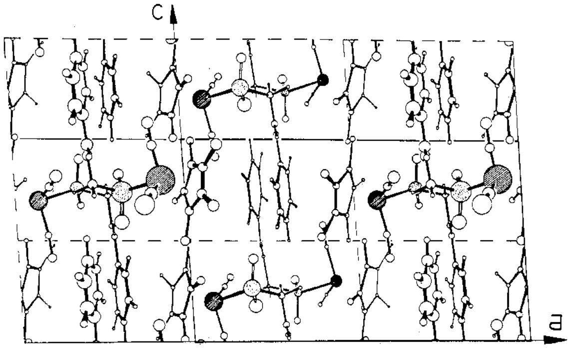

Figure 3.—Packing of $[\pi\text{-}C_5(CH_3)_5]Fe(CO)_2SO_2CH_2CH{=}CH\text{-}(C_6H_5)$ molecules within the unit cell, viewed down *b*. The dashed lines represent the half-periods in the unit cell.

(6) Å. These distances are closely similar to the S=O bond length of 1.480 (8) Å in $\pi\text{-}C_5H_5Fe(CO)_2\text{-}C_4H_5SO_2$.[1,37] The present sulfur–sp^3 carbon bond, S–C(1), is 1.840 (8) Å long; this is consistent with the sulfur–sp^2 carbon distance of 1.781 (9) Å found in $\pi\text{-}C_5H_5Fe(CO)_2C_4H_5SO_2$,[1,37] since there is a difference of 0.03–0.04 Å in the covalent radii of sp^2- and sp^3-hybridized carbon atoms.

As may be seen from Tables V–VII, distances within the phenylallyl moiety are in keeping with the structure as illustrated in Figures 1 and 2.

TABLE VIII

INTERMOLECULAR CONTACTS TO 3.5 Å[a]

Atoms	Dist, Å	Trans[b]	Atoms	Dist, Å	Trans[b]
O(1)···H(6)	2.42	I	C(16)···H(2)	3.34	II
H(1)···H(7)	2.72	I	S···H(6)	3.43	I
H(1)···H(6)	2.87	I	C(17)···H(6)	3.46	III
C(17)···H(2)	3.20	II	O(1)···C(6)	3.47	II
O(3)···H(7)	3.23	I	H(1)···C(7)	3.48	I
H(2)···H(6)	3.25	I	C(11)···H(6)	3.49	III
C(1)···H(6)	3.31	I	C(11)···C(6)	3.50	III

[a] Note that hydrogen atoms belonging to methyl groups of the $\pi\text{-}C_5(CH_3)_5$ ligand have not been located and are not included in these calculations. [b] The translations are as follows: (I) x, y, $1 + z$; (II) $-\frac{1}{2} + x$, $\frac{1}{2} - y$, $-\frac{1}{2} + z$; (III) $-\frac{1}{2} + x$, $\frac{1}{2} - y$, $\frac{1}{2} + z$.

Crystal Packing

The packing of molecules in the crystal is shown in Figure 3; intermolecular contacts are collected in Table VIII. The shortest contact is O(1)···H(6) $[x, y, 1 + z]$ = 2.42 Å. This and all other contacts are greater than the sum of the appropriate van der Waals radii.

Acknowledgments.—We thank Professor A. Wojcicki for supplying the sample. This work has been generously supported by the National Science Foundation (Grant GP-8077). J. W. acknowledges, with gratitude, the receipt of a Graduate National Fellowship from Harvard University for 1967–1970.

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The Bonding of Molecular Nitrogen. III. The Crystal and Molecular Structure of Chlorodinitrogentetrakis(dimethylphenylphosphine)rhenium(I)

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The crystal and molecular structure of the molecular nitrogen complex chlorodinitrogentetrakis(dimethylphenylphosphine)-rhenium(I), $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$, has been determined from three-dimensional X-ray data collected by counter techniques. The central rhenium atom is octahedrally coordinated to four phosphorus atoms, to the chlorine atom, and to a nitrogen atom of the molecular nitrogen group. The chlorine and nitrogen atoms are *trans*. The Re–Cl bond distance is 2.521 (4) Å, the Re–N bond distance is 1.97 (2) Å, and the four Re–P bond distances have a mean value of 2.422 (10) Å. The molecular nitrogen group is linear with an Re–N–N bond angle of 177 (1)° and a Cl–Re–N bond angle of 175.6 (4)°. Owing to partial disorder between the chlorine atom and the molecular nitrogen entity, a precise determination of the N–N distance has not been possible. Crystal data are as follows: triclinic, space group $C_i^1\text{-}P\bar{1}$; $a = 12.730$ (6) Å, $b = 12.771$ (6) Å, $c = 11.523$ (6) Å, $\alpha = 103.25$ (3)°, $\beta = 103.96$ (2)°, $\gamma = 95.37$ (2)° (temperature 22°), $Z = 2$; $d_{\text{obsd}} = 1.57$ (3) g/cm^3, $d_{\text{calcd}} = 1.53$ g/cm^3. The structure was refined using 1968 independent reflections for which $F^2 > 3\sigma(F^2)$ and the refinement converged to a conventional R factor (on F) of 3.7%.

Introduction

In the previously reported structures of transition metal complexes which contain molecular nitrogen as a coordinating ligand, $CoH(N_2)(P(C_6H_5)_3)_3$, $Ru(N_2)(NH_3)_5{}^{2+}$, and $[Ru(N_3)(N_2)(NH_2CH_2CH_2NH_2)_2][PF_6]$, it has been shown that molecular nitrogen bonds in a manner similar to the isoelectronic species carbon monoxide.[1-3] In continuing our studies and collaboration with the Unit of Nitrogen Fixation at the University of Sussex, Brighton, England, to determine factors con-

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cerned in the bonding of nitrogen to transition metals, we report here a determination of the structure of chlorodinitrogentetrakis(dimethylphenylphosphine)rhenium-(I).[4] The existence[4] of the carbonyl analog $ReCl(CO)(P(CH_3)_2C_6H_5)_4$ was an important factor in our choice of the present dinitrogen compound. Eventual comparison of the structures of the dinitrogen compound and its carbonyl analog should provide increased understanding of the bonding of molecular nitrogen to transition metals. Moreover, this dinitrogen compound is of intrinsic interest because it exhibits a very low infrared N–N stretching frequency[4] (1922 cm^{-1}) and reacts with $MoCl_4 \cdot 2(C_2H_5)_2O$ to form a complex with an N_2 stretching frequency of 1680 cm^{-1}. The grouping Re–N–N–Mo[5] is proposed in this complex. Finally, this work bears directly on our previous studies of metal–nitrogen multiple bonds.[6]

Collection and Reduction of Intensity Data

A sample of $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$ was kindly supplied by Professor J. Chatt and Dr. J. R. Dilworth. Suitable crystals were obtained by recrystallization from a benzene–methanol solution. A series of Weissenberg and precession photographs taken with Cu K$\bar{\alpha}$ radiation revealed no symmetry elements. Hence, the crystals have been assigned to the triclinic system.

The cell constants and their standard deviations were determined at 22° by a least-squares refinement of the setting angles of 12 reflections that had been centered on a Picker four-circle automatic X-ray diffractometer, using procedures previously described.[7] The results (Mo Kα_1 radiation, λ 0.7093 Å) are a = 12.730 (6) Å, b = 12.771 (6) Å, c = 11.523 (6) Å, α = 103.25 (3)°, β = 103.96 (2)°, γ = 95.37 (2)°. A Delauney reduction to obtain this cell revealed no hidden symmetry. The calculated density of 1.53 g/cm^3 for two formula units in the cell is in reasonable agreement with the observed density of 1.57 (3) g/cm^3 obtained by the flotation method. An optical study of the prismatic platelike crystal used in the data collection showed that the prominent faces are $\bar{1}01$ and $10\bar{1}$ and the other faces are $0\bar{1}0$, $\bar{1}00$, 110, and $\bar{1}10$.

This crystal was approximately 0.45 × 0.35 × 0.20 mm along the [100], [010], and [101] directions, respectively. It was wedged into a thin-walled glass capillary and mounted on the diffractometer along its long direction [100]. Several ω scans with a narrow source and wide-open counter were taken to determine the mosaicity of the crystal. The average width at half-height for a strong reflection was 0.15°.

