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THE CRYSTAL AND MOLECULAR STRUCTURE OF BIS (2, 4-PENTANEDIONATO) BIS (PYRIDINE N-OXIDE) NICKEL(II), $Ni(C_5H_7O_2)_2(C_5H_5NO)_2$

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The Crystal and Molecular structure of Bis(2,4-pentanedionato)bis(pyridine N-oxide)nickel(II), $Ni(C_5H_7O_2)_2(C_5H_5NO)_2$ [1a]

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ABSTRACT

The structure of bis(2,4-pentanedionato)bis(pyridine N-oxide)nickel(II), $Ni(C_5H_7O_2)_2(C_5H_5NO)_2$ has been determined by single crystal X-ray diffraction. The crystals are monoclinic in space group C2/c, with $\underline{a}$ = 14.653 ± 0.005A, $\underline{b}$ = 16.972 ± 0.005A, $\underline{c}$ = 18.344 ± 0.005A, and $\underline{\beta}$ = 100.74 ± 0.05°. For Z = 8 the measured and calculated densities are 1.32 and 1.324 g/cm^3 respectively. Counter data were collected for 2319 independent reflections by the θ-2θ scan technique. The structure was refined, including hydrogens, by least squares methods to a conventional R value of 0.097. Individual molecular units, which involve a <u>cis</u> configuration of pyridine N-oxide and acetylacetonate chelate rings coordinated to the nickel in a nearly regular octahedral disposition, make up the structure. The pyridine N-oxide molecules are coordinated in an angular fashion with an average Ni-O-N angle of 121°.

INTRODUCTION

Heterocyclic amine N-oxides act as oxygen donor ligands in a variety of transition metal coordination compounds.[2] Very recently structural studies have been reported for compounds which involve pyridine N-oxide acting as a bridging ligand between copper atoms,[3-5] however, no other structural work dealing with complexes of this class of ligand appears to have been done. Not long ago Kluiber and Horrocks[6,7] synthesized and studied complexes of the type bis(2,4-pentanedionato)bis(heterocyclic amine N-oxide)metal(II), hereafter referred to as $M(AA)_2(ligand)_2$, were M = Co,Ni. These complexes belong to the class of neutral donor adducts of $M(AA)_2$ of which the dihydrates,[8,9] $M(AA)_2(H_2O)_2$, and dipyridinates,[10] $M(AA)_2(C_5H_5N)_2$, are known and which involve <u>trans</u> octahedral coordination of the metal in the solid state. On the basis of an analysis of the dipolar (pseudocontact) contribution to the isotropic proton magnetic resonance shifts in solution in the complexes $M(AA)_2(L)_2$, M = Co,Ni, L = pyridine N-oxide or γ-picoline N-oxide, Kluiber and Horrocks[6] estimated an average M-O-N angle in the range 115-130° for the coordinated heterocyclic amine N-oxides.[11] These results were based on a <u>trans</u> octahedral model for coordination which was suggested by the known solid state structures[8-10] for the compounds with L = H_2O, C_5H_5N. Clearly the detailed geometry of the coordination of heterocyclic amine N-oxides in general and the stereochemistry of $M(AA)_2(C_5H_5NO)_2$ in particular are of interest. The present article reports the results of the crystal and molecular structure determination of $Ni(AA)_2(C_5H_5NO)_2$. Earlier powder x-ray work[6] showed the analogous cobalt complex to crystallize in two modifications one of which was isomorphous and presumably isostructural with the nickel compound.

EXPERIMENTAL SECTION

Crystals of bis(2,4-pentanedionato)bis(pyridine N-oxide)nickel(II), $Ni(C_5H_7O_2)_2(C_5H_5NO)_2$, were prepared by the method of Kluiber and Horrocks.[6] A crystal of approximate dimensions .16 × .15 × .08 mm was chosen for intensity measurements and was mounted on a quartz fiber with the b axis (unique) of the monoclinic cell parallel to the spindle axis of the instrument. The unit cell dimensions were determined at room temperature on a General Electric XRD-5 unit equipped with a manual goniostat, scintillation counter, and pulse height discriminator using unfiltered molybdenum radiation (λ = 0.70926 for $K\alpha_1$). They are a = 14.653 ± 0.005A, b = 16.972 ± 0.005A, c = 18.344 ± 0.005A and β = 100.74 ± 0.05 . Systematic absences for reflections $hk\ell$, h+k = odd and $h0\ell$, ℓ = odd, observed on Weissenberg film layers: $h0\ell$, $h1\ell$, $h2\ell$, and $h3\ell$, suggested space groups Cc or C2/c. The density measured by flotation in a carbontetrachloride-methylcyclohexane mixture was 1.32 ± 0.01 g/cm^3 which compares favorably with the calculated density of 1.324 for Z = 8. With eight molecules per unit cell and the appearance of 2x, 2y, 2z peaks for nickel in the Patterson function, the centric space group C2/c(C_{2h}^6, No 15) was chosen and this choice was confirmed by the subsequent refinement of the structure. All atoms occupy general positions and no molecular symmetry conditions are imposed by crystallographic symmetry.

