lutidine N-oxide)copper(II) complex,[9] the plane of the chlorine and copper atoms makes an angle of 54.4° with the plane of the copper and oxygen atoms. The Zn–Cl bond length of 2.246 Å and the Zn–O bond length of 2.01 Å are comparable to those found in the copper complex where Cu–Cl = 2.221 and 2.247 Å and Cu–O = 1.93 and 1.97 Å. The oxygen–oxygen separation is 2.952 Å compared to 2.68 Å in the copper complex. A plane was least-squares-fitted to the six-ring atoms of the 2,6-lutidine molecule with all atoms weighted equally. The largest deviation was 0.018 Å which is less than the estimated standard deviations for the positions of the individual atoms. The N–O bond length of 1.35 Å compares with 1.36 and 1.31 Å found in the copper complex. The average C–N distance is 1.38 Å, and the average C–C distance around the ring is 1.39 Å.

The Zn–O–N angle, 118.6°, is slightly less than that found in the corresponding copper(II) complex where the angles are 118.6 and 121.6°. The N–O bond makes an angle of 3.1° with the 2,6-lutidine ring which leaves the oxygen atom 0.08 Å out of the plane of the ring. The two 2,6-lutidine rings make an angle of 61° relative to each other. This is greater than the angle of 53° found for the copper complex.

The zinc and copper complexes are not isostructural. Since the molecular packing imposes no restrictions on the chlorine atoms through strong nonbonding interactions, they are free to achieve the most stable configuration relative to the oxygen atoms. The copper complex should fit into the zinc lattice with a minimum of distortion of the N-oxide ligand. This slight rearrangement of the 2,6-lutidine N-oxide ligand should not be too energetically unfavorable. All zinc sites are equivalent in projection down the *b* axis. This need not be the case for the copper ion when substituted into the zinc lattice. Two nonequivalent sites would result if random statistical substitution occurred.

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The Structure of Tris(ethylenediamine)chromium(III) Pentacyanonickelate(II) Sesquihydrate, $[Cr(NH_2CH_2CH_2NH_2)_3][Ni(CN)_5]\cdot 1.5H_2O$

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The crystal and molecular structure of tris(ethylenediamine)chromium(III) pentacyanonickelate(II) sesquihydrate, $[Cr(NH_2CH_2CH_2NH_2)_3][Ni(CN)_5]\cdot 1.5H_2O$, has been determined from three-dimensional X-ray data collected by counter methods. The structure has been refined on F to a final conventional R factor of 9.4% and a weighted R factor of 6.9% for the 2758 observed reflections. The salt crystallizes in space group C_{2h}^5-$P2_1/c$ of the monoclinic system, with eight formula units in a cell of dimensions $a = 14.883$ (4), $b = 15.748$ (4), $c = 16.464$ (5) Å, $\beta = 94.88$ (1)°. The calculated density of 1.55 g/cm^3 agrees well with the observed density of 1.56 ± 0.02 g/cm^3. The structure consists of discrete $Cr(C_2H_8N_2)_3{}^{3+}$ and $Ni(CN)_5{}^{3-}$ ions linked by intermolecular hydrogen bonds. The waters of crystallization participate in some of these bonds. There are two crystallographically independent $Ni(CN)_5{}^{3-}$ ions in the compound: one is a regular square pyramid and the other is a distorted trigonal bipyramid. The square pyramid has axial and average equatorial Ni–C bond lengths of 2.168 (14) and 1.862 (6) Å, respectively. The average C–Ni–C angle between the opposing basal carbon atoms is 159.5 (4)°, so that the nickel atom is 0.34 Å above the basal plane of carbon atoms. The distorted trigonal-bipyramidal $Ni(CN)_5{}^{3-}$ group has Ni–C axial bonds that are significantly shorter than the Ni–C equatorial bonds. The average axial Ni–C bond length is 1.837 (9) Å. The C–Ni–C angle between the axial carbon atoms is 172.8 (5)°. There are two equivalent equatorial Ni–C bonds of average length 1.907 (9) Å and one longer equatorial bond of 1.992 (14) Å. This longer bond and the large C–Ni–C angle, 141.2 (5)°, between the other two equatorial carbon atoms are the primary deviations from a regular trigonal-bipyramidal geometry. The observed C_2 geometry is apparently not due to crystal-packing interactions but is rather an energy minimum of the free ion. The isolation of both geometries in the same crystal demonstrates the very small energy difference between them. The conformations of the two tris(ethylenediamine)chromium cations are different. For the Λ configuration of each, one is $\Lambda\lambda\lambda\delta$ and the other is $\Lambda\delta\delta\lambda$.

Introduction

It has long been known that pale yellow solutions of $Ni(CN)_4{}^{2-}$ form a cyanide adduct in concentrated aqueous cyanide solutions.[1] In a series of careful spectroscopic studies, Coleman, Peterson, and Penneman[1] showed that the complex formed in aqueous solution is $Ni(CN)_5{}^{3-}$. Repeated efforts to isolate this anion were unsuccessful, but recently stable salts of $Cr(NH_3)_6{}^{3+}$ and $Cr(en)_3{}^{3+}$ (en = $NH_2CH_2CH_2NH_2$) have been obtained.[2] Moreover, the unstable potassium salt has been isolated at low temperatures.[3]

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(1) J. S. Coleman, H. Peterson, Jr., and R. A. Penneman, *Inorg. Chem.*, **4**, 135 (1965), and references therein.

(2) K. N. Raymond and F. Basolo, *ibid.*, **5**, 949 (1966).

(3) W. C. Anderson and R. H. Harris, *Inorg. Nucl. Chem. Letters*, **2**, 315 (1966).

Although there are now a great many five-coordinate transition metal complexes known,[4] there are still relatively few that have been the subject of detailed structural investigations.[5] There are even fewer such complexes that have been studied which are formed from identical, unidentate ligands. These are of special interest because their geometry must be determined by electronic, rather than steric, effects. Thus, the geometry of such complexes leads to important insight into the chemical bonding in five-coordinate complexes. As part of a series of structural studies of five-coordinate transition metal complexes we report here on the structure of $[Cr(en)_3][Ni(CN)_5]\cdot 1.5H_2O$.

Space Group and Lattice Parameters

Large, red crystals of $[Cr(en)_3][Ni(CN)_5]\cdot 1.5H_2O$ were prepared as described earlier.[2] This salt was initially characterized as a dihydrate, but the analytical data fit a sesquihydrate equally well and the subsequent structure determination confirms this formulation. The crystals were, in general, of equant habit with well-developed faces. Very sharp extinction was observed under the polarizing microscope and the crystals appeared to be of high quality. The crystals were observed to be deliquescent at low temperature but efflorescent in low humidity at room temperature. Because of this, all of the crystals examined were sealed in glass capillaries.

Precession photographs of zero-level and upper-level zones indicated monoclinic symmetry and had systematic absences $h0l$ when $l \neq 2n$ and $0k0$ when $k \neq 2n$. The absences are consistent with space group $P2_1/c$. In addition, there were systematically weak reflections such as $hk2h$ when $k \neq 4n$ and $hk0$ when $h + k \neq 4n$. These indicated the presence of considerable pseudosymmetry in the crystal. Preliminary cell constants were measured from the films. The density was determined to be 1.56 ± 0.02 g/cm^3 by flotation in carbon tetrachloride–methylene chloride solutions.

For eight formula units in the cell the calculated density is 1.55 g/cm^3. Since the order of $P2_1/c$ is four, there are two crystallographically independent $Cr(en)_3^{3+}$ and $Ni(CN)_5^{3-}$ ions in the structure and three independent waters of crystallization.

Collection of Intensity Data

A nearly spherical crystal was mounted on a eucentric goniometer head and carefully measured under a microscope with a micrometer attachment. Many of the possible projections were examined. The minimum and maximum diameters are 0.215 and 0.295 mm. Two protuberances on the sphere were opposite one another. With a linear absorption coefficient for Cu $K\alpha$ radiation of 63.1 cm^{-1}, in this one direction there could be a 20% variation in F^2. However, the observed variation is less than 5% for intense reflections, indicating that this particular orientation was never reached. The mean diameter is 0.23 mm, corresponding to a volume of approximately 6.4×10^{-3} mm^3 and a mass of 10 μg.

The lattice parameters, obtained by a least-squares refinement involving the setting angles of 20 reflections which had been carefully centered on a Picker automatic X-ray diffractometer in the manner previously described,[6,7] are a = 14.883 (4), b = 15.748 (4), c = 16.464 (5) Å, β = 94.88 (1)°. These parameters were obtained at 21° with the use of $CuK\alpha_1$ radiation (λ 1.54056 Å).