A total of 2207 independent reflections were collected in the range $0° \leq 2\theta$ (Mo Kα_1) $\leq 35°$. The diffracted beams were filtered through 3-mil Nb foil. A takeoff angle of 1.6° was used. At this angle, the peak intensity of a strong reflection was about 80% of the maximum value as a function of takeoff angle. The counter aperture selected was 4 mm × 5 mm and was positioned 29 cm from the crystal. The pulse height analyzer was set for approximately a 90% window, centered on the Mo K$\bar{\alpha}$ peak. The data were collected by the θ–2θ scan technique at a scan rate of 1°/min. An asymmetric scan range of 0.70° on the low side and 1.20° on the high side of the calculated 2θ values was used. Stationary counter, stationary crystal background counts of 10 sec were taken at each end of the scan. Attenuators were inserted automatically when the intensity of the diffracted beam exceeded about 7000 counts/sec during the scan; the attenuators inserted were Cu foil, their thickness being chosen to give attenuator factors of approximately 2.2.

Throughout the collection of the data, the intensities of four reference reflections were measured every 100 reflections as a check on electronic and crystal stability. The average intensity of the reference reflections had dropped approximately 10% after these 2207 reflections had been scanned. For this reason data collection was terminated at a 2θ of 35°. No attempt was made to correct for the average 10% drop in intensity because the decomposition was not isotropic. The minimum change in a reference intensity was 5% and the maximum was 20%.

The data were processed in a manner previously described.[7] The value of p in the calculation of $\sigma(I)$ was selected as 0.04. The values of I and $\sigma(I)$ were corrected for Lorentz–polarization effects and absorption.[8] The linear absorption coefficient of this compound for Mo Kα radiation is 39.6 cm^{-1}, and for the crystal chosen transmission coefficients ranged from 0.662 to 0.485. Of the 2207 reflections, only the 1968 which obeyed the condition $F^2 > 3\sigma(F^2)$ were used in subsequent calculations.

Solution and Refinement

All least-squares refinements were carried out on F, the function minimized being $\Sigma w(|F_o| - |F_c|)^2$, where $|F_o|$ and $|F_c|$ are the observed and calculated structure amplitudes and the weight w is $4F_o^2/\sigma^2(F_o^2)$. In all calculations of F_c, the atomic scattering factors for rhenium and hydrogen were those calculated by Cromer and Waber[9] and by Stewart, Davidson, and Simpson,[10] respectively; scattering factors for chlorine, phosphorus, carbon, and nitrogen were taken from the usual tabulation.[11] The effects of anomalous dispersion of the rhenium, chlorine, and phosphorus atoms were included in the calculation of F_c;[12] the values of $\Delta f'$ and $\Delta f''$ used were those calculated by Cromer.[13]

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[8] In addition to various local programs, Patterson functions and Fourier syntheses were calculated using a local version of Zalkin's FORDAP. Absorption corrections were arrived at by a modification of W. C. Hamilton's GONO9. Refinement and structure factor calculations were carried out by our least-squares program, NUCLS, which, in its nongroup form, resembles the Busing–Levy ORFLS. Errors in derived quantities were obtained from the Busing–Levy ORFFE program, and drawings were made with use of Johnson's ORTEP program.

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TABLE I

POSITIONAL, THERMAL, AND GROUP PARAMETERS FOR $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$

Atom	x	y	z	β_{11}[a]	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Re	0.22640 (4)[b]	0.22963 (4)	0.27108 (4)	0.00652 (6)	0.00472 (5)	0.00742 (7)	0.00128 (4)	0.00171 (4)	0.00193 (4)
Cl[c]	0.3799 (3)	0.2561 (3)	0.4651 (4)	0.0084 (6)	0.0081 (4)	0.0122 (7)	0.0014 (3)	0.0013 (5)	0.0045 (4)
Cl′	0.0729[d]	0.2032	0.0771	0.0084	0.0081	0.0122	0.0014	0.0013	0.0045
P1	0.3354 (3)	0.3893 (3)	0.2531 (3)	0.0070 (3)	0.0055 (3)	0.0094 (4)	0.0014 (2)	0.0024 (3)	0.0022 (3)
P2	0.3162 (3)	0.1180 (3)	0.1378 (3)	0.0076 (3)	0.0064 (3)	0.0091 (4)	0.0017 (3)	0.0017 (3)	0.0023 (3)
P3	0.1524 (3)	0.0745 (3)	0.3304 (3)	0.0072 (3)	0.0051 (3)	0.0088 (4)	0.0014 (2)	0.0021 (3)	0.0022 (3)
P4	0.1223 (3)	0.3447 (3)	0.3803 (3)	0.0082 (3)	0.0056 (3)	0.0098 (4)	0.0016 (3)	0.0022 (3)	0.0014 (3)
N1	0.1005 (14)	0.2008 (10)	0.1242 (17)	0.0087 (15)	0.0073 (12)	0.0082 (17)	0.0044 (11)	0.0022 (13)	0.0059 (12)
N2	0.0304 (16)	0.1864 (12)	0.0484 (14)	0.0054 (14)	0.0088 (13)	0.0097 (18)	0.0003 (11)	0.0004 (12)	0.0025 (12)
N1′	0.3523	0.2584	0.4180	0.0087	0.0073	0.0082	0.0044	0.0022	0.0059
N2′	0.4224	0.2728	0.4937	0.0054	0.0088	0.0097	0.0003	0.0004	0.0025
C11	0.3666 (11)	0.5092 (10)	0.3845 (12)	0.0095 (14)	0.0070 (12)	0.0128 (17)	0.0004 (10)	0.0020 (12)	0.0020 (12)
C12	0.4778 (11)	0.3739 (10)	0.2617 (13)	0.0102 (15)	0.0071 (12)	0.0143 (18)	0.0006 (10)	0.0031 (13)	0.0038 (12)
C21	0.4416 (12)	0.0762 (11)	0.2133 (13)	0.0109 (15)	0.0098 (14)	0.0167 (20)	0.0037 (11)	0.0055 (14)	0.0065 (14)
C22	0.2381 (12)	−0.0111 (11)	0.0395 (13)	0.0128 (15)	0.0067 (12)	0.0148 (18)	−0.0001 (11)	0.0065 (14)	0.0006 (12)
C31	0.1498 (11)	0.0987 (10)	0.4916 (12)	0.0118 (15)	0.0080 (12)	0.0114 (17)	0.0030 (11)	0.0053 (13)	0.0031 (12)
C32	0.0113 (10)	0.0135 (10)	0.2482 (13)	0.0084 (13)	0.0064 (12)	0.0167 (20)	0.0000 (10)	0.0021 (12)	0.0039 (12)
C41	0.1858 (12)	0.4128 (11)	0.5431 (13)	0.0111 (15)	0.0097 (14)	0.0132 (19)	0.0018 (11)	0.0052 (14)	−0.0001 (13)
C42	0.0799 (11)	0.4585 (11)	0.3163 (14)	0.0112 (14)	0.0092 (14)	0.0175 (20)	0.0043 (11)	0.0056 (13)	0.0050 (14)

Group	x_c[e]	y_c	z_c	δ	ϵ	η
Ring 1	0.2597 (5)	0.4899 (5)	0.0179 (6)	−1.276 (6)	3.000 (6)	−2.295 (6)
Ring 2	0.3715 (5)	0.1999 (4)	−0.0896 (5)	−1.916 (6)	3.137 (5)	−2.093 (6)
Ring 3	0.2815 (5)	−0.1332 (5)	0.3204 (5)	1.975 (6)	2.475 (5)	−2.915 (7)
Ring 4	−0.1246 (5)	0.2524 (5)	0.3785 (6)	−2.139 (16)	−1.922 (6)	0.773 (17)

[a] The form of the thermal ellipsoid is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$ [b] Numbers in parentheses given here and in other tables are estimated standard deviations in the least significant digits. [c] The atoms Cl, N1, and N2 have a multiplicity of 0.88 (2) and the atoms Cl′, N1′, and N2′ have a multiplicity of 0.12. [d] The coordinates of Cl′, N1′, and N2′ were derived from the coordinates of Cl, N1, and N2 such that the Re–Cl′ distance equals the Re–Cl distance, the Cl′–Re–Cl angle is 180°, etc. The thermal parameters of Cl, N1, and N2 were assigned to those of Cl′, N1′, and N2′, respectively. [e] x_c, y_c, and z_c are fractional coordinates of the ring center; δ, ϵ, and η (in radians) have been defined previously.[14]

The rhenium and four phosphorus atoms were found from a Patterson function calculation. The eight methyl carbon atoms and four phenyl rings were found on a subsequent difference Fourier map. A least-squares refinement cycle was carried out in which the rhenium, four phosphorus, and eight methyl carbon atoms were refined with isotropic thermal parameters; the four phenyl rings were treated as rigid groups and restricted to their known geometry (D_{6h} symmetry, C–C = 1.392 Å). The variable parameters for a ring included an overall isotropic thermal parameter, the coordinates of the ring center, and three orientation angles which have been described previously.[14] The usual agreement factors $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and R_2 (or weighted R factor) $= (\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2)^{1/2}$ were 16.5 and 20.6%, respectively. A difference Fourier synthesis revealed the positions of the chlorine atom and the molecular nitrogen group. The atoms of the molecular nitrogen entity were not resolved in the electron density map but appeared as an elongated peak with a single-peak maximum. The two nitrogen atoms were assigned positions 0.5 Å on each side of the peak maximum, resulting in an N–N distance of 1.0 Å, an Re–N distance of 2.0 Å, and an Re–N–N angle of 177°.

