

CRYSTAL STRUCTURE AND CHARACTERIZATION OF NEUTRAL COBALT(III) 2,3-PYRIDINEDICARBOXYLATE COMPLEX

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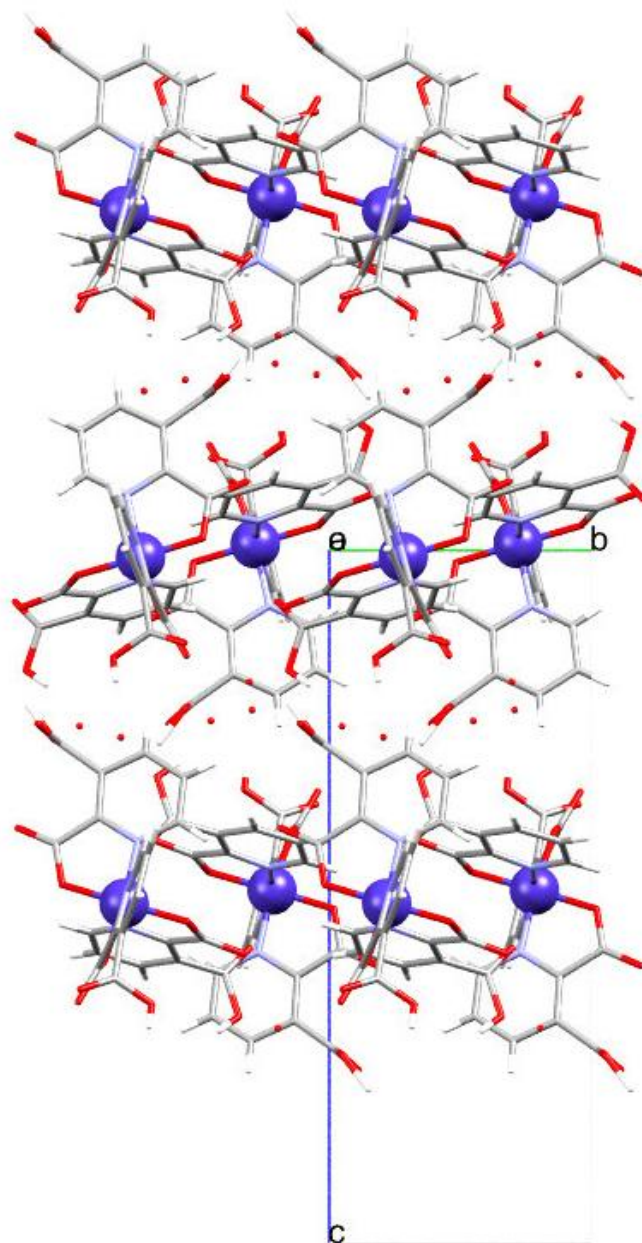


Figure S1. Packing diagram along *a* axis.

