ACTA CHEMICA SCANDINAVICA 25 (1971) 1758–1766

The Molecular and Crystal Structure of Diimidazole Silver(I) Nitrate, $Ag(C_3H_4N_2)_2NO_3$

CARL-JOHAN ANTTI and BRUNO K. S. LUNDBERG

Department of Inorganic Chemistry, University of Umeå, S-901 87 Umeå, Sweden

The crystal structure of $Ag(C_3H_4N_2)_2NO_3$ has been determined from three-dimensional X-ray data, collected by the equi-inclination Weissenberg method with the linear diffractometer PAILRED, using Mo$K\alpha$ radiation. There are four formula units in the orthorhombic unit cell, and the cell dimensions are $a = 10.927$ Å, $b = 18.215$ Å, and $c = 4.999$ Å. The space group is $P2_12_12_1$. The coordination of the silver atom is almost linear ($172.0 \pm 0.32°$), and the bond distances Ag–N are 2.120 and 2.132 Å ($\sigma = 0.008$ Å).

The bonding of imidazole with transition metal ions is of interest because of this ligand's close relationship with biological systems of more complex nature involving histidine residues. A list of previously determined structures is to be found in the paper presenting $Co(C_3H_4N_2)_6CO_3(H_2O)_5$[1]. The structure presented in this paper is a part of a research program, being carried out in this department.

EXPERIMENTAL

Preparation of the crystals. The crystals were prepared by dissolving 1.2 g (0.007 mol) $AgNO_3$ in 35 ml of H_2O. 2 g (0.03 mol) of imidazole was added, and the white precipitate that appeared was dissolved by adding HNO_3 to pH = 5.5. The colourless crystals were obtained by slow evaporation of the solution at room temperature.

Analysis. The silver content of the crystals was determined electrolytically (exp. weight %: 34.5, calc. weight %: 35.3). The presence of $C_3H_4N_2$ and NO_3^-, and the absence of H_2O was determined with the aid of IR-spectroscopy.[2]

Unit cell data. From rotation photographs (around [001] and [100]) and the corresponding Weissenberg photographs (zero, first and second layers), taken with Cu$K\alpha$-radiation, it was concluded that the crystals are orthorhombic with $a = 10.92$ Å, $b = 18.20$ Å, and $c = 5.00$ Å. More accurate values for the unit cell dimensions were calculated from a powder photograph, taken with monochromatic Cu$K\alpha$-radiation in a focusing camera of Guinier type, using $Pb(NO_3)_2$ as an internal standard substance. The following result was obtained: $a = 10.927 \pm 0.002$ Å, $b = 18.215 \pm 0.005$ Å, $c = 4.999 \pm 0.001$ Å, and $V = 994.90$ Å^3. The errors given are the standard deviations (Table 1). By the flotation method, using the liquids bromoform and acetone, the density was determined to 2.06 g/cm^3. Four formula units $Ag(C_3H_4N_2)NO_3$ in the unit cell give a calculated density of 2.04 g/cm^3.

Space group. The following conditions limiting possible reflections were found:

hkl		
0*kl*	No conditions	*h*00: *h* = 2*n*
*h*0*l*		0*k*0: *k* = 2*n*
*hk*0		00*l*: *l* = 2*n*

which is characteristic for the space group $P2_12_12_1$ (No. 19).[3]

Table 1. Observed and calculated theta values.

H	*K*	*L*	θ_{obs}	θ_{calc}
1	1	0	4.720	4.719
2	0	0	8.100	8.112
0	1	1	9.205	9.202
1	1	1	10.055	10.067
1	2	1	10.927	10.926
2	1	1	12.319	12.314
3	1	1	15.384	15.384
3	2	1	15.979	15.975
4	1	0	16.575	16.581
4	0	1	18.756	18.760
1	2	2	19.125	19.119
4	2	1	19.426	19.424
2	2	2	20.469	20.462
4	5	0	20.652	20.655
3	7	0	21.356	21.352
3	1	2	22.114	22.115
0	9	1	24.256	24.263
4	1	2	24.835	24.847

The intensity material. With the linear diffractometer PAILRED 1500 independent reflections were recorded on data-tape from the *hk*0 – *hk*4. They were corrected for background radiations and tabulated with the relative counting statistic errors. Reflections with an error ($\Delta I/I$) greater than 0.5 were omitted. From the intensity values of the 1021 remaining reflections, F^2 values were then calculated in the ordinary way.

Computer programs used. The Lorentz-, polarization-, and absorption corrections were computed by using a program originally written by P. Coppens, L. Leiserowitz and D. Rabinovich. The Fourier summations were computed with a program originally written by A. Zalkin. A modified version of a program written by Gantzel, Sparks and Trueblood was used for refinement of structural parameters. For the calculations of distances and angles, a program first written by A. Zalkin was used. To draw the figures we used a plot program ORTEP written by C. Johnson. The computers used were CD 3600 and CD 3200.

STRUCTURE DETERMINATION

There are four formula units in the unit cell, which means that in $P2_12_12_1$ all atoms occupy general fourfold positions.

To determine the position of the silver atom, a three-dimensional Patterson synthesis was calculated. Because silver is a very heavy atom, compared with the others in the molecule, we could easily find the Ag – Ag vectors and determine the *x*-, *y*-, and *z*-coordinates for the Ag atoms.

Table 2. Observed and calculated structure factors.

