# Supporting materials

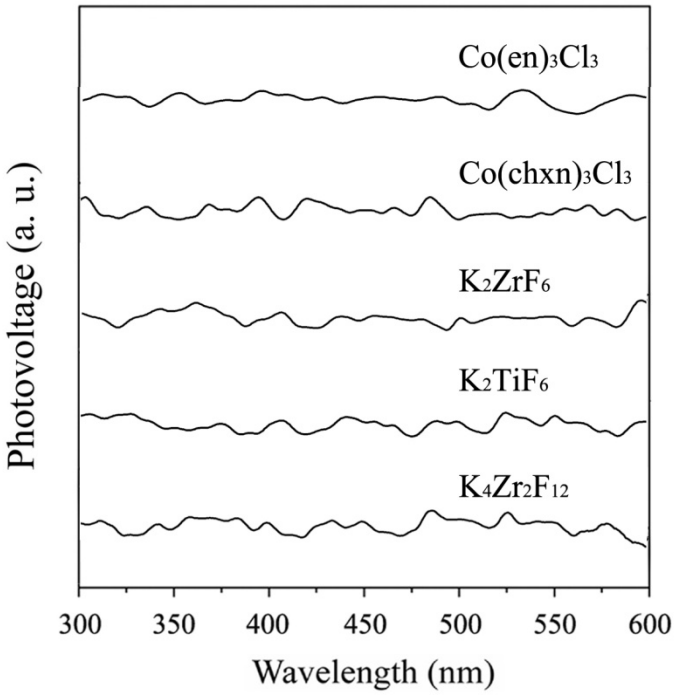
Co(en)3Cl3
Co(chxn)3Cl3
K2ZrF6
K2TiF6
K4Zr2F12
Photovoltage (a. u.)
300
350
400
450
500
550
600
Wavelength (nm)

Figure 1S

Table 1S the selected bond distances and bond angles of **1**.

| | | | |
|---|---|---|---|
| Ti(1)-F(6) | 1.772(5) | Co(1)-N(6) | 2.015(10) |
| Ti(1)-F(1) | 1.773(4) | Co(1)-N(5) | 2.017(9) |
| Ti(1)-F(2) | 1.812(4) | Co(1)-N(1') | 2.039(9) |
| Ti(1)-F(5) | 1.865(4) | C(1)-C(2) | 1.493(11) |
| Ti(1)-F(3) | 1.881(4) | C(1)-N(1) | 1.570(12) |
| Ti(1)-F(4) | 1.9490(14) | C(1)-N(1') | 1.587(13) |
| Ti(2)-F(8) | 1.795(4) | C(2)-N(2') | 1.359(13) |
| Ti(2)-F(9) | 1.804(5) | C(2)-N(2) | 1.566(12) |
| Ti(2)-F(10) | 1.820(4) | C(3)-C(4) | 1.477(10) |
| Ti(2)-F(11) | 1.848(4) | C(3)-N(3) | 1.534(12) |
| Ti(2)-F(7) | 1.850(4) | C(3)-N(3') | 1.558(12) |
| Ti(2)-F(12) | 1.9417(13) | C(4)-N(4') | 1.508(12) |
| Co(1)-N(6') | 1.888(9) | C(4)-N(4) | 1.556(11) |
| Co(1)-N(2) | 1.904(9) | C(5)-C(6) | 1.438(11) |
| Co(1)-N(5') | 1.923(9) | C(5)-N(5) | 1.465(12) |
| Co(1)-N(3) | 1.930(10) | C(5)-N(5') | 1.591(12) |
| Co(1)-N(1) | 1.942(10) | C(6)-N(6) | 1.351(12) |
| Co(1)-N(3') | 1.960(10) | C(6)-N(6') | 1.561(12) |
| Co(1)-N(4') | 1.981(9) | F(4)-Ti(1)#1 | 1.9490(14) |
| Co(1)-N(2') | 1.991(11) | F(12)-Ti(2)#2 | 1.9417(14) |
| Co(1)-N(4) | 2.013(9) | | |

