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The Crystal and Molecular Structure of Dibromo-1-(2-pyridyl)-2,5-diaza-5-methyl-hexa-1-enezinc(II)

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The crystal structure of dibromo-1-(2-pyridyl-2,5-diaza-5-methyl-hexa-1-enezinc(II), $C_{10}H_{15}N_3ZnBr_2$*, has been determined from three-dimensional X-ray diffraction data collected on a Picker automatic single crystal diffractometer with MoKα radiation. The cell has dimensions* $a = 10.730(2)$, $b = 11.248(2)$, $c = 7.433(2)$ Å, *alpha* $= 102.69(2)$, *beta* $= 91.36(2)$, *gamma* $= 110.70(1)^\circ$*, belongs to the space group* $P\bar{1}$*, and contains two molecules. 3701 independent reflections have been measured and the structure has been refined by least squares to a final R value of .072. The coordination configuration can be described as a distorted trigonal bipyramid. The zinc-to-ligand bond distances are:* Zn–Br(1) = 2.396(1), Zn–Br(2) = 2.410(1), Zn–N(1) = 2.245(8), Zn–N(2) = 2.087(6), Zn–N(3) = 2.236(7) Å.

Introduction

A great deal of synthetic chemistry research has been performed recently on pentacoordinated complexes, resulting in hundreds of new complexes utilizing a variety of ligand and donor atoms. The general stereochemistry as determined by X-ray crystallographic studies on a considerable number of these complexes is trigonal bipyramidal or tetragonal pyramidal or a distortion of one of these configurations. The present structural determination of dibromo-1-(2-pyridyl)-2,5-diaza-5-methyl-hexa-1-enezinc(II) was performed to verify the proposed pentacoordination of the complex and to examine the details of the structure, although spectral information from corresponding nickel(II) and cobalt(II) complexes implied the pentacoordination.[1]

Experimental Section

Equimolar amounts of reagent grade N,N-dimethylethylenediamine and pyridine-2-aldehyde in boiling ethanol were added to the calculated amount of zinc bromide dissolved in ethanol to obtain the 1:1 zinc-to-ligand adduct. The microcrystalline, white solid was found to be noncoduncting in solutions of chloroform and dichloroethane. Carbon, nitrogen, and metal analyses indicated the empirical formula to be identical with the expected 1:1 adduct of the formula $C_{10}H_{15}N_3ZnBr_2$.

The compound was recrystallized from a mixture of chloroform and acetone to obtain a crystal of usable size. The crystal chosen was a plate with dimensions $0.14 \times 0.11 \times 0.19$ mm along a, b, and c, respectively. Oscillation and Weissenberg photographs showed the crystal to be triclinic.

The cell constants were determined at 27°, with the chrystal mounted with the $0\bar{1}\bar{3}$ reciprocal lattice vector parallel to the Φ axis of the diffractometer, from the least squares fit for the measurements of 26 two-theta values in the range 16.5 to 35.8°. These were measured by the $+2\theta$, -2θ technique on a Picker four-angle automatic single crystal diffractometer using MoKα radiation filtered with .001 inch niobium metal foil. The cell constants are a = 10.730(2), b = 11.248(2), c = 7.433(2) Å, alpha = 102.69(2), beta = 91.36(2), gamma = 110.70(1)°. The unit cell contains two molecules and has a volume of 813.65 Å.[3] The density measured by the flotation method is 1.666 g/cm^3 while the calculated density is 1.642 g/cm^3. F(000) = 392.