Intensity data were collected in the manner previously described.[6,7] The take-off angle used was 1.0°. At this take-off angle the peak intensity of a typical strong reflection is 70% of the maximum value as a function of the angle. Data were collected by the θ–2θ method. A 2θ scan rate of 1°/min and upper and lower background counts of 20 sec were used throughout the data collection. A symmetrical scan width of 1.8° was used for the first 3308 reflections ($0 < 2\theta \leq 55°$) and a width of 1.6° was used thereafter. The smaller scan widths at higher angles were possible in spite of broadening and α_1–α_2 splitting because of the weaker peaks in that region. The pulse height analyzer was set to pass about 90% of the Cu $K\alpha$ radiation. The receiving aperture size selected to minimize extraneous background was 5.0 mm high by 4.5 mm wide and was positioned 21 cm from the crystal. The effects of multiple reflections should be minimal as the symmetry axis of the crystal was far from the spindle axis.[8]

The intensities of four reflections at different positions in reciprocal space were monitored as standards. All four showed a large, uniform drop in intensity with time. The intensities at the end of data collection were only 35% of their initial values. The measured intensities were adjusted to what their values would have been at the beginning of the data collection by taking into account this uniform decrease of the monitored intensities.

In a centrosymmetric monoclinic system there are four equivalent reflections in $\{hkl\}$: hkl, $\bar{h}k\bar{l}$, $\bar{h}\bar{k}\bar{l}$, and $h\bar{k}l$. All four of these were collected for the first 6932 reflections ($0 < 2\theta \leq 72°$), but only two forms ($\bar{h}k\bar{l}$ and $\bar{h}\bar{k}\bar{l}$) were collected for the remaining reflections ($72 < 2\theta \leq 86°$), since relatively few reflections at such high angles had significant intensities. The non-Friedel pairs were chosen since reflections related by the center of symmetry were found to be in much closer agreement than the non-Friedel pairs. The mean of the latter two was found to be very close to the mean for all four reflections in most cases. In all, 8891 reflections were observed.

The intensity data were corrected for background and were assigned standard deviations according to the formula[6]

$$\sigma(I) = [CT + 0.25(t_c/t_b)^2(B_1 + B_2) + (pI)^2]^{1/2}$$

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[4] E. L. Muetterties and R. A. Schunn, *Quart. Rev.* (London), **20**, 245 (1966).

[5] J. A. Ibers, *Ann. Rev. Phys. Chem.*, **16**, 380 (1965).

[6] P. W. R. Corfield, R. J. Doedens, and J. A. Ibers, *Inorg. Chem.*, **6**, 197 (1967).

[7] R. J. Doedens and J. A. Ibers, *ibid.*, **6**, 204 (1967).

[8] W. H. Zachariasen, *Acta Cryst.*, **18**, 705 (1965).

The quantity CT is the total integrated count in time t_c; B_1 and B_2 are the background counts above and below the peak, each obtained in time t_b; p is a factor introduced to avoid overweighting the very strong reflections (since for very strong reflections $\sigma(I) = pI$), and I, the intensity, is given by

$$I = CT - 0.5(t_c/t_b)(B_1 + B_2)$$

The factor p was initially chosen to be 0.04 but, on the basis of a statistical analysis of the agreement factors calculated for ranges of intensity, was ultimately changed to 0.07. Values of I were next reduced to values of F^2 by application of Lorentz-polarization and absorption factors. The intensities of equivalent reflections were then averaged to yield the intensities of 2758 independent reflections. The standard deviation of an average intensity was taken as the larger of the individual estimate or the range estimate.[6] A total of 2154 intensities were greater than their standard deviations. Owing to the very large number of structure parameters in this problem, all independent reflections were used in the refinements.

Solution and Refinement of the Structure

An unsharpened Patterson function[9] was calculated, using the 861 independent reflections of lowest θ. (At a later stage, a sharpened Patterson function was obtained using all of the data, and it showed essentially the same features as the initial Patterson function.) The Patterson map had two peaks at $0, {}^1/_4, {}^1/_2$ and $0, {}^1/_2, 0$ that were half as large as the origin peak. In addition, there were three peaks at ${}^1/_2, 0, 0$; ${}^1/_4, {}^1/_2, {}^3/_8$; and $-{}^1/_4, {}^1/_4, {}^1/_8$ that were approximately one-fourth as high as the origin peak. The 30 strongest peaks all had x and y of 0, ${}^1/_2$, or $\pm{}^1/_4$; and z of 0, ${}^1/_2$, $\pm{}^1/_4$, or $\pm{}^1/_8$. The general pseudo-symmetry of the Patterson map and the positions of the several extremely strong peaks implied that the metal atoms lie at noncrystallographic special positions, and this was later verified.

Trial parameters for the metal atoms were refined by least-squares techniques, use being made of the 861 low-angle reflections. In this and succeeding refinements the function minimized was $\Sigma w(|F_o| - |F_c|)^2$, where $|F_o|$ and $|F_c|$ are the observed and calculated structure amplitudes and where the weights, w, were taken as $4F_o^2/\sigma^2(F_o^2)$. The atomic scattering factors tabulated by Ibers[10] were used for neutral Ni, Cr, O, N, and C, and those of Stewart, *et al.*,[11] for H. The effects of both real and imaginary anomalous scattering by Ni and Cr were included in the calculated structure factors.[12] The anomalous scattering factors of Cromer[13] were used for Ni and Cr. This first refinement of the proposed positions of the metal atoms led to values of $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and of the weighted R factor or $R_2 = (\Sigma w(|F_o| - |F_c|)^2/\Sigma w F_o^2)^{1/2}$ of 55 and 56%. A difference Fourier map, calculated using the phases of the inner 861 reflections, could not be readily interpreted. The high R factor at this stage and the lack of resolution of the structure are not surprising since the metal atoms contribute only 22% of the total electron density. Three more cycles of least-squares refinement of the initial set of parameters of the metal atoms were then performed using all 2758 independent reflections. The values of R_1 and R_2 dropped slightly to 53 and 51%, respectively. Another difference Fourier map was computed and, with imagination, one or two cyanide groups could be discerned. Once these were located, the choice as to whether a metal atom was nickel or chromium could be made. Other cyanide groups were found by carefully looking in chemically reasonable places. Since the coordination around the chromium atoms was expected to be octahedral, a set of peaks in the electron density map was sought, near the presumed chromium atoms, which formed a rough octahedron for each chromium. In this way, 7 carbon and 15 nitrogen positions were chosen. Two cycles of least-squares refinement of coordinates and isotropic temperature factors reduced the values of R_1 and R_2 to 39.9 and 41.2%. Two of the atoms were incorrectly located and showed very large temperature factors. Another difference Fourier map was then computed which clearly showed the remaining structure. The metal coordinates and isotropic temperature factors and the coordinates of the carbon, nitrogen, and three oxygen atoms were carried through two cycles of least-squares refinement. The carbon and nitrogen temperature factors were held equal and the over-all temperature factor was refined. The values of R_1 and R_2 decreased to 13.1 and 10.6%. Up until this time the compound had been characterized as a dihydrate.[2] When no new atoms could be found in the Fourier maps the compound was reformulated as a sesquihydrate.

A small program, FINDH, was written at this point to compute the positions of the 48 hydrogen atoms of the ethylenediamine ligands. Let X denote the C or N atom and let Y denote the nonhydrogen atoms bonded to X. Then the H atoms were placed such that the H–X–H plane bisects the Y–X–Y angle and the Y–X–Y plane bisects the H–X–H angle. The parameters assumed were C–H = 1.09 Å, N–H = 1.03 Å, and H–X–H = 109° 28′. The structure factor contributions from these hydrogens were added as fixed contributions to the calculated structure factors in subsequent least-squares refinements. There were many hydrogen atom structure factors in the range of 20–30 electrons for low-angle reflections. These were very important in many cases as evidenced by an immediate drop in the values of R_1 and R_2 to 12.2 and 9.4%.

If we neglect hydrogen atoms, there are 51 atomic positions to be located. If these atoms are restricted to isotropic motion, there are 205 variable parameters to be determined. Limitations of speed and core size

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[9] In addition to various local programs, local modifications of Zalkin's FORDAP Fourier program, the Levy–Busing ORFLS least-squares and ORFFE error function programs, and the Johnson ORTEP thermal ellipsoid plotting program were used on a CDC 3400 computer.

[10] J. A. Ibers, "International Tables for X-Ray Crystallography," Vol. 3, The Kynoch Press, Birmingham, England, 1962, Table 3.3.1A.

[11] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, **42**, 3175 (1965).

[12] J. A. Ibers and W. C. Hamilton, *Acta Cryst.*, **17**, 781 (1964).

[13] D. T. Cromer, *ibid.*, **18**, 17 (1965).

on our computer prevented us from refining all of these variables simultaneously. The remaining refinement was, of necessity, accomplished by refining a fraction of these parameters in each cycle so that after two or three cycles each parameter had been varied and one approximate, full least-squares cycle was finished. This corresponds to factoring the complete matrix of all variables into subblocks that lie along the full-matrix diagonal (*i.e.*, the cross terms for certain parameters are assumed to be zero). To make this as good an approximation as possible, the subblocks were chosen so that the parameters of atoms bonded together were refined simultaneously. At this stage the two $Ni(CN)_5^{3-}$ ions and the waters were refined in one block and the two $Cr(en)_3^{3+}$ ions in another. The scale factor was refined with each block. After four half-cycles (two complete cycles) and allowance for small changes in the calculated positions of the hydrogen atoms, the values of R_1 and R_2 were 10.8 and 7.8%. Next, anisotropic vibrations were permitted to the metal and oxygen atoms. Two full cycles of refinement resulted in values of R_1 and R_2 of 10.5 and 7.5%. This improvement in R_2 has a significance level of 0.5% on the assumption that there are only random errors in the data.[14]

At this point a difference Fourier map was computed. The highest peak on this map was 0.9 electron/Å^3. The coordinates of the 100 highest peaks on this map along with the coordinates of the atoms already located were included in a calculation of bond distances and angles in order to determine if any electron density peaks came at holes in the structure. None did, and so the possibility was excluded of another water molecule, or any atom other than those already found, being in the structure. The positions of the missing six hydrogen atoms of the water molecules were not obvious on this map.