Next the absorption correction was applied, and, after subsequent isotropic refinement, the hydrogen atoms of the methyl groups were located from electron density maps calculated in planes perpendicular to the phosphorus–carbon vectors. The observed hydrogen atoms were idealized using a C–H bond distance of 1.0 Å and an H–C–H bond angle of 109.5°. The positions of the hydrogen atoms of the phenyl rings were calculated from the known geometry of the ring and a C–H distance of 0.90 Å. The fixed contribution to F_c of these 44 hydrogen atoms (with isotropic thermal parameters of 5.0 Å^2) was included in subsequent calculations.

In the next cycle of refinement, the sixteen nongroup atoms were refined anisotropically and the four phenyl rings were refined as rigid groups with individual isotropic thermal parameters on each carbon atom; the resulting values of R_1 and R_2 were 3.7 and 4.7%, respectively.

However, in the resulting structure the N–N bond distance was only 0.94 Å and the Re–N bond distance was 2.02 Å. From previous work we expected an N–N bond distance greater than 1.10 Å and an Re–N bond distance less than 2.00 Å.[1,3] The Co–N distance is 1.807 (23) Å in $CoH(N_2)(P(C_6H_5)_3)_3$[1] and the Ru–N distance is 1.894 (9) Å in $[Ru(N_3)(N_2)(NH_2CH_2CH_2NH_2)_2][PF_6]$.[3] We believe that a plausible explanation for this short N–N bond distance is a partial disorder between the molecular nitrogen group and the chlorine atom. Because of the distances involved (Re–Cl = 2.5 Å, Re–N1 = 1.9 Å, Re–N2 = 3.0 Å), if there is partial disorder, the nitrogen atoms will refine inward toward the N–N center in an attempt to compensate for chlorine scattering. This will lead to a short N–N bond

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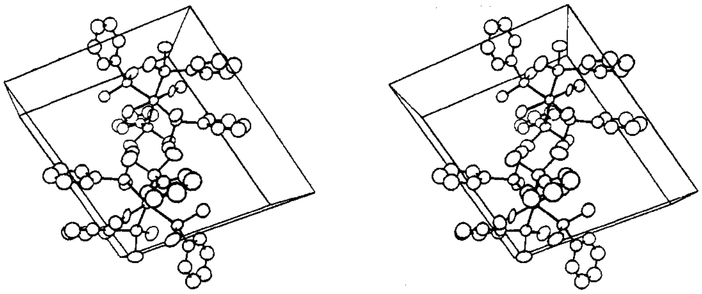

Figure 1.—A stereoscopic pair of views of the contents of a unit cell of $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$.

distance and a long Re–N bond distance. Such a model of disorder is feasible, as the steric pockets above and below the plane of the rhenium and four phosphorus atoms are very similar. Therefore in an attempt to account for this disorder the following model was used. The atoms Cl, N1, and N2 were assigned a variable occupancy factor α. Three additional atoms Cl′, N1′, and N2′ were assigned the occupancy factor $1 - \alpha$. The positions of these atoms were derived in the calculations from the positions of Cl, N1, and N2 in such a way that the Re–X bond length was equal to the Re–X′ bond length and the X–Re–X′ bond angle was 180°. The thermal parameter of X was assigned to X′ (X = Cl, N1, N2). In the ensuing least-squares refinement the only additional variable was α, and appropriate relationships among the derivatives were taken into account in its refinement. This refinement converged to values of R_1 and R_2 of 3.7 and 4.7% and to a value of α of 0.88 (2). The resultant Re–N and N–N distances are 1.966 (21) and 1.055 (30) Å. Although no clear distinction can be made on the basis of R_2, we favor this disordered model because both the derived distances and the value of α are reasonable and because of the lack of resolution of the nitrogen atoms on electron density maps. Although the Re–N–N portion of the molecule is not well defined in this study, the rest of the molecule is. Even the Re–Cl portion is unaffected by assumptions about the nature of the disorder.

A statistical analysis of R_2 shows no unusual trends with $|F_o|$, $\lambda^{-1} \sin \theta$, or various combinations of Miller indices. For the 194 variables and 1968 observations, the error in an observation of unit weight is 1.97 e^-. On a final difference Fourier synthesis, the highest peaks (1.0 and 0.79 $e^-/Å^3$) were associated with the rhenium atom. The agreement factors based on F_o^2 are $R_1 = 6.6$ and $R_2 = 9.4\%$. For the 239 reflections omitted from the refinement for which $F_o^2 < 3\sigma(F_o^2)$, three had $|F_o^2 - F_c^2| > 3\sigma(F_o^2)$.

The positional, thermal, and group parameters derived from the last cycle of refinement are presented in Table I along with the associated standard deviations, as derived from the inverse matrix. The positional and thermal parameters of the ring carbon atoms and the idealized positional parameters of the methyl and phenyl hydrogen atoms are listed in Tables II and III. The final values of $10|F_o|$ and $10|F_c|$ (in electrons) are given in Table IV for the 1968 reflections which were used in the refinement.

TABLE II

PARAMETERS FOR RING CARBON ATOMS

Atom	x	y	z	B,[a] $Å^2$
		Ring 1		
C1[b]	0.2933 (7)[c]	0.4484 (7)	0.1202 (7)	4.6 (3)
C2	0.3702 (5)	0.5078 (8)	0.0825 (8)	6.0 (3)
C3	0.3367 (8)	0.5493 (7)	−0.0197 (9)	7.4 (4)
C4	0.2262 (9)	0.5314 (8)	−0.0843 (7)	7.3 (4)
C5	0.1493 (6)	0.4720 (8)	−0.0467 (8)	7.2 (4)
C6	0.1828 (6)	0.4305 (7)	0.0556 (8)	5.5 (3)
		Ring 2		
C1	0.3527 (7)	0.1679 (7)	0.0122 (7)	4.0 (3)
C2	0.4552 (6)	0.1664 (7)	−0.0108 (8)	5.9 (3)
C3	0.4740 (6)	0.1984 (8)	−0.1126 (9)	7.1 (4)
C4	0.3903 (9)	0.2319 (8)	−0.1915 (7)	7.1 (4)
C5	0.2878 (7)	0.2334 (8)	−0.1685 (8)	7.8 (4)
C6	0.2690 (6)	0.2014 (7)	−0.0667 (9)	5.2 (3)
		Ring 3		
C1	0.2233 (7)	−0.0461 (6)	0.3245 (8)	4.1 (3)
C2	0.1809 (6)	−0.1438 (7)	0.2340 (7)	5.3 (3)
C3	0.2392 (8)	−0.2310 (6)	0.2299 (8)	6.4 (4)
C4	0.3398 (7)	−0.2204 (6)	0.3164 (9)	6.7 (4)
C5	0.3821 (6)	−0.1227 (8)	0.4069 (8)	6.2 (4)
C6	0.3239 (7)	−0.0355 (6)	0.4109 (7)	5.0 (3)
		Ring 4		
C1	−0.0176 (6)	0.2904 (7)	0.3815 (8)	4.1 (3)
C2	−0.0424 (7)	0.2793 (7)	0.4898 (6)	5.5 (3)
C3	−0.1494 (8)	0.2414 (9)	0.4869 (8)	7.4 (4)
C4	−0.2316 (6)	0.2145 (9)	0.3755 (10)	8.1 (4)
C5	−0.2068 (7)	0.2256 (8)	0.2672 (8)	7.3 (4)
C6	−0.0998 (8)	0.2635 (8)	0.2702 (6)	5.8 (3)

[a] B is the refined isotropic thermal parameter for the individual ring carbon atoms. [b] Ring atoms are numbered sequentially, with C1 attached to the P. [c] The estimated standard deviations are derived from those of the group parameters.

