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Five-Coordinate Nickel(III). The Crystal and Molecular Structure of $NiBr_3(P(C_6H_5)(CH_3)_2)_2 \cdot 0.5NiBr_2(P(C_6H_5)(CH_3)_2)_2 \cdot C_6H_6$

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The crystal and molecular structure of the 1:0.5:1 adduct of tribromobis(phenyldimethylphosphine)nickel(III), dibromobis(phenyldimethylphosphine)nickel(II), and benzene has been determined from three-dimensional X-ray data collected by counter methods. The structure has been refined by least-squares techniques to a final R factor on F of 0.054. The material crystallizes in space group C_i^1-$P\bar{1}$ of the triclinic system, with two molecules of $NiBr_3(P(C_6H_5)(CH_3)_2)_2$, one molecule of $NiBr_2(P(C_6H_5)(CH_3)_2)_2$, and two molecules of benzene in a cell of dimensions $a = 9.021$ (5), $b = 17.951$ (10), $c = 11.181$ (6) Å; $\alpha = 98° 52$ (1)$'$, $\beta = 94° 29$ (1)$'$, $\gamma = 90° 44$ (1)$'$. The observed and calculated densities are 1.67 ± 0.02 and 1.68 g/cm^3, respectively. The four- and five-coordinate molecules are well separated. The *trans*-planar complex $NiBr_2(P(C_6H_5)(CH_3)_2)_2$ is crystallographically required to possess a center of inversion; the Ni–P and Ni–Br bond lengths are 2.251 (3) and 2.297 (2) Å, respectively. The five-coordinate Ni(III) complex $NiBr_3(P(C_6H_5)(CH_3)_2)_2$ possesses a trigonal-bipyramidal geometry with axial phosphine groups. There is a slight distortion of the molecule in the plane of the Ni and three Br atoms, which could arise from Jahn–Teller effects. The Ni–P bond distances are 2.263 (3) and 2.273 (3) Å, and the Ni–Br bond distances are 2.349 (2), 2.375 (2), and 2.339 (2) Å.

Introduction

The preparation of a nickel(III) complex, $NiBr_3(P(C_2H_5)_3)_2$, was first reported by Jensen[1] in 1936. From dipole moment data, Jensen and coworkers[2] inferred that complexes of this type possess a trigonal-bipyramidal rather than a square-pyramidal geometry, as they had earlier suggested.[3] Several other complexes containing trivalent nickel with a variety of donor atoms have been suggested,[4-6] largely on the basis of observed magnetic moments consistent with low-spin Ni(III). There has been much discussion as to whether the complexes $Ni(mnt)_2^-$ and $Ni(diars)_2Cl_2^+$ (mnt^{2-} and diars are $(CN)_2C_2S_2^{2-}$ and o-$C_6H_4(As(CH_3)_2)_2$, respectively) can properly be considered as complexes of trivalent nickel.[5,7-10] The recent X-ray structure determination[11] of $Ni(diars)_2Cl_2^+$ showed that this cation possesses a nearly octahedral geometry; electron spin resonance studies indicate[11] that the complex could be more correctly considered as a Ni(II) complex, with the unpaired electron spending a significant amount of time on the As atoms.

Tribromobis(phenyldimethylphosphine)nickel(III), $NiBr_3(P(C_6H_5)(CH_3)_2)_2$, has been prepared by Alyea and Meek.[12] The determination of the structure of $NiBr_3(P(C_6H_5)(CH_3)_2)_2$ was undertaken to substantiate its formulation as a monomeric complex of trivalent nickel. A preliminary account of this work has appeared.[13] Furthermore, structures of five-coordinate transition metal complexes are being extensively investigated in this laboratory; we have found that complexes of the type MX_3Y_2 frequently exhibit distortions from an idealized geometry. Two Ni(II) complexes, $Ni(CN)_2(P(C_6H_5)(OC_2H_5)_2)_3$ and $Ni(CN)_2(P(C_6H_5)(CH_3)_2)_3$, have been shown to be distorted from a trigonal-bipyramidal toward a tetragonal-pyramidal geometry.[14,15] The determination of the structure of a five-coordinate Ni(III) complex should provide a useful comparison with the Ni(II) structures.

