Crystal Structure of *trans*-Diaquabis(3-aminobenzoato-*O*)-bis(nicotinamide-*N*)cobalt(II)

Tuncer HÖKELEK* and Hacali NECEFOĞLU**

**Hacettepe University, Department of Physics, 06532 Beytepe-Ankara, Turkey*
***Kafkas University, Department of Chemistry, Kars, Turkey*

Nicotinamide (NA) is one form of niacin. The deficiency of this vitamin leads to a loss of copper from the body, known as pellagra disease. The nicotinic acid derivative, *N*,*N*-diethylnicotinamide (DENA), is an important respiratory stimulant.

The title compound was prepared by dissolving $CoSO_4 \cdot 7(H_2O)$ (2.81 g, 0.01 mol) and NA (2.44 g, 0.02 mol) in water (75 ml) and sodium-3-aminobenzoate (3.18 g, 0.02 mol) in water (25 ml) and then adding the solutions. The mixture was set aside for crystallization at ambient temperature for a few days.

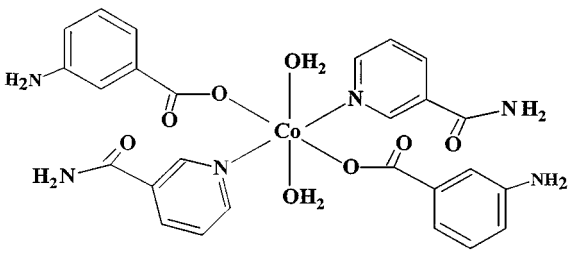

Fig. 1 Chemical structure.

Table 1 Crystal and experimental data

Formula: $C_{26}H_{28}CN_6O_8$	
Formula weight=611.48	
Crystal system: monoclinic	
Space group: $P2_1/n$	Z=2
a=7.383(1)Å	
b=17.956(1)Å	
c=10.417(2)Å	
β=107.72(2)°	
V=1315.5(3)Å^3	
D_x=1.544 g/cm^3	R=0.056
wR=0.064	
$(\Delta/\sigma)_{max}$=0.01	
$(\Delta\rho)_{max}$=0.52 eÅ^{-3}	
$(\Delta\rho)_{min}$=–0.78 eÅ^{-3}	
No. of reflection used=1970	
Measurement: Enraf-Nonius CAD-4 diffractometer	
Program system: CAD-4-EXPRESS software	
Structure determination: SHELXS86	
Refinement: full matrix	

† To whom correspondence should be addressed.

A structure determination of the title compound was undertaken in order to determine the ligand properties of NA and benzoate ligands, and to compare the coordination geometries when the NA ligands are substituted for water in complexes $[Co(p\text{-}O_2NC_6H_4COO)_2(H_2O)_4]$[1] (I) and $[Co(p\text{-}H_2NC_6H_4COO)_2(H_2O)_4]$[2] (II). The title compound is a monomeric complex with cobalt in a center of symmetry. All ligands are monodentate and the O atoms of each water molecule and benzoate group form a slightly distorted square-planar coordination around the Co atom, which is completed to a Jahn-Teller distorted octahedron by the pyridine N atoms of NA at 2.153(3)Å (Fig. 2). There are intra- and inter-molecular hydrogen bonds between the nicotinamide N3 and O4 atoms [N···O 2.236(6)Å], and the non-coordinated $O3^i$ atom and the water O2 atom [O···O 2.583(6)Å, symmetry code: (i) *–x*, *–y*, *–z*], respectively. Similar hydrogen bonds are observed in (I) [2.59 Å], (II) [2.592(3) Å], $[Co(C_7H_5O_2)_2(C_6H_6N_2O)_2(H_2O)_2]$[3] (III) [2.580(2)Å] and $[Co(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]$[4] (IV) [2.634(5)Å].

The configuration around the Co atom is given by the torsion angles (Table 4). The Co atom is out of the C1, O1, O3 plane by 0.645(2)Å. The dihedral angle between the carboxyl group and the phenyl ring is 24.1(4)°. The corresponding ones are 13.0(2) and 23.7(3)° in complexes (III) and (IV), respectively. Most

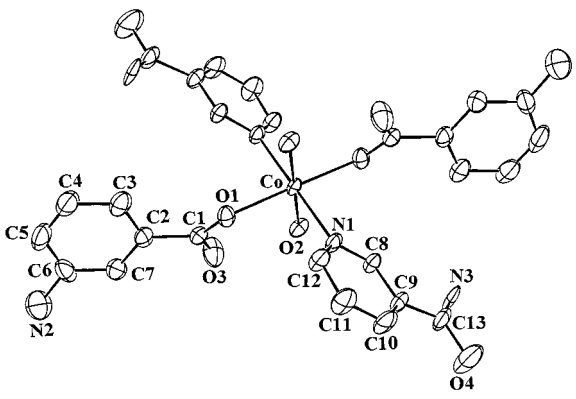

Fig. 2 Molecular structure of the title compound with atom-numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