The large error in an observation of unit weight (1.42) and a marked increase in the R_2 values for weak reflections indicated that the weighting scheme applied up to this point ($p = 0.04$) could be improved. The introduction of a value of p of 0.07 led to essential constancy in the function $\Sigma(|F_o| - |F_c|)^2/\sigma^2(F_o)$ when summed over ranges of $|F_o|$. The absolute weights resulting from this modification were also modified to take into account the number of times reflections of a given form had been observed. An additional cycle of refinement with this weighting scheme resulted in values of R_1 and R_2 of 10.1 and 7.8% and in the error of an observation of unit weight of 1.11.

Because of the ease with which the ligand–metal–ligand angles may be changed relative to ligand–metal bond lengths in five-coordinated complexes, a least-squares refinement was carried out on a model in which all except the ethylenediamine atoms were allowed to vibrate anisotropically. The number of variables (340) required factoring the matrix into three subblocks. The first contained one $Ni(CN)_5^{3-}$ anion and the two oxygen atoms involved in strong hydrogen bonds with it, the second included the remaining $Ni(CN)_5^{3-}$ anion and oxygen, and the third block contained the $Cr(en)_3^{3+}$ ions. Three complete cycles of least-squares refinement were performed for this model. The average parameter shift in the final refinement was 7% of the standard deviation of the parameter, and the largest was 23%. The final values of R_1 and R_2 are 9.4 and 6.9% and the error in an observation of unit weight, corrected for the total number of variables, is 1.03. Application of the usual statistical tests[14] on R_2 indicates that highly significant improvement was obtained in this refinement in which the cyanide atoms were allowed to vibrate anisotropically. Since there was no evidence of the effects of extinction, no correction was applied.

A comparison of the bond lengths computed for the final structure and those of the preceding model gives an insight into how much the weighting scheme and anisotropic factors can affect atom positions. The largest changes occurred in the C–N bond lengths for the axial cyanides in the trigonal bipyramid. The first values were 1.224 and 1.245 Å. Cyanide bond lengths are remarkably constant for a wide range of compounds and average about 1.16 Å. For this reason the unusually long values obtained were suspect. After changing the weighting scheme and allowing the cyanides to vibrate anisotropically, the two C–N bond lengths dropped to normal values of 1.178 and 1.158 Å. An earlier partial refinement with changed weights but isotropic cyanide atoms made it possible to estimate the relative importance of the change in weights and the change in model. The two changes were found to be about equal in importance and, in the case of the C–N bond lengths quoted above, added up to give shifts of 0.04 and 0.05 Å. These are about three or four standard deviations. The remaining shifts, however, were much less than this. It is impossible to judge whether or not this same effect would have occurred had we been able to perform the refinements with a full matrix.

The final values of $|F_o|$ and $|F_c|$ (in electrons × 10) are given in Table I. The final atomic parameters are given in Table II.

Discussion of Structure

The salt consists of two nearly identical, although crystallographically independent, $Cr(en)_3^{3+}$ groups, a five-coordinate $Ni(CN)_5^{3-}$ ion with a nearly perfect square-pyramidal configuration, and another five-coordinate $Ni(CN)_5^{3-}$ ion with a distorted trigonal-bipyramidal coordination. All are involved to some extent in hydrogen bonds to one or more of the twelve waters of hydration in the cell. This appears to be the first compound known in which two different five-coordinate geometries of the same metal complex exist together in the solid. It also is the only example of a square-pyramidal nickel complex with five equivalent ligands. The few other ML_5 complexes are all trigonal bipyramidal, except for the recent, as yet unpublished, $MnCl_5^{2-}$ ion.[15]

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[14] W. C. Hamilton, *Acta Cryst.*, **18**, 502 (1965).

[15] I. Bernal, private communication.

TABLE I

OBSERVED AND CALCULATED STRUCTURE AMPLITUDES (×10) (IN ELECTRONS) FOR $[Cr(C_2H_8N_2)_3][Ni(CN)_5]\cdot 1.5H_2O$

K	L	FO	FC
***** H = 0 *****			
0	2	1580	1634
0	4	687	636
0	6	1188	1139
0	8	1421	1456
0	10	538	526
0	12	1307	1308
0	14	188	181
1	-12	569	592
1	-8	577	606
1	-7	635	615
1	-6	90	55
1	-3	588	543
1	1	339	419
1	2	570	605
1	4	422	438
1	5	446	454
1	9	737	778
1	10	935	926
1	11	412	419
1	13	239	271
1	14	292	316
2	-14	233	182
2	-12	364	216
2	-11	1045	1093
2	-4	115	91
2	-3	2668	2715
2	0	245	244
2	1	139	118
2	2	181	189
2	5	715	635
2	6	250	273
2	7	369	404
2	8	201	192
2	9	51	85
2	10	255	266
3	-14	391	330
3	-12	638	645
3	-11	136	99
3	-10	392	359
3	-9	217	256
3	-8	364	346
3	-7	1266	1296
3	-5	327	274
3	-4	694	664
3	-1	46	21
3	2	78	42
3	3	588	543
3	6	576	539
3	13	369	345
4	-13	217	44
4	-12	552	503
4	-10	183	80
4	-8	1472	1544
4	-5	64	40
4	-3	338	339
4	-1	1466	1463
4	0	4195	4218
4	1	682	649
4	4	1293	1311
4	6	1017	1074
4	7	113	151
4	9	152	42
4	11	318	298
5	-13	298	279
5	-9	694	694
5	-8	507	476
5	-5	207	221
5	-3	600	625
5	-1	430	398
5	2	846	867
5	4	1064	1056
5	6	166	170
5	7	432	455
5	10	844	858
5	11	484	529
5	12	407	366
6	-12	395	40
6	-11	546	528
6	-6	480	467
6	-5	1760	1751
6	0	589	569
6	1	1507	1418
6	2	1537	1461
6	3	2012	2109
6	4	399	409
6	7	850	801
6	8	121	78
6	9	169	170
6	10	238	275
6	13	172	126
7	-8	517	485
7	-5	484	492
7	-3	84	65
7	-2	119	55
7	-1	358	363
7	4	714	697
7	5	912	906
7	7	583	600
7	9	187	72
7	10	520	498
7	11	131	128
7	12	494	451
8	-10	238	309
8	-7	33	65
8	-5	237	287
8	-3	135	59
8	0	1822	1899
8	1	224	260
8	2	951	973
8	4	421	415
8	6	993	996
8	8	493	448
8	9	407	455
8	11	145	86
9	-9	973	996
9	-7	526	517
9	-6	154	100
9	-5	288	282
9	-2	1052	1058
9	1	924	941
9	3	666	691
9	4	99	125
9	8	75	43
9	10	690	666
9	11	523	513
10	-10	79	74
10	-9	381	347
10	-7	151	96
10	-3	735	809
10	-2	363	301
10	-1	366	337
10	0	546	541
10	3	1374	1393
10	4	188	67
10	6	243	162
10	8	183	125
11	-4	352	313
11	-3	420	424
11	-2	121	79
11	1	228	133
11	5	161	122
11	6	707	662
11	7	431	432
11	8	142	182
12	-7	228	173
12	-6	707	744
12	-3	535	453
12	-2	396	351
12	0	1144	1168
12	1	324	364
12	4	71	89
13	-5	213	142
13	-4	151	19
13	1	375	392
13	2	393	433
13	3	433	466
***** H = 1 *****			
0	-14	1116	1149
0	-12	1056	1068
0	-10	161	198
0	-8	460	432
0	-6	1376	1364
0	-4	627	640
0	-2	3111	3175
0	0	45	66
0	2	2653	2976
0	4	1479	1447
0	6	785	754
0	8	379	413
0	10	1005	1018
0	12	418	417
0	14	412	385
1	-14	230	117
1	-13	380	271
1	-12	231	215
1	-11	221	207
1	-10	77	48
1	-9	254	285
1	-8	422	393
1	-7	201	194
1	-6	160	178
1	-5	1248	1163
1	-4	563	523
1	-3	492	444
1	-2	88	57
1	-1	328	162
1	0	70	125
1	1	274	296
1	2	332	248
1	3	347	370
1	4	106	49
1	5	382	401
1	6	677	670
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7	0	154	59
7	1	348	191
7	2	152	78
***** H = 12 *****			
0	-6	413	552
0	-4	609	593
0	-2	366	404
0	0	757	681
0	2	546	556
0	4	248	139
1	-7	271	98
1	-5	282	71
1	-4	622	642
1	-3	176	227
1	-2	479	456
1	-1	755	765
1	0	490	544
1	1	511	517
1	2	385	344
1	3	598	675
1	4	422	359
2	-5	152	167
2	-4	308	145
2	-3	271	325
2	-1	225	34
2	0	254	69
2	1	140	129
2	2	194	41
2	3	637	584
2	4	230	176
3	-6	223	138
3	-5	280	220
3	-4	535	534
3	-3	364	377
3	-2	653	686
3	-1	472	476
3	0	439	391
3	1	720	749
3	2	631	618
3	3	336	340
4	-5	235	97
4	-4	555	548
4	-3	267	75
4	-2	73	120
4	-1	279	168
4	0	626	583
4	1	230	264
4	2	695	681
4	3	300	75
5	-4	218	88
5	-3	153	129
5	-2	533	526
5	-1	665	642
5	0	124	157
5	1	877	901
***** H = 13 *****			
0	-2	361	368
0	0	398	317
1	-3	253	203
1	-2	279	49
1	-1	137	140
1	0	82	79
2	-2	273	142
2	-1	769	835