| | | | |
|---|---|---|---|
| F(6)-Ti(1)-F(1) | 94.3(3) | N(3)-Co(1)-N(4') | 67.3(4) |
| F(6)-Ti(1)-F(2) | 92.4(3) | N(1)-Co(1)-N(4') | 130.7(4) |
| F(1)-Ti(1)-F(2) | 95.2(2) | N(3')-Co(1)-N(4') | 84.9(4) |
| F(6)-Ti(1)-F(5) | 96.1(2) | N(6')-Co(1)-N(2') | 93.0(4) |
| F(1)-Ti(1)-F(5) | 90.5(2) | N(2)-Co(1)-N(2') | 37.5(4) |
| F(2)-Ti(1)-F(5) | 169.4(2) | N(5')-Co(1)-N(2') | 93.8(4) |
| F(6)-Ti(1)-F(3) | 93.1(3) | N(3)-Co(1)-N(2') | 125.5(4) |
| F(1)-Ti(1)-F(3) | 170.9(3) | N(1)-Co(1)-N(2') | 65.6(4) |
| F(2)-Ti(1)-F(3) | 89.7(2) | N(3')-Co(1)-N(2') | 168.5(4) |
| F(5)-Ti(1)-F(3) | 83.5(2) | N(4')-Co(1)-N(2') | 87.9(4) |
| F(6)-Ti(1)-F(4) | 176.3(2) | N(6')-Co(1)-N(4) | 52.6(4) |
| F(1)-Ti(1)-F(4) | 86.6(2) | N(2)-Co(1)-N(4) | 90.4(4) |
| F(2)-Ti(1)-F(4) | 83.95(19) | N(5')-Co(1)-N(4) | 132.0(4) |
| F(5)-Ti(1)-F(4) | 87.46(15) | N(3)-Co(1)-N(4) | 86.0(4) |
| F(3)-Ti(1)-F(4) | 86.33(16) | N(1)-Co(1)-N(4) | 178.3(4) |
| F(8)-Ti(2)-F(9) | 94.3(2) | N(3')-Co(1)-N(4) | 68.3(4) |
| F(8)-Ti(2)-F(10) | 92.1(2) | N(4')-Co(1)-N(4) | 48.0(4) |
| F(9)-Ti(2)-F(10) | 93.6(2) | N(2')-Co(1)-N(4) | 112.9(4) |
| F(8)-Ti(2)-F(11) | 172.0(2) | N(6')-Co(1)-N(6) | 7.0(4) |
| F(9)-Ti(2)-F(11) | 93.2(2) | N(2)-Co(1)-N(6) | 91.6(4) |