Table 2 Final atomic coordinates and equivalent isotropic thermal parameters

Atom	*x*	*y*	*z*	B_{eq}/Å^2
Co	0.000	0.000	0.000	1.70(1)
O1	0.0819(5)	0.1007(2)	-0.0646(3)	2.38(7)
O2	0.2960(5)	-0.0300(2)	0.0760(3)	2.55(7)
O3	-0.1977(5)	0.1431(3)	-0.1929(4)	4.23(9)
O4	-0.4237(5)	-0.0027(3)	0.3473(3)	4.13(8)
N1	0.0093(5)	0.0471(2)	0.1920(3)	2.11(8)
N2	-0.0089(8)	0.3690(3)	-0.4161(5)	4.6(1)
N3	-0.3200(7)	0.0741(3)	0.5235(4)	4.2(1)
C1	-0.0202(6)	0.1428(3)	-0.1556(4)	2.18(9)
C2	0.0773(7)	0.1943(3)	-0.2278(4)	2.5(1)
C3	0.2581(8)	0.1786(3)	-0.2331(5)	3.2(1)
C4	0.3440(9)	0.2248(4)	-0.3077(5)	4.0(1)
C5	0.2498(9)	0.2849(4)	-0.3690(5)	4.4(1)
C6	0.0708(9)	0.3032(3)	-0.3631(5)	3.6(1)
C7	-0.0185(8)	0.2559(3)	-0.2930(5)	3.1(1)
C8	-0.1325(6)	0.0335(3)	0.2437(4)	2.18(9)
C9	-0.1409(7)	0.0647(3)	0.3642(4)	2.38(9)
C10	0.0036(8)	0.1117(3)	0.4306(5)	3.2(1)
C11	0.1510(8)	0.1261(3)	0.3792(5)	3.3(1)
C12	0.1493(7)	0.0915(3)	0.2601(5)	2.7(1)
C13	-0.3068(7)	0.0423(3)	0.4100(4)	2.9(1)

$B_{eq}=(8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*(\boldsymbol{a}_i\cdot\boldsymbol{a}_j)$.

Table 3 Bond distances (Å) and angles (˚)

Co-O1	2.082(4)	C2-C3	1.382(8)
Co-O2	2.154(4)	C2-C7	1.376(7)
Co-N1	2.153(3)	C3-C4	1.412(9)
O1-C1	1.266(5)	C4-C5	1.336(9)
O3-C1	1.248(6)	C5-C6	1.381(9)
O4-C13	1.217(6)	C6-C7	1.408(9)
N1-C8	1.338(6)	C8-C9	1.393(7)
N1-C12	1.327(6)	C9-C10	1.371(7)
N2-C6	1.360(7)	C9-C13	1.499(8)
N3-C13	1.343(7)	C10-C11	1.376(9)
C1-C2	1.506(7)	C11-C12	1.384(8)
O1-Co-O2	88.5(1)	N2-C6-C7	121.4(5)
O1-Co-N1	91.7(1)	C5-C6-C7	119.0(6)
O2-Co-N1	90.9(1)	C2-C7-C6	119.3(5)
Co-O1-C1	126.5(3)	N1-C8-C9	123.0(4)
Co-N1-C8	119.7(3)	C8-C9-C10	117.5(4)
Co-N1-C12	122.1(3)	C8-C9-C13	116.4(4)
C8-N1-C12	118.2(4)	C10-C9-C13	126.2(5)
O1-C1-O3	124.4(4)	C9-C10-C11	120.4(5)
O1-C1-C2	118.3(4)	C10-C11-C12	118.2(5)
O3-C1-C2	117.3(4)	N1-C12-C11	122.8(5)
C1-C2-C3	120.6(5)	O4-C13-N3	121.7(4)
C1-C2-C7	119.2(4)	O4-C13-C9	121.5(5)
C3-C2-C7	120.1(5)	N3-C13-C9	116.8(4)
C2-C3-C4	120.2(5)	C4-C5-C6	122.5(6)
C3-C4-C5	118.8(6)	N2-C6-C5	119.4(6)

of the H-atoms were determined from difference synthesis and were refined isotropically. The remaining ones were calculated geometrically, 0.95 Å from the corresponding atoms, and a riding model was used in the refinement process.

Table 4 Torsion angles (˚)

O2-Co-O1-C1	158.3(4)	O1-Co-N1-C12	-42.9(4)
N1-Co-O1-C1	-110.9(4)	O2-Co-N1-C8	-136.5(3)
O1-Co-N1-C8	135.0(3)	O2-Co-N1-C12	45.6(4)

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