The intensity data were collected at a take-off angle of 3.5° by the θ–2θ scan method using MoKα radiation and a Picker automatic single crystal diffractometer equipped with a scintillation counter and pulse-height discriminator. A suitable scan range for each reflection was calculated using the formula of Alexander and Smith,[2] scan range = $1.0 + 1.0 \tan\theta$. Of the 3701 reflections which were measured to 2θ values of 55°, 2431 reflections had an intensity greathe than twice the standard deviation of the intentensity, σ_I. σ_I is defined from $\sigma_I^2 = \sigma_{Is}^2 + k^2$ (total counts);[2] σ_{Is} is the standard deviation due to counting statistics $= p + t^2(B_1 + B_2)$, where p is the peak scan count, t is the peak-scan-to-background ratio (= scan time for peak/2 (scan time for each background)) and B_1 and B_2 are background counts, k is the stability constant which in this case was assigned a vâlue of 0.01. The remaining 1270 reflections, whose intensities were less than $2\sigma_I$, were coded unobserved and assigned intensities of $1 + 2\sigma_I$ for later least squares refinement. Four standard reflections were measured every two hours during data collection and a least squares analysis was performed on the deviations of each of these groups of standards to determine periodic scale factors. The crystal decomposed approximately 14% during data collection and the periodic scale factors ranged from 1.000 to 1.139.

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(1) Zakrzewski and L. Sacconi, *Inorg. Chem.*, *7*, 1034 (1968).

(2) L. E. Alexander and G. S. Smith, *Acta Cryst.*, *17*, 1195 (1964).

Table I. Final Parameters for non-hydrogen atoms as obtained from the least squares refinement. Positions are multiplied by 10^4. Temperature parameters are multiplied by 10^2. Estimated standard deviations are given in parentheses

Atom	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Zn	2742(1)	1479(1)	7125(1)	417(5)	446(5)	249(4)	217(4)	67(3)	92(4)
Br1	1027(1)	1720(1)	9013(1)	459(4)	582(5)	376(4)	271(4)	140(3)	126(4)
Br2	4926(1)	2201(1)	8823(1)	409(4)	635(6)	436(5)	205(4)	−3(3)	110(4)
N1	3048(7)	3274(7)	6071(9)	458(36)	392(36)	353(32)	159(29)	68(26)	132(28)
N2	2793(7)	874(7)	4274(8)	452(36)	497(38)	271(29)	224(30)	62(25)	130(28)
N3	2112(7)	−697(7)	6606(9)	511(41)	408(37)	366(32)	186(32)	82(29)	119(27)
C1	3206(10)	4468(10)	7032(12)	703(60)	596(56)	417(44)	400(48)	144(41)	110(41)
C2	3409(10)	5532(10)	6198(15)	667(62)	687(65)	638(60)	370(51)	131(48)	328(51)
C3	3455(10)	5297(11)	4301(16)	544(57)	679(65)	681(65)	311(49)	29(48)	293(54)
C4	3312(9)	4050(10)	3278(13)	529(52)	547(55)	457(48)	70(43)	−20(39)	280(44)
C5	3105(8)	3048(8)	4211(11)	345(39)	328(40)	365(40)	−26(31)	−17(31)	120(33)
C6	2953(8)	1702(8)	3306(11)	369(41)	422(45)	343(38)	70(34)	45(32)	75(35)
C7	2605(10)	−513(9)	4454(11)	831(63)	563(55)	285(38)	405(48)	214(39)	69(36)
C8	2891(9)	−1046(8)	5082(11)	626(55)	410(42)	329(40)	220(39)	109(37)	111(33)
C9	619(9)	−1367(10)	6032(13)	430(49)	670(60)	625(54)	200(44)	37(41)	177(45)
C10	2460(13)	−1107(11)	8250(13)	1230(88)	763(67)	394(47)	660(65)	160(51)	237(45)
Y	−34(8)	4903(8)	2880(15)	287(41)	229(40)	950(71)	−28(32)	41(43)	212(44)
Z	1533(5)	6062(5)	575(7)	431(28)	275(24)	373(25)	107(21)	4(21)	52(19)

Table II. Parameters ($\times 10^3$) of Hydrogen Atoms from Difference Synthesis

	x/a	y/b	z/c
H1	317	444	860
H2	350	633	688
H3	358	595	373
H4	320	386	185
H5	305	141	206
H70	329	−47	273
H71	176	−96	292
H80	270	−149	484
H81	390	−88	556
H90	0	−141	629
H91	54	−220	582
H92	56	−115	496
H100	213	−84	956
H101	349	−74	828
H102	216	−198	795