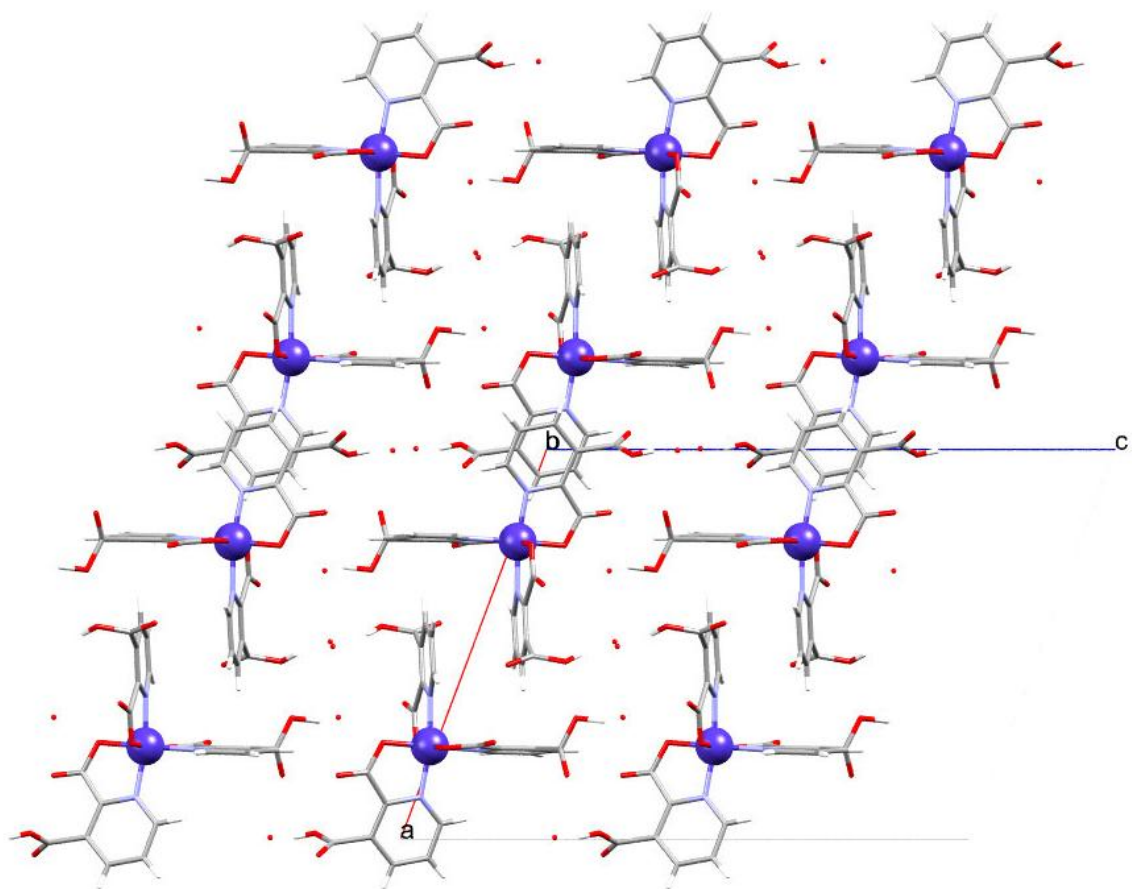


Figure S2. Packing diagram along *b* axis.

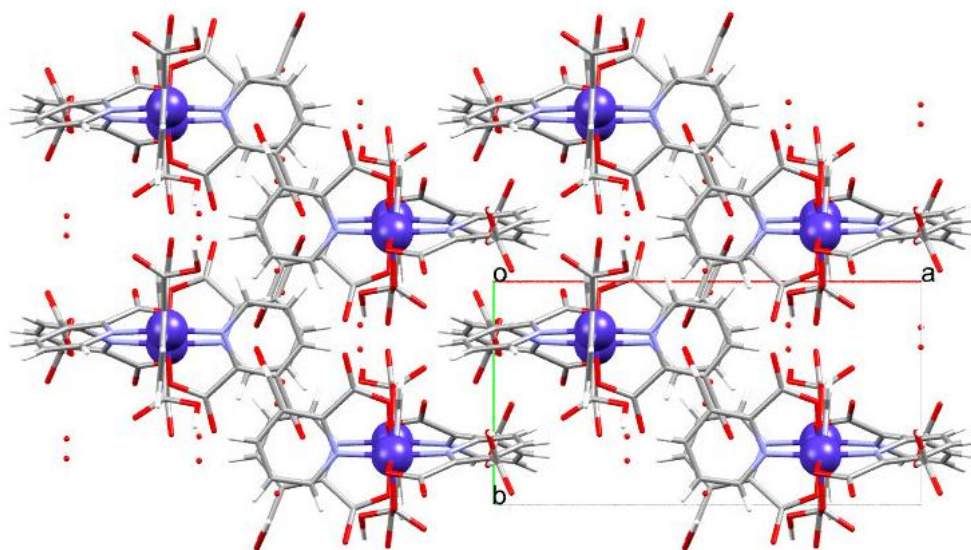


Figure S3. Packing diagram along *c* axis.

Table S1

| Bond lengths (Å). | | | | | |
|-------------------|------|------------|------|------|------------|
| Atom | Atom | Distance | Atom | Atom | Distance |
| Co1 | O1 | 1.887(5) | Co1 | O5 | 1.909(5) |
| Co1 | O9 | 1.875(6) | Co1 | N1 | 1.929(7) |
| Co1 | N2 | 1.908(6) | Co1 | N3 | 1.955(6) |
| O1 | C1 | 1.308 (12) | O2 | C1 | 1.224 (10) |
| O3 | C7 | 1.205(9) | O4 | C7 | 1.322 (11) |
| O5 | C8 | 1.298(8) | O6 | C8 | 1.239 (9) |
| O7 | C14 | 1.342(12) | O8 | C14 | 1.211(12) |
| O9 | C15 | 1.287(11) | O10 | C15 | 1.236(11) |
| O11 | C21 | 1.311 (11) | O12 | C21 | 1.200 (11) |
| N1 | C2 | 1.370 (10) | N1 | C6 | 1.326 (10) |
| N2 | C9 | 1.347 (9) | N2 | C13 | 1.355(9) |
| N3 | C16 | 1.356(11) | N3 | C20 | 1.341(9) |
| C1 | C2 | 1.491 (11) | C2 | C3 | 1.371(12) |
| C3 | C4 | 1.400(12) | C3 | C7 | 1.514(12) |
| C4 | C5 | 1.379(13) | C5 | C6 | 1.373(14) |
| C8 | C9 | 1.509(11) | C9 | C10 | 1.386(9) |
| C10 | C11 | 1.395(11) | C10 | C14 | 1.488(11) |
| C11 | C12 | 1.369(11) | C12 | C13 | 1.380(10) |
| C15 | C16 | 1.484(9) | C16 | C17 | 1.394(11) |
| C17 | C18 | 1.388(10) | C17 | C21 | 1.515(14) |
| C18 | C19 | 1.387(13) | C19 | C20 | 1.385(11) |