TABLE II

POSITIONAL AND THERMAL PARAMETERS FOR $[Cr(C_2H_8N_2)_3][Ni(CN)_5]\cdot 1.5H_2O$

Atom	10^5x	10^5y	10^5z	$10^5\beta_{11}$[a] or 10^2B, Å^2	$10^5\beta_{22}$	$10^5\beta_{33}$	$10^5\beta_{12}$	$10^5\beta_{13}$	$10^5\beta_{23}$
Ni_1	01360(10)[b]	12053(10)	23825(9)	288(10)	260(9)	172(8)	45(8)	40(7)	25(7)
Ni_2	51978(10)	11736(10)	21687(10)	284(10)	230(9)	226(8)	- 12(8)	70(7)	19(7)
Cr_1	-26009(10)	38423(10)	38723(9)	250(10)	205(9)	190(8)	- 13(8)	33(7)	- 6(7)
Cr_2	25286(10)	36404(10)	12018(9)	280(10)	205(9)	199(8)	14(8)	- 2(7)	- 13(7)
O1	-20162(41)	34049(39)	01180(38)	361(42)	231(36)	320(35)	- 18(31)	64(30)	- 34(29)
O2	-36276(49)	04356(49)	53454(41)	764(56)	663(53)	316(37)	22(44)	137(37)	- 11(37)
O3	09185(53)	28830(48)	41128(47)	868(61)	444(47)	571(46)	-109(43)	173(43)	- 83(38)
Ni_1N_1	-05671(65)	-07730(68)	21153(59)	498(68)	383(63)	392(53)	-113(55)	56(46)	42(52)
Ni_1N_2	14979(70)	08402(71)	38077(62)	559(76)	807(77)	314(56)	171(59)	29(50)	- 72(56)
Ni_1N_3	16414(60)	13172(56)	12682(55)	354(58)	320(54)	349(51)	- 1(48)	100(44)	0(43)
Ni_1N_4	-09594(59)	22128(59)	10954(56)	340(62)	472(62)	256(50)	54(47)	- 17(45)	- 53(45)
Ni_1N_5	-11256(62)	17334(57)	36299(55)	472(66)	385(55)	292(51)	197(48)	154(46)	60(44)
Ni_1C_1	-03113(76)	-00904(85)	21618(66)	388(78)	442(80)	165(54)	19(65)	125(52)	63(59)
Ni_1C_2	09773(80)	09683(73)	32599(75)	391(80)	408(76)	320(67)	11(61)	154(58)	- 39(58)
Ni_1C_3	10675(72)	12781(62)	16898(64)	324(69)	66(54)	250(56)	18(54)	14(51)	99(46)
Ni_1C_4	-05435(69)	18253(74)	16082(65)	180(70)	502(77)	135(56)	- 10(56)	44(51)	- 52(51)
Ni_1C_5	-06579(69)	15243(63)	31482(70)	243(70)	143(60)	312(63)	33(50)	- 38(54)	119(49)
Ni_2N_1	50379(54)	31639(65)	23652(52)	262(56)	284(57)	383(50)	109(47)	- 88(39)	- 10(46)
Ni_2N_2	37199(66)	03412(70)	30798(60)	562(73)	753(75)	377(56)	-339(59)	162(51)	-133(50)
Ni_2N_3	38828(58)	12683(53)	06824(56)	289(56)	260(49)	317(49)	45(45)	82(43)	65(45)
Ni_2N_4	-33046(71)	06473(75)	11339(59)	581(76)	1040(86)	359(57)	283(65)	253(53)	157(55)
Ni_2N_5	-33808(66)	09229(57)	35576(57)	480(67)	341(55)	320(53)	-105(49)	26(47)	40(44)
Ni_2C_1	51555(69)	24279(81)	23150(62)	339(72)	260(69)	207(55)	46(59)	- 41(47)	- 14(54)
Ni_2C_2	42700(77)	06943(73)	27615(63)	415(77)	397(72)	172(58)	- 13(60)	60(55)	- 89(51)
Ni_2C_3	44042(70)	12144(69)	12600(66)	247(69)	327(63)	191(57)	- 93(56)	35(51)	43(54)
Ni_2C_4	-38724(70)	08510(71)	15063(65)	151(67)	494(71)	172(57)	82(54)	-113(51)	114(49)
Ni_2C_5	-39519(73)	10031(64)	30404(69)	269(71)	215(62)	261(61)	-114(54)	108(54)	- 58(51)
Cr_1N_1	-21395(46)	44561(45)	28687(42)	196(17)					
Cr_1N_2	-27146(45)	28272(44)	30587(42)	163(16)					
Cr_1N_3	-12933(47)	35467(45)	43321(43)	206(17)					
Cr_1N_4	-23733(46)	48712(44)	46516(41)	174(17)					
Cr_1N_5	-39240(46)	41995(46)	35994(42)	198(17)					
Cr_1N_6	-31589(46)	31344(44)	47663(41)	167(17)					
Cr_1C_1	-18876(65)	38010(65)	22646(60)	328(24)					
Cr_1C_2	-26187(64)	31445(63)	22152(62)	291(24)					
Cr_1C_3	-08539(60)	43064(61)	46865(55)	225(22)					
Cr_1C_4	-15172(60)	47764(59)	51615(56)	209(22)					
Cr_1C_5	-44801(62)	39341(60)	42744(58)	286(24)					
Cr_1C_6	-41529(62)	30915(59)	45851(57)	248(23)					
Cr_2N_1	11670(50)	33005(48)	12296(45)	268(18)					
Cr_2N_2	19787(47)	46542(47)	05506(44)	250(18)					
Cr_2N_3	25182(48)	42939(50)	22963(46)	270(18)					
Cr_2N_4	29568(48)	26453(47)	19515(45)	238(18)					
Cr_2N_5	26849(50)	29002(49)	01734(46)	297(19)					
Cr_2N_6	38192(47)	40407(45)	10050(44)	212(17)					
Cr_2C_1	05977(61)	38463(61)	06488(57)	249(22)					
Cr_2C_2	10024(59)	47294(60)	07035(55)	229(22)					
Cr_2C_3	29590(68)	37578(67)	29671(62)	358(25)					
Cr_2C_4	27106(70)	28375(70)	27888(68)	409(27)					
Cr_2C_5	34857(69)	32274(65)	-02198(62)	342(25)					
Cr_2C_6	42276(63)	34906(60)	03936(59)	266(23)					

Atom[c]	10^3x	10^3y	10^3z
$Cr_1N_1H_1$	-158	482	305
$Cr_1N_1H_2$	-264	484	260
$Cr_1N_2H_1$	-334	254	308
$Cr_1N_2H_2$	-221	239	322
$Cr_1N_3H_1$	-094	333	387
$Cr_1N_3H_2$	-131	309	477
$Cr_1N_4H_1$	-290	491	502
$Cr_1N_4H_2$	-235	542	431
$Cr_1N_5H_1$	-417	391	306
$Cr_1N_5H_2$	-396	485	353
$Cr_1N_6H_1$	-301	342	532
$Cr_1N_6H_2$	-289	253	477
$Cr_2N_1H_1$	098	339	181
$Cr_2N_1H_2$	109	267	106
$Cr_2N_2H_1$	203	456	-006
$Cr_2N_2H_2$	231	520	074
$Cr_2N_3H_1$	186	442	241
$Cr_2N_3H_2$	287	485	226
$Cr_2N_4H_1$	365	258	196
$Cr_2N_4H_2$	265	209	175
$Cr_2N_5H_1$	212	295	-023
$Cr_2N_5H_2$	279	228	034
$Cr_2N_6H_1$	422	402	155
$Cr_2N_6H_2$	379	466	079
$Cr_1C_1H_1$	-124	351	247
$Cr_1C_1H_2$	-184	409	167
$Cr_1C_2H_1$	-325	343	197
$Cr_1C_2H_2$	-244	262	183
$Cr_1C_3H_1$	-064	471	420
$Cr_1C_3H_2$	-027	412	509
$Cr_1C_4H_1$	-163	442	571
$Cr_1C_4H_2$	-125	540	533
$Cr_1C_5H_1$	-519	389	404
$Cr_1C_5H_2$	-441	440	477
$Cr_1C_6H_1$	-447	294	514
$Cr_1C_6H_2$	-432	261	412
$Cr_2C_1H_1$	-009	386	082
$Cr_2C_1H_2$	061	360	003
$Cr_2C_2H_1$	066	514	025
$Cr_2C_2H_2$	094	499	131
$Cr_2C_3H_1$	272	395	355
$Cr_2C_3H_2$	369	383	299
$Cr_2C_4H_1$	308	242	323
$Cr_2C_4H_2$	199	275	282
$Cr_2C_5H_1$	328	377	-060
$Cr_2C_5H_2$	373	273	-060
$Cr_2C_6H_1$	453	293	069
$Cr_2C_6H_2$	473	385	010

[a] The form of the thermal ellipsoid is:

$$\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}\ell^2+2\beta_{12}hk+2\beta_{13}h\ell+2\beta_{23}k\ell)].$$

[b] Numbers in parentheses here and in succeeding tables are the estimated standard deviations in the least significant digits.