Collection and Reduction of the Intensity Data

Crystals of what proved to be $NiBr_3(P(C_6H_5)(CH_3)_2)_2 \cdot 0.5NiBr_2(P(C_6H_5)(CH_3)_2)_2 \cdot C_6H_6$ were kindly supplied by Professor D. W. Meek and Dr. E. C. Alyea. The crystals were obtained by recrystallization of pure $NiBr_3(P(C_6H_5)(CH_3)_2)_2$ from a benzene–hexane solution. However, unit cell and density determinations followed by magnetic and spectral evidence[13] on the recrystallized sample led us to believe that the unit cell contained one diamagnetic molecule of $NiBr_2(P(C_6H_5)(CH_3)_2)_2$ to every two paramagnetic molecules of $NiBr_3(P(C_6H_5)(CH_3)_2)_2$; this formulation was confirmed by the X-ray structural determination, which also indicated the presence of two molecules of benzene in the unit cell. An extremely dark violet, diamond-shaped crystal of approximate dimensions 0.1 × 0.4 × 0.4 mm in the [010], [001], and [101] directions was sealed in a 0.5-mm

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(1) K. A. Jensen, *Z. Anorg. Allgem. Chem.*, **229**, 275 (1936).

(2) K. A. Jensen, B. Nygaard, and C. T. Pederson, *Acta Chem. Scand.*, **17**, 1126 (1963).

(3) K. A. Jensen and B. Nygaard, *ibid.*, **3**, 474 (1949).

(4) N. F. Curtis and D. F. Cook, *Chem. Commun.*, 962 (1967), and references therein.

(5) A. H. Maki, N. Edelstein, A. Davison, and R. H. Holm, *J. Am. Chem. Soc.*, **86**, 4580 (1964).

(6) G. R. Van Hecke and W. D. Horrocks, Jr., *Inorg. Chem.*, **5**, 1968 (1966).

(7) H. B. Gray and E. Billig, *J. Am. Chem. Soc.*, **85**, 2019 (1963).

(8) S. I. Shupack, E. Billig, R. J. H. Clark, R. Williams, and H. B. Gray, *ibid.*, **86**, 4594 (1964).

(9) E. I. Stiefel, J. H. Waters, E. Billig, and H. B. Gray, *ibid.*, **87**, 3016 (1965).

(10) A. H. Maki, T. E. Berry, A. Davison, R. H. Holm, and A. L. Balch, *ibid.*, **88**, 1080 (1966).

(11) P. Kreisman, R. Marsh, J. R. Preer, and H. B. Gray, *ibid.*, **90**, 1067 (1968).

(12) E. C. Alyea and D. W. Meek, *ibid.*, in press.

(13) D. W. Meek, E. C. Alyea, J. K. Stalick, and J. A. Ibers, *ibid.*, **91**, 4920 (1969).

(14) J. K. Stalick and J. A. Ibers, *Inorg. Chem.*, **8**, 1084 (1969).

(15) J. K. Stalick and J. A. Ibers, *ibid.*, **8**, 1090 (1969).

quartz capillary and mounted on a eucentric goniometer head with [101] nearly along the ϕ axis. Weissenberg and precession photographs did not show any special symmetry or systematic absences, suggesting space groups C_1^1-P1 or C_i^1-P$\bar{1}$. A triclinic unit cell was assigned, and a Delaunay reduction of the cell parameters as determined from the films failed to indicate any hidden symmetry. The cell parameters, at 22° as determined from diffractometer measurements (*vide infra*) using Cu Kα radiation (λ 1.54056 Å), are a = 9.021 (5), b = 17.951 (10), c = 11.181 (6) Å; α = 98° 52 (1)′, β = 94° 29 (1)′, γ = 90° 44 (1)′. The observed density of 1.67 ± 0.02 g/cm^3, obtained by flotation in aqueous $ZnCl_2$ solutions, agrees well with the calculated value of 1.68 g/cm^3 for two molecules of $NiBr_3(P(C_6H_5)(CH_3)_2)_2$, one molecule of $NiBr_2(P(C_6H_5)(CH_3)_2)_2$, and two molecules of benzene in the unit cell.

Sixteen reflections were carefully centered using a Picker four-circle automatic diffractometer, and the cell parameters and orientation angles were determined from a least-squares refinement of the setting angles of these reflections using procedures previously described.[16] Cu Kα radiation was used for the data collection, and the diffracted beams were filtered through a 1.0-mil Ni foil. The intensities were collected by the θ–2θ scan technique at a takeoff angle of 1.8°. The peaks were scanned from 0.5° on the low-angle side of the Kα_1 peak to 0.7° on the high-angle side at a scan rate of 1.0°/min. Stationary-crystal, stationary-counter background counts of 10 sec were taken at each end of the scan. The scintillation counter was placed 29 cm from the crystal and had an aperture of 4.0 × 4.0 mm.

A unique data set was initially collected to $2\theta = 70°$, and a second shell to $2\theta = 88°$ was subsequently collected. Four reflections were monitored as standards after every 250 reflections were processed, and each of these remained constant within counting statistics throughout the data collection process. The data were corrected for background and standard deviations were assigned to the intensities as previously described,[16] using a value of 0.04 for p. A later statistical analysis (*vide infra*) of the weighting scheme as a function of $|F_o|$ indicated that this value was too large; the strong reflections had been underweighted. The data were also corrected for Lorentz and polarization effects.