16	7	0	11.02	6.21	5	15	0	35.43	33.88	11	10	1	8.33	8.27	4	4	1	96.47	97.55												
16	4	0	9.16	6.71	5	16	0	20.83	19.93	11	11	1	8.75	8.37	4	3	1	31.00	27.09												
15	3	0	16.88	17.34	5	17	0	16.43	15.99	11	12	1	22.22	22.98	4	2	1	67.16	62.27												
15	6	0	9.48	11.23	5	18	0	9.26	9.25	11	16	1	16.93	14.28	4	1	1	17.67	18.47												
15	9	0	14.47	12.82	5	19	0	15.47	15.22	10	17	1	9.71	6.34	4	0	1	143.84	140.43												
14	14	0	10.80	10.10	5	22	0	12.27	5.38	10	14	1	17.76	14.53	3	0	1	9.77	10.78												
14	10	0	14.05	14.13	5	23	0	12.02	11.25	10	10	1	21.48	22.34	3	1	1	45.86	44.13												
14	8	0	17.84	17.15	4	21	0	15.26	18.80	10	11	1	15.03	13.48	3	2	1	109.32	108.26												
14	4	0	21.33	22.22	4	17	0	19.28	20.56	10	9	1	10.31	10.53	3	3	1	11.79	11.34												
14	0	0	21.32	21.50	4	15	0	12.01	11.49	10	8	1	14.15	10.67	3	4	1	84.48	83.21												
13	2	0	22.53	22.64	4	13	0	9.69	8.88	10	7	1	16.47	16.38	3	5	1	39.52	38.89												
13	4	0	12.03	10.28	4	11	0	44.06	44.40	10	6	1	21.85	22.29	3	6	1	63.98	65.86												
13	5	0	13.60	12.54	4	9	0	13.20	14.24	10	5	1	15.60	16.39	3	7	1	41.05	38.72												
13	6	0	10.69	10.74	4	7	0	70.09	71.94	10	4	1	34.24	33.59	3	8	1	62.87	66.68												
13	8	0	14.16	15.78	4	6	0	12.47	12.33	10	3	1	13.96	14.51	3	9	1	12.13	10.28												
13	9	0	12.07	10.53	4	5	0	49.15	50.48	10	2	1	15.80	15.75	3	10	1	26.48	25.33												
13	10	0	8.61	6.84	4	4	0	18.13	17.47	10	1	1	23.94	23.95	3	11	1	22.11	20.61												
13	12	0	13.42	11.96	4	3	0	118.91	116.58	10	0	1	45.47	46.87	3	12	1	59.69	60.09												
13	13	0	10.39	7.92	4	1	0	108.93	107.79	9	0	1	17.78	17.45	3	13	1	16.65	17.60												
13	14	0	9.53	10.34	4	0	0	51.70	49.50	9	1	1	28.86	29.82	3	14	1	10.58	12.04												
12	17	0	10.43	6.71	3	1	0	66.25	63.67	9	2	1	38.69	37.69	3	15	1	14.32	17.46												
12	13	0	13.22	8.97	3	2	0	20.26	21.09	9	3	1	28.34	23.85	3	16	1	40.55	40.78												
12	11	0	11.07	13.28	3	3	0	19.48	18.64	9	4	1	28.38	27.92	3	17	1	13.19	12.76												
12	9	0	10.27	10.07	3	4	0	31.23	31.69	9	5	1	34.62	35.20	3	18	1	15.49	15.71												
12	7	0	22.79	22.56	3	5	0	134.98	130.29	9	6	1	19.27	20.14	3	22	1	12.69	12.43												
12	6	0	10.60	12.36	3	6	0	27.24	23.64	9	7	1	14.90	14.03	3	26	1	12.28	5.51												
12	5	0	26.77	27.87	3	7	0	12.64	10.41	9	8	1	22.12	22.49	2	27	1	8.58	3.18												
12	1	0	19.66	20.25	3	8	0	21.43	22.53	9	9	1	18.17	14.46	2	21	1	14.08	12.90												
12	0	0	15.16	15.96	3	9	0	84.31	84.07	9	10	1	14.38	14.04	2	20	1	18.67	18.20												
11	1	0	27.64	26.53	3	11	0	47.07	44.38	9	11	1	10.92	11.43	2	19	1	8.36	6.40												
11	2	0	8.99	8.67	3	12	0	19.96	18.93	9	12	1	16.31	18.75	2	18	1	13.25	11.91												
11	3	0	17.05	18.20	3	13	0	38.19	37.44	9	13	1	10.76	11.60	2	17	1	17.43	17.91												
11	5	0	32.57	30.81	3	14	0	9.47	4.74	9	15	1	11.35	12.58	2	16	1	21.48	21.22												
11	9	0	22.69	23.01	3	15	0	28.58	28.87	9	16	1	10.65	12.16	2	14	1	26.42	27.71												
11	11	0	11.94	9.95	3	16	0	9.87	9.36	9	18	1	8.77	7.40	2	13	1	18.68	20.21												
11	13	0	11.21	10.84	3	17	0	15.85	14.91	8	21	1	10.72	10.92	2	12	1	11.66	11.85												
11	14	0	8.36	1.11	3	19	0	13.35	12.55	8	17	1	18.19	17.46	2	11	1	29.78	28.91												
10	14	0	8.93	4.63	3	23	0	8.88	8.85	8	16	1	15.31	14.82	2	10	1	43.24	43.78												
10	14	0	8.91	5.42	2	25	0	9.23	4.57	8	13	1	14.72	14.79	2	8	1	52.82	53.68												
10	13	0	14.68	14.95	2	21	0	10.95	13.97	8	12	1	15.71	13.94	2	7	1	67.05	68.89												
10	11	0	23.60	22.70	2	20	0	10.13	12.12	8	11	1	24.96	24.71	2	6	1	58.94	60.82												
10	10	0	9.03	9.92	2	17	0	26.68	25.44	8	10	1	13.43	13.68	2	5	1	61.86	57.31												
10	8	0	9.08	9.84	2	16	0	13.23	13.73	8	9	1	11.17	12.98	2	4	1	132.57	131.39												
10	6	0	7.89	3.58	2	15	0	19.19	19.55	8	8	1	19.54	18.88	2	3	1	48.89	50.98												
10	7	0	36.69	35.87	2	14	0	40.07	40.37	8	7	1	44.33	44.87	2	2	1	96.75	93.74												
10	5	0	14.92	16.50	2	13	0	37.22	36.91	8	6	1	26.56	27.08	2	1	1	126.41	129.54												
10	4	0	13.64	13.13	2	12	0	7.15	3.53	8	5	1	18.00	19.08	2	0	1	210.61	219.78												
10	3	0	27.80	26.15	2	11	0	63.89	64.43	8	4	1	12.87	13.47	1	3	1	34.96	33.25												
10	1	0	24.54	23.59	2	10	0	67.52	63.87	8	3	1	51.48	51.38	1	4	1	72.68	68.61												
10	0	0	19.37	18.82	2	9	0	21.78	19.91	8	2	1	21.59	21.06	1	5	1	141.53	140.28												
9	1	0	23.04	22.70	2	8	0	43.80	42.76	8	1	1	48.76	47.65	1	6	1	59.17	56.52												
9	2	0	32.50	31.37	2	7	0	101.70	99.82	8	0	1	27.98	28.16	1	7	1	11.94	14.65												
9	3	0	11.30	8.28	2	6	0	88.69	83.84	7	0	1	10.98	11.12	1	8	1	42.17	42.29												
9	4	0	29.95	30.55	2	5	0	32.14	29.30	7	1	1	44.23	42.47	1	9	1	72.69	73.66												
9	5	0	34.41	34.62	2	4	0	16.92	18.06	7	2	1	20.31	20.55	1	10	1	42.57	39.70												
9	8	0	26.49	25.91	2	3	0	11.36	13.85	7	3	1	15.77	14.51	1	11	1	53.73	52.02												
9	7	0	10.99	11.25	2	2	0	10.28	12.47	7	4	1	15.23	13.77	1	12	1	32.31	32.33												
9	8	0	30.98	31.72	2	1	0	54.52	55.77	7	5	1	67.11	64.76	1	13	1	54.85	52.87												
9	9	0	29.92	28.30	2	0	0	99.11	101.51	7	6	1	26.17	26.13	1	14	1	15.43	16.92												
9	11	0	21.08	19.23	1	3	0	24.85	26.00	7	7	1	8.83	9.56	1	15	1	31.18	31.47												