Although the structure was actually solved using data obtained by 10 sec peak counts on the manual goniostat and employing zirconium filtered molybdenum radiation and a 4° take-off angle, intensity data for the final refinement reported here were recorded on an automated GE XRD-5 diffractometer. Nickel filtered (at the receiving slit) copper radiation (λ = 1.54051 for $K\alpha_1$) with a 20 MA source current, a 2° take-off

angle, and a θ-2θ scan technique were employed. Scans commenced at 2θ values 0.7° below the calculated $K\alpha_1$ position, proceeded through the $K\alpha_1$-$K\alpha_2$ separations, and on to 0.7° beyond the $K\alpha_2$ peak position at a rate of 1° per min. A 10 sec background count was taken 0.4° from each end of the peak scan. The background correction for each reflection was obtained from the average of the two background counts pro-rated to the length (sec) of the peak scan. In order to assess the importance of counter saturation, the reflections with $2\theta \leq 50°$ were remeasured with a source current of 6MA. Only the most intense reflection was appreciably affected by errors from this cause. The 6MA data were averaged in with the 20MA data using a scale factor obtained from a comparison of 40 representative reflections of intermediate intensity obtained at both amperages. Of the 2319 non equivalent reflections measured, 2113 were observed to be non-zero. The corrected intensities, I, were assigned standard deviations according to the formula:

$$\sigma(I) = [TC + 0.25(t_c/t_b)^2(B_1+B_2) + (0.05I)^2]^{1/2} ,$$

where TC is the total integrated peak count obtained in a scan time t_c, B_1 and B_2 are the two background counts each obtained in time, t_b, and $I = TC-0.5(t_c/t_b)(B_1+B_2)$. Six standard reflections were recorded every hundred measurements. The constancy of these standard reflections indicated little or no deterioration of the crystal through the course of the data collection. The linear absorption coefficient of the crystal is $\mu = 15.1\ cm^{-1}$. No noticable absorption affects appeared for 0k0 reflections as a function of ϕ and no absorption corrections were applied to the data.

SOLUTION AND REFINEMENT OF THE STRUCTURE

A Patterson[12] synthesis located the nickel and several of the adjacent oxygens. A least squares refinement and subsequent Fourier synthesis[12] disclosed the remaining atoms. Least squares refinement proceeded with all twenty-nine atoms and only the nickel atom treated anisotropically to a conventional R value[13] of 0.117. At this point a difference synthesis disclosed all but one of the twenty four hydrogens. When the hydrogens were included and refined, R dropped to a final value of 0.097 for all reflections. Atomic scattering factors and dispersion corrections were taken from the International Tables.[14] The isotropic thermal parameters have the form $\exp(-B \sin^2\theta/\lambda^2)$ while the anisotropic temperature factor was

$$\exp[-0.25(B_{11}b_1^2\underline{h}^2 + B_{22}b_2^2\underline{k}^2 + B_{33}b_3^2\underline{\ell}^2 + 2B_{12}b_1b_2\underline{hk} + 2B_{13}b_1b_3\underline{h\ell} + B_{23}b_2b_3\underline{k\ell})] ,$$

