ACTA CHEMICA SCANDINAVICA 25 (1971) 1767–1774

The Crystal Structure of Hexaimidazole Cobalt(II) Carbonate Pentahydrate, $Co(C_3H_4N_2)_6CO_3(H_2O)_5$

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The crystal structure of $Co(C_3H_4N_2)_6CO_3(H_2O)_5$ has been determined from three-dimensional X-ray data, collected by the equi-inclination Weissenberg method using Cu$K\alpha$-radiation. There are two formula units in the hexagonal unit cell, and the cell dimensions are $a=b=8.996$ Å, and $c=21.13$ Å. The space group is $P6_3$. There are layers of carbonate ions and water oxygens parallel to the x,y-plane. Halfway between these layers, there are $Co(C_3H_4N_2)_6^{2+}$ ions. The coordination around Co to the binding nitrogen is octahedral, with the bond distances Co–N 2.16 Å and 2.18 Å.

It is well established that metal ions function as mediatory links between enzymes and their substrates in biochemical processes. However, the structural details of this linking are not at present well known. Direct observations in biological systems are time-consuming and difficult to carry out, and investigations are often restricted to model studies. Careful X-ray investigations have thereby shown to give very valuable contributions. Since it has been shown that the imidazole residue of the amino acid histidine is involved in binding metal ions in many metal-enzymes, it is of particular interest to study metal-imidazole complexes.

Of previous crystal structure investigations of metal-imidazole complexes we may mention the following:

$Cu(C_3H_3N_2)_2$,[1] $Zn(C_3H_4N_2)_2Cl_2$,[2] $Zn(C_3H_4N_2)_6Cl_2.4H_2O$,[3] $Cu(C_3H_4N_2)_4I_2$,[4] $Ni(C_3H_3N_2)NO_3.2H_2O$,[5] $Zn(C_3H_3N_2)_2$,[6] $Co(C_3H_4N_2)_2CO_3.(H_2O)_2$[7] and $Ni(C_3H_4N_2)_6(NO_3)_2$.[8]

At this institute, we are carrying out X-ray and solution studies of metal-imidazole complexes, and the following crystal structures have been investigated by X-ray methods:

$Cu(C_3H_4N_2)_2Cl_2$, $Cu(C_3H_3N_2)(C_3H_4N_2)_2Cl$, $Cu(C_3H_4N_2)_4Cl_2$, $Co(C_3H_4N_2)_2Cl_2$ (Bruno K. S. Lundberg), $Cu_3(C_3H_3N_2)_2(C_3H_4N_2)_8(ClO_4)_4$ (G. Ivarsson and Bruno K. S. Lundberg), $Ag(C_3H_4N_2)_2NO_3$ (C.-J. Antti and Bruno K. S. Lundberg), and $Co(C_3H_4N_2)_6CO_3(H_2O)_5$. The last complex is the subject of this publication.

EXPERIMENTAL

In a typical preparation of the crystals, 125 ml of a 0.3 M $CoSO_4$-solution were added to 500 ml of a hot aqueous solution, which was 0.3 M in $C_3H_4N_2$, and 0.8 M with respect to $NaHCO_3$. The solution obtained was then allowed to stand under stirring for 1 h on a water bath (at about 90°C). It was then filtered and placed at room-temperature for crystallization. After a few hours, pink crystals in the shape of very regular hexagonal prisms were obtained. They were not stable in air, and during the X-ray exposures they were enclosed together with part of the mother liquid in a sealed capillary of Lindeman glass.

The cobalt content of the crystals was determined by igniting at 1100°C, storing at 750°C for one day, and finally weighing out as Co_3O_4. The contents of C, N, and H were determined by elemental analysis. (Found: Co 9.7; N 26.5; C 35.3; H 5.6. Calc. for $Co(C_3H_4N_2)_6CO_3(H_2O)_5$: Co 9.5; N 27.2; C 36.9; H 5.5.)