Description of the Structure

The structure consists of discrete molecules of $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$ upon which no crystallographic symmetry is imposed. A stereoscopic pair of views of the contents of a unit cell is given in Figure 1. The inner coordination sphere of the molecule is displayed in Figure 2 and an overall view of the molecule, with the exclusion of hydrogen atoms, is presented in Figure 3. A selection of intramolecular bond distances and bond angles, together with estimated standard deviations as derived with the inclusion of correlation effects, is given in Tables V and VI. The root-mean-square amplitudes of vibration along the principal axes of vibration for atoms refined anisotropically are

TABLE III

DERIVED PARAMETERS FOR HYDROGEN ATOMS[a]

Atom	x	y	z	Atom	x	y	z
H111[b]	0.391	0.488	0.466	H2*R1*[c]	0.442	0.524	0.124
H112	0.428	0.563	0.381	H3*R1*	0.385	0.591	−0.045
H113	0.301	0.546	0.387	H4*R1*	0.203	0.558	−0.152
H121	0.484	0.318	0.186	H5*R1*	0.079	0.458	−0.090
H122	0.524	0.444	0.268	H6*R1*	0.135	0.391	0.079
H123	0.512	0.347	0.337	H2*R2*	0.509	0.146	0.039
H211	0.437	0.051	0.287	H3*R2*	0.540	0.198	−0.129
H212	0.468	0.021	0.155	H4*R2*	0.403	0.253	−0.259
H213	0.506	0.144	0.246	H5*R2*	0.234	0.256	−0.221
H221	0.163	−0.003	−0.003	H6*R2*	0.203	0.204	−0.053
H222	0.276	−0.043	−0.026	H2*R3*	0.127	−0.153	0.178
H223	0.233	−0.066	0.089	H3*R3*	0.214	−0.296	0.172
H311	0.091	0.143	0.510	H4*R3*	0.379	−0.277	0.314
H312	0.135	0.028	0.516	H5*R3*	0.448	−0.116	0.463
H313	0.223	0.140	0.551	H6*R3*	0.351	0.027	0.469
H321	0.004	−0.015	0.155	H2*R4*	0.010	0.297	0.562
H322	−0.012	−0.052	0.277	H3*R4*	−0.166	0.234	0.557
H323	−0.040	0.066	0.257	H4*R4*	−0.301	0.190	0.374
H411	0.192	0.354	0.594	H5*R4*	−0.261	0.208	0.196
H412	0.263	0.448	0.556	H6*R4*	−0.085	0.270	0.200
H413	0.143	0.465	0.577				
H421	0.032	0.430	0.229				
H422	0.037	0.502	0.368				
H423	0.145	0.508	0.316				

[a] All atoms have $B = 5.0$ Å^2. [b] H111, H112, and H113 are attached to C11; H121, H122, and H123 are attached to C12; etc. [c] H2*R1* is attached to C2 of ring 1, H3*R1* to C3 of ring 1, etc.

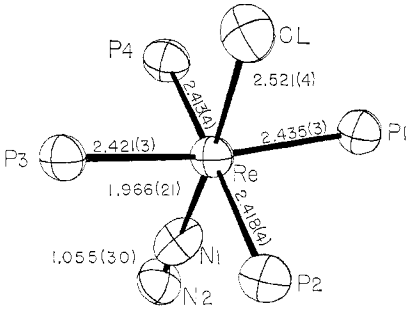

Figure 2.—The inner coordination sphere of $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$.

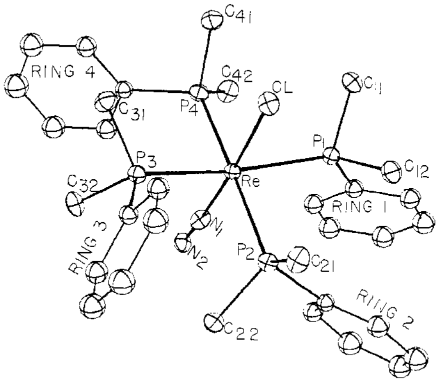

Figure 3.—An overall view of the $ReCl(N_2)(P(CH_3)_2C_6H_5)$ molecule.

given in Table VII. The directions of vibration of atoms may be discerned from Figures 2 and 3. These figures also display the numbering scheme employed.

The molecular nitrogen group in this structure is not well defined because of the disorder between it and the chlorine atom. The Re–N bond distance of 1.97 (2) Å is shorter than the Os–N single-bond distance of 2.136 (9) Å found in $OsCl_3(NH_3)(P(C_6H_5)_3)_2$[15] but not as short as the Re–N formal double-bond distance of 1.709 (4) Å found in $ReCl_3(NC_6H_4OCH_3)(P(C_2H_5)_2C_6H_5)_2$.[16] The N–N bond distance of 1.06 (3) Å is somewhat shorter than expected in view of the low N–N infrared stretching frequency but the uncertainty in the distance is large. On the basis of the Re–N1–N2 bond angle of 177 (1)° we conclude that the bonding of dinitrogen in this complex is similar to that found in other transition metal complexes of molecular nitrogen.[1-3]

The Re–P mean distance of 2.422 (10) Å compares well with the Os–P distance of 2.411 (2) Å found in $OsCl_3(NH_3)(P(C_6H_5)_3)_2$[15] but is slightly shorter than the distance of 2.470 (1) Å found in $ReCl_3(NC_6H_4OCH_3)(P(C_2H_5)_2C_6H_5)_2$.[16] The least-squares plane through the rhenium and four phosphorus atoms is given in Table VIII. Two phosphorus atoms are below this plane and two are above it. It is also clear from the P···N, P···Cl distances and the P–Re–N, P–Re–Cl bond angles that P1 and P3 are bent toward the chlorine atom and P2 and P4 are bent toward the molecular nitrogen group.

The Re–Cl distance of 2.521 (4) Å, though long, is slightly shorter than the Re–Cl distance of 2.563 (4) Å found in $ReNCl_2(P(C_2H_5)_2C_6H_5)_3$.[7]

The bond distances in the present structure may be explained in a manner discussed previously.[6] Where there is a short M–N (M = metal) bond length, the steric hindrance caused by a close approach of the nitrogen atom to the metal may be relieved either by

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(15) D. Bright and J. A. Ibers, *Inorg. Chem.*, **8**, 1078 (1969).

(16) D. Bright and J. A. Ibers, *ibid.*, **7**, 1099 (1968).

TABLE IV

OBSERVED AND CALCULATED STRUCTURE AMPLITUDES × 10 (IN ELECTRONS) FOR $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$