[c] Temperature factors for the hydrogen atoms are chosen to be 3.0 Å^2.

Square-Pyramidal $Ni(CN)_5{}^{3-}$.—A perspective drawing of the first $Ni(CN)_5{}^{3-}$ group (involving Ni_1) is shown in Figure 1. A view down the noncrystallographic fourfold axis of the ion is shown in Figure 2. The ion is virtually a perfect square pyramid, whose coordination consists of four equivalent cyanides below the nickel atom and an apical cyanide at a greater distance above the nickel atom. The nickel atom is 0.34 Å above the plane of the four carbon atoms and 0.55 Å above the plane of the four nitrogen atoms. The bond lengths, angles, and standard deviations estimated from the inverse matrix for this ion are in Table III. The root-mean-square amplitudes of vibration along the principal axes of the thermal ellipsoids are given for each atom in Table IV. The orientations of these ellipsoids can be seen in the figures. The relatively large errors in the anisotropic thermal parameters probably account for the one or two very distorted thermal ellipsoids.

There is no weak coordination of the nickel atom below the basal plane. The nearest atom (excluding those of cyanide) is 3.99 Å away.

The basal cyanides are all linearly coordinated to within one or two standard deviations (Table III), but the apical Ni–C–N angle of 173.9° is significantly less than 180°. This is consistent with the greater ease of distortion accompanying the longer bond length. The equations for best weighted least-squares planes (in

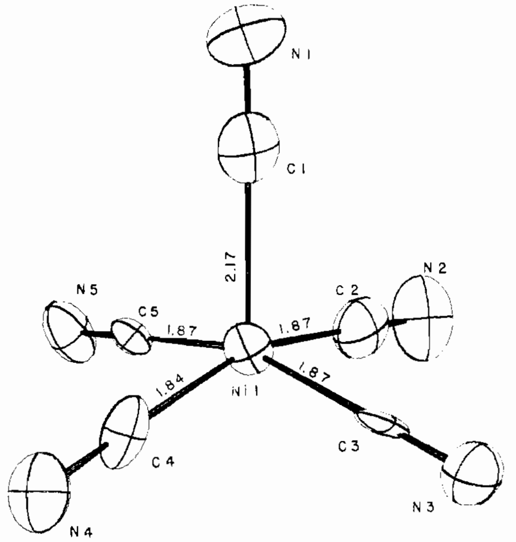

Figure 1.—A perspective drawing of the square-pyramidal $Ni(CN)_5^{3-}$ ion. The shapes of the atoms in this and following drawings, unless noted otherwise, represent 50% probability contours of the thermal motion.

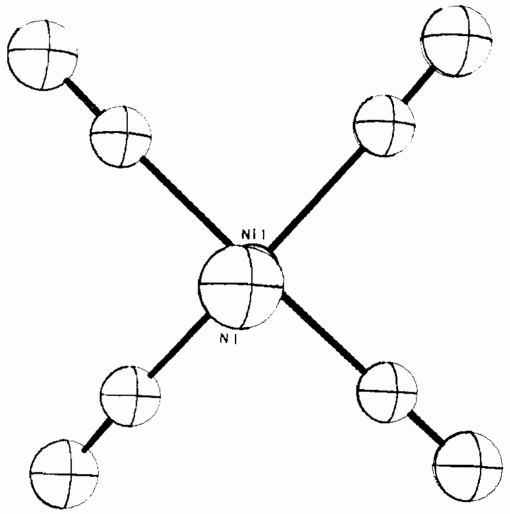

Figure 2.—A view down the noncrystallographic fourfold axis of the square-pyramidal $Ni(CN)_5^{3-}$ ion. Atoms are plotted as spheres for clarity.

monoclinic fractional coordinates) through various combinations of the atoms are shown in Table V. The close adherence to molecular symmetry C_{4v} can be seen from the several interplanar angles in Table VI.

Trigonal-Bipyramidal $Ni(CN)_5^{3-}$.—The second $Ni(CN)_5^{3-}$ ion (involving Ni_2) is approximately related to the first by a translation along the *a* axis of $^1/_2$ and reflection about the plane $y = {}^1/_8$. It is an intermediate between trigonal-bipyramidal and square-pyramidal coordination. The molecular symmetry of this $Ni(CN)_5^{3-}$ ion is very nearly C_2. The distortions in bond lengths and angles from a regular trigonal bipyramid are much less than from a square pyramid. Therefore, it will be referred to as a trigonal bipyramid. A perspective drawing of this ion is shown in Figure 3. In this view, the threefold axis of the idealized trigonal bipyramid runs from left to right toward the viewer. This perspective is chosen since it is closest to the best view for a square pyramid and therefore gives the fairest comparison between the two different $Ni(CN)_5^{3-}$ groups. A view nearly down the "threefold axis" is shown in Figure 4. The coordination consists of two axial cyanides at equal distances and three equatorial

TABLE III

BOND DISTANCES (Å) AND BOND ANGLES (DEG) IN THE TWO $Ni(CN)_5^{3-}$ GROUPS

Bond	Distance Ni_1	Distance Ni_2
$Ni-C_1$	2.168 (14)	1.992 (14)
$Ni-C_2$	1.867 (14)	1.913 (13)
$Ni-C_3$	1.872 (12)	1.827 (12)
$Ni-C_4$	1.839 (13)	1.902 (13)
$Ni-C_5$	1.869 (13)	1.851 (13)
$Ni-N_1$	3.304 (11)	3.162 (11)
$Ni-N_2$	3.023 (12)	3.061 (11)
$Ni-N_3$	3.019 (10)	3.004 (11)
$Ni-N_4$	3.013 (11)	3.034 (11)
$Ni-N_5$	3.015 (10)	3.006 (11)
C_1-N_1	1.141 (12)	1.176 (12)
C_2-N_2	1.156 (12)	1.152 (11)
C_3-N_3	1.147 (11)	1.178 (11)
C_4-N_4	1.175 (12)	1.132 (11)
C_5-N_5	1.147 (11)	1.158 (11)
C_1-C_2	3.023 (19)	3.146 (18)
C_1-C_3	3.120 (17)	2.755 (16)
C_1-C_4	3.162 (18)	3.219 (18)
C_1-C_5	3.084 (18)	2.821 (18)
C_2-C_3	2.645 (17)	2.628 (16)
C_2-C_4	3.646 (19)	3.598 (17)
C_2-C_5	2.578 (17)	2.691 (17)
C_3-C_4	2.541 (16)	2.626 (16)
C_3-C_5	3.682 (18)	3.670 (18)
C_4-C_5	2.599 (16)	2.550 (16)

Atoms	Angle Ni_1	Angle Ni_2
C_1-Ni-C_2	96.76 (49)	107.35 (46)
C_1-Ni-C_3	100.86 (43)	92.25 (48)
C_1-Ni-C_4	103.92 (46)	111.48 (47)
C_1-Ni-C_5	99.40 (42)	94.40 (45)
C_2-Ni-C_3	90.05 (47)	89.27 (46)
C_2-Ni-C_4	159.31 (50)	141.17 (40)
C_2-Ni-C_5	87.29 (47)	91.30 (46)
C_3-Ni-C_4	86.41 (44)	89.49 (44)
C_3-Ni-C_5	159.74 (45)	172.83 (49)
C_4-Ni-C_5	89.01 (44)	85.58 (44)
$Ni-C_1-N_1$	173.9 (11)	172.9 (11)
$Ni-C_2-N_2$	178.5 (12)	174.0 (12)
$Ni-C_3-N_3$	179.5 (10)	177.7 (10)
$Ni-C_4-N_4$	177.8 (10)	177.8 (11)
$Ni-C_5-N_5$	178.0 (11)	175.6 (11)

Wtd av bond distances

Bond type	No.	Av distance
Basal Ni_1-C	4	1.862 (6)
Basal Ni_1-N	4	3.017 (5)
C–N (Ni_1)	5	1.153 (5)
Axial Ni_2-C	2	1.837 (9)
Equatorial Ni_2-C (equivalent)	2	1.907 (9)
Equatorial Ni_2-C	3	1.94[a]
C–N (Ni_2)	5	1.158 (5)
C–N ($Ni_1 + Ni_2$)	10	1.156 (4)

[a] Nonequivalent bonds.