In all, 2735 reflections were observed; only 97 of these were less than their standard deviations. The 2514 reflections for which $F_o^2 \geq 3\sigma(F_o^2)$ were used in the solution and refinement of the structure. The crystal was measured by means of a micrometer eyepiece for application of a numerical absorption correction, and the six faces of the forms {010}, {001}, and {101} were identified by optical and X-ray means.

Solution and Refinement of the Structure

The positions of the two Ni, four Br, and three P atoms were determined by direct methods using Sayre's equation[17] in the form of a modified version of Long's computer program,[18] assuming the centric space group P$\bar{1}$. One cycle of least-squares refinement,[19] assigning isotropic temperature factors to all 9 atoms, resulted in discrepancy factors $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $R_2 = (\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2)^{1/2}$ of 0.346 and 0.448, respectively, where the weights w were taken as $4F_o^2/\sigma^2(F_o^2)$. In this and succeeding refinements the function minimized was $\Sigma w(|F_o| - |F_c|)^2$. The atomic scattering factors for Ni, Br, P, and C were from the usual tabulation[20] and those of Stewart, *et al.*,[21] were used for H. The anomalous scattering factors of Cromer[22] for Ni, Br, and P were used for the real and imaginary scattering contributions to F_c.[23] A difference Fourier map gave the positions of the methyl and phenyl group carbon atoms. These were included in two cycles of least-squares refinement in which the phenyl rings were treated as rigid groups[24] of known geometry and dimension (C–C = 1.392 Å) with a single group temperature factor. The resultant discrepancy factors were $R_1 = 0.210$ and $R_2 = 0.304$. A difference Fourier map at this point indicated the presence of a molecule of solvent benzene in the asymmetric unit; when this was included in a cycle of least-squares refinement, the discrepancy factors were lowered to $R_1 = 0.175$ and $R_2 = 0.261$.

The observed intensities were next corrected for the effects of absorption, using a calculated absorption coefficient of 82.75 cm^{-1}; transmission coefficients ranged from 0.40 to 0.09. One cycle of least-squares refinement led to a significant improvement in the overall agreement, with $R_1 = 0.138$ and $R_2 = 0.240$. This calculation was followed by two cycles of refinement in which anisotropic thermal parameters were assigned to all nongroup atoms and individual isotropic thermal parameters were assigned to group carbon atoms (except for the solvent benzene molecule); the resultant discrepancy factors were 0.063 and 0.116. A difference Fourier map was computed using only those reflections for which $\lambda^{-1} \sin\theta < 0.3$ Å^{-1}, and all phenyl and methyl group hydrogen atoms were located. The methyl hydrogen atom positions were idealized to conform to the known geometry (C–H = 1.09 Å, $\angle$H–C–H = 109° 28′) in best agreement with the observed positions and were added as fixed contributions to the calculated structure factors, assuming B = 5.0 Å^2. The idealized positions of the phenyl ring H atoms (C–H = 1.0 Å, B = B of C atom to which H atom is bonded) were also added. Two

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(16) P. W. R. Corfield, R. J. Doedens, and J. A. Ibers, *Inorg. Chem.*, **6**, 167 (1967).

(17) D. Sayre, *Acta Cryst.*, **5**, 60 (1952).

(18) R. E. Long, Ph.D. Thesis, part III, University of California, Los Angeles, Calif., 1965.

(19) Programs used for this analysis included local modifications of Zalkin's FORDAP Fourier program, the Busing-Levy ORFFE error function program, Johnson's ORTEP plotting program, and Hamilton's GONO9 absorption program. Our least-squares program NUCLS in its nongroup form resembles the Busing-Levy ORFLS program.

(20) J. A. Ibers, "International Tables for X-Ray Crystallography," Vol. 3, The Kynoch Press, Birmingham, England, 1962, Table 3.3.1A.

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

(22) D. T. Cromer, *Acta Cryst.*, **18**, 17 (1965).

(23) J. A. Ibers and W. C. Hamilton, *ibid.*, **17**, 781 (1964).

(24) S. J. La Placa and J. A. Ibers, *ibid.*, **18**, 511 (1965); R. Eisenberg and J. A. Ibers, *Inorg. Chem.*, **4**, 773 (1965).