K	L	FO	FC
***** H = -10 *****			
-3	3	594	591
-2	2	246	210
-2	3	446	434
-2	4	434	430
-2	5	200	169
-1	1	154	126
-1	2	669	695
-1	3	235	193
-1	4	516	269
-1	5	210	227
0	1	631	677
0	3	651	715
0	5	399	371
1	0	425	449
1	1	158	171
1	2	566	615
1	4	514	527
1	5	156	125
2	-1	482	544
2	1	373	421
2	3	369	385
2	5	526	507
3	0	277	295
4	0	221	193
4	1	465	461
4	3	578	553
***** H = -9 *****			
-4	4	350	316
-4	5	374	360
-4	6	268	272
-3	3	447	430
-3	4	510	509
-3	5	211	202
-3	6	135	150
-2	2	738	731
-2	3	372	416
-2	4	521	531
-2	5	268	270
-2	6	246	254
-2	7	392	340
-1	1	762	624
-1	3	659	663
-1	4	219	221
-1	5	434	426
-1	7	366	325
0	1	227	234
0	2	1027	1057
0	3	149	149
0	6	502	510
0	7	539	480
1	0	232	270
1	1	697	737
1	3	622	560
1	4	143	122
1	5	463	480
1	6	162	170
2	-1	176	223
2	1	167	162
2	2	550	535
2	4	261	257
2	6	602	617
3	-2	341	308
3	-1	636	703
3	0	215	231
3	1	465	440
3	3	390	394
3	5	456	443
3	6	163	160
4	-3	623	621
4	-2	476	480
4	-1	632	644
4	0	416	384
4	1	362	365
4	2	530	515
4	3	127	98
4	4	463	471
5	-2	531	525
5	0	559	529
5	1	389	394
5	2	515	506
5	3	619	570
5	4	220	221
6	-1	430	445
6	1	614	573
6	2	564	549
6	3	532	492
***** H = -8 *****			
-5	5	461	464
-5	6	355	336
-4	4	267	262
-4	5	307	296
-4	6	368	324
-3	3	350	376
-3	4	446	433
-3	5	425	406
-3	6	344	344
-3	7	305	296
-2	3	854	855
-2	4	265	301
-2	5	611	609
-2	6	365	354
-2	7	210	220
-2	8	319	281
-1	1	254	221
-1	2	1006	1077
-1	4	879	867
-1	5	220	216
-1	6	522	517
-1	7	417	416
-1	8	419	369
0	1	966	1041
0	3	870	946
0	5	614	619
0	6	225	192
0	7	406	407
0	8	416	398
1	0	590	660
1	1	196	146
1	2	729	786
1	4	410	440
1	6	629	641
1	7	341	317
2	0	372	435
2	1	696	759
2	3	200	202
2	4	131	94
2	5	262	240
2	7	662	635
3	-2	342	334
3	-1	643	649
3	0	606	676
3	1	425	406
3	2	356	375
3	4	367	366
3	6	506	456
4	-2	778	815
4	-1	371	367
4	0	857	886
4	1	527	555
4	2	372	387
4	3	269	279
4	4	272	266
4	5	640	604
5	-3	654	646
5	1	472	447
5	2	356	340
5	3	464	440
5	4	542	510
5	5	307	283
6	-3	374	359
6	-2	466	492
6	0	459	470
6	1	178	207
6	2	548	544
6	3	516	494
6	4	608	569
7	-2	146	131
7	-1	476	461
7	0	130	83
7	1	522	490
7	2	319	312
7	3	495	439
***** H = -7 *****			
-6	6	464	443
-6	7	878	808
-5	5	312	307
-5	6	576	580
-5	7	388	375
-4	4	308	302
-4	5	360	390
-4	6	528	526
-4	7	401	393
-4	8	125	121
-3	3	471	508
-3	5	848	828
-3	6	637	634
-3	7	426	416
-3	8	370	346
-2	2	1151	1142
-2	4	1031	1092
-2	5	379	384
-2	6	953	952
-2	7	397	390
-2	8	204	221
-1	1	979	987
-1	2	278	305
-1	3	950	979
-1	5	1130	1190
-1	6	421	406
-1	7	390	415
-1	8	464	427
0	1	133	140
0	2	1020	1100
0	3	236	236
0	4	849	901
0	5	147	160
0	6	705	803
0	7	412	395
0	8	406	390
1	0	225	259
1	1	966	1083
1	3	583	624
1	5	637	654
1	6	205	195
1	7	447	451
1	8	248	235
2	-1	549	587
2	0	788	842
2	1	363	370
2	2	644	698
2	4	322	335
2	6	418	399
2	8	570	533
3	-2	758	755
3	-1	450	450
3	0	1203	1254
3	1	905	867
3	2	390	385
3	3	361	370
3	4	216	204
3	5	526	531
3	7	415	389
4	-3	803	760
4	-1	1303	1282
4	0	654	634
4	1	917	924
4	2	290	300
4	3	407	416
4	4	626	642
4	5	339	339
4	6	670	630
5	-4	665	655
5	-2	866	855
5	-1	143	136
5	0	998	963
5	1	443	438
5	2	365	397
5	3	379	365
5	4	595	595
5	5	826	797
5	6	272	261
6	-4	317	305
6	-3	691	705
6	-2	214	195
6	-1	714	699
6	0	152	161
6	1	401	377
6	2	299	320
6	3	491	485
6	4	573	526
6	5	569	563
7	-4	607	588
7	-2	665	645
7	0	426	419
7	2	291	305
7	3	362	339
7	4	532	512
8	-3	363	371
8	-2	220	192
8	-1	540	533
8	1	357	333
8	2	217	213
***** H = -6 *****			
-7	7	601	556
-6	6	494	498
-6	7	325	334
-5	5	242	230
-5	6	499	490
-5	7	333	324
-5	8	460	434
-4	4	214	204
-4	5	569	598
-4	6	454	430
-4	7	501	466
-4	8	160	155
-3	3	258	247
-3	4	939	931
-3	5	500	497
-3	6	1062	1110
-3	7	416	417
-3	8	427	385
-3	9	226	204
-2	2	418	449
-2	3	910	950
-2	4	120	130
-2	5	1160	1214
-2	6	364	364
-2	7	759	737
-2	8	332	312
-2	9	349	305
-1	1	321	303
-1	2	624	671
-1	3	224	225
-1	4	1314	1361
-1	6	990	1046
-1	7	299	290
-1	8	310	310
-1	9	456	434
0	1	551	610
0	2	396	398
0	3	698	756
0	4	105	95
0	5	1075	1160
0	7	371	366
0	8	351	343
0	9	463	424
1	0	359	400
1	1	260	246
1	2	739	803
1	3	357	388
1	4	877	905
1	6	545	561
1	8	345	358
2	-1	362	401
2	0	859	923
2	1	628	658
2	2	676	674
2	3	562	569
2	7	223	225
3	-2	156	185
3	-1	1215	1187
3	0	743	747
3	1	1249	1250
3	2	629	647
3	3	434	425
3	4	916	904
3	5	217	243
3	6	389	355
3	7	131	135
3	8	562	545
4	-3	193	177
4	-2	1023	1021
4	-1	237	233
4	0	1405	1399
4	1	588	595
4	2	997	1002
4	3	531	515
4	4	742	731
4	5	828	848
4	6	208	219
4	7	563	513
5	-3	663	640
5	-2	122	108
5	-1	1291	1215
5	0	299	297
5	1	657	651
5	2	273	286
5	3	623	643
5	4	796	779
5	6	788	781
6	-4	635	627
6	-3	154	166
6	-2	881	890
6	-1	177	172
6	0	681	697
6	2	434	422
6	3	364	367
6	4	590	550
6	5	508	465
6	6	454	427
7	-5	561	580
7	-4	366	315
7	-3	691	664
7	-2	142	142
7	-1	646	645
7	0	113	73
7	1	181	174
7	3	386	374
7	4	347	327
7	5	361	340
8	-4	412	442
8	-3	507	494
8	-2	619	629
8	-1	206	188
8	0	346	331
8	2	424	411
8	3	213	191
9	-3	370	362
9	-2	525	547
9	-1	567	539
9	0	243	237
9	1	526	502
***** H = -5 *****			
-7	7	143	136
-6	6	203	201
-6	7	259	257
-6	8	207	205
-5	5	563	531
-5	6	214	252
-5	7	501	484
-5	8	257	255
-4	4	671	693
-4	5	452	450
-4	6	457	477
-4	7	204	165
-4	8	615	585
-4	9	299	274
-3	3	869	861
-3	5	1318	1330
-3	7	741	761
-3	8	372	383
-3	9	492	472
-2	2	564	567
-2	3	287	293
-2	4	1116	1176
-2	6	1117	1181
-2	7	165	177
-2	8	617	622
-2	9	485	487
-1	1	213	201
-1	2	97	118
-1	3	678	715
-1	5	1198	1286
-1	7	756	772
-1	8	357	356
-1	9	469	450
0	1	176	165
0	2	258	289
0	3	646	682
0	4	1169	1269
0	5	356	341
0	6	731	762
0	8	437	439
0	9	268	260
1	0	587	650
1	1	199	217
1	2	744	801
1	3	879	953
1	4	510	522
1	6	712	743
1	7	307	330
1	9	445	421
2	-1	1189	1231
2	0	294	315
2	1	595	595
2	2	784	832
2	3	851	906
2	4	871	904
2	5	298	292
2	6	284	303
2	7	146	136
2	8	424	434
3	-2	985	956
3	-1	421	399
3	0	1252	1255
3	1	922	903
3	2	1012	1017
3	3	785	795
3	4	561	583
3	5	732	737
3	6	152	143
3	7	449	428
4	-3	696	650
4	-2	160	161
4	-1	1164	1153
4	1	1202	1167
4	2	531	520
4	3	1072	1074
4	4	870	876
4	5	591	568
4	6	612	599
4	7	208	210
5	-4	507	485
5	-3	199	201
5	-2	1047	1007
5	-1	243	219
5	0	809	796
5	1	221	238
5	2	849	850
5	3	378	374
5	4	693	710
5	5	498	511
5	6	411	412
5	7	750	729
6	-5	364	330
6	-4	255	245
6	-3	813	796
6	-1	1170	1131
6	1	553	530
6	3	478	460
6	4	262	236
6	5	564	542
6	6	385	365
7	-6	231	223
7	-5	644	610
7	-4	625	616
7	-3	602	617
7	-2	1078	1061
7	0	408	421
7	2	451	455
7	4	374	354
7	5	154	125
8	-5	312	317
8	-4	781	770
8	-3	729	727
8	-2	523	514
8	-1	685	684
8	0	207	179
8	1	473	460
8	2	123	97
8	3	751	736
8	4	192	171
9	-4	427	437
9	-3	710	713
9	-2	603	638
9	-1	561	598
9	0	438	460
9	1	248	255
9	2	787	769
10	-1	342	352
***** H = -4 *****			
-7	7	331	319
-7	8	284	255
-6	6	169	176
-6	7	131	137
-6	8	310	296
-5	5	193	176
-5	6	477	462
-5	8	471	461
-5	9	453	414
-4	4	192	207
-4	5	606	622
-4	6	178	204
-4	7	444	449
-4	8	236	205
-4	9	600	591
-3	3	309	297
-3	4	1251	1284
-3	5	628	604
-3	6	893	913
-3	7	440	441
-3	8	873	878
-3	9	382	360
-2	3	1044	1053
-2	4	316	340
-2	5	940	1005
-2	6	116	89
-2	7	971	1019
-2	8	363	365
-2	9	667	648
-1	1	206	184
-1	2	524	517
-1	4	1037	1132
-1	5	157	152
-1	6	722	774
-1	7	141	139
-1	9	378	386
0	1	149	137
0	2	761	829
0	3	1075	1145
0	4	438	454
0	5	812	866
0	6	538	527
0	7	528	540
0	9	418	423
1	1	531	550
1	2	792	861
1	3	1156	1235
1	4	997	1046
1	5	257	276
1	6	351	365
1	7	142	159
1	8	406	405
2	-1	155	152
2	0	981	980
2	1	550	549
2	2	1445	1448
2	3	1065	1114
2	4	634	656
2	5	610	610
2	6	168	179
2	7	425	423
2	8	161	146
3	-2	278	271
3	-1	866	855
3	0	345	335
3	1	1123	1130
3	2	1165	1183
3	3	1363	1347
3	4	759	772
3	5	337	340
3	6	403	412
3	7	139	139
3	8	656	614
4	-3	438	434
4	-2	574	575
4	0	853	827
