | 88.34(15) |
| O(6)-Sr(1)-O(2) | 86.73(13) | O(1)-Co(1)-O(5)#3 | 91.66(15) |
| O(4)#1-Sr(1)-O(7) | 78.76(14) | O(1)#3-Co(1)-O(5) | 91.66(15) |
| O(6)-Sr(1)-O(7) | 81.03(16) | O(1)-Co(1)-O(5) | 88.34(15) |
| O(2)-Sr(1)-O(7) | 68.95(12) | O(5)#3-Co(1)-O(5) | 180 |
| O(4)#1-Sr(1)-O(8) | 77.43(12) | O(1)#3-Co(1)-N(1)#3 | 78.26(14) |
| O(6)-Sr(1)-O(8) | 133.40(12) | O(1)-Co(1)-N(1)#3 | 101.74(14) |
| O(2)-Sr(1)-O(8) | 69.71(11) | O(5)#3-Co(1)-N(1)#3 | 92.39(16) |
| O(7)-Sr(1)-O(8) | 122.65(13) | O(5)-Co(1)-N(1)#3 | 87.61(16) |
| O(4)#1-Sr(1)-O(9) | 71.60(12) | O(1)#3-Co(1)-N(1) | 101.74(14) |
| O(6)-Sr(1)-O(9) | 79.97(12) | O(1)-Co(1)-N(1) | 78.26(14) |
| O(2)-Sr(1)-O(9) | 139.65(11) | O(5)#3-Co(1)-N(1) | 87.61(16) |
| O(7)-Sr(1)-O(9) | 71.41(11) | O(5)-Co(1)-N(1) | 92.39(16) |
| O(8)-Sr(1)-O(9) | 142.53(12) | N(1)#3-Co(1)-N(1) | 180 |
| O(4)#1-Sr(1)-O(3)#2 | 107.10(12) | Sr(1)#4-O(4)-Sr(1)#2 | 116.34(13) |
| O(6)-Sr(1)-O(3)#2 | 75.89(13) | Sr(1)-O(8)-Sr(1)#2 | 111.91(13) |

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 -x+1,-y+1,-z #3 -x+1,-y+1,-z+1 #4 x-1,y,z #5 -x+2,-y+1,-z

Compound **3**

| | | | |
|---|---|---|---|
| Ba(1)-O(1)#1 | 2.733(3) | O(5)-Ba(1)-O(8) | 142.99(11) |
| Ba(1)-O(9)#2 | 2.746(3) | O(6)-Ba(1)-O(8) | 94.28(9) |
| Ba(1)-O(4) | 2.786(3) | O(7)-Ba(1)-O(8) | 76.21(11) |
| Ba(1)-O(5) | 2.788(4) | O(1)#1-Ba(1)-O(6)#1 | 80.74(9) |
| Ba(1)-O(6) | 2.811(3) | O(9)#2-Ba(1)-O(6)#1 | 142.55(9) |
| Ba(1)-O(7) | 2.855(4) | O(4)-Ba(1)-O(6)#1 | 132.79(9) |
| Ba(1)-O(8) | 2.856(3) | O(5)-Ba(1)-O(6)#1 | 133.66(11) |
| Ba(1)-O(6)#1 | 2.895(3) | O(6)-Ba(1)-O(6)#1 | 71.56(10) |
| Ba(1)-O(9) | 2.909(3) | O(7)-Ba(1)-O(6)#1 | 68.10(9) |
| Co(1)-O(2)#3 | 2.069(3) | O(8)-Ba(1)-O(6)#1 | 61.76(9) |
| Co(1)-O(2) | 2.069(3) | O(1)#1-Ba(1)-O(9) | 134.42(9) |
| Co(1)-O(3)#3 | 2.106(3) | O(9)#2-Ba(1)-O(9) | 64.64(10) |
| Co(1)-O(3) | 2.106(3) | O(4)-Ba(1)-O(9) | 81.82(9) |
| Co(1)-N(1)#3 | 2.117(3) | O(5)-Ba(1)-O(9) | 141.04(11) |
| Co(1)-N(1) | 2.117(3) | O(6)-Ba(1)-O(9) | 65.27(9) |
| O(1)-Ba(1)#1 | 2.733(3) | O(7)-Ba(1)-O(9) | 120.61(11) |
| O(6)-Ba(1)#1 | 2.895(3) | O(8)-Ba(1)-O(9) | 44.69(8) |
| O(9)-Ba(1)#2 | 2.746(3) | O(6)#1-Ba(1)-O(9) | 85.25(8) |
| O(1)#1-Ba(1)-O(9)#2 | 104.07(10) | O(2)#3-Co(1)-O(2) | 180 |
| O(1)#1-Ba(1)-O(4) | 137.05(9) | O(2)#3-Co(1)-O(3)#3 | 88.85(12) |
| O(9)#2-Ba(1)-O(4) | 67.09(9) | O(2)-Co(1)-O(3)#3 | 91.15(12) |

| | | | |
|---|---|---|---|
| O(1)#1-Ba(1)-O(5) | 67.19(11) | O(2)#3-Co(1)-O(3) | 91.15(12) |
| O(9)#2-Ba(1)-O(5) | 79.63(11) | O(2)-Co(1)-O(3) | 88.85(12) |
| O(4)-Ba(1)-O(5) | 69.86(11) | O(3)#3-Co(1)-O(3) | 180 |
| O(1)#1-Ba(1)-O(6) | 69.15(9) | O(2)#3-Co(1)-N(1)#3 | 78.29(12) |
| O(9)#2-Ba(1)-O(6) | 75.64(9) | O(2)-Co(1)-N(1)#3 | 101.71(12) |
| O(4)-Ba(1)-O(6) | 138.25(9) | O(3)#3-Co(1)-N(1)#3 | 91.68(13) |
| O(5)-Ba(1)-O(6) | 121.77(11) | O(3)-Co(1)-N(1)#3 | 88.32(13) |
| O(1)#1-Ba(1)-O(7) | 93.67(11) | O(2)#3-Co(1)-N(1) | 101.71(12) |
| O(9)#2-Ba(1)-O(7) | 146.10(9) | O(2)-Co(1)-N(1) | 78.29(12) |
| O(4)-Ba(1)-O(7) | 80.18(9) | O(3)#3-Co(1)-N(1) | 88.32(13) |
| O(5)-Ba(1)-O(7) | 81.09(12) | O(3)-Co(1)-N(1) | 91.68(13) |
| O(6)-Ba(1)-O(7) | 138.19(9) | N(1)#3-Co(1)-N(1) | 180 |
| O(1)#1-Ba(1)-O(8) | 142.35(9) | Ba(1)-O(6)-Ba(1)#1 | 108.44(10) |
| O(9)#2-Ba(1)-O(8) | 103.96(9) | Ba(1)#2-O(9)-Ba(1) | 115.36(10) |
| O(4)-Ba(1)-O(8) | 77.68(9) | | |