A coincidence loss correction was applied by taking the results of a least squares line analysis performed on a group of reflections whose intensities were measured both at a filament current of 14 and 4 milliamps and then plotted as intensity ratio *vs.* intensity. The correction was $n_t = n_o/(1-n_o \text{ tau})$; in this expression n_o is the observed count in a scan and n_t is the true count and tau is the fraction of time lost per scan per count, 7.01×10^{-8} in the present case. Since the linear absorption coefficient was equal to 67.94 cm^{-1}, a correction was made for absorption using the absorption program described by J. Meulenaer and H. Tompa[3] and adapted for the University of Washington crystallographic system by D. Cullen.[4] Comparison of the observed and calculated structure factors by the method of Housty and Clastre,[5] near the end of the refinement, showed no evidence of secondary extinction effects.

Structure determination

All calculations were carried out on an IBM 7040-7094 direct couple system computer using a set of programs written or adapted by Stewart.[6] The atomic scattering factors used were those of Cromer and Waber[7] for zinc ion, bromide ion, nitrogen, carbon and oxygen atoms, and those of Stewart, Davidson and Simpson[8] for hydrogen. In later stages of the refinement of the structure, a correction was applied for anomalous dispersion using the corrections for zinc io n($\Delta f' = 0.3$, $\Delta f'' = 1.5$) and bromide ion ($\Delta f' = 0.3$, $\Delta f'' = 2.5$) described in the International Tables for X-ray Crystallography.[9]. The positions of the zinc and bromide ions were found from a Patterson synthesis. The space group $P\bar{1}$ was assumed and in the following Fourier syntheses all of the atoms of the proposed structure were located. The R value at this point was 0.235, where R is defined as $\Sigma||F_o|-|F_c||/\Sigma|F_o|$. Further refinement was performed using the full-matrix least squares program of Busing and Levy,[10] as modified by Stewart.[6] The function minimized was $\Sigma w(F_o-F_c)^2$, where initially $w = 1.0$ for observed reflections and unobserved reflections for which $F_c > F_o$, and $w = 0$ for unobserved reflections for which $F_c < F_o$. Isotropic temperature factors were used in the form $\exp(-(B \sin^2\theta/\lambda^2))$ and anisotropic temperature factors in the form $\exp(-1/4 \sum_{i=1}^{3} \sum_{j=1}^{3} h_i h_j a_i^* a_j^* B_{ij})$. Three cycles of isotropic refinement lowered R from 0.235 to 0.156 and two cycles of anisotropic refinement lowered R to 0.124. A difference synthesis was calculated and a pair of peaks with peak heights of 8.6 and 4.6 electrons/Å^3 were found, with a considerable amount of diffuse electron density between 1 and 1.9 electrons/Å^3 between them. Other peaks with peak heights less than 1 electron/Å^3, presumably the hydrogen atoms, were not considered at this

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(3) J. DeMeulenaer and H. Tompa, *Acta, Cryst.*, *19*, 1014 (1965).
(4) D. Cullen, Ph. D. dissertation, University of Washington (1969).
(5) J. Housty and J. Clastre, *Acta Cryst.*, *10*, 695 (1957).

(6) J. M. Stewart (1964) *Crystal Structure Calculations System X-ray-63*, University of Maryland TR-64-6.
(7) D. Cromer and J. Waber, *Acta Cryst.*, *18*, 104 (1965).
(8) R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, *42*, 3175 (1965).
(9) *International Tables for X-ray Crystallography*, Vol. III, the Kynoch Press, Birmingham, England (1962), p. 213-16.
(10) W. Busing and H. Levy, « *ORFLS, A Fortran Crystallographic Least Squares Program* » *ORNL-TM-305*, Oak Ridge National Laboratory, Oak Ridge, Tennessee 1962.