4	2	1461	1419
4	3	689	688
4	4	803	797
4	5	435	425
4	6	317	320
4	7	615	615
5	-4	386	342
5	-3	474	478
5	-1	736	714
5	0	115	114
5	1	738	740
5	3	696	705
5	4	426	442
5	5	419	415
5	6	287	301
5	7	507	469
6	-5	450	452
6	-4	318	316
6	-3	748	709
6	-2	990	960
6	0	765	746
6	1	118	92
6	2	918	920
6	4	114	105
6	6	606	607
7	-6	666	653
7	-4	796	798
7	-3	854	830
7	-2	564	548
7	-1	940	955
7	1	591	608
7	2	124	41
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6	-2	205	206
6	-1	640	632
6	0	650	644
6	1	547	546
6	2	801	786
6	3	492	502
6	4	847	858
6	5	148	145
7	-6	468	442
7	-4	908	903
7	-2	761	732
7	0	393	416
7	1	424	416
7	2	650	677
7	3	710	728
7	4	321	317
8	-7	668	650
8	-6	192	162
8	-5	479	501
8	-4	172	159
8	-3	469	483
8	-1	325	337
8	2	288	286
8	3	636	672
9	-7	539	520
9	-6	702	669
9	-5	345	330
9	-4	502	512
9	-3	323	331
9	-2	412	412
9	0	544	595
10	-5	440	430
10	-4	527	526
10	-3	573	562
10	-1	610	645
***** H = 3 *****			
-7	7	749	705
-6	6	674	666
-6	7	292	271
-5	6	538	527
-5	7	706	685
-5	8	432	449
-4	4	403	383
-4	5	761	738
-4	6	399	398
-4	7	691	706
-4	8	475	456
-3	3	314	330
-3	4	1395	1356
-3	5	486	492
-3	6	805	806
-3	7	294	326
-3	8	379	392
-2	2	276	289
-2	3	1565	1559
-2	4	195	225
-2	5	779	841
-2	6	264	292
-2	7	554	573
-2	8	165	191
-1	2	1463	1585
-1	4	1116	1174
-1	5	625	633
-1	6	503	494
-1	7	331	372
0	0	349	360
0	1	968	963
0	2	590	570
0	3	1727	1695
0	4	143	119
0	5	931	879
0	6	393	410
0	7	378	366
0	8	469	471
1	0	410	390
1	1	896	882
1	2	1346	1299
1	3	395	391
1	4	955	916
1	5	239	247
1	6	663	643
1	7	312	344
2	-1	769	754
2	0	551	534
2	1	1019	995
2	2	998	959
2	3	945	889
2	5	508	469
2	6	235	228
2	7	706	693
3	-2	963	920
3	-1	862	850
3	0	867	842
3	1	870	840
3	2	648	637
3	3	366	369
3	6	535	526
4	-3	373	364
4	-2	1445	1429
4	-1	1060	1024
4	0	677	640
4	1	743	703
4	2	520	480
4	3	751	705
4	4	172	184
4	5	642	661
4	6	225	242
5	-4	151	117
5	-3	1495	1465
5	-2	485	465
5	-1	1051	1026
5	0	377	384
5	1	955	896
5	2	745	727
5	3	349	357
5	4	758	772
5	5	266	268
6	-5	234	237
6	-4	1172	1140
6	-2	772	764
6	-1	124	130
6	0	525	503
6	1	336	334
6	2	526	524
6	3	674	643
6	4	364	360
7	-6	239	259
7	-5	676	640
7	-4	254	276
7	-3	1066	1063
7	-1	265	249
7	1	571	598
7	2	239	261
7	3	536	559
8	-7	525	507
8	-6	473	496
8	-5	375	373
8	-4	600	591
8	-3	274	250
8	-2	229	215
8	0	311	312
8	1	162	153
8	2	591	625
9	-6	599	553
9	-5	609	622
9	-4	451	464
9	-3	498	493
9	-2	115	69
9	-1	331	355
9	1	612	620
10	-4	516	524
10	-3	308	314
10	-2	499	510
***** H = 4 *****			
-6	6	254	252
-6	7	662	634
-5	5	265	237
-5	6	315	333
-5	7	625	597
-4	4	469	471
-4	5	161	140
-4	6	746	721
-4	7	375	353
-3	3	1199	1130
-3	4	310	324
-3	5	776	781
-3	6	183	199
-3	7	647	672
-2	2	1167	1163
-2	3	526	502
-2	4	817	837
-2	5	165	236
-2	6	799	873
-2	7	237	249
-1	2	155	150
-1	3	1377	1345
-1	4	180	172
-1	5	871	842
-1	6	339	331
-1	7	469	505
0	0	399	426
0	1	827	855
0	2	1450	1436
0	3	425	410
0	4	984	926
0	6	630	603
0	7	343	345
1	0	892	889
1	1	559	532
1	2	530	518
1	3	1107	1083
1	4	343	320
1	5	534	516
1	7	490	456
2	-1	620	620
2	0	813	808
2	1	1038	1023
2	2	820	787
2	3	344	336
2	4	292	261
2	5	271	284
2	6	517	503
3	-2	1374	1346
3	-1	732	704
3	0	836	824
3	1	944	900
3	2	749	722
3	3	561	533
3	5	396	379
3	6	226	212
4	-3	1074	1049
4	-2	526	514
4	-1	1207	1174
4	0	885	860
4	1	1001	976
4	2	942	891
4	3	274	296
4	4	515	486
4	5	165	190
5	-4	942	925
5	-3	163	154
5	-2	1020	1006
5	-1	354	346
5	0	1399	1338
5	1	560	541
5	2	443	447
5	3	574	577
5	4	340	343
5	5	491	485
6	-5	444	460
6	-4	245	261
6	-3	1068	1057
6	-2	120	155
6	-1	666	674
6	1	607	602
6	2	306	315
6	3	361	397
6	4	376	393
7	-6	337	329
7	-5	556	568
7	-4	929	936
7	-3	235	236
7	-2	693	660
7	0	440	445
7	2	444	445
7	3	151	160
8	-7	362	335
8	-6	624	602
8	-5	674	700
8	-4	475	487
8	-2	124	104
8	-1	375	374
8	0	141	136
8	1	455	477
9	-6	606	581
9	-5	665	669
9	-4	720	727
9	-3	335	324
9	-2	415	436
***** H = 5 *****			
-6	6	420	400
-5	6	445	427
-5	7	414	376
-4	4	297	276
-4	5	369	329
-4	7	558	533
-3	3	513	519
-3	4	767	753
-3	5	262	275
-3	6	807	832
-3	7	188	222
-2	2	131	103
-2	3	949	977
-2	4	145	119
-2	5	812	865
-2	6	319	364
-2	7	631	655
-1	1	367	371
-1	2	1179	1271
-1	3	195	186
-1	4	1072	1007
-1	6	771	765
-1	7	375	400
0	0	606	726
0	1	610	640
0	2	514	521
0	3	1097	1035
0	4	437	446
0	5	769	715
1	0	255	265
1	1	793	801
1	2	465	497
1	3	546	494
1	4	568	586
1	6	516	491
2	0	965	959
2	1	692	686
2	2	717	720
2	3	562	551
2	4	473	469
2	5	556	532
2	6	217	213
3	-1	909	880
3	0	651	631
3	1	1202	1151
3	2	833	800
3	3	424	388
3	4	409	378
3	5	123	40
4	-2	760	774
4	-1	207	181
4	0	1544	1469
4	1	675	659
4	2	636	625
4	3	646	650
4	4	297	298
4	5	510	525
5	-4	268	272
5	-3	469	470
5	-2	240	215
5	-1	1057	1050
5	1	659	645
5	2	446	443
5	3	304	281
5	4	259	239
6	-5	436	433
6	-4	408	478
6	-2	490	497
6	-1	267	285
6	0	734	774
6	1	133	99
6	2	273	267
7	-6	508	499
7	-5	464	430
7	-4	330	339
7	-3	745	726
7	-2	250	260
7	-1	544	551
7	0	116	115
7	1	361	357
8	-6	276	280
8	-5	674	670
8	-4	657	676
8	-3	390	394
8	-2	502	525
8	-1	187	223
8	0	526	536
9	-4	544	565
9	-3	541	521
***** H = 6 *****			
-5	5	510	471
-5	6	149	149
-4	4	665	625
-4	6	464	440
-3	3	628	629
-3	4	225	221
-3	5	744	695
-3	6	254	261
-2	2	622	690
-2	6	754	625
-1	1	658	720
-1	2	165	169
-1	3	530	524
-1	4	302	273
-1	5	760	746
-1	6	144	129
0	1	485	510
0	2	517	546
0	3	423	430
0	4	661	617
0	5	436	427
0	6	541	532
1	0	471	467
1	1	345	352
1	2	360	343
1	3	525	526
1	4	764	696
1	5	503	461
2	-1	667	676
2	0	742	695
2	1	761	765
2	2	550	550
2	3	717	695
2	4	480	475
2	5	367	377
3	-2	625	734
3	0	1106	1097
3	1	677	650
3	2	816	814
3	3	564	544
4	-3	364	364
4	-2	117	94
4	-1	695	625
4	0	299	269
4	1	1064	1137
4	2	522	530
4	3	515	490
4	4	425	447
5	-4	271	260
5	-3	160	164
5	-2	595	562
5	-1	216	241
5	0	834	807
5	1	164	160
5	2	436	410
5	3	150	175
6	-5	215	170
6	-3	361	362
6	-2	202	167
6	-1	554	540
6	0	162	150
6	1	456	469
6	2	125	175
7	-6	243	265
7	-5	364	350
7	-4	472	475
7	-3	232	225
7	-2	597	607
7	-1	261	200
7	0	614	659
8	-5	335	323
8	-4	524	522
8	-3	556	543
8	-2	510	511
***** H = 7 *****			
-4	4	193	200
-4	5	602	548
-3	4	505	576
-3	5	232	232
-2	2	206	201
-2	3	369	431
-2	4	175	177
-2	5	566	546
-1	1	400	393
-1	2	239	204
-1	3	344	336
-1	4	422	400
-1	5	271	250
0	0	756	753
0	1	231	225
0	2	309	290
0	3	325	322
0	4	556	537
0	5	509	406
1	0	468	464
1	1	272	257
1	2	267	269
1	3	606	640
1	4	513	510
2	-1	332	320
2	0	660	667
2	1	528	540
2	2	655	644
2	3	376	357
2	4	663	643
3	-2	175	150
3	-1	677	634
3	0	345	361
3	1	734	710
3	2	275	305
3	3	724	683
4	-3	204	201
4	-2	454	474
4	-1	192	191
4	0	671	670
4	2	765	754
4	3	201	265
5	-4	175	191
5	-3	166	193
5	-2	356	300
5	-1	516	459
5	0	145	157
5	1	522	514
5	2	149	140
6	-5	270	322
6	-4	217	224
6	-3	241	262
6	-2	506	534
6	-1	315	316
6	0	466	495
6	1	195	175
7	-5	307	257
7	-4	295	250
7	-3	457	470
7	-2	472	483
7	-1	564	566
***** H = 8 *****			
-4	4	567	604
-3	3	508	565
-2	2	266	273
-2	3	264	320
-2	4	342	370
-1	1	254	261
-1	2	346	342
-1	3	190	166
-1	4	206	259
0	0	350	404
0	1	406	403
0	2	229	233
0	3	341	353
0	4	316	315
1	0	605	590
1	1	334	345
1	2	225	197
1	3	297	326
2	-1	663	699
2	0	375	360
2	1	323	326
2	2	277	264
2	3	524	511
3	-2	416	367
3	0	457	496
3	1	217	235
3	2	445	401
4	-3	241	234
4	-2	277	270
4	-1	297	316
4	1	501	523
5	-4	219	225
5	-3	279	262
5	-2	411	400
5	-1	239	274
5	0	265	240
6	-5	255	246
6	-4	304	316
6	-3	337	329
6	-2	266	263
***** H = 9 *****			
-3	3	351	377
-2	3	335	380
-1	2	194	160
-1	3	540	530
0	0	671	714
0	1	150	199
0	2	446	440
1	0	161	139
1	1	513	558
1	2	215	222
2	0	464	527
2	1	125	131
3	-2	307	307
3	-1	595	561
3	1	412	397
4	-3	409	412
4	-2	296	305
5	-4	495	484
5	-3	356	330
***** H = 10 *****			
1	0	542	504
2	-1	531	529