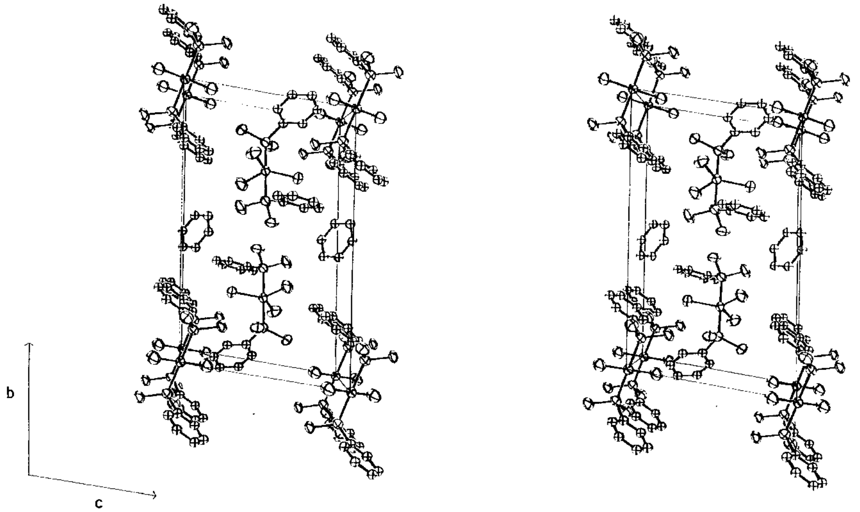

Figure 1.—A stereoscopic view of the unit cell of $NiBr_3(P(C_6H_5)(CH_3)_2)_2 \cdot 0.5NiBr_2(P(C_6H_5)(CH_3)_2)_2 \cdot C_6H_6$.

TABLE I

FINAL ATOMIC AND GROUP PARAMETERS FOR $NiBr_3(P(C_6H_5)(CH_3)_2)_2 \cdot 0.5NiBr_2(P(C_6H_5)(CH_3)_2)_2 \cdot C_6H_6$

Atom[a]	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_2
Ni_1	0	0	0	0.0106 (4)	0.0028 (1)	0.0070 (2)	0.0004 (1)	0.0002 (2)	0.0001 (1)
Ni_2	−0.30091 (19)	0.26330 (9)	0.50779 (14)	0.0135 (3)	0.0029 (1)	0.0062 (2)	0.0000 (1)	0.0016 (2)	0.0002 (1)
Br_1	−0.18289 (16)	0.00772 (7)	−0.15214 (13)	0.0222 (3)	0.0043 (1)	0.0130 (2)	0.0017 (1)	−0.0067 (2)	−0.0003 (1)
Br_2	−0.39635 (13)	0.26668 (7)	0.30718 (10)	0.0146 (2)	0.0042 (1)	0.0071 (1)	−0.0001 (1)	0.0006 (1)	0.0010 (1)
Br_3	−0.46253 (17)	0.32408 (8)	0.64783 (12)	0.0281 (3)	0.0046 (1)	0.0117 (2)	−0.0002 (1)	0.0109 (2)	−0.0010 (1)
Br_4	−0.08448 (16)	0.21372 (8)	0.59026 (14)	0.0185 (3)	0.0049 (1)	0.0167 (2)	−0.0013 (1)	−0.0067 (2)	0.0031 (1)
P_1	−0.02529 (31)	0.12269 (15)	0.07386 (25)	0.0128 (5)	0.0029 (1)	0.0080 (3)	0.0003 (2)	0.0017 (3)	−0.0002 (1)
P_2	−0.42617 (31)	0.15318 (15)	0.50691 (24)	0.0127 (5)	0.0029 (1)	0.0079 (3)	−0.0001 (2)	0.0022 (3)	0.0006 (1)
P_3	−0.17949 (34)	0.37531 (16)	0.51002 (26)	0.0165 (5)	0.0030 (1)	0.0086 (3)	−0.0006 (2)	0.0025 (3)	−0.0004 (2)
C_1	−0.2001 (12)	0.1671 (6)	0.0366 (10)	0.0140 (20)	0.0038 (5)	0.0125 (14)	0.0019 (8)	0.0018 (13)	−0.0002 (7)
C_2	0.0000 (12)	0.1513 (6)	0.2383 (9)	0.0195 (20)	0.0039 (5)	0.0067 (11)	−0.0008 (8)	0.0057 (12)	−0.0013 (6)
C_3	−0.4190 (13)	0.1237 (6)	0.6540 (10)	0.0185 (21)	0.0040 (5)	0.0095 (12)	−0.0010 (8)	0.0042 (13)	0.0015 (6)
C_4	−0.6234 (13)	0.1566 (6)	0.4617 (12)	0.0147 (21)	0.0039 (5)	0.0152 (16)	−0.0005 (8)	0.0018 (14)	0.0013 (7)
C_5	−0.2998 (14)	0.4477 (6)	0.4656 (11)	0.0225 (24)	0.0025 (4)	0.0153 (16)	0.0008 (8)	0.0073 (16)	0.0007 (7)
C_6	−0.0961 (15)	0.4149 (7)	0.6602 (11)	0.0246 (26)	0.0053 (6)	0.0096 (14)	−0.0044 (10)	0.0018 (15)	−0.0030 (8)