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1 #2 -x,-y+2,-z+1 #3 -x+1,-y+2,-z+2

Compound **4**

| | | | |
|---|---|---|---|
| Ni(1)-N(2)#1 | 2.040(2) | O(6)-Ca(1)-O(4)#2 | 161.16(8) |
| Ni(1)-N(2) | 2.040(2) | O(6)-Ca(1)-O(7) | 89.13(9) |
| Ni(1)-O(1)#1 | 2.052(2) | O(4)#2-Ca(1)-O(7) | 97.85(8) |
| Ni(1)-O(1) | 2.052(2) | O(6)-Ca(1)-O(5) | 93.43(10) |
| Ni(1)-O(11)#1 | 2.101(2) | O(4)#2-Ca(1)-O(5) | 86.34(9) |
| Ni(1)-O(11) | 2.101(2) | O(7)-Ca(1)-O(5) | 158.90(10) |
| Ca(1)-O(6) | 2.357(2) | O(6)-Ca(1)-O(4) | 128.93(8) |
| Ca(1)-O(4)#2 | 2.3602(19) | O(4)#2-Ca(1)-O(4) | 69.44(7) |
| Ca(1)-O(7) | 2.371(2) | O(7)-Ca(1)-O(4) | 84.28(8) |
| Ca(1)-O(5) | 2.448(3) | O(5)-Ca(1)-O(4) | 77.83(10) |
| Ca(1)-O(4) | 2.472(2) | O(6)-Ca(1)-O(8) | 78.82(8) |
| Ca(1)-O(8) | 2.476(2) | O(4)#2-Ca(1)-O(8) | 82.96(7) |
| Ca(1)-O(10) | 2.504(2) | O(7)-Ca(1)-O(8) | 126.15(8) |
| Ca(1)-O(3) | 2.592(2) | O(5)-Ca(1)-O(8) | 74.81(10) |
| O(4)-Ca(1)#2 | 2.3602(19) | O(4)-Ca(1)-O(8) | 142.04(7) |
| N(2)#1-Ni(1)-N(2) | 180 | O(6)-Ca(1)-O(10) | 80.90(9) |
| N(2)#1-Ni(1)-O(1)#1 | 80.76(8) | O(4)#2-Ca(1)-O(10) | 83.90(8) |
| N(2)-Ni(1)-O(1)#1 | 99.24(8) | O(7)-Ca(1)-O(10) | 75.66(8) |
| N(2)#1-Ni(1)-O(1) | 99.24(8) | O(5)-Ca(1)-O(10) | 125.43(10) |
| N(2)-Ni(1)-O(1) | 80.76(8) | O(4)-Ca(1)-O(10) | 144.02(8) |
| O(1)#1-Ni(1)-O(1) | 180 | O(8)-Ca(1)-O(10) | 50.75(7) |
| N(2)#1-Ni(1)-O(11)#1 | 90.98(9) | O(6)-Ca(1)-O(3) | 77.76(8) |
| N(2)-Ni(1)-O(11)#1 | 89.02(9) | O(4)#2-Ca(1)-O(3) | 120.63(7) |
| O(1)#1-Ni(1)-O(11)#1 | 91.48(8) | O(7)-Ca(1)-O(3) | 79.64(8) |
| O(1)-Ni(1)-O(11)#1 | 88.52(8) | O(5)-Ca(1)-O(3) | 80.45(9) |
| N(2)#1-Ni(1)-O(11) | 89.02(9) | O(4)-Ca(1)-O(3) | 51.22(6) |
| N(2)-Ni(1)-O(11) | 90.98(9) | O(8)-Ca(1)-O(3) | 144.57(8) |
| O(1)#1-Ni(1)-O(11) | 88.52(8) | O(10)-Ca(1)-O(3) | 147.40(7) |
| O(1)-Ni(1)-O(11) | 91.48(8) | Ca(1)#2-O(4)-Ca(1) | 110.56(7) |
| O(112)#1-Ni(1)-O(11) | 180 | | |