point. The largest peak (Y) was assigned an atomic scattering factor equal to that of oxygen and the second peak (Z) was assigned an atomic scattering factor equal to that of carbon. A structure factor calculation performed including these two « solvent molecule » atoms gave R = 0.072. A new difference synthesis was calculated but did not further resolve the diffuse electron density between X and Y. All hydrogen atoms were located in this difference synthesis and were assigned isotropic temperature factors of 6.0 after two cycles of isotropic refinement on their positions and temperature factors were unsuccessful. The positions of the hydrogen atoms found from the difference synthesis were used as fixed atom contributions for all further refinement. At this time a weight of $1/\sigma_F^2$, where $\sigma_F = (F^2+\sigma_I Lp)^{1/2} - F$ and F is the structure factor, Lp is the Lorentz-polarization factor and σ_I is the standard deviation of the inten-

Table III. Observed and calculated structure factors. Columns are h, 10F$_o$, and 10F$_c$. Unobserved reflections are marked by*

Table III. (Continued)

sity, was introduced for each reflection. Since the number of variables for further refinement exceeded the maximum of 172 variables which can be refined using the full-matrix least squares program as adapted to the University of Washington crystallographic system, it was necessary to perform fixed atom contribution refinement, in which most of the atoms are refined in each cycle with the other atoms providing a fixed atom contribution to the calculation. Four cycles of anisotropic refinement gave the final R value of .072 with a weighted R, defined as $R_w = \left\{\frac{\Sigma w(F_o-F_c)^2}{\Sigma_w F_o^2}\right\}^{1/2}$, of .064. The maximum shift/error for the last cycle of least squares was less than 1.0 with the average shift error being 0.321. The final positional and thermal parameters are listed in Tables I and II. The list of observed and calculated structure factors is given in Table III.

Discussion

The crystal structure consists of discrete monomeric units of dibromo-1-(2-pyridyl)-2,5-diaza-hexa-1-enezinc(II) (Figure 1). Interatomic distances and angles are given in Table IV. Pentacoordinated complexes whose structures have been determined have been found to possess trigonal bipyramidal, tetragonal pyramidal, or a distortion of one of these stereochemistries. If this complex is considered to be a trigonal bipyramid in which Br(1), Br(2), and N(2) constitute the equatorial plane with N(1) and N(3) being the apical donor atoms, the angles of the coordination can be explained on the basis of the restrictions which the tridentate ligand places on certain angles and on the basis of other steric effects.

Table IV. Interatomic Distances and angles. Estimated Standard deviations are given in Parentheses

Zn—N(1)	2.245(8) Å
Zn—N(2)	2.087(6)
Zn—N(3)	2.236(7)
Zn—Br(1)	2.396(1)
Zn—Br(2)	2.410(1)
N(1)—C(1)	1.324(12)
C(1)—C(2)	1.418(17)
C(2)—C(3)	1.382(16)
C(3)—C(4)	1.394(15)
C(4)—C(5)	1.405(15)
C(5)—C(6)	1.464(12)
C(6)—N(2)	1.266(13)
N(2)—C(7)	1.484(12)
C(7)—C(8)	1.533(14)
C(8)—N(3)	1.489(12)
N(3)—C(9)	1.514(11)
N(3)—C(10)	1.480(14)
N(1)—Zn—N(2)	75.4(3)°
N(1)—Zn—N(3)	150.2(2)
N(2)—Zn—N(3)	76.4(3)
N(1)—Zn—Br(1)	95.3(2)
N(1)—Zn—Br(2)	97.8(2)
N(2)—Zn—Br(1)	133.9(2)
N(2)—Zn—Br(2)	111.8(2)
N(3)—Zn—Br(1)	97.6(2)
N(3)—ZnBr(2)	101.2(2)
Br(1)—Zn—Br(2)	114.2(1)
N(1)—C(1)—C(2)	122.9(9)
C(1)—C(2)—C(3)	117.7(10)
C(2)—C(3)—C(4)	120.0(12)
C(3)—C(4)—C(5)	118.7(9)
C(4)—C(5)—N(1)	121.4(8)
C(5)—N(1)—C(1)	119.4(8)
C(4)—C(5)—C(6)	121.4(8)
C(6)—C(5)—N(1)	114.5(8)
C(6)—N(2)—C(7)	122.6(7)
C(6)—N(2)—Zn	118.5(6)
C(7)—N(2)—Zn	118.9(6)
N(2)—C(7)—C(8)	105.5(6)
C(7)—C(8)—N(3)	108.4(9)
C(8)—N(3)—Zn	104.1(5)
C(8)—N(3)—C(9)	111.3(6)
C(10)—N(3)—Zn	112.4(5)
C(9)—N(3)—C(10)	108.8(7)