TABLE IV

ROOT-MEAN-SQUARE AMPLITUDES OF VIBRATION (Å)[a]

Atom	Min	Intermed	Max
Ni_1	0.149 (4)	0.164 (4)	0.196 (3)
C_1	0.119 (32)	0.214 (20)	0.243 (22)
C_2	0.161 (25)	0.226 (22)	0.242 (21)
C_3	0.053 (67)	0.190 (21)	0.199 (21)
C_4	0.121 (31)	0.149 (29)	0.253 (20)
C_5	0.093 (40)	0.169 (24)	0.228 (21)
N_1	0.188 (21)	0.235 (17)	0.257 (16)
N_2	0.202 (20)	0.233 (19)	0.334 (15)
N_3	0.182 (18)	0.201 (18)	0.229 (16)
N_4	0.177 (20)	0.195 (18)	0.252 (16)
N_5	0.154 (22)	0.188 (19)	0.281 (15)
Ni_2	0.152 (4)	0.174 (4)	0.192 (3)
C_1	0.156 (26)	0.174 (26)	0.213 (20)
C_2	0.135 (30)	0.214 (22)	0.234 (21)
C_3	0.134 (28)	0.168 (25)	0.220 (20)
C_4	0.031 (113)	0.192 (24)	0.260 (19)
C_5	0.120 (32)	0.159 (25)	0.226 (22)
N_1	0.129 (25)	0.200 (19)	0.250 (15)
N_2	0.184 (20)	0.213 (18)	0.356 (15)
N_3	0.165 (21)	0.170 (18)	0.226 (17)
N_4	0.163 (24)	0.249 (18)	0.389 (16)
N_5	0.181 (19)	0.211 (18)	0.251 (16)
O_1	0.167 (14)	0.192 (12)	0.218 (12)
O_2	0.197 (13)	0.287 (12)	0.297 (12)
O_3	0.225 (13)	0.264 (12)	0.328 (12)
Cr_1	0.157 (4)	0.158 (4)	0.172 (4)
Cr_2	0.157 (4)	0.162 (4)	0.183 (3)

[a] The directions of these principal axes of vibration are displayed in the various figures.

TABLE V

BEST WEIGHTED LEAST-SQUARES PLANES. EQUATIONS OF PLANES OF THE FORM $AX + BY + CZ = D$ (MONOCLINIC COORDINATES)

Atoms	Plane no.	A	B	C	D
Ni_1, C_1, C_2, C_4	1	11.36	−1.953	−11.47	−2.815
Ni_1, C_1, C_3, C_5	2	8.838	−4.992	11.30	2.211
N_2, N_3, N_4, N_5 of Ni_1	3	4.778	14.53	3.035	3.087
Ni_2, C_1, C_2, C_4, N_1, N_2, N_4	4	8.454	−0.786	12.68	7.050
Ni_2, C_1, C_2, C_4	5	8.573	−1.156	12.55	7.042
Ni_2, C_2, C_3, C_5	6	3.910	−14.40	−5.419	−0.828
Ni_2, C_1, C_3, C_5	7	11.91	1.734	−10.79	4.058
Ni_2, C_3, C_4, C_5	8	4.012	15.10	−1.849	3.453

Distances of Atoms from Planes (Å)

	Plane No.							
Atom	1	2	3	4	5	6	7	8
Ni	0.0002 (15)	−0.0003 (16)		+0.002 (2)	+0.000 (2)	−0.005 (2)	−0.002 (2)	0.004 (2)
C_1	−0.002 (11)	0.002 (12)		0.053 (11)	0.002 (11)		0.007 (11)	
C_2	−0.005 (11)			0.007 (11)	0.004 (11)	0.001 (11)		
C_3		0.004 (10)				0.119 (11)	0.040 (10)	−0.085 (11)
C_4	−0.004 (10)			−0.027 (10)	0.003 (10)			0.012 (12)
C_5		0.004 (10)				0.101 (11)	0.041 (10)	−0.074 (10)
N_1				−0.041 (9)				
N_2			0.005 (12)	−0.027 (10)				
N_3			−0.003 (9)	−0.003 (11)				
N_4			0.003 (9)					
N_5			−0.004 (10)					

TABLE VI

INTERPLANAR ANGLES FOR SQUARE-PYRAMIDAL $Ni(CN)_5^{3-}$

Plane 1	Plane 2	Angle, deg
C_2, Ni, C_4	C_3, Ni, C_5	91.40 (34)
C_2, Ni, C_4	C_2, C_4, C_5	89.9 (13)
C_2, Ni, C_4	C_2, C_3, C_4	89.7 (13)
C_3, Ni, C_5	C_3, C_4, C_5	92.8 (13)
C_3, Ni, C_5	C_2, C_3, C_5	87.4 (13)

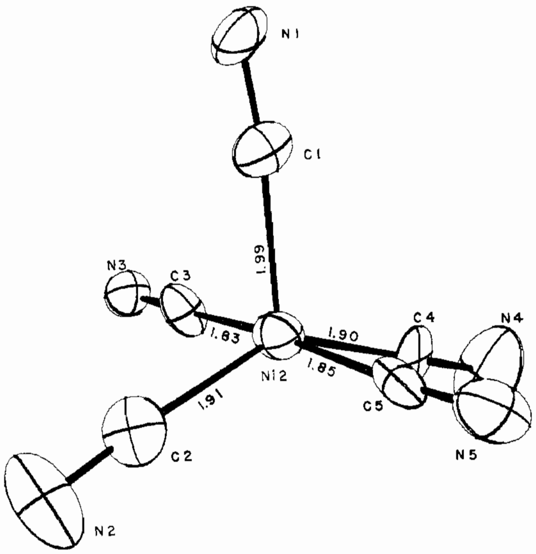

Figure 3.—A perspective drawing of the trigonal-bipyramidal $Ni(CN)_5^{3-}$ ion.

cyanides, one of which is further from the nickel atom than are the other two. The bond lengths and angles with their standard deviations are given in Table III. The root-mean-square amplitudes of vibration along the principal axes of the thermal ellipsoids are given for each atom in Table IV.

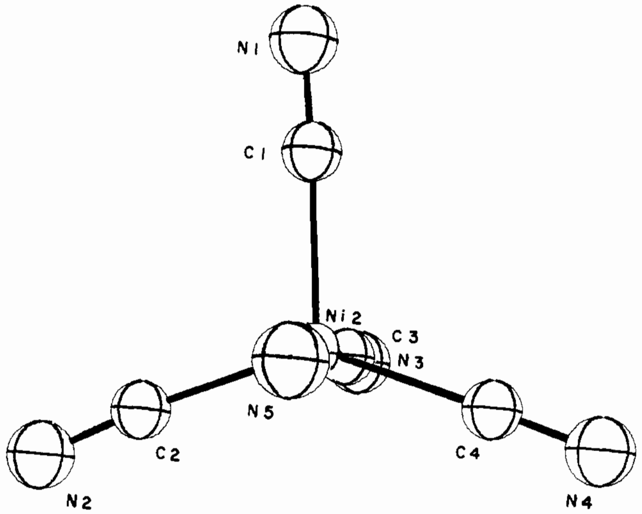

Figure 4.—A perspective view down the pseudo-threefold axis of the distorted trigonal-bipyramidal $Ni(CN)_5^{3-}$ ion. Atoms are plotted as spheres for clarity.

The important distortions from regular trigonal-bipyramidal coordination are: (1) the one longer equatorial bond length of 1.99 Å; (2) the corresponding increase in the opposite angle to 141° (ideal, 120°); (3) the axial cyanide–nickel–cyanide angle of 173° (ideal, 180°). These deviations from D_{3h} coordination symmetry are also observed in the compound $[Ni(P(OC_2H_5)_2(C_6H_5))_3(CN)_2]$.[16] The remarkable similarity in the observed geometry of that compound and the trigonal-bipyramidal $Ni(CN)_5^{3-}$ indicates that the C_2 geometry is not due to distortion by crystal-packing forces but is rather an energy minimum for the free ion. When the idealized trigonal-bipyramidal coordination is considered, the most important point is the shorter, average axial bond length (1.84 Å) *vs.* the average equatorial bond length (1.94 Å). This is more fully

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(16) J. K. Stalick and J. A. Ibers, unpublished results.

discussed elsewhere.[17] The closest noncyanide atom approach to the nickel atom is from a hydrogen atom of one of the ethylenediamine rings (2.95 Å).

The cyanides are all nearly linearly coordinated (Table III). As in the first anion, the greatest distortion from linearity occurs with the longest Ni–C bond. The equations for best weighted least-squares planes through various atoms are in Table V.

$Cr(en)_3^{3+}$ Ions.—In both cations the chromium ions have their expected, distorted octahedral coordination. Figure 5 shows the coordination about each of the Cr atoms. The configurations around the metals in this figure are arbitrarily chosen as Λ, since the centrosymmetric space group requires that both the Λ and the Δ configurations of each cation be present in equal numbers. The conformation of the Cr_1 cation (Figure 5a) is Λ∂λλ; the conformation of the Cr_2 cation (Figure 5b) is Λ∂∂λ. These are the first examples of conformations for tris(ethylenediamine)metal complexes that differ from Λ∂∂∂. This matter is discussed more fully elsewhere.[18]

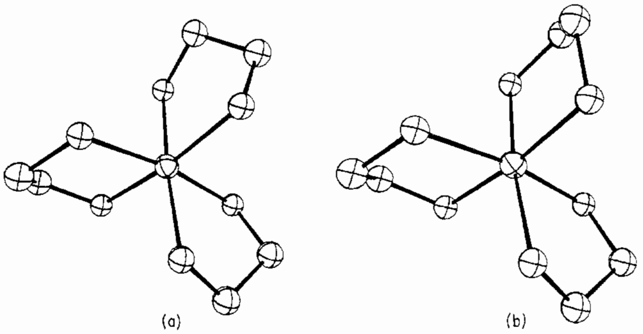

Figure 5.— perspective drawing of the $Cr(en)_3^{3+}$ cations: (a) Cr_1; (b) Cr_2.