pushing the ligands cis to the nitrogen toward the trans chlorine atom (leading to a long M–Cl bond distance) or by lengthening the bonds cis to the metal–nitrogen bond (Table IX).

The $OsCl_3(NH_3)(P(C_6H_5)_3)_2$[15] (F of Table IX) system is not strained sterically. The Os–N bond distance is long, 2.136 (9) Å, and the Os–P, Os–Cl(cis), and Os–Cl(trans) bond lengths are normal. Also, there are no

TABLE V

INTRAMOLECULAR ANGLES IN $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$

Atoms	Angles, deg		Atoms	Angles, deg	
Re–N1–N2	177 (1)		Re–P1–C11	116.2 (5)	116 (1) (av)
Cl–Re–N1	175.6 (4)		Re–P1–C12	113.6 (4)	
Cl–Re–P1	82.1 (1)		Re–P2–C21	116.6 (5)	
Cl–Re–P2	94.7 (1)		Re–P2–C22	117.0 (5)	
Cl–Re–P3	84.8 (1)		Re–P3–C31	116.0 (4)	
Cl–Re–P4	92.2 (1)		Re–P3–C32	116.4 (3)	
N1–Re–P1	102.2 (4)		Re–P4–C41	117.6 (5)	
N1–Re–P2	86.3 (4)		Re–P4–C42	115.8 (5)	
N1–Re–P3	91.0 (4)		C11–P1–C1*R1*	102.2 (5)	100 (4) (av)
N1–Re–P4	87.0 (4)		C12–P1–C1*R1*	104.0 (5)	
N2–Re–P1	102.6 (3)		C21–P2–C1*R2*	103.4 (5)	
N2–Re–P2	87.3 (3)		C22–P2–C1*R2*	95.9 (5)	
N2–Re–P3	90.6 (3)		C31–P3–C1*R3*	97.0 (5)	
N2–Re–P4	86.0 (3)		C32–P3–C1*R3*	102.3 (5)	
P1–Re–P2	88.2 (1)		C41–P4–C1*R4*	102.3 (5)	
P1–Re–P4	90.5 (1)		C42–P4–C1*R4*	94.8 (5)	
P2–Re–P3	92.2 (1)		C11–P1–C12	95.6 (6)	100 (3) (av)
P3–Re–P4	90.7 (1)		C21–P2–C22	101.6 (7)	
Re–P1–C1*R1*	121.5 (3)	120 (1) (av)	C31–P3–C32	102.1 (7)	
Re–P2–C1*R2*	119.0 (3)		C41–P4–C42	102.3 (7)	
Re–P3–C1*R3*	119.8 (3)				
Re–P4–C1*R4*	120.3 (3)				

TABLE VI

INTRAMOLECULAR DISTANCES IN $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$

Atoms	Distance, Å	Atoms	Distance, Å	
Re–Cl	2.521 (4)	P3–N1	3.144 (17)	
Re–P1	2.435 (3)	P4–N1	3.031 (16)	
Re–P2	2.418 (4)	P1–N2	4.272 (20)	
Re–P3	2.421 (3)	P2–N2	3.777 (19)	
Re–P4	2.413 (4)	P3–N2	3.889 (16)	
Re–N1	1.966 (21)	P4–N2	3.733 (16)	
Re–N2	3.020 (19)	P1–C11	1.824 (14)	1.822 (10)[b] (av)
N1–N2	1.055 (30)[a]	P1–C12	1.823 (15)	
P1–P2	3.377 (5)	P2–C21	1.814 (14)	
P1–P4	3.442 (5)	P2–C22	1.812 (14)	
P2–P3	3.487 (5)	P3–C31	1.821 (13)	
P3–P4	3.439 (5)	P3–C32	1.819 (13)	
P1–Cl	3.257 (5)	P4–C41	1.822 (15)	
P2–Cl	3.633 (6)	P4–C42	1.843 (14)	
P3–Cl	3.332 (5)	P1–C1*R1*	1.847 (8)	1.850 (4) (av)
P4–Cl	3.557 (5)	P2–C1*R2*	1.847 (8)	
P1–N1	3.437 (17)	P3–C1*R3*	1.853 (8)	
P2–N1	3.016 (16)	P4–C1*R4*	1.854 (8)	

[a] See text. [b] The standard deviation for the average quantity is that for an individual estimate as derived from the collection of values assumed to be equivalent. On this basis, it appears that individual standard deviations derived from the inverse matrix are reasonable.