In a regular trigonal bipyramid, equatorial donor atom-to metal ion-to apical donor atom angles of 90° would be expected. However, the condensed ethylenediamine group (one nitrogen atom of which forms the Schiff base imine nitrogen) does not have the flexibility for 90° N—M—N angles (as shown by small corresponding angles in similar structures[11,12,13]) and reduces the N(2)—Zn—N(3) bond angle to 76.4(3)°. Likewise, for the planar system formed by the pyridine ring, C(6), and N(2), the chelate ring requires an angle less than 90° (this angle is equal to 75.4(3)°) as is shown in the similar structure of dichloro(pyridine-2- aldehyde-2-pyridylhydrazone)Co(III).[11] Since these angles are less than 90°, the N(1)—Zn—Br(1) (95.3(2)°), N(3)—Zn—Br(1) (97.6(2)°), and N(3)—Zn—Br(2) (101.2(2)°) bond angles must be greater than 90°.

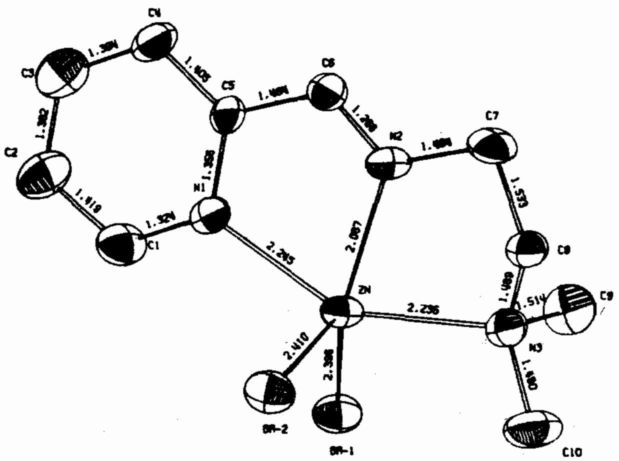

Figure 1. Interatomic Distances and 30% Probability Thermal Ellipsoids

The equatorial bond angles are Br(2)—Zn—N(2) = 111.8(2)°, Br(1)—Zn—N(2) = 133.9(2)°, and Br(1)—Zn—Br(2) = 114.2(1) and may be explained to differ from 120° if the steric interaction between the methyl carbon atoms bonded to N(3) (on the ethylenediamine) and the bromine atoms in the equatorial plane are considered. The sum of the Van der Waals radii for a bromine-to-methyl group interaction is 3.95 Å[14], while for this compound the distances are Br(1)—C(9) = 3.56 Å, Br(1)—C(10) = 3.93 Å, Br(2)—C(9) = 4.96 Å, and Br(2)—C(10) = 3.65 Å. This seems to indicate that the steric hindrance of the methyl group interaction, C(9) with Br(1) and C(10) with Br(2) pushes the Br(1) and Br(2) atoms down from the equatorial plane. These atoms are found to be distorted in this direction slightly, but they cannot be pushed down from the plane to a great extent due to the steric repulsion of the N(1) atom. The sum of the Van der Waals radii for bromine and nitrogen atoms is 3.45 Å, while the Br(1)—N(1) distance is 3.43 Å and Br(2)—N(1) distance is 3.51 Å. Thus the steric interaction between the methyl groups and bromine atoms must be relieved by a rotation of the bromine atoms in the equatorial plane. The C(9) group (which has the greatest steric interaction with the bromine atoms) is found in such a position above the Br(1) atom that an angular rotation of the Br(1)