In some experiments, we also measured the uptake of protons when the crystals were dissolved in an acidic solution of known H^+-concentration. This uptake should occur according to the reaction:

$$Co(C_3H_4N_2)_6CO_3(H_2O)_5(s) + 8H^+ \rightarrow Co^{2+} + 6C_3H_5N_2^+ + H_2CO_3 + 5H_2O$$

These titrations gave the expected result of eight H^+-uptake per cobalt atom.

From rotation photographs (around [001] and [100]) and the corresponding Weissenberg photographs (zero, first and second layer lines), taken with Cu$K\alpha$-radiation, it was concluded that the crystals are hexagonal. The dimensions were refined from powder data. Systematic extinctions were found for $00l$-reflections with l odd. This is characteristic for the three space groups $P6_322$, $P6_3/m$ and $P6_3$. However, from the diffraction symmetry $P6_322$ could be rejected. The other two space groups differ only in centrosymmetry. Precession photographs were taken as a check, to confirm the Laue group.

Equi-inclination Weissenberg films, $0kl - 8kl$, were taken with Cu$K\alpha$-radiation. The intensities of 822 independent reflections were estimated visually with multiple film technique. No correction was applied for absorption. Since the content of cobalt in the crystals is small, the fluorescence-radiation was not strong and therefore not disturbing.

The Lorentz- and polarization corrections and Fourier summations were computed, using a program originally written by A. Zalkin. A modified version of a program, written by Gantzel, Sparks and Trueblood, was used for structure factor calculations and refinement of the structural parameters. For the calculations of distances and angles, a program first written by A. Zalkin was used. The computers used were CD 3600 and CD 3200.

Crystal data:

$Co(C_3H_4N_2)_6CO_3(H_2O)_5$ F.w. = 616.9
Hexagonal, $P6_3$ $Z = 2$
$a = b = 8.996 \pm 0.001$ Å
$c = 21.13 \pm 0.01$ Å
$V = 1479.9$ Å^3 $\mu = 50.0$ cm^{-1} (Cu$K\alpha$)
$d_{calc} = 1.39$ g/cm^3
$d_{exp} = 1.38 \pm 0.02$ g/cm^3 (flotation method)

STRUCTURE DETERMINATION AND REFINEMENT

The structure determination was initiated assuming the space group $P6_3/m$. Since there are two formula units in the unit cell, the Co-atoms must occupy one of the two-fold positions. They are:

2*a*	0,0,$\frac{1}{4}$;	0,0,$\frac{3}{4}$
2*b*	0,0,0;	0,0,$\frac{1}{2}$
2*c*	$\frac{1}{3}$,$\frac{2}{3}$,$\frac{1}{4}$;	$\frac{2}{3}$,$\frac{1}{3}$,$\frac{3}{4}$
2*d*	$\frac{2}{3}$,$\frac{1}{3}$,$\frac{1}{4}$;	$\frac{1}{3}$,$\frac{2}{3}$,$\frac{3}{4}$

Thus in a Patterson space, the Co-atoms may give Co – Co vectors at either $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ and $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ or $0,0,\frac{1}{2}$. In a three-dimensional Patterson synthesis, $P(u\,v\,w)$, it was found that besides the high peak ($P(u\,v\,w)=999$) at $u=0$, $v=0$, $w=0$, there were two high peaks, one at $u=0$, $v=0$, $w=\frac{1}{2}$ with a height of 500, and another one at $u=0$, $v=0$, $w=\frac{1}{4}$ with a height of 150. All other peaks had heights <100. Now, if the peak at $u=0$, $v=0$, $w=\frac{1}{2}$ is taken as a Co – Co vector, the two Co-atoms must occupy the positions of either 2*a* or 2*b*. The other two possibilities, 2*c* and 2*d*, must be ruled out, since the peaks at $u=\frac{1}{3}$, $v=\frac{2}{3}$, $w=\frac{1}{2}$, and $u=\frac{2}{3}$, $v=\frac{1}{3}$, $w=\frac{1}{2}$ are too low (heights ≈ 40).