9	12	0	27.51	27.09	1	4	0	122.57	123.49	7	8	1	18.09	18.20	1	16	1	18.64	20.15												
9	13	0	12.94	12.93	1	5	0	84.10	82.47	7	9	1	49.04	48.78	1	17	1	18.91	18.95												
9	14	0	12.91	12.59	1	6	0	112.19	110.60	7	10	1	28.69	29.57	1	18	1	8.78	7.79												
9	15	0	15.90	13.91	1	8	0	74.02	71.80	7	11	1	30.96	29.78	1	19	1	14.25	12.85												
9	16	0	8.54	5.30	1	9	0	40.54	41.70	7	13	1	25.25	24.55	1	23	1	9.11	8.60												
8	16	0	12.38	13.46	1	10	0	15.82	14.36	7	14	1	14.94	13.86	0	27	1	8.83	5.53												
8	14	0	7.95	8.08	1	11	0	36.83	34.41	7	15	1	24.08	23.16	0	26	1	13.86	1.79												
8	14	0	23.33	23.75	1	12	0	88.50	87.86	7	17	1	15.07	10.24	0	21	1	17.93	18.17												
8	13	0	9.96	9.44	1	13	0	19.97	19.61	7	19	1	14.01	13.86	0	18	1	12.83	12.51												
8	12	0	9.38	7.08	1	15	0	21.78	22.23	7	20	1	9.14	3.46	0	17	1	23.54	23.83												
8	10	0	47.80	46.28	1	16	0	41.63	40.71	7	21	1	8.16	1.12	0	15	1	27.88	29.71												
8	8	0	18.60	18.10	1	18	0	19.02	20.14	7	23	1	15.69	7.44	0	14	1	8.11	8.36												
8	7	0	21.63	21.29	1	19	0	13.35	13.36	6	23	1	8.96	3.79	0	13	1	48.99	39.89												
8	6	0	50.27	48.89	1	20	0	11.65	13.34	6	18	1	10.45	9.64	0	12	1	29.65	28.76												
8	5	0	12.97	12.40	1	22	0	10.99	12.23	6	17	1	15.55	16.62	0	11	1	70.41	70.90												
8	4	0	58.30	58.33	1	23	0	12.04	9.14	6	14	1	14.72	16.04	0	9	1	31.45	33.88												
8	3	0	16.43	16.99	1	26	0	8.90	7.31	6	13	1	15.48	15.92	0	8	1	15.62	14.61												
8	2	0	25.66	25.24	0	22	0	10.19	9.03	6	12	1	16.97	17.20	0	7	1	130.11	133.66												
8	1	0	31.93	30.81	0	20	0	27.41	28.17	6	11	1	33.68	34.93	0	6	1	46.88	47.71												
8	0	0	87.93	87.55	0	18	0	21.38	21.90	6	10	1	43.99	43.49	0	5	1	27.97	24.84												
7	1	0	7.19	3.77	0	16	0	25.06	24.49	6	9	1	11.11	9.19	0	4	1	24.96	21.15												
7	2	0	100.62	100.56	0	14	0	41.42	43.23	6	8	1	23.56	23.11	0	3	1	47.38	45.78												
7	4	0	55.73	52.84	0	12	0	6.51	3.33	6	7	1	56.18	56.26	16	4	2	10.13	7.81												
7	6	0	68.63	67.56	0	10	0	48.19	46.38	6	6	1	29.13	27.48	16	0	2	12.36	6.98												
7	8	0	54.72	53.22	0	8	0	91.69	92.12	6	5	1	31.77	31.84	15	2	2	12.22	10.18												
7	10	0	21.22	20.15	0	6	0	130.16	135.80	6	4	1	55.76	52.13	15	6	2	11.21	8.14												
7	11	0	10.10	7.36	0	4	0	197.22	211.57	6	3	1	57.96	56.96	15	7	2	10.32	7.76												
7	12	0	48.54	50.35	16	3	1	9.54	9.20	6	2	1	41.56	39.03	15	10	2	10.93	6.12												
7	14	0	28.70	28.97	15	1	1	10.91	9.64	6	1	1	56.94	54.85	14	14	2	11.24	3.85												
7	18	0	12.68	13.29	15	9	1	10.38	8.36	6	0	1	40.25	40.63	14	10	2	9.28	4.88												
7	22	0	12.89	9.72	14	11	1	11.61	9.76	5	0	1	61.73	61.06	14	4	2	11.87	10.77												
6	21	0	10.68	9.76	14	7	1	14.91	14.84	5	1	1	42.49	41.78	14	0	2	12.82	14.94												
6	20	0	12.48	12.61	14	4	1	8.33	6.55	5	2	1	86.74	86.03	13	1	2	11.11	8.33												
6	18	0	14.86	14.17	14	3	1	15.64	15.63	5	3	1	22.21	23.06	13	1	2	11.88	11.97												
6	17	0	18.51	19.79	14	1	1	10.50	8.78	5	4	1	60.11	60.13	13	2	2	13.62	11.88												
6	16	0	20.77	20.25	13	0	1	8.28	6.21	5	5	1	58.23	57.11	13	3	2	10.61	10.62												
6	14	0	35.75	37.09	13	1	1	10.10	11.14	5	6	1	71.90	70.77	13	4	2	9.31	6.12												
6	13	0	13.41	12.17	13	2	1	14.70	14.12	5	7	1	13.66	15.18	13	5	2	12.94	11.89												
6	11	0	35.84	36.98	13	5	1	14.63	14.86	5	8	1	65.07	62.26	13	7	2	11.79	9.17												
6	10	0	55.77	58.02	13	6	1	14.96	16.28	5	9	1	36.45	36.02	12	11	2	13.25	13.33												
6	9	0	22.00	20.15	13	8	1	10.93	10.27	5	10	1	30.09	30.20	12	9	2	13.55	8.92												
6	8	0	40.13	40.14	13	9	1	11.35	14.04	5	11	1	24.04	23.97	12	8	2	11.13	10.58												
6	7	0	26.64	26.92	13	12	1	9.07	8.15	5	12	1	43.98	44.59	12	7	2	14.54	14.66												
6	6	0	50.10	48.05	13	13	1	8.56	5.80	5	14	1	17.25	16.28	12	6	2	11.73	10.45												
6	5	0	33.57	31.72	12	14	1	11.77	11.37	5	15	1	13.58	13.94	12	5	2	12.45	14.33												
6	4	0	80.43	80.68	12	11	1	8.99	5.93	5	16	1	28.40	29.59	12	3	2	12.40	14.61												
6	3	0	59.83	58.56	12	10	1	15.41	17.21	5	22	1	10.80	9.86	12	2	2	16.08	19.28												
6	1	0	31.51	28.78	12	8	1	13.42	14.79	4	20	1	12.80	16.00	12	1	2	15.62	15.91												
6	0	0	11.95	114.04	12	7	1	8.81	10.37	4	16	1	17.02	18.70	11	0	2	21.38	22.29												
5	1	0	61.14	62.44	12	6	1	17.45	17.88	4	8	1	29.99	24.59	11	1	2	22.83	22.69												
5	2	0	23.03	24.24	12	5	1	8.90	7.55	4	14	1	41.37	40.61	11	3	2	12.42	13.49												
5	3	0	32.48	32.50	12	4	1	21.11	23.41	4	13	1	17.98	16.08	11	4	2	24.08	24.59												
5	4	0	44.68	42.65	12	3	1	12.94	17.06	4	12	1	13.35	13.23	11	5	2	27.19	27.03												
5	5	0	83.38	81.21	12	2	1	12.45	10.53	4	11	1	15.16	14.61	11	6	2	12.36	11.64												
5	6	0	16.78	18.07	12	0	1	29.61	30.34	4	10	1	76.24	76.11	11	7	2	9.33	5.35												
5	8	0	29.25	31.13	11	2	1	31.96	32.08	4	9	1	23.83	24.18	11	9	2	14.98	18.58												
5	9	0	57.58	57.10	11	1	1	10.35	12.85	4	8	1	29.99	29.16	11	10	2	15.66	14.88												
5	11	0	25.60	23.85	11	4	1	23.86	23.13	4	7	1	23.73	22.60	11	14	2	11.98	8.58												
5	12	0	36.32	36.14	11	5	1	19.79	20.79	4	6	1	72.68	74.62	11	15	2	10.47	11.20												
5	13	0	22.13	21.78	11	8	1	27.78	27.88	4	5	1	29.05	28.98	11	16	2	9.79	4.69												