Table S2

| Bond angles (°). | | | | | | | |
|------------------|------|------|----------|------|------|------|----------|
| Atom | Atom | Atom | Angle | Atom | Atom | Atom | Angle |
| O1 | Co1 | O5 | 178.0(3) | O1 | Co1 | O9 | 89.1(2) |
| O1 | Co1 | N1 | 84.6(3) | O1 | Co1 | N2 | 93.5(2) |
| O1 | Co1 | N3 | 93.8(2) | O5 | Co1 | O9 | 92.2(2) |
| O5 | Co1 | N1 | 94.0(3) | O5 | Co1 | N2 | 85.1(2) |
| O5 | Co1 | N3 | 87.7(2) | O9 | Co1 | N1 | 173.7(2) |
| O9 | Co1 | N2 | 86.5(3) | O9 | Co1 | N3 | 85.3(3) |
| N1 | Co1 | N2 | 93.0(3) | N1 | Co1 | N3 | 95.9(3) |
| N2 | Co1 | N3 | 168.9(3) | Co1 | O1 | C1 | 115.5(5) |
| Co1 | O5 | C8 | 113.7(5) | Co1 | O9 | C15 | 114.6(4) |
| Co1 | N1 | C2 | 111.8(5) | Co1 | N1 | C6 | 128.1(6) |
| C2 | N1 | C6 | 120.0(7) | Co1 | N2 | C9 | 113.4(5) |
| Co1 | N2 | C13 | 128.1(5) | C9 | N2 | C13 | 118.2(5) |
| Co1 | N3 | C16 | 109.8(4) | Co1 | N3 | C20 | 130.0(6) |
| C16 | N3 | C20 | 119.8(7) | O1 | C1 | O2 | 125.1(8) |
| O1 | C1 | C2 | 113.6(7) | O2 | C1 | C2 | 121.3(9) |
| N1 | C2 | C1 | 113.7(7) | N1 | C2 | C3 | 120.5(7) |
| C1 | C2 | C3 | 125.8(7) | C2 | C3 | C4 | 118.9(7) |
| C2 | C3 | C7 | 123.6(7) | C4 | C3 | C7 | 117.5(8) |
| C3 | C4 | C5 | 119.7(9) | C4 | C5 | C6 | 118.6(8) |
| N1 | C6 | C5 | 122.3(8) | O3 | C7 | O4 | 122.9(9) |
| O3 | C7 | C3 | 124.1(8) | O4 | C7 | C3 | 112.8(6) |
| O5 | C8 | O6 | 124.2(7) | O5 | C8 | C9 | 115.3(6) |
| O6 | C8 | C9 | 120.4(6) | N2 | C9 | C8 | 112.5(6) |
| N2 | C9 | C10 | 123.4(7) | C8 | C9 | C10 | 124.1(7) |
| C9 | C10 | C11 | 116.8(7) | C9 | C10 | C14 | 123.5(7) |
| C11 | C10 | C14 | 119.7(6) | C10 | C11 | C12 | 120.4(7) |
| C11 | C12 | C13 | 119.3(7) | N2 | C13 | C12 | 121.6(7) |
| O7 | C14 | O8 | 118.7(7) | O7 | C14 | C10 | 118.6(8) |
| O8 | C14 | C10 | 122.4(9) | O9 | C15 | O10 | 123.9(6) |
| O9 | C15 | C16 | 115.0(8) | O10 | C15 | C16 | 121.1(8) |
| N3 | C16 | C15 | 114.0(7) | N3 | C16 | C17 | 121.2(6) |
| C15 | C16 | C17 | 124.8(8) | C16 | C17 | C18 | 118.5(8) |
| C16 | C17 | C21 | 120.3(6) | C18 | C17 | C21 | 121.0(7) |
| C17 | C18 | C19 | 120.0(8) | C18 | C19 | C20 | 118.5(7) |
| N3 | C20 | C19 | 122.0(8) | O11 | C21 | O12 | 125.5(9) |
| O11 | C21 | C17 | 109.6(8) | O12 | C21 | C17 | 124.9(8) |

Table S3

Torsion Angles(°).