In order to find C- and N-atoms in the imidazole rings coordinated to the Co-atoms we used the Patterson synthesis, and looked for the vectors corresponding to Co-N and Co-C. We found that it was possible to find the atoms of six imidazole rings around each of the Co-atoms. Furthermore, the octahedral Co-imidazole arrangement gave acceptable distances Co – N, C – C and C – N. At this stage of the determination, no decision could be made whether the Co-atoms were placed in 2*a* or 2*b*.

In order to find the oxygens in H_2O and CO_3^{2-}, two three-dimensional Fourier synthesis were performed. In one of them, we assumed that the Co-atoms in the $Co(C_3H_4N_2)_6^{2+}$-molecules were placed in 2*a*, and in the other one in 2*b*. Additional peaks, besides those corresponding to the input atoms, were then found in the Fourier maps, and they were readily identified as oxygens. From distance considerations, these oxygen peaks could then easily be separated in O-peaks arising from water-molecules and O-peaks from CO_3^{2-} groups. However, for the case with Co in 2*a*, the H_2O and CO_3^{2-} found were not in agreement with the experimentally determined composition $Co(C_3H_4N_2)_6CO_3(H_2O)_5$ and the density $d=1.38$ g/cm³. In order to be able to explain this Fourier electron density map, it would be necessary to assume the formula $Co(C_3H_4N_2)_6(HCO_3)_2(H_2O)_7$ and a density $d=1.61$ g/cm³. Considering the experimental accuracy in analysis and density determinations, this formula and density are improbable, and thus the possibility of Co in 2*a* was ruled out. However, by placing Co in 2*b*, 0,0,0, and $0,0,\frac{1}{2}$, both the electron density maps, the analysis and the density determinations can be well explained. With this model, all vectors in the Patterson space could also be explained. By using the least-squares-method, the various atomic parameters were refined, and the resulting *R*-value was 0.131.

$$R=\frac{\sum||F_o|-|F_c||}{\sum|F_o|}$$

The scattering factors used were those given in *International Tables for X-ray Crystallography* (1962) Vol. III, where account was taken of the real part of the dispersion correction. The weighting scheme used was that proposed by Cruickshank: $\omega=1/(a+|F_o|+c|F_o|^2+d|F_o|^3)$ with the final values for the constants $a=10.0$, $c=0.03$, and $d=0$.

The refinement was then continued, assuming the structure to be non-centrosymmetric (space-group $P6_3$), and this gave $R=10.6$ %. By using anisotropic temp. factors, the *R*-value was 8.8 %. The final isotropic atomic parameters of the non-centrosymmetric structure and corresponding standard deviations are shown in Table 1.

Table 1. Atomic positional fractional coordinates and the isotropic thermal parameters with their standard deviations.

	X	$\sigma(X)$	Y	$\sigma(Y)$	Z	$\sigma(Z)$	B	$\sigma(B)$
Co	0	0	0	0	0	0	2.55	0.05
N(1)	0.9911	0.0015	0.1925	0.0015	0.0602	0.0005	4.18	0.21
N(2)	0.9451	0.0018	0.3136	0.0018	0.1388	0.0006	5.17	0.27
N(3)	0.0041	0.0016	0.8058	0.0016	0.9414	0.0006	2.55	0.21
N(4)	0.0608	0.0019	0.6767	0.0019	0.8609	0.0006	3.18	0.26
C(1)	0.0581	0.0019	0.3589	0.0020	0.0457	0.0007	4.48	0.26
C(2)	0.0549	0.0019	0.4485	0.0019	0.1039	0.0007	4.37	0.26
C(3)	0.9102	0.0013	0.1713	0.0013	0.1128	0.0004	2.35	0.16
C(4)	0.9064	0.0021	0.6246	0.0022	0.9484	0.0008	3.39	0.27
C(5)	0.9651	0.0026	0.5547	0.0025	0.9087	0.0009	4.42	0.36
C(6)	0.0790	0.0032	0.8342	0.0032	0.8816	0.0011	5.18	0.46
C(7)	0.6667	0	0.3333	0	0.2547	0.0011	2.17	0.24
O(1)	0.5624	0.0011	0.1724	0.0011	0.2543	0.0006	3.37	0.16
O(2)	0.2728	0.0015	0.3337	0.0015	0.2339	0.0006	4.94	0.26
O(3)	0	0	0	0	0.2557	0.0016	5.82	0.44
O(4)	0.3333	0	0.6667	0	0.2326	0.0014	7.86	0.62