Table 2. Continued.

10	20	2	10.01	3.57	3	1	2	37.79	30.48	4	11	3	17.49	17.46	7	0	3	26.49	28.19
10	13	2	11.57	9.02	3	4	2	80.99	89.21	4	14	3	12.45	7.81	1	3	3	40.41	40.21
10	12	2	14.76	14.50	3	5	2	96.41	93.85	4	15	3	10.18	9.73	1	4	3	71.00	70.15
10	11	2	13.65	14.05	3	6	2	86.37	86.70	4	16	3	10.30	6.04	1	5	3	57.75	56.08
10	10	2	14.77	13.58	3	7	2	13.01	6.61	4	20	3	13.04	3.62	1	6	3	46.11	45.74
10	8	2	21.69	21.46	3	8	2	43.88	40.55	4	17	3	9.86	7.47	1	7	3	36.99	35.21
10	7	2	27.12	27.01	3	9	2	69.06	67.69	4	16	3	10.53	11.06	1	8	3	24.39	24.01
10	6	2	23.72	23.37	3	10	2	53.06	50.84	4	13	3	16.43	10.76	1	9	3	31.91	30.61
10	4	2	20.42	19.12	3	11	2	32.87	32.86	4	12	3	17.30	16.13	1	10	3	56.04	54.15
10	3	2	33.22	32.88	3	12	2	17.12	16.48	4	11	3	15.93	16.35	1	11	3	28.49	27.75
10	2	2	30.86	31.07	3	13	2	22.65	22.92	4	10	3	9.28	9.71	1	14	3	27.98	29.21
10	1	2	23.73	23.70	3	14	2	31.58	31.16	4	9	3	15.02	15.25	1	15	3	21.72	22.57
10	0	2	27.14	27.42	3	15	2	29.66	30.79	4	8	3	26.32	24.35	1	16	3	12.34	12.88
9	0	2	11.41	11.01	3	16	2	11.57	9.00	4	7	3	24.92	20.31	1	18	3	13.98	12.72
9	1	2	15.74	15.31	3	17	2	15.40	13.02	4	6	3	21.84	21.95	1	19	3	13.92	8.00
9	2	2	29.65	30.52	3	19	2	14.01	13.08	4	5	3	21.06	22.38	0	22	3	13.61	11.41
9	3	2	21.89	22.44	3	23	2	13.04	8.25	4	4	3	19.47	20.02	0	18	3	9.78	9.35
9	4	2	28.01	30.72	2	21	2	9.81	11.01	4	3	3	29.56	27.74	0	17	3	15.44	13.09
9	5	2	19.77	20.27	2	20	2	11.71	11.04	4	2	3	43.28	44.35	0	16	3	22.47	22.03
9	7	2	32.78	32.57	2	18	2	1.49	44.33	4	1	3	39.18	40.67	0	15	3	9.31	9.91
9	8	2	13.98	12.58	2	17	2	13.70	13.74	4	0	3	17.30	17.30	0	12	3	30.17	30.41
9	8	2	24.26	24.23	2	16	2	10.58	10.47	7	0	3	35.84	35.98	0	11	3	35.12	36.01
9	9	2	20.78	20.60	2	15	2	18.49	17.61	7	1	3	21.19	23.24	0	10	3	21.10	19.65
9	10	2	24.64	27.12	2	14	2	24.04	23.85	7	2	3	18.30	19.10	0	9	3	32.95	30.64
9	11	2	15.65	13.31	2	13	2	19.95	19.72	7	3	3	10.06	10.71	0	8	3	56.33	55.84
9	12	2	25.32	24.16	2	12	2	28.65	27.63	7	4	3	39.29	40.07	0	7	3	62.17	63.76
9	14	2	13.22	13.06	2	11	2	34.75	34.74	7	5	3	30.71	32.39	0	6	3	53.10	52.25
9	16	2	12.32	12.58	2	10	2	43.93	44.33	7	6	3	37.40	39.60	0	5	3	11.39	10.63
8	19	2	9.88	4.77	2	9	2	45.51	43.44	7	8	3	18.64	18.82	0	4	3	32.58	33.35
8	17	2	9.11	4.68	2	8	2	25.30	25.30	7	9	3	19.76	20.94	0	3	3	51.61	53.85
8	16	2	12.03	10.46	2	7	2	49.68	49.68	7	10	3	37.36	40.68	14	1	4	16.95	11.72
8	14	2	19.68	21.82	2	6	2	76.04	74.65	7	11	3	13.98	13.98	14	3	4	12.28	8.45
8	13	2	10.99	10.17	2	5	2	32.62	31.62	7	12	3	16.13	11.64	14	11	4	13.23	6.06
8	10	2	30.66	31.57	2	4	2	50.81	50.25	7	13	3	8.34	9.78	13	7	4	12.87	12.69
8	9	2	22.64	22.07	2	3	2	67.67	68.33	7	14	3	22.42	23.95	13	3	4	18.44	15.39
8	8	2	22.04	23.92	2	2	2	77.31	75.98	7	15	3	12.15	11.85	13	1	4	18.21	16.56
8	6	2	25.73	24.80	2	1	2	67.57	65.86	6	16	3	17.52	16.28	12	2	4	13.33	17.13
8	5	2	25.81	24.96	2	0	2	101.93	99.97	6	13	3	15.49	15.57	12	5	4	11.26	9.39
8	4	2	29.59	28.46	1	3	2	55.73	54.01	6	12	3	27.88	29.94	12	10	4	13.85	6.07
8	3	2	15.17	16.17	1	4	2	53.14	57.18	6	10	3	21.38	21.95	12	16	4	12.08	5.65
8	2	2	12.51	8.69	1	5	2	28.52	30.33	6	9	3	17.93	20.28	11	6	4	17.49	13.35
8	1	2	23.73	23.95	1	6	2	56.81	57.54	6	8	3	34.93	38.82	11	4	4	13.17	15.24
8	0	2	44.24	42.79	1	7	2	35.93	35.68	6	7	3	25.03	26.42	11	3	4	10.87	2.06
7	0	2	9.47	9.05	1	8	2	44.14	45.15	6	5	3	35.21	36.60	11	0	4	16.89	10.67
7	1	2	25.28	25.77	1	9	2	24.05	23.00	6	5	3	21.24	21.34	10	2	4	21.77	21.91
7	2	2	48.33	48.22	1	10	2	26.01	24.87	6	4	3	14.35	13.70	10	3	4	9.56	3.11
7	3	2	36.12	34.60	1	11	2	35.81	35.19	6	3	3	29.27	28.81	10	6	4	18.59	17.51
7	4	2	26.70	26.06	1	12	2	41.42	43.75	6	2	3	38.38	37.10	10	8	4	11.35	17.05
7	5	2	21.70	20.12	1	13	2	13.73	12.44	6	1	3	28.90	27.57	10	9	4	9.16	8.22
7	6	2	30.47	32.02	1	14	2	14.47	17.61	6	0	3	22.72	23.59	10	10	4	11.59	8.78
7	7	2	25.34	26.27	1	15	2	21.65	21.55	5	0	3	39.77	39.28	10	11	4	10.79	2.69
7	8	2	21.27	20.99	1	16	2	28.75	30.74	5	1	3	30.01	28.39	10	12	4	15.32	13.32
7	10	2	10.74	10.03	1	17	2	14.44	13.82	5	2	3	37.30	38.42	10	18	4	13.96	3.43
7	11	2	18.13	17.82	1	18	2	12.85	9.61	5	3	3	40.15	40.25	9	11	4	14.95	12.45
7	12	2	22.46	22.74	1	21	2	10.39	7.54	5	4	3	41.53	39.27	9	10	4	18.86	17.67
7	13	2	13.28	12.08	1	22	2	11.65	8.27	5	5	3	13.41	13.25	9	7	4	18.77	18.83
7	14	2	16.56	15.95	0	26	2	12.81	0	5	6	3	36.56	34.41	9	6	4	20.80	17.32
7	24	2	11.53	.73	0	22	2	10.27	3.70	5	7	3	37.75	39.53	9	5	4	10.60	3.41
6	22	2	9.18	3.47	0	20	2	16.66	15.82	5	8	3	16.18	17.46	9	4	4	20.64	20.80
6	20	2	10.28	7.54	0	19	2	13.66	11.99	5	9	3	18.06	18.83	9	3	4	14.56	16.16
