

|                                     |        |                       |
|-------------------------------------|--------|-----------------------|
| $\text{Au}_2\text{Co}[\text{CN}]_4$ | $hP66$ | (180) $P6_222 - k^5f$ |
|-------------------------------------|--------|-----------------------|

**Co[Au(CN)<sub>2</sub>]<sub>2</sub> [1]**

Structural features:  $\text{CoN}_4$  tetrahedra and C-Au-C linear units are interconnected via C-N bonds (cyanide units) to form three non-intersecting 3D-frameworks with approximately linear Co-N-C-Au-C-N-Co segments.

Abrahams S.C. et al. (1982) [1]

$\text{Au}_2\text{C}_4\text{CoN}_4$

$a = 0.8434$ ,  $c = 2.0695$  nm,  $c/a = 2.454$ ,  $V = 1.2749$  nm<sup>3</sup>,  $Z = 6$

| site | Wyck. | sym. | $x$           | $y$     | $z$     | occ. | atomic environment          |
|------|-------|------|---------------|---------|---------|------|-----------------------------|
| Au1  | $12k$ | 1    | 0.0058        | 0.31633 | 0.2926  |      | non-colinear C <sub>2</sub> |
| C2   | $12k$ | 1    | 0.1796        | 0.3976  | 0.11347 |      | single atom N               |
| N3   | $12k$ | 1    | 0.2919        | 0.4319  | 0.14947 |      | single atom C               |
| C4   | $12k$ | 1    | 0.3937        | 0.2035  | 0.02843 |      | single atom N               |
| N5   | $12k$ | 1    | 0.4484        | 0.1589  | 0.06943 |      | single atom C               |
| Co6  | $6f$  | 2..  | $\frac{1}{2}$ | 0       | 0.1259  |      | tetrahedron N <sub>4</sub>  |

Transformation from published data ( $P6_422$ ): new axes -a,-b,-c; origin shift 0 0  $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.036$ ,  $T = 298$  K

References: [1] Abrahams S.C., Zyontz L.E., Bernstein J.L. (1982), J. Chem. Phys. 76, 5458-5462.