DESCRIPTION OF THE STRUCTURE

The cobalt atom binds to the nitrogens of six imidazole rings yielding $Co(C_3H_4N_2)_6^{2+}$ ions. The coordination to the binding nitrogens is octahedral (Fig. 1). Halfway between the $Co(C_3H_4N_2)_6^{2+}$ ions, there are layers of car-

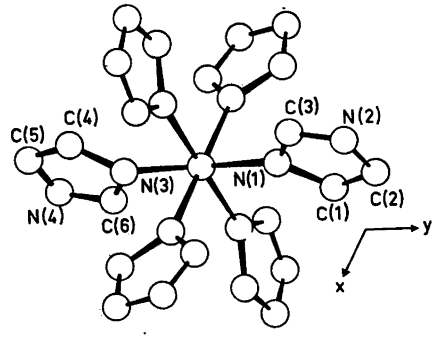

Fig. 1. The structure of the hexaimidazole-cobalt(II)-ion.

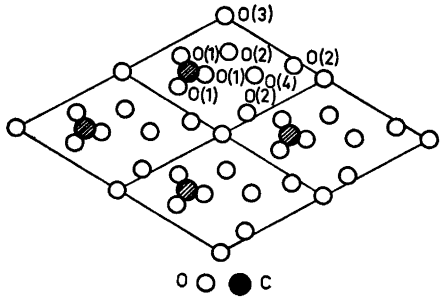

Fig. 2. A layer of carbonate ions and water oxygens.

bonate ions and water oxygens (Fig. 2). The Co-atoms lie on the z-axis, which is a six-fold screw-axis, and the layers are perpendicular to this, *i.e.* parallel to the x,y-plane.

In the imidazole rings, the bond distances range from 1.28 to 1.48 Å, and the angles from 100.0° to 112.6° (Fig. 1 and Table 2). The bond distances Co – N are 2.16 and 2.18 Å, and the C – O distance in the carbonate ions is 1.27 Å.

Table 2. Bond distances and angles in the imidazole rings.

	Distance		Angle
N(1) – C(1)	1.34 Å	N(1) – C(1) – C(2)	107.3°
C(1) – C(2)	1.48	C(1) – C(2) – N(2)	100.0
C(2) – N(2)	1.34	C(2) – N(2) – C(3)	111.7
N(2) – C(3)	1.28	N(2) – C(3) – N(1)	112.6
C(3) – N(1)	1.29	C(3) – N(1) – C(1)	105.6
N(3) – C(4)	1.42	N(3) – C(4) – C(5)	108.5
C(4) – C(5)	1.31	C(4) – C(5) – N(4)	108.6
C(5) – N(4)	1.42	C(5) – N(4) – C(6)	106.0
N(4) – C(6)	1.41	N(4) – C(6) – N(3)	107.1
C(6) – N(3)	1.40	C(6) – N(3) – C(4)	105.6

Table 3. Interatomic distances O – O and N – O shorter than 3 Å.

O(1) – O(2)	2.73 Å
O(2) – O(3)	2.81
O(2) – O(4)	2.77
O(1) – N(2)	2.88
O(1) – N(4)	2.65

DISCUSSION

The centrosymmetric space-group was ruled out, while refinement in the non-centrosymmetric space-group gave on one hand a better R-value (10.6 % against 13.1 %), and on the other more probable temperature factors for the oxygen atoms: O(2) 4.94 *v.* 7.95, O(3) 5.82 *v.* 6.66, and O(4) 7.86 *v.* 14.63.

In most structures with Co – N bonds, which have been determined so far, cobalt has the oxidation number three. Then the bond distances often range from 1.95 to 2.00 Å. If cobalt has the oxidation number two, the distances increase by about 0.15 Å[9]. Examples of compounds with Co(II) – N bonds are (bond distances in parenthesis):
α-$CoPy_2Cl_2$ (2.14 Å);[10] $Co(NH_3)_6Cl_2$ (2.114 Å);[11] $Co(C_3H_4N_2)_6CO_3(H_2O)_5$ (2.16 and 2.18 Å).