6	19	2	10.48	10.04	0	18	2	10.16	10.06	5	10	3	21.03	20.66	9	0	4	16.57	19.58
6	17	2	9.95	9.06	0	16	2	20.72	20.22	5	11	3	25.85	26.88	8	0	4	17.86	16.59
6	16	2	13.00	8.30	0	15	2	15.07	16.71	5	12	3	12.35	12.23	8	1	4	25.99	27.03
6	15	2	11.47	12.51	0	14	2	28.00	27.82	5	13	3	14.45	15.83	8	2	4	12.01	11.76
6	14	2	17.19	17.56	0	13	2	15.64	16.38	5	14	3	13.11	13.90	8	3	4	14.35	12.39
6	13	2	10.65	8.10	0	12	2	10.69	10.60	5	15	3	18.81	17.12	8	5	4	28.58	27.56
6	12	2	11.13	15.38	0	11	2	10.55	9.57	5	16	3	11.92	10.80	8	8	4	11.95	12.24
6	11	2	16.19	15.58	0	10	2	41.69	42.58	5	17	3	10.34	11.40	8	9	4	20.01	22.04
6	10	2	25.25	26.15	0	9	2	34.24	34.49	5	20	3	13.33	6.47	8	13	4	14.03	12.28
6	9	2	22.28	21.19	0	8	2	46.26	45.25	5	21	3	10.04	6.87	8	17	4	11.27	3.49
6	8	2	23.10	21.40	0	7	2	8.40	9.19	4	19	3	14.49	14.15	8	19	4	12.69	8.74
6	7	2	23.97	23.95	0	6	2	19.49	19.63	4	15	3	13.11	15.16	7	17	4	16.62	15.52
6	6	2	34.36	33.47	0	5	2	61.54	59.33	4	14	3	15.68	16.35	7	15	4	11.19	10.06
6	5	2	35.92	36.14	0	4	2	82.22	85.17	4	13	3	15.14	14.72	7	13	4	19.42	16.69
6	4	2	40.31	41.75	0	3	2	46.55	44.55	4	12	3	13.31	12.96	7	11	4	19.97	21.52
6	3	2	46.91	46.29	16	1	3	12.76	8.22	4	11	3	10.91	12.54	7	9	4	11.77	9.39
6	2	2	30.55	27.89	15	0	3	11.29	11.02	4	10	3	28.36	28.36	7	7	4	30.85	31.05
6	1	2	59.50	60.26	14	4	3	12.59	10.57	4	9	3	28.34	28.11	7	6	4	10.47	11.07
6	0	2	63.94	64.17	14	1	3	9.81	5.30	4	8	3	17.91	18.62	7	5	4	16.70	17.08
5	0	2	52.62	50.47	13	0	3	12.13	12.15	4	6	3	28.34	27.41	7	4	4	7.56	7.47
5	1	2	38.90	39.95	13	4	3	13.03	11.49	4	5	3	53.10	52.39	7	3	4	42.20	43.15
5	2	2	45.52	43.30	13	6	3	14.49	12.23	4	4	3	31.81	33.16	7	2	4	9.88	10.12
5	3	2	14.62	15.45	13	7	3	11.38	8.14	4	3	3	26.95	27.88	7	1	4	26.59	30.28
5	4	2	41.50	40.75	13	8	3	10.51	8.80	4	2	3	26.73	27.07	6	1	4	46.88	48.55
5	5	2	61.70	60.33	13	11	3	10.10	2.76	4	1	3	44.35	44.51	6	2	4	19.71	22.56
5	6	2	42.06	40.34	13	16	3	14.98	4.25	3	0	3	7.53	9.82	6	3	4	25.28	27.55
5	7	2	31.91	32.61	12	9	3	12.95	12.00	4	0	3	46.87	47.06	6	4	4	20.80	14.29
5	8	2	27.37	28.45	12	6	3	10.16	10.74	3	1	3	31.49	31.18	6	5	4	38.42	37.80
5	9	2	35.66	37.10	12	5	3	12.89	14.04	3	2	3	48.26	47.22	6	6	4	15.20	16.47
5	10	2	30.16	29.27	12	1	3	11.22	11.18	3	3	3	42.96	43.80	6	7	4	18.96	19.72
5	11	2	30.14	31.79	12	0	3	14.37	15.12	3	4	3	31.33	33.03	6	8	4	14.91	16.53
5	12	2	19.73	19.26	11	1	3	14.66	11.10	3	5	3	14.80	20.36	6	9	4	28.71	27.25
5	13	2	21.42	22.14	11	2	3	15.38	14.25	3	6	3	29.50	28.19	6	11	4	15.25	13.58
5	14	2	20.17	18.54	11	3	3	20.28	20.13	3	7	3	41.39	43.54	6	12	4	14.51	16.68
5	15	2	27.72	27.85	11	5	3	15.07	6.21	3	8	3	22.22	21.44	6	15	4	12.75	15.49
5	16	2	15.73	14.53	11	6	3	11.24	12.24	3	9	3	16.92	17.78	5	15	4	12.91	11.74
5	17	2	15.68	11.84	11	7	3	17.75	17.90	3	10	3	14.17	14.77	5	16	4	15.87	18.67
4	22	2	11.12	6.91	11	11	3	16.63	13.42	3	11	3	31.51	32.72	5	13	4	10.46	12.77
4	21	2	12.64	12.80	11	12	3	13.72	9.31	3	12	3	16.28	17.33	5	11	4	18.60	19.98
4	18	2	13.32	10.83	10	15	3	11.91	12.12	3	13	3	25.14	25.26	5	10	4	24.69	24.73
4	17	2	22.70	22.85	10	13	3	10.29	10.47	3	15	3	21.20	20.88	5	9	4	17.36	16.92
4	16	2	12.93	13.99	10	12	3	11.39	6.41	3	16	3	17.49	16.34	5	8	4	22.31	22.99
4	14	2	9.47	7.96	10	11	3	14.96	11.21	3	17	3	15.95	17.51	5	7	4	19.95	19.86
4	13	2	28.72	28.72	10	9	3	16.35	17.66	2	17	3	14.75	12.33	5	6	4	22.74	22.20
4	12	2	32.50	34.16	10	7	3	13.85	11.65	2	16	3	13.97	12.41	5	5	4	26.49	25.30
4	11	2	51.99	53.11	10	5	3	17.80	18.72	2	15	3	18.23	19.72	5	4	4	32.65	32.40
4	10	2	15.27	15.53	10	4	3	11.42	11.18	2	13	3	26.66	26.13	5	3	4	31.93	31.37
4	9	2	21.33	22.93	10	3	3	16.53	15.81	2	14	3	12.11	13.05	5	2	4	11.89	7.17
4	8	2	42.79	40.66	10	1	3	21.71	22.66	2	12	3	18.05	14.72	5	1	4	14.63	16.39
4	7	2	70.31	69.32	10	0	3	15.70	15.43	2	11	3	31.86	30.64	5	0	4	39.18	37.88
4	6	2	57.03	56.38	9	0	3	21.53	20.48	2	10	3	22.82	22.96	4	1	4	18.85	17.60
4	5	2	49.57	47.59	9	1	3	28.21	28.43	2	9	3	48.15	47.75	4	2	4	42.15	42.62
4	4	2	38.54	38.55	9	2	3	8.88	8.17	2	8	3	22.87	22.91	4	3	4	14.95	14.89
4	3	2	70.86	68.88	9	3	3	29.67	29.59	2	7	3	31.95	32.87	4	4	4	19.28	20.06
4	2	2	77.35	77.28	9	4	3	17.45	19.80	2	6	3	34.78	34.71	4	5	4	11.48	12.26
4	1	2	56.46	58.22	9	5	3	31.26	29.96	2	5	3	56.05	53.31	4	6	4	31.76	32.48
4	0	2	19.99	18.37	9	6	3	11.20	6.82	2	4	3	27.30	26.82	4	7	4	20.51	19.13
3	0	2	97.39	95.61	9	7	3	14.44	15.86	2	3	3	42.99	43.66	4	8	4	33.94	33.60
3	1	2	71.23	70.40	9	8	3	10.38	9.26	2	2	3	49.92	51.18	4	9	4	16.10	17.36
3	2	2	39.52	39.75	9	10	3	9.47	9.19	2	1	3	57.30	56.67	4	10	4	13.02	14.50