where b_i is the $\underline{i}$th reciprocal axis. The values of the hydrogen coordinates and their temperature factors obtained from the final refinement are as follows: Hydrogen, x, y, z (temp. factor); R1H1A, 0.272, -0.183, 0.104(12.6); R1H1B, 0.348, -0.143, 0.099(-1.1); R1H1C, 0.278, -0.117, 0.141(1.1); R1H3, 0.179, -0.177, -0.013(2.9); R1H5A, 0.038, -0.170, -0.114(5.4); R1H5B, 0.058, -0.132, -0.176(1.2); R1H5C, 0.112, -0.187, -0.164(4.5); R2H1A, 0.424, 0.047, -0.189(-1.5); R2H1B, 0.485, 0.114, -0.136(1.8); R2H1C, 0.435, 0.148, -0.197(5.0); R2H3, 0.307, 0.191, -0.193(4.8); R2H5A, 0.065, 0.246, -0.196(6.0); R2H5B, 0.167, 0.250, -0.232(10.8); R2H5C, 0.112, 0.218, -0.227(-1.2); P1H1, 0.043, -0.030, 0.069(-1.5); P1H2, 0.048, -0.079, 0.168(-0.7); P1H3, 0.157, -0.022, 0.263(5.9); P1H4, 0.205, 0.082, 0.278(2.6); P1H5, 0.200, 0.115, 0.127(0.9); P2H1, 0.363, 0.271, -0.001(1.1); P2H2, 0.509, 0.274, 0.008(5.0); P2H3, 0.586, 0.183, 0.076(1.0); P2H4, 0.542, 0.106, 0.081(1.7); P2H5, 0.418, 0.074, 0.065(10.5).

The hydrogen labeling should be obvious from Fig. 1, however, not much significance should be attached to the numerical values of these parameters. In some instances considerable displacement of the hydrogen from the position expected on the basis of the heavy atom structure was noted. Since the hydrogen positions in the present structure are of no particular chemical interest no further consideration will be given to them here.

Table I gives the final observed and calculated structure factors. On the final full matrix least squares cycle the largest variation of a heavy atom positional parameter was 0.0006 while the largest temperature factor shift was 0.1, in all cases the shifts were smaller than the estimated standard deviations. The final heavy atom parameters are given in Table II.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The crystal is composed of discrete molecules, $Ni(AA)_2(C_5H_5NO)_2$, in which the six oxygens are coordinated to the nickel in a very nearly regular octahedral array. The bond distances and angles internal to these molecules are indicated in Table III. In Fig. 1 the overall molecular geometry is illustrated along with the atom labeling and average values of chemically equivalent bond distances are given. A pair of stereoscopic representations is provided in Fig. 2 to permit the reader to appreciate the details of the geometry. The closest Ni-Ni approach is 6.882 A which occurs within the unit cell for molecules related by x, y, z and 1/2-x, 1/2-y, -z. This juxtaposition is achieved by efficient molecular packing and no specific intermolecular interactions are indicated.

The two pyridine N-oxide molecules occupy positions <u>cis</u> to one another in the coordination sphere of the nickel. This contrasts with the solid state

structures of $M(AA)_2(H_2O)_2$ [8,9] and $M(AA)_2(C_5H_5N)_2$,[10] M = Co,Ni, in which the neutral monodentate ligands occupy trans positions. However precedents for a cis coordination geometry in divalent metal acetylacetonate compounds are provided by the crystal structures of $[Ni(AA)_2]_3$,[15] $[Co(AA)_2]_4$,[16] and $[Co(AA)_2H_2O]_2$.[17] These polymeric complexes involve a cis octahedral arrangement of the terminal chelate rings. Also, complex anions of the type $[M(AA)_3^-]$[18-22] necessarily involve coordination of this sort. These findings, taken together, suggest that there is very little energy difference between cis and trans structures of this type. Crystal packing forces may very well determine the solid state conformation in any particular example. The problem of the structures of $M(AA)_2L_2$ complexes in solution is of course not solved, but the present results suggest that the possibility of a cis structure in solution should not be ignored. For $Ni(AA)_2(C_5H_5N)_2$ in solution Hashagen and Fackler[10] averred that their electronic spectral data were consistent with a trans structure, but their data do not rule out a cis configuration, or what is even more likely, an equilibrium mixture of the two forms. Complexes of this type are quite labile and exchange their monodentate ligands rapidly with excess ligand molecules present in solution.[6,7] Thus a facile mechanism for converting between cis and trans forms is readily available through ligand exchange, although an isomerization mechanism without bond rupture is also quite possible. Complexes of the type $Ti(AA)_2X_2$, X = halogen, have been shown to exhibit a cis octahedral structure in solution,[23,24] however the higher oxidation state and negatively charged monodentate ligands make the analogy with the present system inexact.