The chemically equivalent bond lengths and angles for both ions are equal within experimental error and are given in Tables VII and VIII. The weighted averages and the standard deviations of the mean bond lengths are also given in Table VII. The usual quantity $\Sigma(\Delta_i/\sigma_i)^2$, where Δ_i and σ_i are the deviation from the mean and the estimated standard deviation from the inverse matrix, should be distributed as χ^2 if the individual observations are from the same population. Thus, by examination of this quantity, one can test the hypotheses that the bonds being averaged are really chemically equivalent and that the assigned standard deviations are correct. Only for the 12 Cr–N bonds is there an indication that these hypotheses are not valid. Here there is one unusually short and one unusually long Cr–N bond. This indicates that these bonds are not chemically equivalent or that they have been affected by systematic errors in the data or the model. We believe that this second possibility is more likely. These results also indicate that the assigned standard deviations are reasonable and that factoring of the full least-squares matrix has not led to a serious underestimate of these quantities.

Table VII

Bond Lengths for $Cr(en)_3^{3+}$ Cations

Bond	Cr_1 distance, Å	Cr_2 distance, Å
$Cr–N_1$	2.080 (7)	2.100 (8)
$Cr–N_2$	2.083 (7)	2.054 (8)
$Cr–N_3$	2.079 (8)	2.076 (8)
$Cr–N_4$	2.077 (7)	2.062 (8)
$Cr–N_5$	2.062 (7)	2.085 (8)
$Cr–N_6$	2.076 (7)	2.073 (7)
	Wtd av 2.076 (3)	Wtd av 2.075 (3)
	Wtd av for all 12 Cr–N bonds	2.075 (2)
$C_1–N_1$	1.503 (12)	1.495 (12)
$C_2–N_2$	1.494 (12)	1.500 (10)
$C_3–N_3$	1.461 (11)	1.497 (12)
$C_4–N_4$	1.473 (11)	1.487 (13)
$C_5–N_5$	1.500 (11)	1.496 (12)
$C_6–N_6$	1.486 (11)	1.496 (12)
	Wtd av 1.485 (5)	Wtd av 1.496 (5)
	Wtd av for all 12 C–N bonds	1.490 (3)
$C_1–C_2$	1.498 (13)	1.515 (13)
$C_3–C_4$	1.505 (12)	1.518 (14)
$C_5–C_6$	1.489 (13)	1.490 (13)
	Wtd av 1.498 (7)	Wtd av 1.507 (8)
	Wtd av for all 6 C–C bonds	1.502 (5)
en ring	Conformation[a]	Conformation[a]
1–2	λ	∂
3–4	λ	∂
5–6	∂	λ

[a] For Λ configuration around Cr atom.

Table VIII

Bond Angles (deg) in $Cr(en)_3^{3+}$ Cations

	$[Cr(en)_3]^{3+}$ group	
Atoms	1	2
$N_1–Cr–N_2$	81.97 (29)	82.36 (30)
$N_1–Cr–N_3$	91.84 (29)	91.66 (30)
$N_1–Cr–N_4$	94.64 (29)	92.46 (31)
$N_1–Cr–N_5$	94.21 (29)	92.85 (31)
$N_1–Cr–N_6$	172.62 (29)	171.67 (31)
$N_2–Cr–N_3$	94.88 (29)	92.04 (31)
$N_2–Cr–N_4$	174.99 (28)	172.90 (31)
$N_2–Cr–N_5$	92.57 (28)	94.46 (31)
$N_2–Cr–N_6$	91.60 (29)	90.89 (30)
$N_3–Cr–N_4$	81.49 (29)	83.22 (31)
$N_3–Cr–N_5$	170.99 (30)	172.53 (31)
$N_3–Cr–N_6$	92.32 (29)	93.46 (30)
$N_4–Cr–N_5$	91.36 (29)	90.63 (31)
$N_4–Cr–N_6$	92.00 (28)	94.67 (30)
$N_5–Cr–N_6$	82.41 (30)	82.78 (31)
$Cr–N_1–C_1$	108.93 (56)	109.6 (57)
$Cr–N_2–C_2$	109.39 (56)	108.8 (55)
$Cr–N_3–C_3$	109.58 (56)	109.0 (60)
$Cr–N_4–C_4$	111.12 (55)	108.2 (62)
$Cr–N_5–C_5$	109.87 (56)	107.9 (60)
$Cr–N_6–C_6$	109.53 (55)	111.3 (57)
$N_1–C_1–C_2$	106.8 (8)	106.8 (8)
$N_2–C_2–C_1$	107.9 (8)	107.7 (8)
$N_3–C_3–C_4$	108.6 (8)	108.2 (9)
$N_4–C_4–C_3$	109.1 (8)	107.4 (9)
$N_5–C_5–C_6$	108.5 (8)	112.0 (8)
$N_6–C_6–N_5$	108.6 (8)	107.3 (8)

The average Cr–N bond length of 2.075 (2) Å is longer than that in $[Cr(NH_3)_6][CuCl_5]$ of 2.064 (3) Å.[17] This difference, if real, is not indicated by the absorption spectra of the two cations in aqueous solution, which

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(17) K. N. Raymond, D. W. Meek, and J. A. Ibers, *Inorg. Chem.*, in press.

(18) K. N. Raymond, P. W. R. Corfield, and J. A. Ibers, *ibid.*, **7**, 842 (1968).

have band maxima at nearly identical energies. Indeed, the maxima are at slightly higher energies for the $Cr(en)_3^{3+}$ salt. The greater intensity of the $Cr(en)_3^{3+}$ bands is consistent with the significant distortion from octahedral symmetry.

The average C–C bond length in the ethylenediamine rings, 1.502 (5) Å, is very significantly shorter than that for a paraffin C–C bond, 1.54 Å. The average C–N bond length in the ethylenediamine rings is 1.490 (3) Å. This is only slightly greater than the usual paraffin–quaternary amine bond length of 1.479 (5) Å.[19]

Intermolecular Packing and Hydrogen Bonding. The coordinates of the nickel atoms are very close to $(0, {}^1/_8, {}^1/_4)$ and $({}^1/_2, {}^1/_8, {}^1/_4)$, and those of the chromium atoms are close to $(-{}^1/_4, {}^3/_8, {}^3/_8)$ and $({}^1/_4, {}^3/_8, {}^1/_8)$. With these idealized coordinates, the metal atoms alone can be described in terms of an idealized cell with $\beta = 90°$ and a "b" axis of half of the length of the "b" axis for the true cell. The idealized cell has symmetry Amma, an alternative setting for Cmcm, and its origin is at $(0, {}^1/_8, {}^1/_4)$ in the true cell. The positions of the metal atoms in the idealized cell are shown in Figure 6. The idealized structure can be regarded as built up of layers perpendicular to "c" with the nickel atoms lying in the mean plane of the layers. Each nickel atom is surrounded by four chromium atoms in the same layer, each at 5.8 Å, and by two further chromium atoms from neighboring layers at 7.2 Å, which complete an elongated octahedron. Each chromium atom lies 2.1 Å above the center of a planar group of four nearest nickel atoms in the same layer, each 5.8 Å from the chromium, and there are two more distant nickel neighbors in the next layer at 7.2 Å. This description emphasizes the closely similar intermolecular environments of the two independent nickel ions and of the independent chromium ions, since in the idealized cell, atoms Ni_1 and Ni_2 and atoms Cr_1 and Cr_2 are equivalent. The actual nickel–chromium distances deviate no more than 0.8 Å from the above idealized geometry, and all but two distances are within 0.5 Å. The similarity in environment extends to the hydrogen-bonding scheme, described in more detail below. Each metal ion apparently forms at least one N···N hydrogen bond with each of its four nearest neighbors and with one of the more distant ones, and the hydrogen bonding of O_1 to Ni_1 ions and a Cr_1 ion is paralleled by that of O_2 to Ni_2 ions and a Cr_2 ion.

Thus there are only slight differences in the arrangements of hydrogen bonds around the trigonal-bipyramidal and square-pyramidal $Ni(CN)_5^{3-}$ groups. Since the energy of formation of these weak hydrogen bonds is small and since only a fraction of this energy can be used for stabilizing one geometry relative to the other, we conclude that the energy of conversion from the trigonal bipyramid to the square pyramid is very small, probably only a few kilocalories per mole.