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

Compound **5**

| | | | |
|---|---|---|---|
| Sr(1)-O(4)#1 | 2.597(4) | O(7)-Sr(1)-O(3)#2 | 94.72(13) |
| Sr(1)-O(2) | 2.608(3) | O(8)-Sr(1)-O(3)#2 | 75.70(13) |
| Sr(1)-O(7) | 2.614(4) | O(6)-Sr(1)-O(3)#2 | 142.09(13) |
| Sr(1)-O(8) | 2.619(5) | O(9)-Sr(1)-O(3)#2 | 74.78(12) |
| Sr(1)-O(6) | 2.619(4) | O(4)#1-Sr(1)-O(4)#2 | 63.61(14) |
| Sr(1)-O(9) | 2.658(4) | O(2)-Sr(1)-O(4)#2 | 138.15(12) |
| Sr(1)-O(3)#2 | 2.730(4) | O(7)-Sr(1)-O(4)#2 | 67.65(13) |
| Sr(1)-O(4)#2 | 2.769(4) | O(8)-Sr(1)-O(4)#2 | 122.94(13) |
| Sr(1)-O(7)#2 | 2.848(4) | O(6)-Sr(1)-O(4)#2 | 137.76(13) |
| Ni(1)-O(1) | 2.055(3) | O(9)-Sr(1)-O(4)#2 | 79.14(12) |
| Ni(1)-O(1)#4 | 2.055(3) | O(3)#2-Sr(1)-O(4)#2 | 47.64(11) |
| Ni(1)-N(1) | 2.059(4) | O(4)#1-Sr(1)-O(7)#2 | 141.50(12) |
| Ni(1)-N(1)#4 | 2.059(4) | O(2)-Sr(1)-O(7)#2 | 77.35(13) |
| Ni(1)-O(5) | 2.086(4) | O(7)-Sr(1)-O(7)#2 | 67.87(15) |
| Ni(1)-O(5)#4 | 2.086(4) | O(8)-Sr(1)-O(7)#2 | 67.59(13) |
| O(1)-Sr(1)#2 | 2.730(4) | O(6)-Sr(1)-O(7)#2 | 135.05(13) |
| O(4)-Sr(1)#5 | 2.597(4) | O(9)-Sr(1)-O(7)#2 | 130.04(13) |
| O(4)-Sr(1)#2 | 2.769(4) | O(3)#2-Sr(1)-O(7)#2 | 61.13(12) |
| O(7)-Sr(1)#2 | 2.848(4) | O(4)#2-Sr(1)-O(7)#2 | 87.16(11) |
| O(4)#1-Sr(1)-O(2) | 107.22(13) | O(1)-Ni(1)-O(1)#4 | 180 |
| O(4)#1-Sr(1)-O(7) | 77.62(13) | O(1)-Ni(1)-N(1) | 80.09(14) |
| O(2)-Sr(1)-O(7) | 70.49(13) | O(1)#4-Ni(1)-N(1) | 99.91(14) |
| O(4)#1-Sr(1)-O(8) | 149.11(13) | O(1)-Ni(1)-N(1)#4 | 99.91(14) |
| O(2)-Sr(1)-O(8) | 86.67(14) | O(1)#4-Ni(1)-N(1)#4 | 80.09(14) |
| O(7)-Sr(1)-O(8) | 133.26(13) | N(1)-Ni(1)-N(1)#4 | 180 |
| O(4)#1-Sr(1)-O(6) | 78.23(14) | O(1)-Ni(1)-O(5) | 89.11(14) |
| O(2)-Sr(1)-O(6) | 68.50(12) | O(1)#4-Ni(1)-O(5) | 90.89(14) |
| O(7)-Sr(1)-O(6) | 122.69(15) | N(1)-Ni(1)-O(5) | 91.30(16) |
| O(8)-Sr(1)-O(6) | 81.76(16) | N(1)#4-Ni(1)-O(5) | 88.70(16) |
| O(4)#1-Sr(1)-O(9) | 71.16(13) | O(1)-Ni(1)-O(5)#4 | 90.89(14) |
| O(2)-Sr(1)-O(9) | 139.41(12) | O(1)#4-Ni(1)-O(5)#4 | 89.11(14) |
| O(7)-Sr(1)-O(9) | 141.97(12) | N(1)-Ni(1)-O(5)#4 | 88.70(16) |
| O(8)-Sr(1)-O(9) | 80.34(13) | N(1)#4-Ni(1)-O(5)#4 | 91.30(16) |
| O(6)-Sr(1)-O(9) | 71.64(13) | O(5)-Ni(1)-O(5)#4 | 180 |
| O(4)#1-Sr(1)-O(3)#2 | 107.01(11) | Sr(1)#5-O(4)-Sr(1)#2 | 116.39(14) |
| O(2)-Sr(1)-O(3)#2 | 138.40(12) | Sr(1)-O(7)-Sr(1)#2 | 112.13(15) |

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z  #2 -x,-y+2,-z+1  #3 -x-1,-y+2,-z+1  #4 -x,-y+2,-z  #5 x+1,y,z

Compound **6**

| | | | |
|---|---|---|---|
| Ba(1)-O(4)#1 | 2.732(4) | O(6)-Ba(1)-O(3)#2 | 77.35(11) |
| Ba(1)-O(2) | 2.738(3) | O(9)-Ba(1)-O(3)#2 | 142.50(12) |
| Ba(1)-O(6) | 2.781(3) | O(7)-Ba(1)-O(3)#2 | 94.16(10) |
| Ba(1)-O(9) | 2.792(4) | O(8)-Ba(1)-O(3)#2 | 75.54(12) |
| Ba(1)-O(7) | 2.816(3) | O(4)#1-Ba(1)-O(7)#2 | 142.65(10) |

| | | | |
|---|---|---|---|
| Ba(1)-O(8) | 2.852(4) | O(2)-Ba(1)-O(7)#2 | 81.04(11) |
| Ba(1)-O(3)#2 | 2.855(4) | O(6)-Ba(1)-O(7)#2 | 132.68(10) |
| Ba(1)-O(7)#2 | 2.886(4) | O(9)-Ba(1)-O(7)#2 | 133.46(13) |
| Ba(1)-O(4)#2 | 2.925(4) | O(7)-Ba(1)-O(7)#2 | 71.62(12) |
| Ba(1)-C(7)#2 | 3.242(5) | O(8)-Ba(1)-O(7)#2 | 68.32(11) |
| Ni(1)-O(1) | 2.049(3) | O(3)#2-Ba(1)-O(7)#2 | 61.95(11) |
| Ni(1)-O(1)#3 | 2.049(3) | O(4)#1-Ba(1)-O(4)#2 | 64.44(12) |
| Ni(1)-N(1)#3 | 2.058(4) | O(2)-Ba(1)-O(4)#2 | 134.14(11) |
| Ni(1)-N(1) | 2.058(4) | O(6)-Ba(1)-O(4)#2 | 81.79(11) |
| Ni(1)-O(5)#3 | 2.083(4) | O(9)-Ba(1)-O(4)#2 | 141.14(13) |
| Ni(1)-O(5) | 2.083(4) | O(7)-Ba(1)-O(4)#2 | 64.80(10) |
| O(3)-Ba(1)#2 | 2.855(4) | O(8)-Ba(1)-O(4)#2 | 120.08(11) |
| O(4)-Ba(1)#4 | 2.732(4) | O(3)#2-Ba(1)-O(4)#2 | 44.85(10) |
| O(4)-Ba(1)#2 | 2.925(4) | O(7)#2-Ba(1)-O(4)#2 | 85.34(10) |
| O(7)-Ba(1)#2 | 2.886(4) | O(1)-Ni(1)-O(1)#3 | 180 |
| O(4)#1-Ba(1)-O(2) | 103.90(12) | O(1)-Ni(1)-N(1)#3 | 99.98(15) |
| O(4)#1-Ba(1)-O(6) | 66.91(11) | O(1)#3-Ni(1)-N(1)#3 | 80.02(14) |
| O(2)-Ba(1)-O(6) | 137.05(11) | O(1)-Ni(1)-N(1) | 80.02(15) |
| O(4)#1-Ba(1)-O(9) | 79.93(13) | O(1)#3-Ni(1)-N(1) | 99.98(15) |
| O(2)-Ba(1)-O(9) | 67.24(11) | N(1)#3-Ni(1)-N(1) | 180 |
| O(6)-Ba(1)-O(9) | 69.83(11) | O(1)-Ni(1)-O(5)#3 | 89.09(14) |
| O(4)#1-Ba(1)-O(7) | 75.67(11) | O(1)#3-Ni(1)-O(5)#3 | 90.91(14) |
| O(2)-Ba(1)-O(7) | 69.34(11) | N(1)#3-Ni(1)-O(5)#3 | 89.19(15) |
| O(6)-Ba(1)-O(7) | 137.97(11) | N(1)-Ni(1)-O(5)#3 | 90.81(15) |
| O(9)-Ba(1)-O(7) | 122.36(13) | O(1)-Ni(1)-O(5) | 90.91(14) |
| O(4)#1-Ba(1)-O(8) | 145.39(12) | O(1)#3-Ni(1)-O(5) | 89.09(14) |
| O(2)-Ba(1)-O(8) | 94.88(13) | N(1)#3-Ni(1)-O(5) | 90.81(15) |
| O(6)-Ba(1)-O(8) | 79.48(11) | N(1)-Ni(1)-O(5) | 89.19(15) |
| O(9)-Ba(1)-O(8) | 81.00(15) | O(5)#3-Ni(1)-O(5) | 180 |
| O(7)-Ba(1)-O(8) | 138.77(11) | Ba(1)#4-O(4)-Ba(1)#2 | 115.56(12) |
| O(4)#1-Ba(1)-O(3)#2 | 103.70(11) | Ba(1)-O(7)-Ba(1)#2 | 108.38(12) |
| O(2)-Ba(1)-O(3)#2 | 142.82(12) | | |