The distances and angles in the imidazole rings, as well as in the carbonate ion, are in agreement with those found in other structures (Table 2).

In the layers, the O – O distances are 2.73 – 2.81 Å, *i.e.* the same as distances found in hexagonal ice.[12] The distances between carbonate oxygens and water oxygens are shorter than the other O – O distances (4 – 5 standard deviations). This indicates that the carbonate ions are hydrated.

Table 4. Observed and calculated structure factors.

Table 4. Continued.

2	1	12	12.34	13.29	3	1	6	12.49	13.31	4	1	14	9.76	10.26	5	3	0	7.66	6.63
2	1	10	28.16	27.27	3	1	4	42.38	35.03	4	1	16	27.45	26.43	5	4	14	11.12	10.19
2	1	8	35.09	36.30	3	1	2	18.46	16.27	4	1	12	11.23	10.15	5	4	6	7.52	7.90
2	1	6	44.38	46.72	3	1	0	69.40	64.35	4	1	10	13.35	7.79	5	4	2	14.83	18.80
2	1	4	8.88	4.72	3	2	24	7.46	6.85	4	1	8	18.52	16.52	5	4	0	25.26	28.45
2	1	2	17.97	19.53	3	2	22	3.69	2.69	4	1	4	31.21	28.36	5	5	12	7.50	7.47
2	1	0	12.08	10.83	3	2	20	11.16	12.26	4	1	6	7.22	6.80	5	5	4	15.02	17.79
2	2	22	4.38	9.79	3	2	18	18.58	18.21	4	1	0	62.23	55.80	5	5	2	4.63	8.04
2	2	20	8.44	8.06	3	2	16	12.63	12.12	4	1	2	40.12	34.39	5	5	0	16.28	14.51
2	2	18	4.80	2.38	3	2	14	10.25	9.79	4	2	22	5.76	5.40	5	6	4	5.65	6.82
2	2	16	12.33	13.17	3	2	12	18.53	18.42	4	2	20	9.46	9.16	5	6	2	8.77	9.76
2	2	14	18.86	18.29	3	2	10	42.99	42.16	4	2	18	18.29	17.28	5	6	0	4.96	5.75
2	2	12	17.80	18.28	3	2	8	39.29	35.33	4	2	16	15.80	15.05	6	1	21	2.16	1.46
2	2	10	7.35	6.68	3	2	6	7.43	9.37	4	2	14	7.51	6.17	6	1	19	3.60	3.00
2	2	8	32.66	34.72	3	2	4	7.59	8.66	4	2	12	5.09	4.67	6	1	17	6.73	7.98
2	2	6	20.80	17.95	3	2	2	38.46	35.95	4	2	10	12.05	10.56	6	1	11	13.68	13.53
2	2	4	27.74	33.20	3	2	0	55.99	51.30	4	2	8	8.31	8.77	6	1	7	5.66	5.02
2	2	2	6.40	5.38	3	3	22	5.33	4.35	4	2	6	19.86	18.03	6	1	5	6.69	8.49
2	2	0	38.68	40.82	3	3	20	6.59	6.62	4	2	4	20.76	17.66	6	1	3	15.15	14.61
2	2	20	8.78	7.40	3	3	18	3.86	3.70	4	2	2	41.12	40.91	6	2	13	10.19	15.08
2	2	18	7.32	8.18	3	3	16	11.90	12.16	4	2	0	34.29	32.99	6	2	7	14.53	13.03
2	2	16	8.63	8.55	3	3	14	8.62	7.40	4	3	20	3.40	2.92	6	2	11	6.35	4.92
2	2	14	4.74	5.43	3	3	12	14.54	15.57	4	3	16	3.73	3.96	6	2	9	21.30	21.95
2	2	12	12.60	13.01	3	3	10	10.73	11.03	4	3	14	6.30	5.99	6	3	3	6.80	6.80