(Those having bond angles > 160 or < 20 degrees are excluded.)

| <i>Atom1</i> | <i>Atom2</i> | <i>Atom3</i> | <i>Atom4</i> | <i>Angle</i> | <i>Atom1</i> | <i>Atom2</i> | <i>Atom3</i> | <i>Atom4</i> | <i>Angle</i> |
|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| O1 | Co1 | O9 | C15 | -89.6(4) | O9 | Co1 | O1 | C1 | -170.7(3) |
| O1 | Co1 | N1 | C2 | -5.6(3) | O1 | Co1 | N1 | C6 | 177.3(4) |
| N1 | Co1 | O1 | C1 | 8.5(3) | O1 | Co1 | N2 | C9 | 176.3(4) |
| O1 | Co1 | N2 | C13 | -11.0(6) | N2 | Co1 | O1 | C1 | -84.2(4) |
| O1 | Co1 | N3 | C16 | 92.2(4) | O1 | Co1 | N3 | C20 | -95.6(5) |
| N3 | Co1 | O1 | C1 | 104.1(3) | O5 | Co1 | O9 | C15 | 91.8(4) |
| O9 | Co1 | O5 | C8 | 87.9(4) | O5 | Co1 | N1 | C2 | 172.9(3) |
| O5 | Co1 | N1 | C6 | -4.2(4) | N1 | Co1 | O5 | C8 | -91.1(4) |
| O5 | Co1 | N2 | C9 | -2.2(4) | O5 | Co1 | N2 | C13 | 170.4(6) |
| N2 | Co1 | O5 | C8 | 1.6(4) | O5 | Co1 | N3 | C16 | -89.0(4) |
| O5 | Co1 | N3 | C20 | 83.2(5) | N3 | Co1 | O5 | C8 | 173.1(4) |
| O9 | Co1 | N2 | C9 | -94.8(5) | O9 | Co1 | N2 | C13 | 77.9(6) |
| N2 | Co1 | O9 | C15 | 176.8(4) | O9 | Co1 | N3 | C16 | 3.4(3) |
| O9 | Co1 | N3 | C20 | 175.6(5) | N3 | Co1 | O9 | C15 | 4.3(4) |
| N1 | Co1 | N2 | C9 | 91.6(5) | N1 | Co1 | N2 | C13 | -95.8(6) |
| N2 | Co1 | N1 | C2 | 87.6(3) | N2 | Co1 | N1 | C6 | -89.4(4) |
| N1 | Co1 | N3 | C16 | 177.1(3) | N1 | Co1 | N3 | C20 | -10.7(5) |
| N3 | Co1 | N1 | C2 | -98.9(3) | N3 | Co1 | N1 | C6 | 84.0(4) |
| Co1 | O1 | C1 | O2 | 171.6(5) | Co1 | O1 | C1 | C2 | -9.1(6) |
| Co1 | O5 | C8 | O6 | -178.0(6) | Co1 | O5 | C8 | C9 | -0.7(9) |
| Co1 | O9 | C15 | O10 | 168.0(6) | Co1 | O9 | C15 | C16 | -10.6(8) |
| Co1 | N1 | C2 | C1 | 2.3(6) | Co1 | N1 | C2 | C3 | -177.4(4) |
| Co1 | N1 | C6 | C5 | 177.3(4) | C2 | N1 | C6 | C5 | 0.5(9) |
| C6 | N1 | C2 | C1 | 179.7(5) | C6 | N1 | C2 | C3 | -0.1(8) |
| Co1 | N2 | C9 | C8 | 2.4(8) | Co1 | N2 | C9 | C10 | 179.3(5) |
| Co1 | N2 | C13 | C12 | -176.3(5) | C9 | N2 | C13 | C12 | -3.9(12) |
| C13 | N2 | C9 | C8 | -171.1(7) | C13 | N2 | C9 | C10 | 5.9(12) |
| Co1 | N3 | C16 | C15 | -9.5(6) | Co1 | N3 | C16 | C17 | 171.5(4) |
| Co1 | N3 | C20 | C19 | -171.8(4) | C16 | N3 | C20 | C19 | -0.3(10) |
| C20 | N3 | C16 | C15 | 177.4(6) | C20 | N3 | C16 | C17 | -1.6(10) |
| O1 | C1 | C2 | N1 | 4.3(8) | O1 | C1 | C2 | C3 | -176.0(5) |
| O2 | C1 | C2 | N1 | -176.4(5) | O2 | C1 | C2 | C3 | 3.3(10) |
| N1 | C2 | C3 | C4 | 1.0(9) | N1 | C2 | C3 | C7 | -176.8(5) |
| C1 | C2 | C3 | C4 | -178.7(5) | C1 | C2 | C3 | C7 | 3.5(10) |
| C2 | C3 | C4 | C5 | -2.4(10) | C2 | C3 | C7 | O3 | 79.3(10) |
| C2 | C3 | C7 | O4 | -105.5(8) | C4 | C3 | C7 | O3 | -98.5(10) |
| C4 | C3 | C7 | O4 | 76.6(8) | C7 | C3 | C4 | C5 | 175.6(6) |