Table 2. Continued.

4	11	4	9.76	8.49	3	1	4	12.47	12.52	2	15	4	14.61	12.84	1	4	4	32.53	31.91
4	12	4	27.15	26.46	3	0	4	41.79	43.30	2	16	4	11.27	11.98	1	3	4	56.07	58.45
4	14	4	13.44	14.08	2	0	4	9.52	9.77	2	20	4	11.92	6.49	0	3	4	28.84	28.45
4	17	4	12.22	5.11	2	1	4	31.54	32.51	2	23	4	10.88	3.24	0	5	4	58.15	58.69
3	20	4	10.77	6.74	2	2	4	50.74	53.39	2	24	4	11.55	3.36	0	6	4	10.48	9.39
3	15	4	17.61	8.30	2	3	4	17.66	17.64	1	17	4	10.44	17.84	0	7	4	9.76	10.93
3	14	4	21.43	22.64	2	4	4	12.92	12.94	1	15	4	12.04	12.77	0	8	4	9.88	3.84
3	10	4	33.10	35.90	2	5	4	30.77	32.16	1	14	4	13.14	11.16	0	9	4	50.65	48.41
3	9	4	13.03	7.51	2	6	4	38.15	37.39	1	13	4	21.02	21.15	0	10	4	14.44	15.99
3	8	4	23.96	23.11	2	7	4	17.18	17.16	1	11	4	33.06	33.13	0	11	4	17.35	17.18
3	7	4	12.67	12.34	2	8	4	25.38	25.41	1	10	4	18.43	17.08	0	12	4	10.13	12.88
3	6	4	36.03	34.70	2	9	4	30.83	30.47	1	9	4	17.13	15.23	0	13	4	18.28	20.82
3	5	4	13.62	14.31	2	11	4	14.33	15.49	1	7	4	43.23	42.14	0	15	4	24.73	26.89
3	4	4	41.37	43.74	2	12	4	20.21	19.62	1	6	4	22.50	22.45	0	19	4	13.37	14.91
3	3	4	19.99	20.32	2	13	4	15.03	14.51	1	5	4	17.70	18.14	0	23	4	12.36	6.83
3	2	4	19.58	18.38															