2	2	8	13.52	12.78	3	3	8	39.35	39.71	4	3	14	8.85	9.23	6	1	20	6.05	6.79
2	2	10	7.89	8.26	3	3	6	20.91	20.74	4	3	12	14.60	13.75	6	1	18	5.59	5.65
2	2	6	7.24	8.56	3	3	4	23.69	27.58	4	3	10	23.64	22.52	6	1	16	5.10	5.68
2	2	4	27.27	31.89	3	3	2	5.74	4.88	4	3	8	12.47	12.11	6	1	14	13.97	13.98
2	2	2	10.03	11.26	3	3	0	31.19	28.99	4	3	6	23.65	25.60	6	1	12	15.61	14.69
2	2	0	20.99	19.18	3	4	20	6.36	6.80	4	3	4	23.16	21.62	6	1	10	11.06	10.63
2	4	18	3.23	2.23	3	4	18	3.61	4.39	4	3	2	17.46	15.73	6	1	8	12.93	13.50
2	4	16	10.02	9.43	3	4	16	3.78	2.51	4	3	0	15.51	11.48	6	1	6	15.96	16.06
2	4	14	5.30	5.52	3	4	14	7.69	6.74	4	4	18	3.23	3.22	6	1	4	20.42	20.47
2	4	12	6.93	8.78	3	4	12	21.27	21.42	4	4	16	11.12	10.28	6	1	2	9.41	8.25
2	4	10	9.26	10.42	3	4	10	25.82	28.67	4	4	14	7.07	8.22	6	1	0	12.85	12.29
2	4	8	24.39	28.57	3	4	8	19.93	19.99	4	4	12	13.15	15.63	6	2	18	5.88	5.12
2	4	6	12.35	14.27	3	4	6	12.50	11.82	4	4	10	4.32	5.70	6	2	16	2.42	2.02
2	4	4	4.22	6.32	3	4	4	17.58	16.53	4	4	8	19.56	18.97	6	2	14	7.33	7.00
2	4	2	4.22	2.34	3	4	2	8.48	9.17	4	4	6	10.14	11.54	6	2	12	9.34	11.87
2	4	0	18.22	18.72	3	4	0	7.34	8.17	4	4	4	23.61	22.43	6	2	10	13.99	15.26
2	7	16	5.65	5.21	3	5	18	6.69	5.77	4	4	2	5.03	4.20	6	2	8	8.86	8.71
2	7	12	3.48	1.81	3	5	16	4.46	3.71	4	4	0	16.20	17.00	6	2	6	18.06	17.30
2	7	10	9.92	10.28	3	5	14	7.06	8.02	4	5	16	7.42	8.22	6	2	4	19.77	18.58
2	7	8	11.83	14.32	3	5	12	8.15	11.09	4	5	14	8.64	9.46	6	2	2	9.28	9.73
2	7	6	10.93	11.53	3	5	10	16.01	17.81	4	5	12	4.61	4.72	6	2	0	8.30	5.36
2	7	2	7.21	8.32	3	5	8	10.20	9.02	4	5	8	8.43	9.58	6	3	16	7.66	8.65
2	7	0	10.99	12.65	3	5	6	16.41	16.90	4	5	4	14.71	15.88	6	3	12	12.39	11.73
2	8	10	4.29	3.69	3	5	4	12.16	13.86	4	5	2	14.33	15.76	6	3	10	9.56	8.31
2	8	8	3.67	5.58	3	5	2	12.95	13.17	4	5	0	14.87	14.16	6	3	8	17.65	18.63
2	8	6	10.56	11.95	3	5	0	3.77	3.43	4	6	12	6.12	6.66	6	3	6	12.98	13.98
2	8	2	5.65	5.75	3	6	16	4.40	5.60	4	6	10	4.90	4.09	6	3	2	4.82	6.89
2	9	8	7.34	7.22	3	6	14	4.16	3.79	4	6	4	6.77	10.09	6	3	0	15.51	14.86
3	1	17	6.59	7.22	3	6	12	9.76	9.41	4	6	6	5.03	4.98	6	4	18	9.92	11.83
3	1	15	6.81	7.73	3	6	10	11.18	12.06	4	6	2	10.02	11.01	6	4	8	5.66	7.69
3	1	11	5.87	4.92	3	6	8	9.89	10.53	4	6	0	6.97	8.68	6	4	2	10.37	11.64
3	1	9	10.65	9.85	3	6	6	5.03	5.08	4	7	6	7.53	8.73	6	4	0	11.61	12.51