Kluiber and Horrocks,[6] in their analysis of isotropic dipolar pmr shifts in solutions of paramagnetic complexes of the type $M(AA)_2(C_5H_5NO)_2$, M = Co,Ni, assumed a trans structure in solution and, on the basis of this determined that pyridine N-oxide and certain of its derivatives coordinate in an angular fashion with a M-O-N angle in the range 115-130°. While this angular mode of coordination is substantiated for the solid state by the present results (vide infra), the use of a trans model is called to question. The answer to the problem of which form is present or predominates (if both forms occur as seems likely) in solution must await further studies.

The nickel to ligand atom distances appear normal. The average Ni-acetylacetonate oxygen distance found here (2.02A) is in excellent agreement with those found for trans $Ni(AA)_2(H_2O)_2$(2.02A)[9] and for the terminal chelate oxygens of $[Ni(AA)_2]_3$(2.01A).[15] The average distance from the nickel to the pyridine N-oxide oxygen found here is 2.10A. This is slightly, but perhaps significantly, shorter than the nickel to water oxygen distance of 2.14A in $Ni(AA)_2H_2O)_2$.[9] This indicates that of the two neutral oxygen donor ligands, pyridine N-oxide is the more strongly coordinating.

In the present structure the two independent pyridine N-oxide molecules, P1 and P2, coordinate with Ni-O-N angles of 119.2° and 122.4° respectively. This angular coordination is to be expected from a consideration of the directional properties of the lone pair electrons on the oxygen which form the coordinate bond to the nickel. The angle of approximately 120° suggests that a reasonable description of the bonding in pyridine N-oxide involves sp^2 hybridization on the oxygen (two lone pairs and the N-O bond pair) with the third lone in a pure p orbital and available for $p\pi$-$p\pi$ interaction with the π-system of the pyridine ring. If this π-interaction were very important one would expect

the Ni-O-N plane and the plane of the pyridine ring to be coincident. The angles between the Ni-O-N planes and the least squares planes of the pyridine rings for ligands P1 and P2 are 67.5° and 48.4° respectively (The stereoscopic view provided by Fig. 2 illustrates this twist well). This suggests that π-interaction of this sort is not of paramount importance in determining the configuration of the coordination. A description of the bonding in terms of a distortion from sp^3 hybridization on the oxygen is of course equally valid. The angular coordination is consistent with the apparent angular hydrogen bond found for the hydrochloride of the ligand.[25] Angular coordination has also been observed in phosphine oxide coordination compounds.[26,27]

The internal distances and angles of the pyridine N-oxide ligand, in particular the average N-O bond distance of 1.33A, agree well with those recently reported[4] for the bridging ligand in $[CuCl_2(C_5H_5NO)]_2$. The present N-O bond distance is 0.05A shorter than that found in the hydrochloride,[25] but considering the probable uncertainty of that determination no conclusions can be drawn from this difference. Tsoucaris[25] estimated that the N-O linkage in $C_5H_5NO \cdot HCl$ had ~20% π-character. While the literature data[28,29] available on N-O bond lengths do not permit as smooth a plot of bond lengths vs bond order to be drawn as was obtained by Cotton and Wing[30] for the C-O bond, a reasonable curve of similar character can be constructed. The N-O bond length for coordinated pyridine N-oxide (1.33A) falls in the steep portion of the curve where bond order is relatively insensitive to bond length, but suggests that the π-bond character is small, on the order of 10-20%. This conclusion is consistent with the observed sizeable twist of the pyridine rings out of the Ni-O-N planes. A further useful comparison is with the N-O bond length of 1.39A[29] in the aliphatic amine N-oxide, $(CH_3)_3NO$; where π-bonding is impossible and the effect of charge separation[29] should roughly correspond to the present case. The pyridine N-oxide oxygens P10 and P20 are respectively 0.06 and 0.07A out of the

least squares planes through the pyridine rings. Similar deviations from planarity have been found for the N-oxide moiety in $C_5H_5NO \cdot HC\ell$[25] and $[CuC\ell_2(C_5H_5NO)]_2$.[4]

The bond lengths and angles of the acetylacetonate chelate rings appear normal and compare well with those in the literature. The methyl carbons fall within 0.15A of the least squares planes defined by the oxygens and carbons 2, 3, and 4 of the chelate rings. As has been noted in other acetylacetonate complexes,[9] the central metal does not lie exactly in the plane of the chelate ring. In the present structure the nickel atom falls 0.17 and 0.46A from the least squares planes of rings R1 and R2 respectively.

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(13) $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.