Group[b]	x_c	y_c	z_c	δ	ϵ	η	B_1 or B, Å²	B_2, Å²	B_3, Å²	B_4, Å²	B_5, Å²	B_6, Å²
Ring 1	0.2268 (6)	0.2115 (3)	−0.0399 (4)	1.078 (5)	2.456 (4)	2.495 (6)	3.5 (2)	4.8 (3)	5.9 (3)	5.8 (3)	5.8 (3)	5.0 (3)
Ring 2	−0.2955 (6)	0.0206 (3)	0.3242 (5)	−2.060 (7)	−2.381 (5)	1.948 (7)	4.1 (2)	5.6 (3)	8.2 (4)	7.6 (4)	7.1 (3)	5.4 (3)
Ring 3	0.0817 (6)	0.3636 (3)	0.3327 (5)	−1.998 (6)	−2.364 (4)	1.258 (7)	3.9 (2)	4.8 (2)	6.2 (3)	6.4 (3)	6.8 (3)	5.3 (3)
Benzene	−0.3096 (8)	0.4716 (4)	0.0715 (6)	2.816 (7)	2.827 (6)	0.847 (7)	8.7 (2)					

[a] x, y, and z are fractional coordinates. The form of the anisotropic thermal ellipsoid is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$. The estimated standard deviations of the least significant digits are given in parentheses. [b] x_c, y_c, and z_c are the fractional coordinates of the ring centers. The angles δ, ϵ, and η (in radians) which bring about alignment (except for translation) of an internal coordinate system within the ring with a fixed external coordinate system are those previously described.[24] B_i is the isotropic thermal parameter of atom i in a given ring. The rings are numbered so that C_1 is attached to P; C_4 is *para* to C_1.

TABLE II

DERIVED PARAMETERS FOR GROUP CARBON ATOMS[a]

Atom	x	y	z
		Ring 1	
C_1	0.1163 (7)	0.1752 (5)	0.0115 (6)
C_2	0.2630 (8)	0.1766 (4)	0.0609 (5)
C_3	0.3734 (6)	0.2129 (5)	0.0095 (7)
C_4	0.3373 (8)	0.2479 (6)	−0.0914 (7)
C_5	0.1906 (9)	0.2465 (4)	−0.1407 (5)
C_6	0.0801 (6)	0.2102 (5)	−0.0893 (6)
		Ring 2	
C_1	−0.3562 (12)	0.0765 (5)	0.4051 (6)
C_2	−0.4116 (10)	0.0631 (6)	0.2838 (7)
C_3	−0.3508 (10)	0.0072 (5)	0.2029 (5)
C_4	−0.2347 (13)	−0.0353 (6)	0.2433 (7)
C_5	−0.1794 (10)	−0.0219 (5)	0.3646 (8)
C_6	−0.2401 (8)	0.0340 (4)	0.4454 (5)
		Ring 3	
C_1	−0.0321 (7)	0.3700 (7)	0.4106 (6)
C_2	−0.0622 (7)	0.3782 (6)	0.2894 (6)
C_3	0.0516 (9)	0.3717 (4)	0.2114 (5)
C_4	0.1955 (8)	0.3572 (7)	0.2548 (7)
C_5	0.2256 (7)	0.3490 (6)	0.3760 (7)
C_6	0.1118 (8)	0.3555 (4)	0.4539 (5)
		Benzene	
C_1	−0.4183 (11)	0.4783 (7)	0.1541 (9)
C_2	−0.3231 (12)	0.5392 (5)	0.1492 (9)
C_3	−0.2144 (12)	0.5325 (5)	0.0667 (10)
C_4	−0.2009 (10)	0.4649 (7)	−0.0110 (9)
C_5	−0.2961 (12)	0.4040 (5)	−0.0061 (9)
C_6	−0.4047 (12)	0.4107 (5)	0.0764 (10)

[a] Estimated standard deviations are derived from those of the group parameters. Intra-ring distances are fixed (C–C = 1.392 Å).

cycles of least-squares refinement yielded discrepancy factors of $R_1 = 0.055$ and $R_2 = 0.093$.

As analysis of the weighting scheme applied showed no systematic variation of the function $\Sigma w(|F_o| - |F_c|)^2$ with $\lambda^{-1} \sin \theta$, but indicated that the reflections with a large value of $|F_o|$ were being underweighted. The weights were modified empirically to give a constant value of $\Sigma w(|F_o| - |F_c|)^2$ over all ranges of $|F_o|$, and one cycle of least-squares refinement resulted in final discrepancy factors of $R_1 = 0.054$ and $R_2 = 0.070$ and an error in an observation of unit weight of 0.99. A difference Fourier map showed no peak greater than 1.1 e$^-$/Å^3, approximately 30% of the height of a carbon atom.