In order to find the nitrogen and the carbon atoms of the imidazole rings and the nitrogen and the oxygen atoms of the nitrate ion, we calculated a three-dimensional Fourier synthesis based on these preliminary Ag-parameters. Assuming the formula $Ag(C_3H_4N_2)_2NO_3$, it was possible to explain all peaks in that electron density map. By using the least-squares-method, the various atomic parameters could be refined to an R-value equal to 0.106

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

The above R-value stands for the isotropic type of refinement. When we used anisotropic type of refinement and all weights equal to 1 for the reflections where $0.75 \leq F_o/F_c \leq 1.25$, we obtained $R = 0.039$. In the same refinement, we obtained R (including zeroweight reflections) $= 0.061$.

The scattering factors used were those given in *International Tables for X-ray Crystallography* (1962) Vol. III,[4] and accounts were taken of the real part of the dispersion correction for the silver atom.

DESCRIPTION OF THE STRUCTURE

The silver atom binds to the pyrrole nitrogens of two imidazole rings giving rise to $Ag(C_3H_4N_2)_2^+$ ions. The coordination to the binding nitrogens is almost linear ($172.0 \pm 0.3°$) (Fig. 1). The NO_3^- ion is situated with its nitrogen atom 3.41 Å away from the nearest silver atom, and the closest Ag – O distance is 2.96 Å. The position of the NO_3^- ion is stabilized by two hydrogen bonds

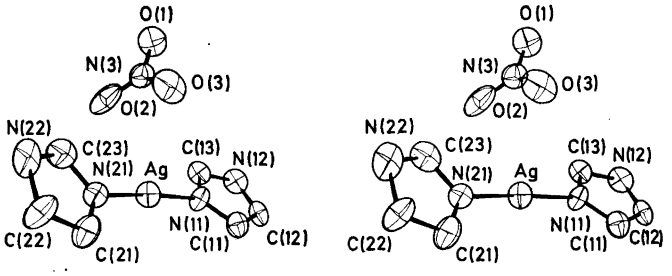

Fig. 1. One formula unit of $Ag(C_3H_4N_2)_2NO_3$. The representations of the atoms are the 50 per cent probability ellipsoids, according to the anisotropic vibrational parameters.

from the pyridine nitrogen atoms in the imidazole rings to two of the oxygen atoms in the nitrate ion. The distances N–H···O are 2.87 Å ±0.01 for both.

The bond distances in the two imidazole rings vary between 1.32–1.38 Å, and 1.31–1.42 Å, and the angles vary between 106–110° and 104–111°. The bond distances and angles in the nitrate ion vary between 1.22–1.24 Å, and 118–122°. For a list of interatomic distances and bond angles in the molecule, see Table 3.

Table 3. Interatomic distances and bond angles in the molecule.

	Distance (Å)	σ		Angles (°)
Ag–N(11)	2.120	0.008	Ag–N(11)–C(11)	127.66
Ag–N(21)	2.132	0.008	Ag–N(11)–C(13)	124.94
N(11)–C(11)	1.367	0.013	N(11)–C(11)–C(12)	109.66
C(11)–C(12)	1.335	0.017	C(11)–C(12)–N(12)	107.03
C(12)–N(12)	1.387	0.015	C(12)–N(12)–C(13)	106.28
N(12)–C(13)	1.364	0.013	N(12)–C(13)–N(11)	110.09
C(13)–N(11)	1.322	0.015	C(13)–N(11)–C(11)	106.94
N(21)–C(21)	1.360	0.014	Ag–N(21)–C(21)	131.22
C(21)–C(22)	1.385	0.017	Ag–N(21)–C(23)	121.38
C(22)–N(22)	1.422	0.016	N(21)–C(21)–C(22)	109.21
N(22)–C(23)	1.307	0.017	C(21)–C(22)–N(22)	103.95
C(23)–N(21)	1.324	0.013	C(22)–N(22)–C(23)	107.90
N(3)–O(1)	1.234	0.011	N(22)–C(23)–N(21)	111.72
N(3)–O(2)	1.218	0.012	C(23)–N(21)–C(21)	107.21
N(3)–O(3)	1.239	0.014	N(11)–Ag–N(21)	172.02
			O(1)–N(3)–O(2)	121.99
			O(1)–N(3)–O(3)	119.95
			O(2)–N(3)–O(3)	118.04

DISCUSSION

The crystal structure of $Ag(C_3H_4N_2)_2NO_3$ may be described as some kind of a sheet structure. On looking down the z-axis of the unit cell, the sheets can be seen repeating themselves in the direction of the y-axis in the following order:
$Ag(C_3H_4N_2)_2^+$, NO_3^-, $Ag(C_3H_4N_2)_2^+$; $Ag(C_3H_4N_2)_2^+$, NO_3^-, $Ag(C_3H_4N_2)_2^+$, and so on (Fig. 2).

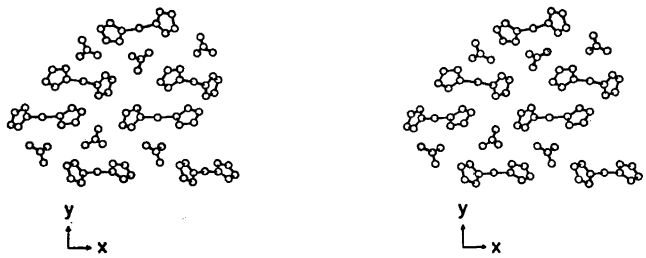

Fig. 2. A view down the z-axis, showing the sheets along the y-axis.

In the z-direction, the ions in each sheet are held together by hydrogen bonds between two of the oxygen atoms of the NO_3^- ion and the pyridine nitrogens of two imidazole rings. These imidazole rings are situated in different unit cells (Fig. 3). The $N-H\cdots O$ distance is 2.87 ± 0.01 Å for both bonds.

Fig. 3. The H-bonds between the oxygen atoms in the NO_3^- ion and the pyridine nitrogen in two imidazole rings.

These values can be compared with the average distance in hydrogen bonds $N-H\cdots O$ which, according to *International Tables*, is 2.88 Å. The two oxygen atoms that are hydrogen bonded are at the distances 2.96 Å and 3.12 Å from the closest silver atom. Again according to *International Tables*, the value of the bond distance between the N-atom and the O-atoms in NO_3^- varies over a range $1.22-1.27$ Å. In $Ag(C_3H_4N_2)_2NO_3$ we have found the $N-O$ distances to be 1.24 Å, 1.23 Å, and 1.22 Å ($\sigma = 0.01$).