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Table I

Observed and Calculated Structure Factors (×3) for $Ni(AA)_2(C_5H_5NO)_2$

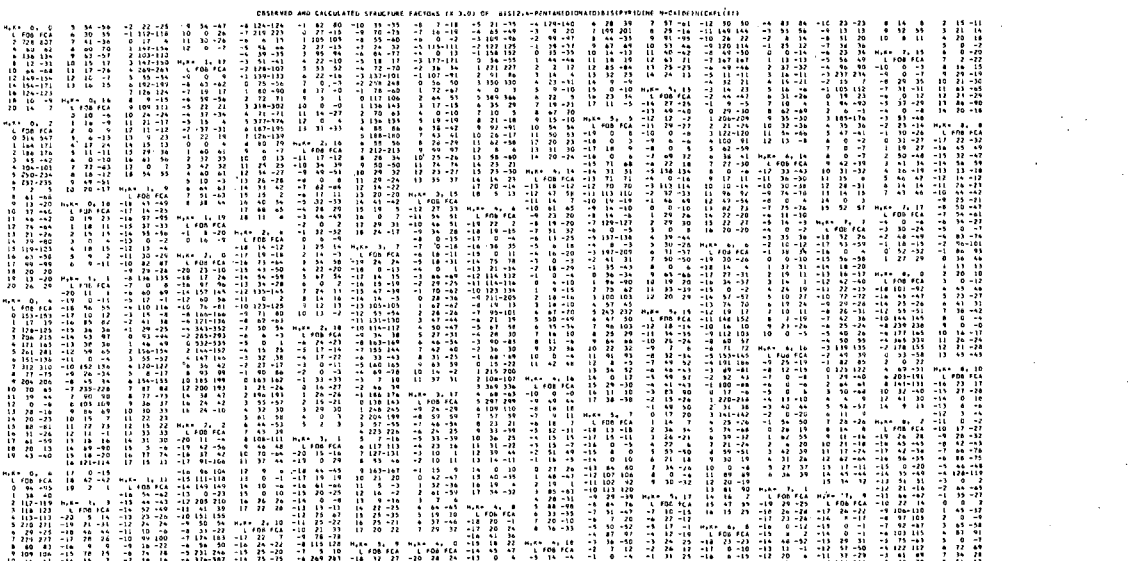

Table II
Final Positional and Thermal Parameters for $Ni(AA)_2(C_5H_5NO)_2$ [a,b]

	x/a	y/b	z/c	B
NI	.2180(1)	.0537(1)	-.0443(1)	c
R1O1	.2769(3)	-.0262(2)	.0311(2)	3.3(1)
R1O2	.1454(3)	-.0321(2)	-.1040(2)	3.4(1)
R1C1	.2933(11)	-.1409(6)	.1043(6)	5.0(2)
R1C2	.2517(5)	-.0987(4)	.0340(4)	3.3(1)
R1C3	.1900(6)	-.1354(4)	-.0208(4)	3.4(2)
R1C4	.1417(5)	-.1037(4)	-.0856(4)	3.7(1)
R1C5	.0766(9)	-.1547(6)	-.1392(7)	5.2(2)
R2O1	.3239(4)	.0460(2)	-.1017(2)	4.1(1)
R2O2	.1535(3)	-.1340(2)	-.1184(2)	3.3(1)
R2C1	.4329(11)	.0913(9)	-.1724(8)	9.1(3)
R2C2	.3399(7)	.0997(5)	-.1457(4)	5.2(2)
R2C3	.2837(8)	.1616(5)	-.1725(5)	4.6(2)
R2C4	.1946(6)	.1740(4)	-.1602(4)	3.7(1)
R2C5	.1391(10)	.2433(6)	-.1991(5)	5.3(2)
P1O	.1104(3)	.0723(2)	.0155(2)	3.2(1)
P1N	.1198(4)	.0447(3)	.0848(3)	2.9(1)
P1C1	.0668(6)	-.0142(4)	.0997(4)	3.4(2)
P1C2	.0730(7)	-.0408(4)	.1712(4)	4.0(2)
P1C3	.1344(7)	-.0098(5)	.2262(5)	4.8(2)
P1C4	.1918(7)	.0476(5)	.2111(5)	5.2(2)
P1C5	.1851(7)	.0754(5)	.1387(5)	4.5(2)