Table I presents the positional, thermal, and group parameters, along with the corresponding standard deviations in these parameters as estimated from the inverse matrix. Table II gives the positional parameters of the group carbon atoms which may be derived from the data in Table I. The final values of $10|F_o|$ and $10|F_c|$ (in electrons) are presented in Table III. For the 221 reflections for which $F_o^2 < 3\sigma(F_o^2)$, none had $|F_o^2 - F_c^2| > 3\sigma(F_o^2)$. These reflections accordingly are omitted from Table III.

The orientations of the thermal ellipsoids can be seen in the figures. Only the C and Br atoms exhibit significant anisotropy, with the root-mean-square amplitudes of vibration ranging from 0.20 to 0.38 Å for C atoms and from 0.18 to 0.39 Å for Br atoms.

Description of the Structure

The structure consists of well-separated four- and five-coordinate molecules, with a four-coordinate *trans*-$NiBr_2(P(C_6H_5)(CH_3)_2)_2$ molecule at the origin of the unit cell and two five-coordinate $NiBr_3(P(C_6H_5)(CH_3)_2)_2$ molecules occupying general positions; the two benzene molecules are located in a rather large hole in the structure. A stereoscopic view of the unit cell is given in Figure 1; it can be seen that layers of five-coordinate molecules alternate with layers of four-coordinate molecules and benzene molecules stacked perpendicular to the c axis. The closest approaches of hydrogen atoms between adjacent molecules are 2.29 and 2.40 Å. Interatomic distances and angles and their standard deviations, as computed from the final parameters and the correlation matrix, are presented in Table IV.

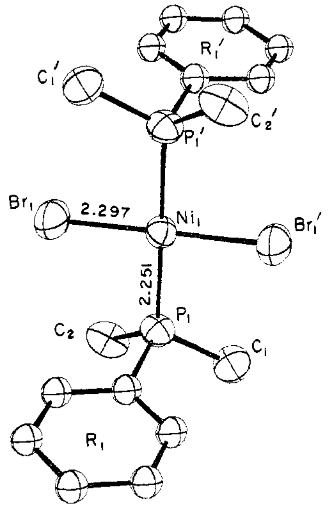

Figure 2.—Perspective drawing of $NiBr_2(P(C_6H_5)(CH_3)_2)_2$.

The four-coordinate $NiBr_2(P(C_6H_5)(CH_3)_2)_2$ molecule is crystallographically required to possess a center of symmetry and hence must have a *trans*-planar structure; Figure 2 illustrates this geometry, and also presents selected bond lengths. The Ni_1–P_1 and Ni_1–Br_1 distances of 2.251 (3) and 2.297 (2) Å, respectively, appear to be normal for planar Ni(II) complexes. The corresponding bond lengths in $NiBr_2(P(C_2H_5)_3)_2$, also with a crystallographic center of symmetry, are 2.26 and 2.30 Å, respectively.[25] The P_1–Ni_1–Br_1 angle is 90.45 (8)°, essentially the same as that reported for $NiBr_2(P(C_2H_5)_3)_2$, 90.5°.

The five-coordinate $NiBr_3(P(C_6H_5)(CH_3)_2)_2$ molecule possesses a trigonal-bipyramidal geometry, as illustrated in Figure 3; Figure 3 also presents selected bond distances. The three bromine atoms occupy the equatorial plane and the two phosphine groups are axial. The P–Ni–P linkage is nearly linear, with a P_2–Ni_2–P_3 angle of 178 8 (1)°. The Ni atom and three Br atoms are coplanar, with the Ni atom 0.004 (2) Å out of the best-weighted least-squares plane. This plane is essentially perpendicular to the P_2–Ni_2–P_3 vector, as can be seen by examination of the P–Ni–Br bond angles.

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(25) V. Scatturin and A. Turco, *J. Inorg. Nucl. Chem.*, **8**, 447 (1958).