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 -x+1,-y+1,-z+1 #3 -x+1,-y+1,-z #4 x+1,y,z #5 -x,-y+1,-z+1

Compound **7**

| | | | |
|---|---|---|---|
| Cu(1)-O(1)#1 | 1.9645(18) | O(3)#2-Ca(1)-O(11) | 85.98(9) |
| Cu(1)-O(1) | 1.9645(18) | O(9)-Ca(1)-O(11) | 156.00(9) |
| Cu(1)-N(1) | 1.990(2) | O(3)#2-Ca(1)-O(10) | 164.78(7) |
| Cu(1)-N(1)#1 | 1.990(2) | O(9)-Ca(1)-O(10) | 95.46(8) |
| Cu(1)-O(5) | 2.538(2) | O(11)-Ca(1)-O(10) | 95.93(9) |
| Ca(1)-O(3)#2 | 2.3203(19) | O(3)#2-Ca(1)-O(8) | 84.24(8) |
| Ca(1)-O(9) | 2.366(2) | O(9)-Ca(1)-O(8) | 77.14(7) |
| Ca(1)-O(11) | 2.380(2) | O(11)-Ca(1)-O(8) | 125.34(8) |
| Ca(1)-O(10) | 2.387(2) | O(10)-Ca(1)-O(8) | 82.35(8) |
| Ca(1)-O(8) | 2.515(2) | O(3)#2-Ca(1)-O(4) | 122.48(7) |
| Ca(1)-O(4) | 2.549(2) | O(9)-Ca(1)-O(4) | 83.98(8) |
| Ca(1)-O(6) | 2.566(2) | O(11)-Ca(1)-O(4) | 79.39(8) |

| | | | |
|---|---|---|---|
| Ca(1)-O(3) | 2.584(2) | O(10)-Ca(1)-O(4) | 72.63(7) |
| Ca(1)-C(6) | 2.903(3) | O(8)-Ca(1)-O(4) | 146.94(8) |
| Ca(1)-N(3) | 2.949(2) | O(3)#2-Ca(1)-O(6) | 80.12(7) |
| O(3)-Ca(1)#2 | 2.3203(19) | O(9)-Ca(1)-O(6) | 126.54(7) |
| O(1)#1-Cu(1)-O(1) | 180 | O(11)-Ca(1)-O(6) | 75.39(8) |
| O(1)#1-Cu(1)-N(1) | 96.91(8) | O(10)-Ca(1)-O(6) | 85.74(7) |
| O(1)-Cu(1)-N(1) | 83.09(8) | O(8)-Ca(1)-O(6) | 49.96(7) |
| O(1)#1-Cu(1)-N(1)#1 | 83.09(8) | O(4)-Ca(1)-O(6) | 144.68(7) |
| O(1)-Cu(1)-N(1)#1 | 96.91(8) | O(3)#2-Ca(1)-O(3) | 71.95(7) |
| N(1)-Cu(1)-N(1)#1 | 180 | O(9)-Ca(1)-O(3) | 79.43(7) |
| O(1)#1-Cu(1)-O(5) | 91.70(7) | O(11)-Ca(1)-O(3) | 76.65(8) |
| O(1)-Cu(1)-O(5) | 88.30(7) | O(10)-Ca(1)-O(3) | 123.21(7) |
| N(1)-Cu(1)-O(5) | 89.18(8) | O(8)-Ca(1)-O(3) | 146.82(7) |
| N(1)#1-Cu(1)-O(5) | 90.82(8) | O(4)-Ca(1)-O(3) | 50.59(6) |
| O(3)#2-Ca(1)-O(9) | 88.53(8) | O(6)-Ca(1)-O(3) | 141.47(7) |
| Cu(1)-O(1)#1 | 1.9645(18) | O(3)#2-Ca(1)-O(11) | 85.98(9) |
| Cu(1)-O(1) | 1.9645(18) | O(9)-Ca(1)-O(11) | 156.00(9) |
| Cu(1)-N(1) | 1.990(2) | O(3)#2-Ca(1)-O(10) | 164.78(7) |
| Cu(1)-N(1)#1 | 1.990(2) | O(9)-Ca(1)-O(10) | 95.46(8) |