Table II (continued)

	x/a	y/b	z/c	B
P2O	.2851(4)	.1457(2)	.0199(2)	3.7(1)
P2N	.3754(5)	.1582(3)	.0272(3)	3.1(1)
P2C1	.4022(7)	.2318(4)	.0176(4)	3.7(2)
P2C2	.4955(9)	.2487(6)	.0314(5)	5.2(2)
P2C3	.5628(9)	.1919(6)	.0480(6)	5.6(3)
P2C4	.5305(12)	.1144(7)	.0570(7)	5.5(3)
P2C5	.4379(9)	.0996(5)	.0466(5)	4.4(2)

[a]Standard deviations indicated in parentheses refer to the least significant digit(s). The atom labeling conforms to Fig. 1. The carbon (C), nitrogen (N), and oxygen (O) atoms are numbered serially within their respective organic moieties. R1 and R2 designate chelate rings 1 and 2, while P1 and P2 refer to pyridine N-oxide ligands 1 and 2. These group designations precede the individual atom element symbols and numbers.

[b]Orthogonal coordinates, X, Y, Z (with the X and Y axes respectively parallel to $\underline{a}$ and $\underline{b}$ and the Z axis perpendicular to both), may be obtained from the fractional coordinates x, y, z, by the transformation $[\underline{X}] = [\underline{x}][\underline{\beta}]$; for the present case the non-zero components of the $[\beta]$ tensor are $\beta_{11} = 14.6530$, $\beta_{22} = 16.9720$, $\beta_{31} = -3.4185$, and $\beta_{33} = 18.0227$. See Ref. 14, Vol. II, p. 66 ff.

[c]Components of the anisotropic thermal tensor for Ni defined as in the text are: $B_{11} = 5.30(10)$, $B_{22} = 4.30(5)$, $B_{33} = 4.62(5)$, $B_{12} = -0.17(5)$, $B_{13} = 1.13(5)$, $B_{23} = 0.24(4)$.

Table III
Bond Distances and Angles of $Ni(AA)_2(C_5H_5NO)_2$ [a]

Distances, Angstroms

NI-R101	2.013(4)	R2C3-R2C4	1.382(4)
NI-R102	2.004(4)	R2C4-R2C5	1.527(10)
NI-R201	2.035(5)	P1O-P1N	1.337(6)
NI-R202	2.029(4)	P1N-P1C1	1.326(7)
NI-P1O	2.105(3)	P1C1-P1C2	1.373(11)
NI-P2O	2.088(4)	P1C2-P1C3	1.328(9)
R101-R1C2	1.289(7)	P1C3-P1C4	1.349(10)
R102-R1C4	1.265(8)	P1C4-P1C5	1.396(12)
R1C1-R1C2	1.502(11)	P1C5-P1N	1.346(7)
R1C2-R1C3	1.370(9)	P2O-P2N	1.321(1)
R1C3-R1C4	1.375(9)	P2N-P2C1	1.331(8)
R1C4-R1C5	1.510(10)	P2C1-P2C2	1.375(3)
R201-R2C2	1.269(9)	P2C2-P2C3	1.373(10)
R202-R2C4	1.258(7)	P2C3-P2C4	1.418(16)
R2C1-R2C2	1.537(8)	P2C4-P2C5	1.359(3)
R2C2-R2C3	1.368(9)	P2C5-P2N	1.354(8)

Table III (continued)

Angles, Degrees

R2C1-R2C2-R2C3	117.9(8)	R102-NI-R202	89.4(2)
R2C2-R2C3-R2C4	125.6(7)	P10-NI-P20	85.0(1)
R202-R2C4-R2C3	126.2(6)	R101-NI-R201	92.4(2)
R202-R2C4-R2C5	115.2(3)	R102-NI-R202	89.4(2)
R2C3-R2C4-R2C5	118.6(6)	R101-NI-P10	90.5(1)
NI-P10-P1N	119.2(2)	R101-NI-P20	91.0(2)
P10-P1N-P1C1	120.0(4)	R102-NI-R201	92.8(2)
P10-P1N-P1C5	119.8(5)	R102-NI-P10	91.2(1)
P1C1-P1N-P1C5	120.2(6)	R202-NI-P10	87.0(1)
P1N-P1C1-P1C2	120.5(5)	R202-NI-P20	89.3(2)
P1C1-P1C2-P1C3	120.7(6)	R201-NI-P20	90.8(2)
P1C2-P1C3-P1C4	119.3(8)	NI-R101-R1C2	125.5(3)
P1C3-P1C4-P1C5	120.3(6)	NI-R102-R1C4	126.6(3)
P1N-P1C5-P1C4	118.8(6)	R101-R1C2-R1C1	114.6(5)
NI-P20-P2N	122.4(3)	R101-R1C2-R1C3	124.1(7)
P20-P2N-P2C1	116.9(3)	R1C1-R1C2-R1C3	121.3(7)
P20-P2N-P2C5	121.6(5)	R1C2-R1C3-R1C4	128.2(7)
P2C1-P2N-P2C5	121.5(3)	R102-R1C4-R1C3	124.6(5)
P2N-P2C1-P2C2	118.7(6)	R102-R1C4-R1C5	115.4(6)
P2C1-P2C2-P2C3	122.9(8)	R1C3-R1C4-R1C5	120.0(7)
P2C2-P2C3-P2C4	115.9(4)	NI-R201-R2C2	122.2(3)
P2C3-P2C4-P2C5	120.1(8)	NI-R202-R2C4	123.7(2)
P2N-P2C5-P2C4	120.7(8)	R201-R2C2-R2C1	114.5(7)
R101-NI-R102	90.2(2)	R201-R2C2-R2C3	127.6(4)