3	1	7	12.16	11.52	3	6	4	8.12	8.30	4	7	2	4.12	4.68	6	5	6	8.75	8.17
3	1	5	15.13	14.18	3	6	2	8.20	9.75	4	7	0	5.92	6.55	6	5	8	7.36	7.52
3	1	1	3.91	8.25	3	6	0	11.63	11.56	5	1	19	4.19	2.52	7	1	15	2.58	1.97
3	1	3	22.83	18.95	3	7	12	5.72	7.13	5	1	15	8.21	6.71	7	1	11	10.84	8.93
3	2	17	5.36	6.45	3	7	10	5.61	5.38	5	1	3	10.24	7.35	7	1	7	8.26	7.62
3	2	23	6.48	3.94	3	7	8	5.77	6.24	5	1	1	6.45	6.53	7	1	5	13.92	12.36
3	2	15	6.55	5.32	3	7	4	8.72	9.64	5	3	15	10.07	8.61	7	1	3	7.11	5.57
3	2	13	12.44	12.28	3	7	2	6.20	7.83	5	3	11	6.65	7.55	7	2	11	6.23	6.27
3	2	9	11.26	9.66	3	7	0	7.66	10.29	5	3	9	13.63	13.56	7	2	5	5.97	7.36
3	2	5	23.65	22.47	4	1	23	4.47	1.90	5	3	5	12.91	13.58	7	3	3	5.42	3.60
3	2	3	18.68	17.47	4	1	17	4.73	1.87	5	3	3	5.76	7.11	7	3	1	8.65	7.67
3	2	1	17.01	12.16	4	1	13	14.97	15.16	5	3	1	14.25	14.23	7	1	16	7.96	7.37
3	3	19	5.29	5.66	4	1	9	11.25	8.56	5	4	17	3.29	3.59	7	1	12	10.19	10.17
3	3	15	4.30	5.08	4	1	7	19.49	16.63	5	4	15	9.46	2.56	7	1	8	11.48	10.79
3	3	13	13.07	14.74	4	1	5	12.82	11.07	5	4	13	5.36	3.77	7	1	6	8.67	8.64
3	3	11	5.74	7.79	4	1	3	6.08	6.14	5	5	13	5.88	3.24	7	1	4	22.93	22.66
3	3	7	10.36	11.95	4	1	1	8.48	9.34	5	1	22	9.55	9.05	7	1	2	8.07	6.56
3	3	5	6.29	7.40	4	2	21	3.35	2.00	5	1	20	7.96	7.95	7	1	0	14.86	12.57
3	3	3	11.33	9.87	4	2	19	5.65	6.78	5	1	18	9.02	9.03	7	2	14	6.68	6.27
3	3	1	5.89	5.21	4	2	13	11.95	12.68	5	1	16	16.21	16.15	7	2	10	11.54	10.05
3	4	19	3.54	5.76	4	2	7	5.02	10.25	5	1	14	25.02	25.80	7	2	8	11.47	11.66
3	4	17	6.11	6.87	4	2	5	12.43	11.84	5	1	12	6.30	4.22	7	2	6	10.38	12.36
3	4	15	4.75	5.27	4	2	1	10.31	7.17	5	1	10	6.08	3.03	7	2	2	10.56	10.68
3	4	13	12.96	12.51	4	3	21	4.86	5.78	5	1	8	14.09	15.19	7	2	0	10.60	10.91
3	4	11	9.46	9.78	4	3	19	6.70	5.90	5	1	6	22.59	20.32	7	3	10	12.03	12.72
3	4	9	7.27	7.77	4	3	17	9.40	10.14	5	1	4	5.66	3.51	7	3	8	9.76	9.95
3	4	7	22.87	21.76	4	3	15	4.06	4.46	5	1	2	30.06	29.93	7	3	6	8.89	9.13
3	4	5	22.20	24.95	4	3	13	10.87	10.96	5	1	0	49.17	50.53	7	3	4	3.95	3.51
3	4	3	15.70	15.53	4	3	11	22.43	20.85	5	2	20	10.87	9.98	7	3	2	6.68	7.59
3	4	1	4.26	4.97	4	3	9	13.47	12.07	5	2	18	3.67	.93	7	4	6	4.89	4.99
3	5	13	3.41	4.99	4	3	7	7.98	9.11	5	2	16	8.45	8.43	7	4	2	5.74	5.88
3	5	9	5.28	4.21	4	3	5	11.90	10.33	5	2	14	4.73	3.51	7	4	0	10.20	11.13
3	5	5	8.68	10.08	4	3	3	8.70	8.76	5	2	12	24.12	25.41	8	2	9	4.65	1.24