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

Compound **8**

| | | | |
|---|---|---|---|
| Sr(1)-O(2) | 2.508(3) | O(9)-Sr(1)-O(1) | 144.65(9) |
| Sr(1)-O(7) | 2.519(3) | O(6)#2-Sr(1)-O(1) | 140.68(11) |
| Sr(1)-O(4)#1 | 2.612(2) | O(4)-Sr(1)-O(1) | 76.12(11) |
| Sr(1)-O(9) | 2.625(3) | O(2)-Sr(1)-O(9)#2 | 71.85(10) |
| Sr(1)-O(6)#2 | 2.647(2) | O(7)-Sr(1)-O(9)#2 | 134.40(8) |
| Sr(1)-O(4) | 2.649(2) | O(4)#1-Sr(1)-O(9)#2 | 137.90(8) |
| Sr(1)-O(1) | 2.713(3) | O(9)-Sr(1)-O(9)#2 | 67.06(10) |
| Sr(1)-O(9)#2 | 2.854(3) | O(6)#2-Sr(1)-O(9)#2 | 74.94(8) |
| Sr(1)-O(3) | 2.921(2) | O(4)-Sr(1)-O(9)#2 | 86.42(8) |
| Cu(1)-O(5)#3 | 1.981(2) | O(1)-Sr(1)-O(9)#2 | 128.98(13) |
| Cu(1)-O(5) | 1.981(2) | O(2)-Sr(1)-O(3) | 73.83(9) |
| Cu(1)-N(1)#3 | 1.995(3) | O(7)-Sr(1)-O(3) | 142.90(8) |
| Cu(1)-N(1) | 1.995(3) | O(4)#1-Sr(1)-O(3) | 109.26(7) |
| Cu(1)-Cl(1) | 2.7480(10) | O(9)-Sr(1)-O(3) | 96.28(8) |
| Cu(1)-Cl(1)#3 | 2.7480(10) | O(6)#2-Sr(1)-O(3) | 133.03(8) |
| O(4)-Sr(1)#1 | 2.612(2) | O(4)-Sr(1)-O(3) | 46.49(7) |
| O(6)-Sr(1)#2 | 2.647(2) | O(1)-Sr(1)-O(3) | 75.59(13) |
| O(9)-Sr(1)#2 | 2.854(3) | O(9)#2-Sr(1)-O(3) | 58.49(7) |
| O(2)-Sr(1)-O(7) | 79.22(9) | O(5)#3-Cu(1)-O(5) | 180 |
| O(2)-Sr(1)-O(4)#1 | 148.12(11) | O(5)#3-Cu(1)-N(1)#3 | 82.02(10) |
| O(7)-Sr(1)-O(4)#1 | 81.44(8) | O(5)-Cu(1)-N(1)#3 | 97.98(10) |
| O(2)-Sr(1)-O(9) | 136.27(11) | O(5)#3-Cu(1)-N(1) | 97.98(10) |
| O(7)-Sr(1)-O(9) | 120.81(9) | O(5)-Cu(1)-N(1) | 82.02(10) |
| O(4)#1-Sr(1)-O(9) | 75.58(8) | N(1)#3-Cu(1)-N(1) | 180 |
| O(2)-Sr(1)-O(6)#2 | 87.11(11) | O(5)#3-Cu(1)-Cl(1) | 94.34(8) |
| O(7)-Sr(1)-O(6)#2 | 69.04(8) | O(5)-Cu(1)-Cl(1) | 85.66(8) |

| | | | |
|---|---|---|---|
| O(4)#1-Sr(1)-O(6)#2 | 109.19(8) | N(1)#3-Cu(1)-Cl(1) | 91.34(8) |
| O(9)-Sr(1)-O(6)#2 | 68.63(8) | N(1)-Cu(1)-Cl(1) | 88.66(8) |
| O(2)-Sr(1)-O(4) | 118.31(9) | O(5)#3-Cu(1)-Cl(1)#3 | 85.66(8) |
| O(7)-Sr(1)-O(4) | 138.91(8) | O(5)-Cu(1)-Cl(1)#3 | 94.34(8) |
| O(4)#1-Sr(1)-O(4) | 64.53(8) | N(1)#3-Cu(1)-Cl(1)#3 | 88.66(8) |
| O(9)-Sr(1)-O(4) | 73.81(8) | N(1)-Cu(1)-Cl(1)#3 | 91.34(8) |
| O(6)#2-Sr(1)-O(4) | 142.14(8) | Cl(1)-Cu(1)-Cl(1)#3 | 180 |
| O(2)-Sr(1)-O(1) | 75.28(13) | Sr(1)#1-O(4)-Sr(1) | 115.47(8) |
| O(7)-Sr(1)-O(1) | 73.22(13) | Sr(1)-O(9)-Sr(1)#2 | 112.94(10) |
| O(4)#1-Sr(1)-O(1) | 74.99(11) | | |