| | | | |
|---|---|---|---|
| F(10)-Ti(2)-F(11) | 90.3(2) | N(5')-Co(1)-N(6) | 68.8(4) |
| F(8)-Ti(2)-F(7) | 89.8(2) | N(3)-Co(1)-N(6) | 169.6(4) |
| F(9)-Ti(2)-F(7) | 93.3(2) | N(1)-Co(1)-N(6) | 92.7(4) |
| F(10)-Ti(2)-F(7) | 172.6(3) | N(3')-Co(1)-N(6) | 126.7(4) |
| F(11)-Ti(2)-F(7) | 86.8(2) | N(4')-Co(1)-N(6) | 113.1(4) |
| F(8)-Ti(2)-F(12) | 87.11(19) | N(2')-Co(1)-N(6) | 64.5(4) |
| F(9)-Ti(2)-F(12) | 178.54(16) | N(4)-Co(1)-N(6) | 87.1(4) |
| F(10)-Ti(2)-F(12) | 86.70(17) | N(6')-Co(1)-N(5) | 72.6(4) |
| F(11)-Ti(2)-F(12) | 85.38(14) | N(2)-Co(1)-N(5) | 173.0(4) |
| F(7)-Ti(2)-F(12) | 86.32(19) | N(5')-Co(1)-N(5) | 46.0(4) |
| N(6')-Co(1)-N(2) | 103.2(4) | N(3)-Co(1)-N(5) | 90.7(4) |
| N(6')-Co(1)-N(5') | 88.5(4) | N(1)-Co(1)-N(5) | 90.3(4) |
| N(2)-Co(1)-N(5') | 129.4(4) | N(3')-Co(1)-N(5) | 54.0(4) |
| N(6')-Co(1)-N(3) | 133.6(4) | N(4')-Co(1)-N(5) | 132.8(4) |
| N(2)-Co(1)-N(3) | 96.2(4) | N(2')-Co(1)-N(5) | 136.0(4) |
| N(5')-Co(1)-N(3) | 110.7(4) | N(4)-Co(1)-N(5) | 91.3(4) |
| N(6')-Co(1)-N(1) | 127.6(4) | N(6)-Co(1)-N(5) | 81.7(4) |
| N(2)-Co(1)-N(1) | 87.9(4) | N(6')-Co(1)-N(1') | 174.3(4) |
| N(5')-Co(1)-N(1) | 49.3(4) | N(2)-Co(1)-N(1') | 75.4(4) |
| N(3)-Co(1)-N(1) | 94.4(4) | N(5')-Co(1)-N(1') | 88.2(4) |
| N(6')-Co(1)-N(3') | 96.3(4) | N(3)-Co(1)-N(1') | 52.1(4) |
| N(2)-Co(1)-N(3') | 132.8(4) | N(1)-Co(1)-N(1') | 47.2(4) |
| N(5')-Co(1)-N(3') | 93.2(4) | N(3')-Co(1)-N(1') | 88.6(4) |
| N(3)-Co(1)-N(3') | 43.1(4) | N(4')-Co(1)-N(1') | 90.8(4) |
| N(1)-Co(1)-N(3') | 113.1(4) | N(2')-Co(1)-N(1') | 82.5(4) |
| N(6')-Co(1)-N(4') | 92.6(4) | N(4)-Co(1)-N(1') | 132.5(4) |
| N(2)-Co(1)-N(4') | 52.0(4) | N(6)-Co(1)-N(1') | 137.2(4) |
| N(5')-Co(1)-N(4') | 177.9(4) | N(5)-Co(1)-N(1') | 108.3(4) |

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x+1,-y+3,-z+1

Table 2S Atomic coordinates and equivalent isotropic displacement parameters of **1**

| Atom | X | Y | Z | U(eq) |
|---|---|---|---|---|
| Ti(1) | 2449(2) | 1940(2) | 259(1) | 44(1) |
| Ti(2) | 4627(1) | 12888(2) | 4193(1) | 43(1) |
| Co(1) | 10605(1) | 16069(1) | 2529(1) | 37(1) |
| F(1) | 3338(8) | 337(8) | 65(4) | 97(2) |
| F(2) | 2210(8) | 1632(7) | 1484(3) | 88(2) |
| F(3) | 1209(7) | 3429(6) | 304(4) | 83(1) |
| F(4) | 0 | 0 | 0 | 88(2) |
| F(5) | 2228(6) | 2150(6) | -1032(3) | 71(1) |
| F(6) | 4660(7) | 3707(7) | 572(4) | 104(2) |
| F(7) | 7127(5) | 13501(7) | 4545(3) | 85(2) |
| F(8) | 4144(6) | 11747(7) | 5214(3) | 87(2) |
| F(9) | 4307(7) | 10960(6) | 3420(3) | 76(1) |
| F(10) | 2232(6) | 12577(6) | 3898(3) | 72(1) |
| F(11) | 5293(6) | 14346(5) | 3260(3) | 69(1) |
| F(12) | 5000 | 15000 | 5000 | 118(3) |
| C(1) | 8690(10) | 12357(9) | 2378(7) | 70(2) |
| C(2) | 7620(10) | 12930(10) | 1658(6) | 66(2) |
| C(3) | 10305(10) | 17818(10) | 4232(5) | 59(2) |
| C(4) | 9324(9) | 18340(9) | 3460(5) | 54(2) |
| C(5) | 14219(10) | 17189(13) | 2130(7) | 79(3) |
| C(6) | 13255(11) | 17690(12) | 1380(6) | 73(2) |
| N(1) | 10716(13) | 13790(14) | 2421(7) | 43(2) |
| N(2) | 8082(13) | 14914(12) | 1958(6) | 36(2) |
| N(3) | 10130(13) | 16006(13) | 3821(7) | 43(2) |
| N(4) | 10417(13) | 18399(12) | 2618(7) | 38(2) |
| N(5) | 13356(12) | 17257(13) | 2974(7) | 39(2) |
| N(6) | 11443(14) | 16580(14) | 1263(7) | 44(2) |
| N(1') | 9519(13) | 13919(13) | 3222(7) | 44(2) |
| N(2') | 8954(14) | 14400(14) | 1420(8) | 48(2) |
| N(3') | 11815(13) | 17478(13) | 3757(7) | 44(2) |
| N(4') | 8539(12) | 16723(13) | 2739(7) | 39(2) |
| N(5') | 12637(13) | 15445(12) | 2375(7) | 38(2) |
| N(6') | 11610(13) | 17905(13) | 1785(7) | 42(2) |