3	5	3	10.81	10.32	4	3	1	14.46	10.86	5	2	10	10.65	9.77	8	2	3	6.95	7.13
3	6	1	3.78	5.38	4	4	13	6.83	4.78	5	2	8	26.97	27.79	8	1	12	5.00	5.24
3	6	9	6.09	6.98	4	4	11	8.58	10.18	5	2	6	6.98	5.19	8	1	10	5.66	4.41
3	6	7	9.68	11.28	4	4	9	6.36	5.99	5	2	4	29.58	28.54	8	1	8	10.04	8.96
3	6	5	7.89	7.49	4	4	7	9.82	13.76	5	2	2	6.24	2.18	8	1	6	9.77	9.33
3	6	1	7.38	8.26	4	4	5	9.13	10.88	5	2	0	37.01	36.71	8	1	4	10.62	9.74
3	7	24	6.27	6.85	4	4	3	4.36	3.91	5	3	16	5.43	3.91	8	1	0	13.61	13.56
3	7	22	4.84	3.88	4	4	1	4.35	8.44	5	3	14	13.86	12.88	8	2	10	4.98	4.58
3	7	20	8.87	6.31	4	5	13	5.86	6.12	5	3	12	7.38	8.56	8	2	8	10.86	10.75
3	7	18	10.20	9.73	4	5	9	5.16	1.71	5	3	10	13.01	14.28	8	2	6	6.69	5.80
3	7	16	19.86	19.98	4	6	3	8.11	9.31	5	3	8	9.88	9.55	8	2	4	7.62	7.86
3	7	14	10.20	10.02	4	6	1	6.68	6.28	5	3	6	23.10	23.48	8	2	2	8.85	9.81
3	7	12	28.78	25.97	4	1	22	6.01	2.95	5	3	4	11.22	10.88	8	3	6	3.88	6.84
3	7	10	21.95	19.12	4	1	18	22.24	20.82	5	3	2	14.81	12.71	8	3	0	6.71	6.53
3	7	8	89.52	83.58	4	1	20	9.88	9.73										

There are hydrogen bonds between N–H in the imidazole rings and O in the carbonate ions too, the distances N–H···O are 2.65 and 2.88 Å. Every carbonate–oxygen binds in this way to two imidazole nitrogens, one above and one below the layer.

The structure is probably an OD-structure.[13] On the photographs there are, in the vicinity of strong reflections, additional reflections, lying on parallel rows in the reciprocal space. Different crystals produce unequal relative intensities of a few reflections. Careful investigations of the degree of disorder in the structure have not yet been carried out.

Further X-ray determinations are being carried out for an isomorphous crystal, containing cadmium instead of cobalt.

Acknowledgements. We wish to thank Professor Nils Ingri for all the facilities placed at our disposal and for his interest in the present work. Thanks are also due to Mr. Sven-Åke Nääs for valuable help with the computer programs. The English of the present paper has been corrected by Dr. Michael Sharp. This work forms a part of a program supported by *Statens Naturvetenskapliga Forskningsråd.*

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Received October 16, 1970.