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x,-y+1,-z+1 #3 -x,-y+1,-z+2

Compound **9**

| | | | |
|---|---|---|---|
| O(1)-Cu(2) | 1.933(3) | O(3)#1-Sr(1)-O(8) | 90.46(11) |
| Sr(1)-O(4) | 2.553(3) | O(4)-Sr(1)-O(6) | 86.54(12) |
| Sr(1)-O(9) | 2.574(3) | O(9)-Sr(1)-O(6) | 77.33(13) |
| Sr(1)-O(11) | 2.612(3) | O(11)-Sr(1)-O(6) | 121.34(10) |
| Sr(1)-O(10) | 2.631(3) | O(10)-Sr(1)-O(6) | 89.74(12) |
| Sr(1)-O(3)#1 | 2.634(3) | O(3)#1-Sr(1)-O(6) | 153.08(11) |
| Sr(1)-O(8) | 2.653(3) | O(8)-Sr(1)-O(6) | 80.08(12) |
| Sr(1)-O(6) | 2.675(3) | O(4)-Sr(1)-O(5) | 76.65(10) |
| Sr(1)-O(5) | 2.781(3) | O(9)-Sr(1)-O(5) | 113.11(12) |
| Sr(1)-O(4)#1 | 2.799(3) | O(11)-Sr(1)-O(5) | 75.37(9) |
| Cu(2)-O(1)#2 | 1.933(3) | O(10)-Sr(1)-O(5) | 73.31(12) |
| Cu(2)-N(1)#2 | 1.978(3) | O(3)#1-Sr(1)-O(5) | 150.39(10) |
| Cu(2)-N(1) | 1.978(3) | O(8)-Sr(1)-O(5) | 119.15(11) |
| O(4)-Sr(1)#1 | 2.799(3) | O(6)-Sr(1)-O(5) | 45.97(10) |
| O(3)-Sr(1)#1 | 2.634(3) | O(4)-Sr(1)-O(4)#1 | 67.10(10) |
| O(4)-Sr(1)-O(9) | 141.05(10) | O(9)-Sr(1)-O(4)#1 | 114.68(11) |
| O(4)-Sr(1)-O(11) | 78.57(9) | O(11)-Sr(1)-O(4)#1 | 67.95(8) |
| O(9)-Sr(1)-O(11) | 139.87(10) | O(10)-Sr(1)-O(4)#1 | 119.05(10) |
| O(4)-Sr(1)-O(10) | 141.30(11) | O(3)#1-Sr(1)-O(4)#1 | 48.12(8) |
| O(9)-Sr(1)-O(10) | 74.56(11) | O(8)-Sr(1)-O(4)#1 | 79.94(10) |
| O(11)-Sr(1)-O(10) | 70.73(10) | O(6)-Sr(1)-O(4)#1 | 150.46(11) |
| O(4)-Sr(1)-O(3)#1 | 115.14(9) | O(5)-Sr(1)-O(4)#1 | 132.20(10) |
| O(9)-Sr(1)-O(3)#1 | 75.75(11) | O(1)#2-Cu(2)-O(1) | 180 |
| O(11)-Sr(1)-O(3)#1 | 80.47(9) | O(1)#2-Cu(2)-N(1)#2 | 83.86(12) |
| O(10)-Sr(1)-O(3)#1 | 82.79(11) | O(1)-Cu(2)-N(1)#2 | 96.14(12) |
| O(4)-Sr(1)-O(8) | 73.88(9) | O(1)#2-Cu(2)-N(1) | 96.14(12) |
| O(9)-Sr(1)-O(8) | 68.58(10) | O(1)-Cu(2)-N(1) | 83.86(12) |
| O(11)-Sr(1)-O(8) | 143.88(9) | N(1)#2-Cu(2)-N(1) | 180 |
| O(10)-Sr(1)-O(8) | 143.06(11) | Sr(1)-O(4)-Sr(1)#1 | 112.90(10) |

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

Compound **10**

| | | | |
|---|---|---|---|
| Ba(1)-O(4)#1 | 2.705(8) | O(4)#1-Ba(1)-O(5) | 84.1(2) |
| Ba(1)-O(3)#2 | 2.782(8) | O(3)#2-Ba(1)-O(5) | 70.9(3) |

| | | | |
|---|---|---|---|
| Ba(1)-O(2) | 2.816(8) | O(2)-Ba(1)-O(5) | 131.7(3) |
| Ba(1)-O(2)#1 | 2.830(8) | O(2)#1-Ba(1)-O(5) | 76.1(2) |
| Ba(1)-O(4)#3 | 2.960(8) | O(4)#3-Ba(1)-O(5) | 153.9(2) |
| Ba(1)-O(3)#3 | 2.968(9) | O(3)#3-Ba(1)-O(5) | 133.9(2) |
| Ba(1)-O(5) | 3.030(8) | O(4)#1-Ba(1)-O(6) | 141.67(18) |
| Ba(1)-O(6) | 3.165(6) | O(3)#2-Ba(1)-O(6) | 69.1(2) |
| Ba(1)-C(6)#3 | 3.318(11) | O(2)-Ba(1)-O(6) | 122.31(17) |
| Ba(1)-Cl(1) | 3.533(8) | O(2)#1-Ba(1)-O(6) | 141.3(2) |
| Cu(1)-O(1) | 1.942(7) | O(4)#3-Ba(1)-O(6) | 110.32(17) |
| Cu(1)-O(1)#4 | 1.942(7) | O(3)#3-Ba(1)-O(6) | 67.01(19) |
| Cu(1)-N(1) | 2.003(9) | O(5)-Ba(1)-O(6) | 81.07(19) |
| Cu(1)-N(1)#4 | 2.003(9) | O(4)#1-Ba(1)-C(6)#3 | 88.4(2) |
| O(6)-Ba(1)#5 | 3.165(6) | O(3)#2-Ba(1)-C(6)#3 | 79.9(3) |
| O(2)-Ba(1)#1 | 2.830(8) | O(2)-Ba(1)-C(6)#3 | 76.9(2) |
| C(6)-Ba(1)#6 | 3.318(11) | O(2)#1-Ba(1)-C(6)#3 | 125.9(2) |
| O(4)-Ba(1)#1 | 2.705(8) | O(4)#3-Ba(1)-C(6)#3 | 22.7(2) |
| O(4)-Ba(1)#6 | 2.960(8) | O(3)#3-Ba(1)-C(6)#3 | 21.8(2) |
| O(3)-Ba(1)#2 | 2.782(8) | O(5)-Ba(1)-C(6)#3 | 150.8(2) |
| O(3)-Ba(1)#6 | 2.968(9) | O(6)-Ba(1)-C(6)#3 | 87.7(2) |
| Cl(1)-Ba(1)#1 | 3.533(8) | O(4)#1-Ba(1)-Cl(1) | 125.53(19) |
| O(4)#1-Ba(1)-O(3)#2 | 72.6(2) | O(3)#2-Ba(1)-Cl(1) | 146.9(2) |
| O(4)#1-Ba(1)-O(2) | 93.7(2) | O(2)-Ba(1)-Cl(1) | 59.4(2) |
| O(3)#2-Ba(1)-O(2) | 153.3(3) | O(2)#1-Ba(1)-Cl(1) | 59.34(19) |
| O(4)#1-Ba(1)-O(2)#1 | 66.2(2) | O(4)#3-Ba(1)-Cl(1) | 119.96(16) |
| O(3)#2-Ba(1)-O(2)#1 | 129.0(2) | O(3)#3-Ba(1)-Cl(1) | 125.6(2) |
| O(2)-Ba(1)-O(2)#1 | 59.4(3) | O(5)-Ba(1)-Cl(1) | 82.97(19) |
| O(4)#1-Ba(1)-O(4)#3 | 72.5(2) | O(6)-Ba(1)-Cl(1) | 87.41(17) |
| O(3)#2-Ba(1)-O(4)#3 | 90.7(3) | C(6)#3-Ba(1)-Cl(1) | 123.60(17) |
| O(2)-Ba(1)-O(4)#3 | 63.0(2) | O(1)-Cu(1)-O(1)#4 | 180 |
| O(2)#1-Ba(1)-O(4)#3 | 103.7(2) | O(1)-Cu(1)-N(1) | 83.2(3) |
| O(4)#1-Ba(1)-O(3)#3 | 100.6(3) | O(1)#4-Cu(1)-N(1) | 96.8(3) |
| O(3)#2-Ba(1)-O(3)#3 | 67.1(3) | O(1)-Cu(1)-N(1)#4 | 96.8(3) |
| O(2)-Ba(1)-O(3)#3 | 94.1(2) | O(1)#4-Cu(1)-N(1)#4 | 83.2(3) |
| O(2)#1-Ba(1)-O(3)#3 | 147.6(2) | N(1)-Cu(1)-N(1)#4 | 180 |
| O(4)#3-Ba(1)-O(3)#3 | 44.3(2) | | |