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(11) M. Gerloch, *J. Chem. Soc., A*, *1966*, 1317.
(12) P. L. Orioli, M. Di Vaira, and L. Sacconi, *J. Am. Chem. Soc.*, *88*, 4383 (1966).
(13) M. Di Vaira and P. L. Orioli, *Inorg. Chem.*, 6, 490 (1967).
(14) L. Pauling, *The Nature of the Chemical Bond*, Cornell University Press, Ithaca, New York, N. Y. p. 260.

Table V. Equations of Least Squares planes in direct space and the deviations of the Atoms from these planes

1) $-1.467X+10.911Y-2.496Z = 1.973$
2) $10.383X-1.661Y+0.484Z = 2.437$
3) $10.334X-1.466Y+0.495Z = 2.475$
4) $10.568X-3.269Y+0.881Z = 2.161$

X, Y, Z are fractional coordinates

	(1)	(2)	(3)	(4)
Zn(1)	0.044 Å	–0.026 Å	*	*
Br(1)	*	1.704	1.715 Å	1.725 Å
Br(2)	*	–2.255	–2.235	–2.221
N(1)	–2.133	0.006*	*	0.357
N(2)	*	–0.041	*	*
N(3)	2.197	0.292	0.358	*
C(1)	–3.173	–0.006*	– .036	0.496
C(2)	–4.512	0.000*	– .049	0.703
C(3)	–4.722	0.005*	– .037	0.744
C(4)	–3.638	–0.004*	– .022	0.578
C(5)	–2.342	–0.001*	– .001	0.386
C(6)	–1.122	–0.023	.004	0.187
C(7)	1.282	–0.037	.032	–0.182
C(8)	2.311	–0.501	– .423	–0.803
C(9)	2.566	1.759	1.831	1.410
C(10)	3.106	–0.217	– .143	–0.646

* = atoms which define plane

atom to relieve this strain must result in increasing the Br(1)–Zn–N(2) bond angle (133.9(2)°). Because of the position of C(10) with respect to Br(2), the strain of the C(10)–Br(2) interaction is relieved by decreasing the N(2)–Zn–Br(2) angle (111.82(20)°). The deviation of the Br(1)–Zn–Br(2) moreover, can be explained in view of the fact that the C(9)–Br(1) (distance = 3.56 Å) interaction is greater than the C(10)–Br(2) (distance = 3.65 Å) interaction.

The zinc to bromine distances of 2.396(1) and 2.410(1) Å agree with the values obtained from previous structural determinations (2.39(1), 2.41(1), and 2.38(1) Å for Cs_2ZnBr_4 [15] and 2.38 for $Zn(NH_3)_2Br_2$[16]), however we can offer no explanation for the fact that these bond distances differ by 14 standard deviations. The Zn–N(2) bond distance of 2.087(6) Å is the expected value for normal zinc to nitrogen bonds (cf. bis(1-histidino zinc(II) dihydrate, 2.049(10), 2.041(10) Å[17]), while the zinc to N(1) and N(3) distances (2.245(8) and 2.236(7) Å) are both significantly longer due to the stereochemical rigidity of the ligand (as in three terpyridine copper acetate structures[18]), which does not allow all of the nitrogen atoms to form equivalent bonds with the metal ion.

If mean C–C and C–N bond lengths and all pyridine ring bond angles are calculated for the pyridine ring by taking the weighted average value of 18 structural determinations containing 23 crystallographically independent pyridine rings the mean bond distances are C–N = 1.344, C(1)–C(2) = 1.378, C(2)–C(3) = 1.385 Å. The weighted average bond angles are C–N–C = 119.0, N–C(1)–C(2) = 121.5, C(1)–C(2)–C(3) = 118.9, and C(2)–C(3)–C(4) = 119.0°. Of the six bond lengths and six bond angles of the pyridine ring of this complex, the C(1)–C(2) bond distance differs from the above corresponding value by 2.3σ, with all of the other bond lengths and angles differing by less than 2σ from the corresponding mean value.