Table 3 Hydrogen bonds of **1**. [Å and deg.]

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1C)...F(2)#3 | 0.90 | 2.21 | 2.870(11) | 129.3 |
| N(1)-H(1C)...F(3)#3 | 0.90 | 2.28 | 3.111(11) | 154.2 |
| N(1)-H(1D)...F(10)#4 | 0.90 | 1.93 | 2.776(10) | 155.8 |
| N(2)-H(2C)...F(11) | 0.90 | 2.11 | 2.974(10) | 161.8 |
| N(2)-H(2D)...F(5)#5 | 0.90 | 2.19 | 2.955(10) | 142.0 |
| N(2)-H(2D)...F(6)#6 | 0.90 | 2.52 | 2.956(10) | 110.5 |
| N(3)-H(3C)...F(7) | 0.90 | 2.01 | 2.832(10) | 150.7 |
| N(3)-H(3D)...F(7)#7 | 0.90 | 2.14 | 2.909(11) | 142.6 |
| N(4)-H(4C)...F(9)#3 | 0.90 | 2.15 | 3.013(11) | 160.4 |
| N(4)-H(4D)...F(5)#5 | 0.90 | 1.95 | 2.803(10) | 156.8 |
| N(5)-H(5C)...F(9)#3 | 0.90 | 2.01 | 2.884(11) | 165.1 |
| N(5)-H(5D)...F(8)#7 | 0.90 | 2.37 | 2.940(10) | 121.0 |
| N(6)-H(6C)...F(3)#3 | 0.90 | 1.92 | 2.816(12) | 171.2 |
| N(6)-H(6D)...F(3)#5 | 0.90 | 2.15 | 2.911(11) | 141.6 |
| N(1')-H(1'1)...F(10)#4 | 0.90 | 2.12 | 2.924(10) | 148.0 |
| N(1')-H(1'2)...F(7) | 0.90 | 1.93 | 2.776(11) | 155.5 |
| N(2')-H(2'1)...F(3)#5 | 0.90 | 2.44 | 3.189(12) | 140.8 |
| N(2')-H(2'2)...F(3)#3 | 0.90 | 1.94 | 2.844(11) | 178.4 |
| N(3')-H(3'1)...F(7)#7 | 0.90 | 2.00 | 2.773(11) | 143.7 |
| N(3')-H(3'1)...F(8)#7 | 0.90 | 2.63 | 3.186(11) | 121.1 |
| N(3')-H(3'2)...F(9)#3 | 0.90 | 2.02 | 2.902(11) | 167.3 |
| N(4')-H(4'1)...F(5)#5 | 0.90 | 1.90 | 2.775(10) | 163.2 |
| N(4')-H(4'2)...F(11) | 0.90 | 1.91 | 2.777(10) | 161.9 |
| N(5')-H(5'1)...F(11)#4 | 0.90 | 2.18 | 2.847(10) | 130.7 |
| N(5')-H(5'2)...F(3)#3 | 0.90 | 2.35 | 3.158(12) | 150.1 |
| N(6')-H(6'1)...F(5)#5 | 0.90 | 2.36 | 3.117(10) | 141.2 |
| N(6')-H(6'2)...F(2)#8 | 0.90 | 2.44 | 3.030(11) | 123.0 |

Symmetry transformations used to generate equivalent atoms:

#3 x+1,y+1,z #4 x+1,y,z #5 -x+1,-y+2,-z #6 x,y+1,z #7 -x+2,-y+3,-z+1 #8 x+1,y+2,z