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2 #2 -x+1,-y+1,-z+1 #3 x,-y+1,z+1/2 #4 -x+3/2,-y+3/2,-z+1 #5 -x+1,y,-z+3/2 #6 x,-y+1,z-1/2

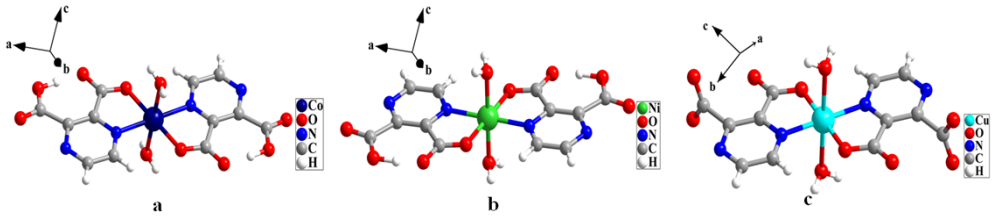


**Fig. S1** The coordination environments of $L_{Co}$ (a), $L_{Ni}$ (b) and $L_{Cu}$ (c), respectively.

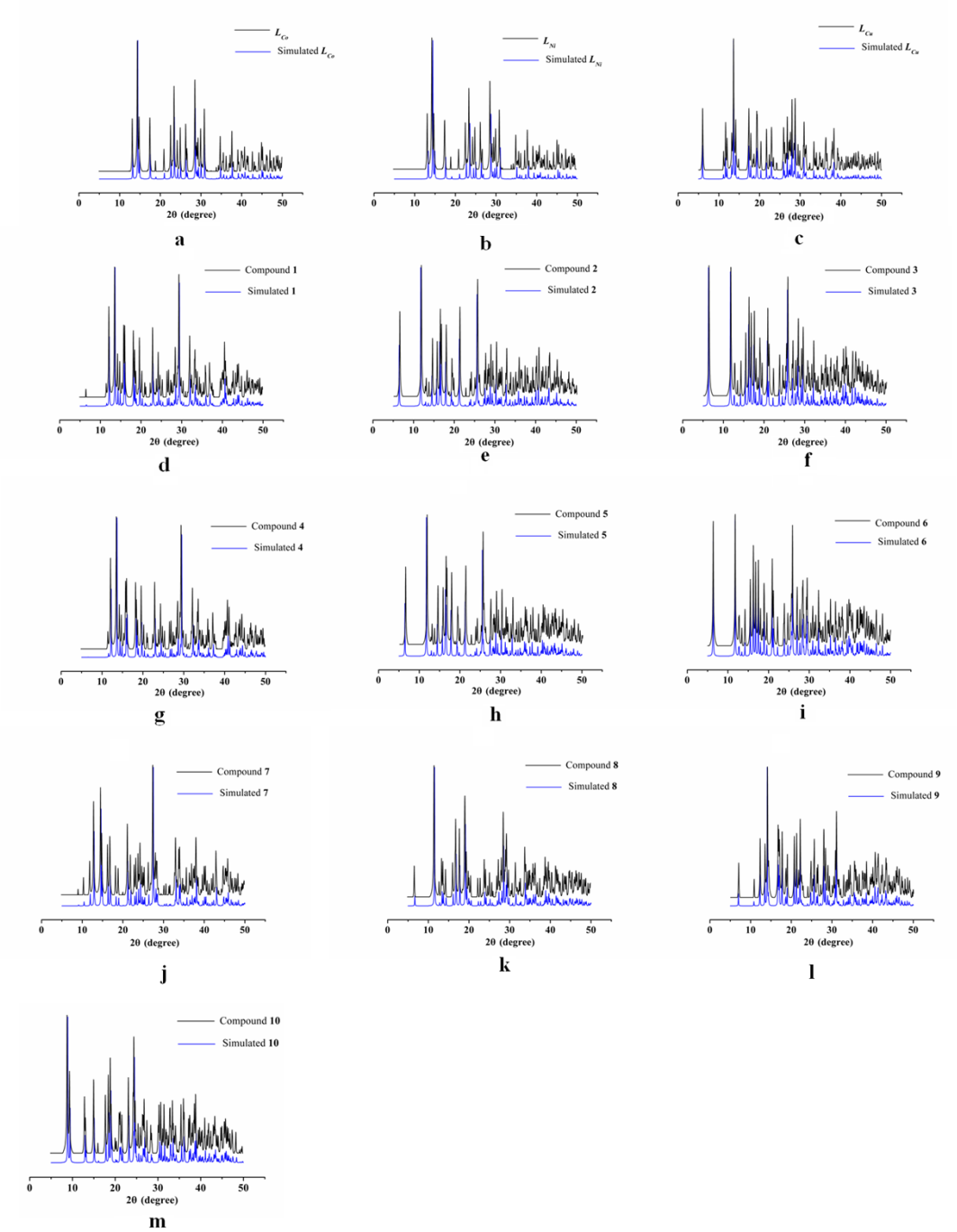


**Fig. S2** The XRPD patterns for $L_{Co}$, $L_{Cu}$, $L_{Ni}$ and **1-10** in **a-m** respectively.

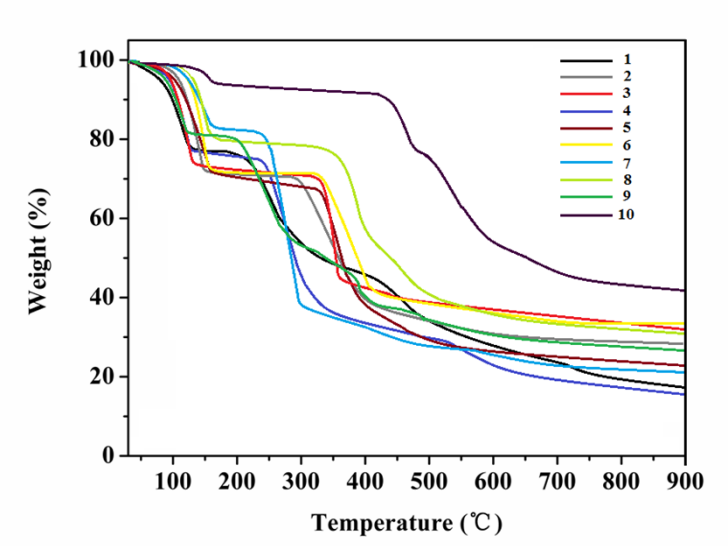