The C(6)–N(2) bond length of 1.266(13) Å and the ring-to-alpha-carbon distance of 1.464(12) agree with the corresponding values for many Schiff base complexes (the average values for 13 salicylaldimine residues are C–N = 1.290 Å and ring-carbon-to-alpha-carbon = 1.403 Å[19]). The C–N single bonds, N(3)–C(8) = 1.498(12), N(3)–C(9) = 1.514(11), N(3)–C(10) = 1.480(14), and N(2)–C(7) = 1.484(12) Å, and the single bond C(7)–C(8) = 1.533(14) Å, are equal to values found in ethylenediamine structures (the average values for 19 ethylenediamine structures are C–N = 1.48 and C–C = 1.535 Å[20]).

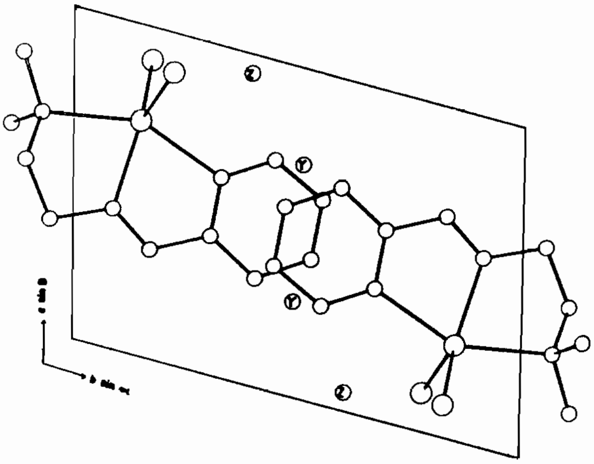

Figure 2. Projection Down (a) Axis.

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(15) B. Morosin and E. C. Lingafelter, *Acta Cryst.*, *12*, 744 (1959).
(16) C. MacGillavry and J. Bijvoet, *Z. Krist.*, *A94*, 249 (1936).
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(18) G. A. Zakrzewski, Ph. D. Dissertation, University of Washington (1969).
(19) R. Braun, Ph. D. dissertation, University of Washington (1966).
(20) J. Weisner, Ph. D. dissertation, University of Washington (1966).

A least-squares plane calculated for the pyridine ring shows the ring to be planar with the greatest deviation from the plane being 0.006 Å and that C(6), N(2), and Zn do not deviate from this plane by more than 0.04 Å (the results of least-squares plane calculations are found in Table V). Similarly, the ring defined by the atoms Zn, N(1), N(2), C(5) and C(6) is completely planar and the two planes are tipped by 1° from each other. A plane was calculated using Zn, N(2), and N(3) as the atoms which define the plane and indicated that C(7) deviates from the plane by –0.18 Å, and C(8) deviates by –0.802 Å, which may be expected since in ethylenediamine structures with metal ions the entire ethylenediamine group and metal ion have never been found to be strictly planar.

The hydrogen atoms were placed in the positions which were found from the difference synthesis and were not refined further. The C–H bond lengths are in the range 0.607 to 1.032 Å.

The packing diagram of the crystal (Figure 2) shows two monomeric units per unit cell with large holes between them, in which the peaks Y and Z and the diffuse electron density were found. We assume that this electron density corresponds to disordered acetone molecules since the distance Y–Z (2.7 Å) and Y–Z′ (at–x, 1–y, –z, 2.8 Å) are only slightly greater than the CH_3–O (2.4 Å) or CH_3–CH_3 (2.7 Å) distances in the acetone molecule. We have, however, made no attempt to investigate this further.

All intermolecular contact distances appear to be normal.

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