[a]Standard deviations indicated in parentheses refer to the least significant digit(s).

Figure Captions

Fig. 1. Geometry of $Ni(AA)_2(C_5H_5NO)_2$ with the average values of chemically equivalent bond lengths indicated.

Fig. 2. Stereoscopic pair of $Ni(AA)_2(C_5H_5NO)_2$ molecules. The labeling of the atoms may be determined by a comparison with Fig. 1.

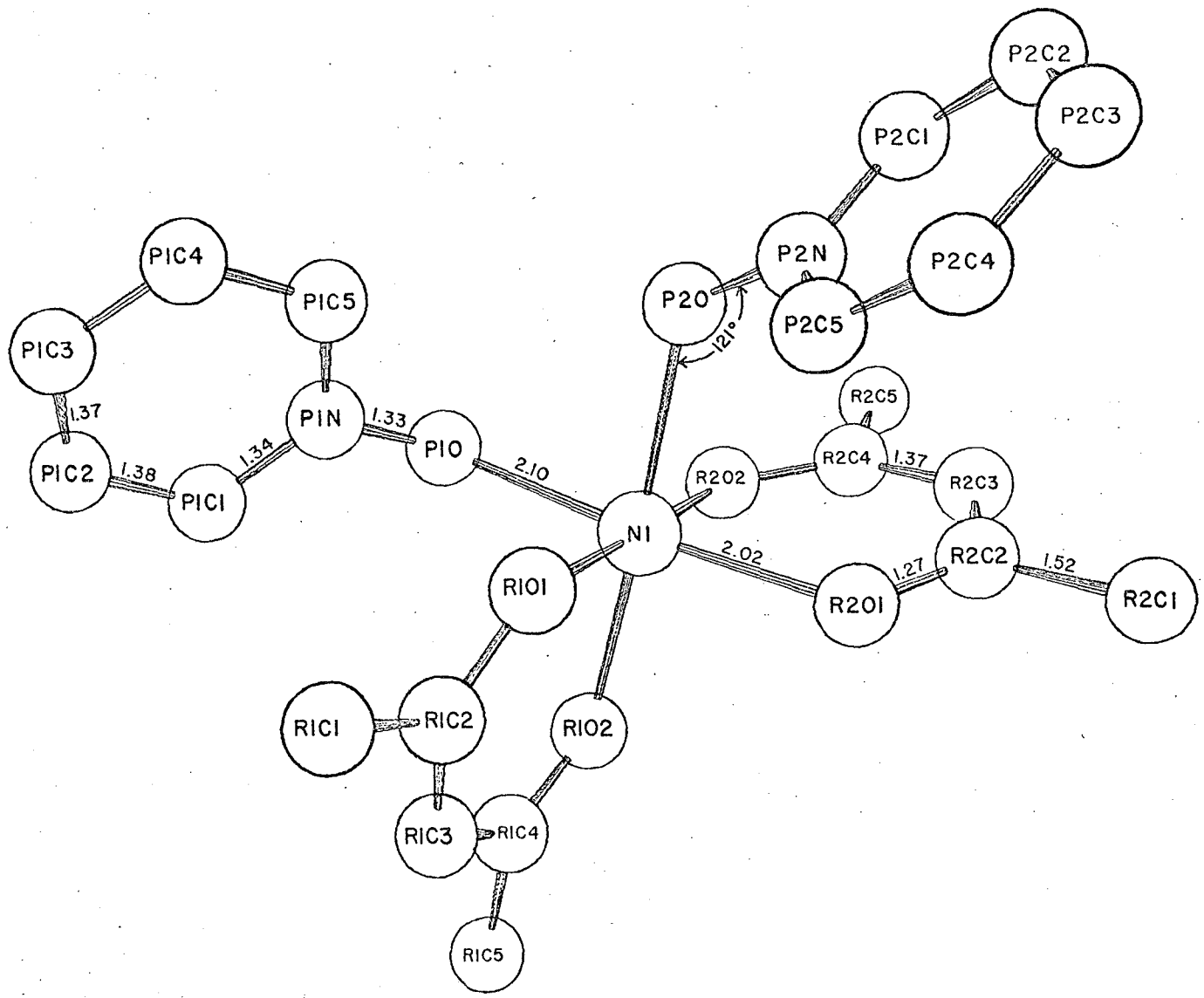

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Fig. 1

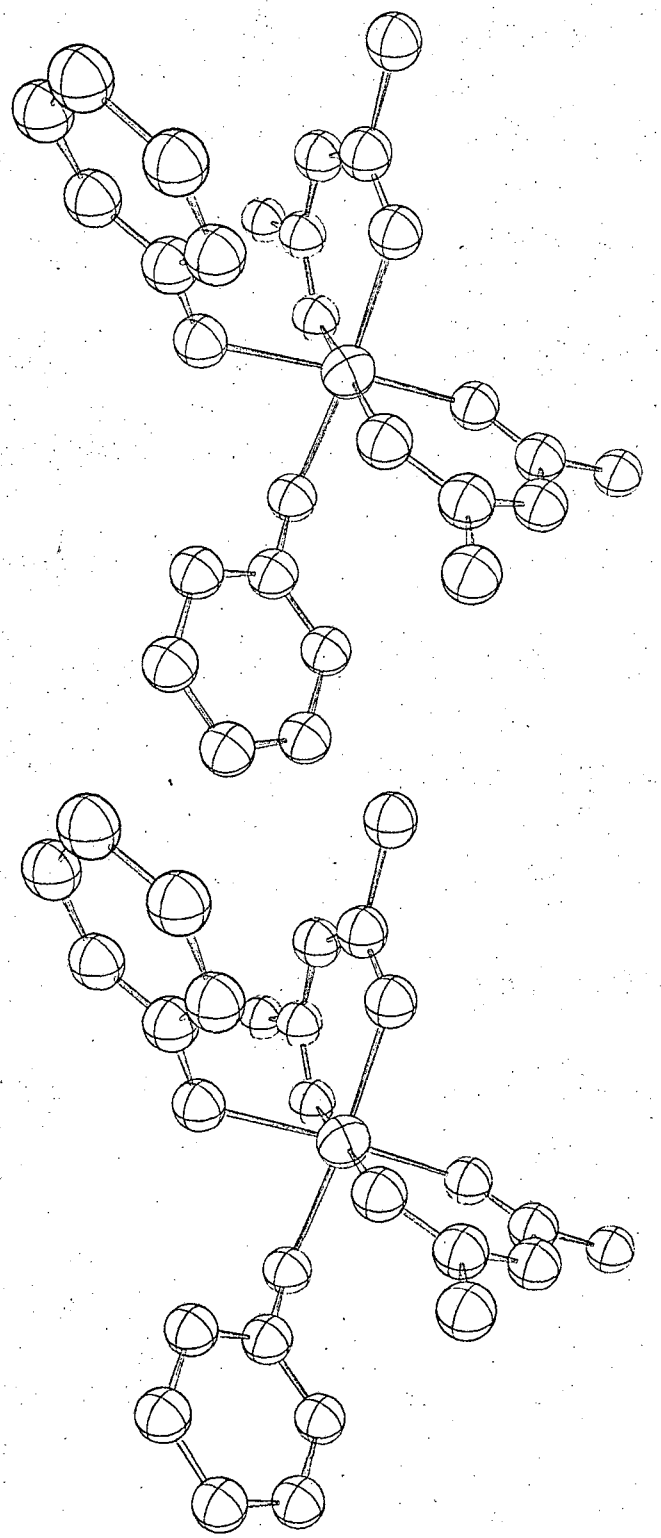

Fig. 2

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