TABLE III

OBSERVED AND CALCULATED STRUCTURE AMPLITUDES (×10) (IN ELECTRONS) FOR $NiBr_3(P(C_6H_5)(CH_3)_2)_2 \cdot 0.5NiBr_2(P(C_6H_5)(CH_3)_2)_2 \cdot C_6H_6$

K	L	FO	FC
***** H = 0 *****			
0	0		8765
0	1	1034	975
0	2	1188	1096
0	3	249	201
0	4	104	73
0	5	580	521
0	6	900	854
0	7	103	108
0	8	214	217
0	9	238	234
1	-10	102	100
1	-9	449	454
1	-8	282	319
1	-7	575	584
1	-6	315	300
1	-5	843	800
1	-4	619	621
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-2	2	116	116
-2	4	223	210
-1	-5	98	102
-1	-4	88	104
-1	-3	78	77
-1	-2	152	157
-1	1	126	102
-1	2	407	404
-1	3	453	447
-1	4	169	154
0	-5	476	477
0	-4	380	429
0	-3	334	296
0	-2	52	61
0	-1	268	254
0	0	56	71
0	1	240	235
0	2	140	167
0	3	149	192
0	4	232	234
1	-4	51	45
1	-2	491	499
1	-1	166	189
1	0	122	113
1	2	296	286
1	3	182	191
1	4	427	430
2	-5	326	322
2	-4	273	294
2	-3	331	362
2	-2	234	249
2	-1	437	468
2	1	374	365
2	2	256	254
3	-4	76	80
3	-3	357	361
3	-2	105	97
3	-1	193	227
3	0	255	287
3	1	208	212
3	2	142	143
3	3	227	235
4	-5	72	66
4	-4	193	177
4	-3	67	99
4	-2	132	131
4	1	260	260
4	2	132	140
4	3	122	125
5	-5	259	253
5	-4	112	126
5	-3	165	155
5	-2	315	355
5	-1	228	241
5	0	512	523
5	1	204	213
5	2	212	198
6	-4	68	77
6	-3	235	236
6	-1	87	86
7	-3	249	261
7	-2	125	104
7	-1	64	57
7	0	453	479
7	1	241	245
8	-2	361	348
***** H = 8 *****			
-2	-1	64	51
-1	-2	94	78
-1	0	129	123
-1	1	81	90
0	-2	156	140
0	0	194	200
0	1	427	409
1	-2	70	54
1	-1	205	237

TABLE IV

SELECTED INTERATOMIC DISTANCES AND ANGLES

Atoms	Distance, Å	Atoms	Angle, deg
	$NiBr_2(P(C_6H_5)(CH_3)_2)_2$		
Ni_1–Br_1	2.297 (2)	Br_1–Ni_1–P_1	90.45 (8)
Ni_1–P_1	2.251 (3)	Ni_1–P_1–C_1	118.4 (4)
P_1–C_1	1.824 (11)	Ni_1–P_1–C_2	117.9 (4)
P_1–C_2	1.826 (11)	Ni_1–P_1–R_1C_1	107.0 (3)
P_1–R_1C_1[a]	1.822 (9)	C_1–P_1–C_2	101.6 (5)
		C_1–P_1–R_1C_1	105.1 (5)
		C_2–P_1–R_1C_1	105.7 (4)
	$NiBr_3(P(C_6H_5)(CH_3)_2)_2$		
Ni_2–Br_2	2.349 (2)	Br_2–Ni_2–Br_3	110.63 (9)
Ni_2–Br_3	2.375 (2)	Br_2–Ni_2–Br_4	132.71 (9)
Ni_2–Br_4	2.339 (2)	Br_3–Ni_2–Br_4	116.66 (9)
Ni_2–P_2	2.263 (3)	P_2–Ni_2–P_3	178.8 (1)
Ni_2–P_3	2.273 (3)	P_2–Ni_2–Br_2	90.3 (1)
P_2–C_3	1.800 (11)	P_2–Ni_2–Br_3	89.3 (1)
P_2–C_4	1.816 (12)	P_2–Ni_2–Br_4	90.6 (1)
P_2–R_2C_1	1.800 (9)	P_3–Ni_2–Br_2	89.7 (1)
P_3–C_5	1.807 (12)	P_3–Ni_2–Br_3	89.6 (1)
P_3–C_6	1.820 (12)	P_3–Ni_2–Br_4	90.3 (1)
P_3–R_3C_1	1.793 (7)	Ni_2–P_2–C_3	113.1 (4)
		Ni_2–P_2–C_4	113.7 (4)
		Ni_2–P_2–R_2C_1	112.6 (3)
		Ni_2–P_3–C_5	113.1 (4)
		Ni_2–P_3–C_6	112.7 (6)
		Ni_2–P_3–R_3C_1	113.8 (4)
		C_3–P_2–C_4	104.5 (6)
		C_3–P_2–R_2C_1	106.4 (5)
		C_4–P_2–R_2C_1	105.9 (5)
		C_5–P_3–C_6	104.8 (6)
		C_5–P_3–R_3C_1	105.5 (6)
		C_6–P_3–R_3C_1	106.2 (5)

[a] R_iC_1 refers to carbon atom 1 on phenyl ring *i*.