Earlier in this paper we mentioned that the coordination of the silver atom is almost linear (172.0°). This non-linear coordination is significant, because the silver atom is situated 0.132 Å away from the plane of one of the imidazole rings, and 0.217 Å away from the plane of the other. These distances are much larger than 3σ of the silver atom's fractional coordinates (Table 4). Table 4 also shows that the nitrate ion, as well as the imidazole rings, is planar.

Table 4. Least squares planes.

	Equations	Mean displacement	Distance to Ag
1st ring	$-0.4086x-0.6289y-0.6615z-1.4702=0$	0.003	0.217 Å
2nd ring	$-0.6826x-0.4109y-0.6044z-1.3221=0$	0.004	0.137 Å
NO_3^- ion	$0.5639x-0.4539y-0.6899z-2.0499=0$	0.003	

The bond distances $Ag-N(11)$ and $Ag-N(21)$ in $Ag(C_3H_4N_2)_2NO_3$ are 2.12 Å and 2.13 Å. They appear somewhat short compared with the $Ag-N$ distance in $Ag-SCN$ chains, that is 2.22 ± 0.05 Å,[5] but the coordination situation in the compared substances differ greatly. However, there seems to be no suitable complex in the literature for comparison. For a study of the bond distances in the imidazole rings, see Table 5.

Table 5. Bond distances in some imidazole rings.

	N_1-C_1	C_1-C_2	C_2-N_2	N_2-C_3	C_3-N_1
$Ag(C_3H_4N_2)_2NO_3$ (1st ring)	1.367	1.335	1.387	1.364	1.322
$Ag(C_3H_4N_2)_2NO_3$ (2nd ring)	1.360	1.385	1.422	1.307	1.324
$Zn(C_3H_4N_2)_2Cl_2$ [6]	1.387	1.367	1.369	1.324	1.349
$Zn(C_3H_4N_2)_6Cl_2.4H_2O$ [7]	1.53	1.24	1.46	1.28	1.33
$Ni(C_3H_4N_2)_6(NO_3)_2$ [8]	1.372	1.366	1.352	1.329	1.310

Table 6. The atomic positional fractional coordinates and their standard deviations ($10^4 \times \sigma$ in parentheses).

	X	*Y*	*Z*
Ag	0.0688 (0.7)	0.1055 (0.4)	0.0518 (2)
N(11)	0.2181 (6)	0.1067 (5)	−0.2185 (19)
N(21)	−0.0651 (7)	0.0961 (4)	0.3601 (17)
C(11)	0.3211 (9)	0.0640 (6)	−0.2112 (29)
C(12)	0.4002 (8)	0.0869 (6)	−0.3971 (26)
N(12)	0.3463 (7)	0.1459 (5)	−0.5272 (21)
C(13)	0.2351 (8)	0.1561 (5)	−0.4089 (24)
C(21)	−0.0854 (9)	0.0425 (6)	0.5442 (27)
C(22)	−0.1781 (10)	0.0646 (6)	0.7153 (29)
N(22)	−0.2100 (8)	0.1358 (6)	0.6219 (23)
C(23)	−0.1418 (10)	0.1504 (6)	0.4138 (29)
N(3)	0.0531 (7)	0.2917 (4)	−0.0122 (19)
O(1)	0.0832 (7)	0.3523 (4)	−0.1009 (19)
O(2)	−0.0372 (8)	0.2593 (5)	−0.0931 (21)
O(3)	0.1138 (9)	0.2627 (5)	0.1685 (25)

Table 7. The final vibrational parameters and their estimated standard deviations ($10^4 \times \sigma$ in parentheses) for Ag, N, C, O. Anisotropic temperature factor:

$$\exp[-(h^2B_{11}+k^2B_{22}+l^2B_{33}+hkB_{12}+hlB_{13}+klB_{23})]$$

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ag	0.007 (0.5)	0.003 (0.2)	0.029 (32)	−0.0001 (0.8)	0.009 (3)	0.002 (2)
N(11)	0.006 (5)	0.003 (3)	0.028 (55)	0.0030 (7)	0.002 (25)	0.002 (22)
N(21)	0.006 (5)	0.003 (2)	0.023 (53)	0.0004 (9)	−0.004 (25)	−0.003 (15)
C(11)	0.006 (8)	0.004 (4)	0.037 (64)	−0.001 (9)	0.003 (37)	−0.002 (24)
C(12)	0.006 (7)	0.004 (4)	0.028 (61)	−0.002 (8)	0.007 (31)	−0.005 (22)
N(12)	0.009 (7)	0.004 (3)	0.020 (53)	−0.002 (8)	0.004 (31)	−0.0004 (20)
C(13)	0.007 (7)	0.003 (3)	0.021 (53)	−0.002 (7)	0.009 (31)	0.002 (21)
C(21)	0.007 (8)	0.004 (3)	0.030 (55)	0.002 (9)	0.001 (39)	−0.002 (24)
C(22)	0.009 (10)	0.004 (4)	0.037 (67)	0.005 (11)	0.005 (41)	−0.002 (25)
N(22)	0.006 (6)	0.006 (4)	0.037 (64)	0.001 (9)	−0.023 (32)	−0.012 (23)
C(23)	0.009 (9)	0.003 (3)	0.035 (61)	−0.001 (10)	−0.013 (45)	0.003 (25)
N(3)	0.008 (7)	0.003 (2)	0.034 (49)	0.002 (7)	−0.009 (31)	0.002 (16)
O(1)	0.010 (7)	0.004 (3)	0.048 (52)	−0.001 (8)	−0.003 (35)	0.006 (18)
O(2)	0.013 (8)	0.004 (3)	0.054 (56)	0.007 (8)	0.025 (38)	0.006 (21)
O(3)	0.016 (11)	0.004 (3)	0.067 (65)	−0.001 (10)	−0.041 (45)	0.012 (23)

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.*

REFERENCES

1. Strandberg, R. and Lundberg, B. K. S. *Acta Chem. Scand.* **25** (1971) 1767.
2. Bellamy, L. J. *The Infrared Spectra of Complex Molecules*, 1964.
3. *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. I.
4. *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. III.
5. Lindqvist, I. *Acta Cryst.* **10** (1957) 29.
6. Lundberg, B. K. S. *Acta Cryst.* **21** (1966) 901.
7. Sandmark, C. and Brändén, C.-I. *Acta Chem. Scand.* **21** (1967) 993.
8. Santoro, A., Mighell, A. D., Zocchi, M. and Reimann, C. W. *Acta Cryst.* **B 25** (1969) 842.

Received October 16, 1970.