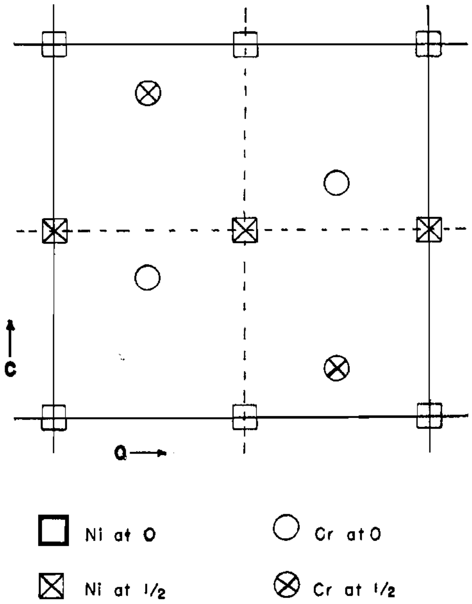

Figure 6.—Packing diagram for $[Cr(en)_3][Ni(CN)_5]\cdot 1.5H_2O$. The geometry is idealized with $\beta = 90°$ and the b axis halved.

Of the four kinds of hydrogen bonds in this compound, the most important interactions are those between the cyanides and either amine groups or waters of crystallization.

Figure 7 shows the hydrogen bonding between the square-pyramidal $Ni(CN)_5^{3-}$ ion and the two waters of crystallization designated O_1 and O_3. The first water molecule (O_1) bonds strongly to two different nitrogens on $Ni(CN)_5^{3-}$ groups related by the glide plane and forms an infinite chain along the c axis. The second water molecule (O_3) bonds only to the apical cyanide. It is relatively unusual that this water molecule apparently does not participate in any other hydrogen

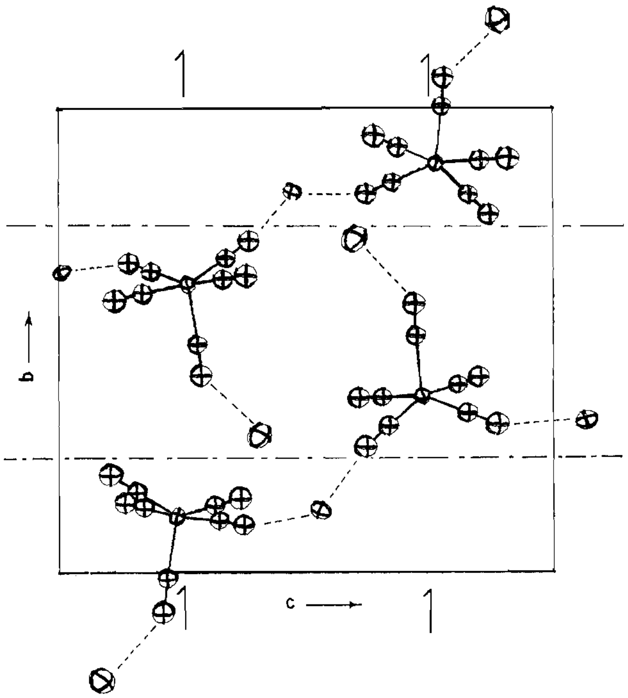

Figure 7.—A perspective drawing of the water hydrogen bonds formed by the square-pyramidal $Ni(CN)_5^{3-}$ ions.

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(19) "Tables of Interatomic Distances and Configurations in Molecules and Ions," The Chemical Society, Burlington House, London, 1958.

bonds, although this is known to occur in $MgSO_4 \cdot 4H_2O$.[20]

The trigonal-bipyramidal $Ni(CN)_5^{3-}$ ions are nearly related to the square-pyramidal ions by a translation along *a* of $^1/_2$, followed by a reflection perpendicular to *b*. Figure 8 shows a projection identical with that in Figure 7, but at $x = {^1/_2}$. Here it is seen that the trigonal-bipyramidal $Ni(CN)_5^{3-}$ groups bond to only one water molecule O_2. The one strong hydrogen bond (2.88 Å) is shown. There is a second, weaker hydrogen bond (3.09 Å) between O_2 and the centrosymmetrically related $Ni(CN)_5^{3-}$ group. These $Ni(CN)_5^{3-}$ groups are thus hydrogen bonded into pairs by the two water molecules O_2 and O_2', where O_2' is related to O_2 by a center of symmetry.

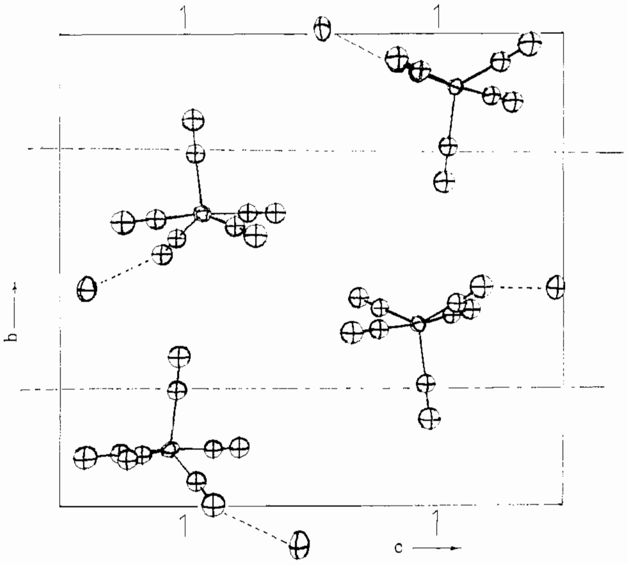

Figure 8—A perspective drawing of the water hydrogen bonds formed by the trigonal-bipyramidal $Ni(CN)_5^{3-}$ ions.

Table IX

Summary of Proposed A–H···B Hydrogen Bonds ≤3.2 Å

B^c	A		H	A–B, Å	Angle around H, deg
Ni_1N_1	O_3[a]	(3)[b]		2.94	
Ni_1N_1	Cr_2N_3	(3)	H_1	3.14	158
Ni_1N_2	Cr_2N_2	(2)	H_1	3.00	151
Ni_1N_3	Cr_1N_4	(3)	H_2	2.99	151
Ni_1N_3	Cr_2N_4	(1)	H_2	3.02	158
Ni_1N_4	O_1	(1)		2.86	
Ni_1N_4	Cr_1N_3	(2)	H_2	3.14	145
Ni_1N_5	O_1	(2)		2.89	
Ni_1N_5	Cr_1N_2	(1)	H_2	3.01	169
Ni_2N_1	Cr_1N_5	(4)	H_1	2.94	156
Ni_2N_1	Cr_2N_6	(1)	H_1	3.09	144
Ni_2N_2	O_2	(6)		2.88	
Ni_2N_2	Cr_1N_1	(3)	H_2	3.05	166
Ni_2N_3	Cr_2N_5	(1)	H_2	3.20	144
Ni_2N_4	Cr_1N_4	(2)	H_1	3.02	139
Ni_2N_4	Cr_1N_6	(5)	H_1	2.98	148
Ni_2N_5	O_2	(1)		3.09	
Ni_2N_5	Cr_2N_2	(3)	H_2	3.16	154
O_1	Cr_1N_6	(7)	H_2	2.99	156
O_2	Cr_2N_2	(3)	H_2	3.12	143
O_2	O_1	(2)		3.06	

[a] The positions of the hydrogen atoms on the water molecules were not located. [b] These numbers correspond to the following transformations of the positions of the A atoms given in Table II: (1) x, y, z; (2) $x, {^1/_2} - y, {^1/_2} + z$; (3) $-x, -{^1/_2} + y, {^1/_2} - z$; (4) $1 + x, y, z$; (5) $x, {^1/_2} - y, -{^1/_2} + z$; (6) $-x, -y, 1 - z$; (7) $x, -{^1/_2} - y, -{^1/_2} + z$. [c] All B atoms are positioned as given in Table II.

The only example of a water–water hydrogen bond in this structure is between O_1 and O_2, which are bonded in the *a* direction with an O–O distance of 3.06 Å.

The vast majority of the hydrogen bonds are formed between amine groups of the coordinated ethylenediamine ligands and the cyanide nitrogens. All of the cyanide nitrogens participate in hydrogen bonds. Table IX summarizes the hydrogen bonds formed in this structure. Most of the hydrogen bond angles around the calculated hydrogen positions differ widely from 180°. These bond angles are, of course, somewhat in error since the hydrogen atom positions were calculated on the assumption of tetrahedral geometry around the atoms of the ethylenediamine rings. Nevertheless, in those hydrates where accurate hydrogen positions are known from neutron diffraction studies it is found that the bond angle in the water molecule differs little from that in free water.[21] Thus hydrogen bond formation would not be expected to alter significantly the assumed tetrahedral configurations about the C and N atoms of the ethylenediamine rings. The average value of the calculated bond angles is 153°. This is less than the average of 160° calculated by Hamilton[22] from the results of various neutron diffraction studies. However, the lower value found here is consistent with the observation that long hydrogen bonds tend to have bond angles farther from 180°. Most of the hydrogen bonded N···N or N···O distances in this structure are long and the hydrogen bonds are weak.

Acknowledgment.—We thank Professor Fred Basolo for his continued interest in this work. K. N. R. expresses his gratitude to the National Institutes of Health for a predoctoral fellowship. We are indebted to the National Science Foundation for its support of this work.

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(20) W. H. Baur, *Acta Cryst.*, **17**, 863 (1964).

(21) W. C. Hamilton and J. A. Ibers, "Hydrogen Bonding in Solids," W. A. Benjamin, Inc., New York, N. Y., 1968.

(22) W. C. Hamilton, *Ann. Rev. Phys. Chem.*, **13**, 19 (1962).