There is, however, a distortion of the molecule in the equatorial plane; the Ni_2–Br_3 bond length of 2.375 (2) Å is significantly longer than the other two Ni–Br distances of 2.339 (2) and 2.349 (2) Å, and the angle opposite this long bond is expanded to 132.71 (9)° from the expected 120°. This distortion is similar to that found for the two $Ni(CN)_2L_3$ complexes[14,15] where L = $P(C_6H_5)(OC_2H_5)_2$ and $P(C_6H_5)(CH_3)_2)_2$ and for one of the $Ni(CN)_5^{3-}$ ions in $[Cr(NH_2CH_2CH_2NH_2)_3][Ni(CN)_5]\cdot 1.5H_2O$,[26] except that in these previous examples the two axial ligands were also bent away from the long bond. The distortion in the present compound could be ascribed to Jahn–Teller effects as the complex contains Ni(III) in a low-spin d^7 electronic configuration. Yet Jahn–Teller effects cannot be invoked to explain the similar distortions found in the Ni(II) complexes.

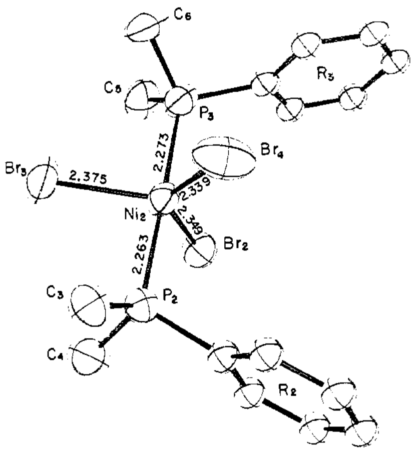

Figure 3.—Perspective drawing of $NiBr_3(P(C_6H_5)(CH_3)_2)_2$.

The Ni–P bond lengths of 2.263 (3) and 2.273 (3) Å cannot be considered significantly longer than that of 2.251 (3) Å found for the four-coordinate complex. However, the Ni–P bond lengths are approximately 0.04 Å shorter than the Ni–P distance found in the high-spin tetrahedral Ni(II) complex $NiBr_2(P(C_6H_5)_3)_2$, 2.33 Å.[27] The Ni–P bond lengths appear to be somewhat longer than those observed in many diamagnetic five-coordinate Ni(II) complexes, for example, 2.18 (1) Å in $Ni(HP(C_6H_5)_2)_3I_2$,[28] 2.206 (8) Å in $[Ni(TAP)CN]ClO_4$ (TAP = $P(CH_2CH_2CH_2As(CH_3)_2)_3$),[29] 2.19 (equatorial P) and 2.15 Å (axial P) in the trigonal-bipyramidal $Ni(P(OCH)_3(CH_2)_3)_5^{2+}$ ion,[30] and 2.223 (3) Å in $Ni(CN)_2(P(C_6H_5)(CH_3)_2)_3$.[15] The Ni–Br distances of 2.349 (2), 2.375 (2), and 2.339 (2) Å are significantly longer than that of 2.297 (2) Å observed in the four-coordinate complex and are more in keeping with the Ni–Br distance of 2.34 Å found in $NiBr_2(P(C_6H_5)_3)_2$.[27] Apparently, the increase in radius resulting from the presence of an unpaired electron in Ni(III) more than compensates for the contraction that would be expected to result from increased nuclear charge. The apparent increase in the nickel covalent radius on going from Ni(II) to Ni(III) complexes is similar to that observed on going from low-spin square-planar Ni(II) to high-spin tetrahedral Ni(II), for which the observed radius expansion is about 0.05 Å.[27]

The C–P bond lengths and C–P–C bond angles in both the four- and five-coordinate complexes appear to be normal. If the four P–CH_3 distances in the five-coordinate molecule are assumed to be equivalent, then the standard deviation of a given distance from the mean of 1.811 Å is 0.009 Å, approximately the same as the computed standard deviations. Thus the reported errors are probably reasonable.

This compound is part of a growing series of trigonal-bipyramidal MX_3Y_2 complexes, where M is a transition metal. Insofar as we are aware, such complexes invariably have the X groups in the equatorial plane, despite widely varying steric and electronic properties of the X and Y ligands.

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(26) K. N. Raymond, P. W. R. Corfield, and J. A. Ibers, *Inorg. Chem.*, **7**, 1362 (1968).

(27) J. A. J. Jarvis, R. H. B. Mais, and P. G. Owston, *J. Chem. Soc., A*, 1473 (1968).

(28) J. A. Bertrand and D. L. Plymale, *Inorg. Chem.*, **5**, 879 (1966).

(29) D. L. Stevenson and L. F. Dahl, *J. Am. Chem. Soc.*, **89**, 3424 (1967).

(30) E. F. Riedel, J. G. Verkade, and R. A. Jacobson, to be submitted for publication. See Abstracts, American Crystallographic Association Meeting, Minneapolis, Minn., 1967, No. P-10.