**Fig. S3** The TGA curves of complexes **1-10**.

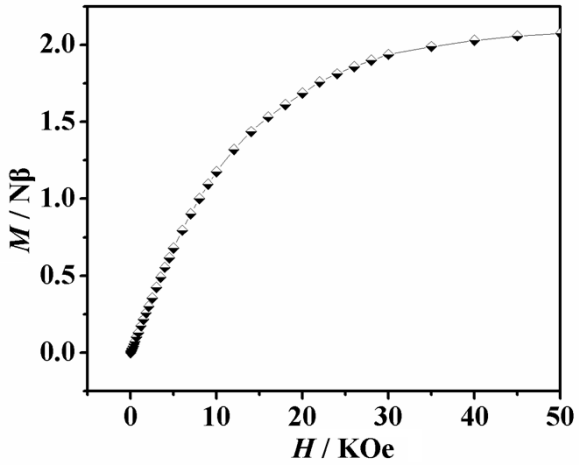


**Fig. S4** Magnetization *vs H* plot for compound **1**.

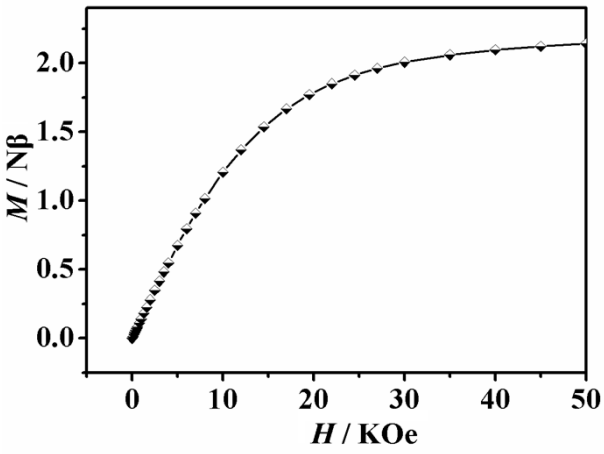


**Fig. S5** Magnetization *vs H* plot for compound **2**.

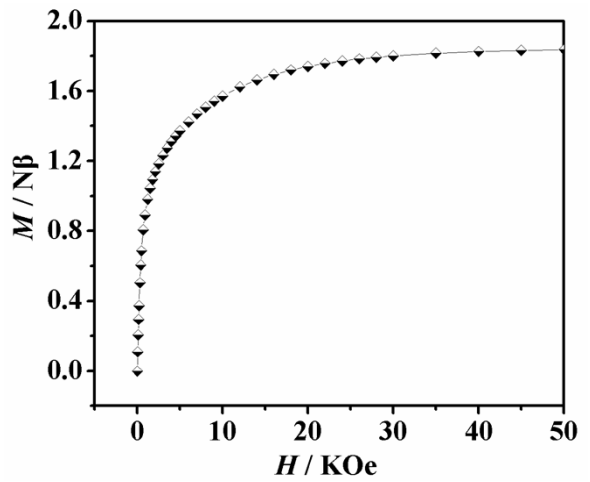


**Fig. S6** Magnetization *vs H* plot for compound **4**.

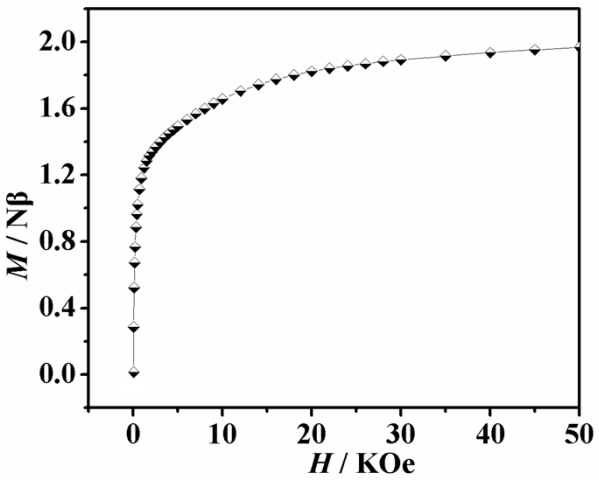


**Fig. S7** Magnetization *vs H* plot for compound **5**.

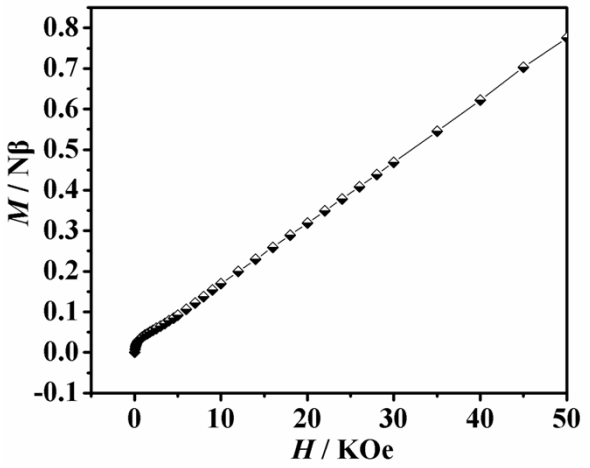


**Fig. S8** Magnetization *vs H* plot for compound **10**.