TABLE VII

ROOT-MEAN-SQUARE AMPLITUDES OF VIBRATION (Å)

Atom	Min	Intermed	Max
Re	0.183 (1)	0.210 (1)	0.224 (1)
Cl	0.215 (9)	0.252 (8)	0.293 (6)
P1	0.200 (5)	0.228 (5)	0.236 (5)
P2	0.210 (6)	0.231 (5)	0.250 (5)
P3	0.192 (6)	0.228 (5)	0.233 (5)
P4	0.203 (6)	0.242 (5)	0.254 (5)
N1	0,11 (4)	0.24 (2)	0.29 (2)
N2	0.19 (3)	0.25 (2)	0.27 (2)
C11	0.23 (2)	0.27 (2)	0.29 (2)
C12	0.22 (2)	0.28 (2)	0.29 (2)
C21	0.23 (2)	0.27 (2)	0.33 (2)
C22	0.22 (2)	0.26 (2)	0.34 (2)
C31	0.23 (2)	0.24 (2)	0.31 (2)
C32	0.21 (2)	0.26 (2)	0.32 (2)
C41	0.23 (2)	0.29 (2)	0.33 (2)
C42	0.23 (2)	0.28 (2)	0.33 (2)

TABLE VIII

WEIGHTED LEAST-SQUARES PLANE[a]

Atom	Dev from plane, Å	Atom	Dev from plane, Å
Re	−0.0069 (5)	P3	0.259 (3)
P1	0.282 (3)	P4	−0.160 (4)
P2	−0.147 (3)		

[a] Equation of plane: $7.106x - 2.176y + 7.661z = 3.193$ (triclinic coordinates).

close Cl(cis)···Cl(trans), N···P, or P···Cl(trans) interactions.

In $OsNCl_5^{2-}$ (A),[4] the Os–N bond is 1.614 (13) Å and there are four chlorine atoms cis to the nitrogen atom. To relieve the steric strain caused by the close approach of the nitrogen atom, the cis chlorine atoms are bent toward the trans chlorine atom leading to a long Os–Cl(trans) bond distance of 2.605 (4) Å.

In the rhenium–imino complexes (C, D, E),[16,17] the Re–N distance, 1.7 Å, is longer than the Os–N distance in $OsNCl_5^{2-}$, but now there are two chlorine atoms and two PR_3 groups cis to the nitrogen atom. Therefore, to relieve steric strain, the Re–P and Re–Cl(cis) bonds are lengthened. The Cl(cis)···Cl(trans), N···P, and P···Cl(trans) interactions are shorter than in $OsCl_3(NH_3)(P(C_6H_5)_3)_2$.

The $ReNCl_2(P(C_2H_5)_2C_6H_5)_3$ (B)[7] system is more sterically strained than the rhenium–imino complexes because of the close approach of the nitrogen atom to the rhenium atom and the placing of one chlorine atom and three PR_3 groups cis to the nitrogen atom. All bond lengths are longer to relieve this strain.

In $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$ (G), we have a situation similar to $ReNCl_2(P(C_2H_5)_2C_6H_5)_3$[7] except that the

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(17) D. Bright and J. A. Ibers, *Inorg. Chem.*, **8**, 703 (1969).

TABLE IX

DISTANCES (Å) BETWEEN ADJACENT ATOMS IN (A) $OsNCl_5^{2-}$, (B) $ReNCl_2(P(C_2H_5)_2C_6H_5)_3$, (C) $ReCl_3(NC_6H_4OCH_3)(P(C_2H_5)_2C_6H_5)_2$, (D) $ReCl_3(NC_6H_4COCH_3)(P(C_2H_5)_2C_6H_5)_2$, (E) $ReCl_3(NCH_3)(P(C_6H_5)_2C_2H_5)_2$, (F) $OsCl_3(NH_3)(P(C_6H_5)_3)_2$, AND (G) $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$

Atoms	A[d]	B[e]	C[f]	D[f]	E[g]	F[h]	G[i]
M[a]–N	1.61	1.79	1.71	1.69	1.69	2.14	1.96
M–Cl(trans)[b]	2.61	2.56	2.43	2.41	2.41	2.36	2.52
M–Cl(cis)	2.37 2.36 2.36	2.45	2.42	2.40 2.43	2.41 2.43	2.36	
M–P[c]		2.44 2.47 2.49	2.47	2.46 2.46	2.48 2.49	2.41	2.44 2.42 2.42 2.41
N···Cl(cis)	3.03 3.00 2.98	3.26	3.04	3.11 2.98	3.11 2.94	3.04	
Cl(cis)···Cl(trans)	3.32 3.27 3.35	3.37	3.34	3.30 3.28	3.34 3.28	3.49	
N···P		3.11 3.16 3.02	3.15	3.02 3.15	3.12 3.12	3.21	3.43 3.01 3.14 3.02
P···Cl(trans)		3.55 3.25 3.58	3.28	3.32 3.32	3.26 3.37	3.38	3.25 3.63 3.33 3.56

[a] M is the metal atom. [b] Cis and trans in the table show positions relative to the nitrogen. [c] All P atoms are cis. [d] See ref 6. [e] See ref. 7. [f] See ref. 16. [g] See ref 17. [h] See ref. 15. [i] This work.

Re–N bond distance is longer and the steric strain results mainly from the placement of four PR_3 groups cis to the nitrogen atom. In $ReNCl_2(P(C_2H_5)C_6H_5)_3$,[7] the cis chlorine atom and one PR_3 group bend toward the trans chlorine atom to give Cl–Re–Cl and P–Re–Cl bond angles of 84.36 (15) and 80.90 (14)°, respectively. The other two PR_3 groups cannot bend toward the nitrogen atom because of the short Re–N bond distance and the N–Re–P bond angles, 91.8 (4) and 89.1 (4)°. This leads to N···P interactions which range from 3.024 (13) to 3.164 (11) Å and P···Cl(trans) interactions which range from 3.249 (6) to 3.578 (6) Å. In the present study of $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$, two PR_3 groups bend toward the chlorine atom to give Cl–Re–P bond angles of 82.1 (1) and 84.8 (1)°, but now the other two PR_3 groups may bend more toward the nitrogen atom resulting in N–Re–P bond angles of 86.3 (4) and 87.0 (4)°. Three of the N···P interactions, 3.016 (16), 3.144 (17), and 3.031 (16) Å, compare well with the range found in $ReNCl_2(P(C_2H_5)_2C_6H_5)_3$,[7] but the N···P1 distance of 3.437 (17) Å is longer. This is the result of the close approach of C6 of ring 1 to the nitrogen atom leading to an N···H6*R1* distance of 2.6 Å. The P···Cl(trans) interactions also compare well with the distances found in $ReNCl_2(P(C_2H_5)_2C_6H_5)_3$,[7] except for the longer P2···Cl(trans) distance of 3.633 (6) Å. Possibly once P1 has made a close approach to the chlorine atom with a P1···Cl(trans) interaction of 3.257 (5) Å, steric balance is achieved with P2 being further from the chlorine atom. The bending of the two PR_3 groups toward the trans chlorine atom prohibits a close approach of this atom to the rhenium atom and results in the long Re–Cl bond length of 2.521 (4) Å. Since now two PR_3 groups may bend toward the nitrogen atom when the other two groups bend toward the trans chlorine atom, there is no need to lengthen the Re–P bonds to relieve steric hindrance. In $ReNCl_2(P(C_2H_5)_2C_6H_5)_3$,[7] the two PR_3 groups which do not bend are found to have Re–P bond distances of 2.490 (5) and 2.469 (5) Å. The PR_3 group which is bent toward the trans chlorine atom has a bond distance of 2.442 (4) Å. In $ReCl(N_2)(P(CH_3)_2C_6H_5)_4$, three of the Re–P distances are 2.418 (4), 2.421 (3), and 2.413 (4) Å, similar to the Os–P distance of 2.411 (2) Å found in the unstrained complex $OsCl_3(NH_3)(P(C_6H_5)_3)_2$.[15] The Re–P1 bond distance of 2.435 (3) Å is slightly longer, possibly because of the close approach of C6 of ring 1 to the nitrogen atom. Just as has been found earlier in our studies of metal–nitrogen multiple bonds,[6] a simple steric explanation will suffice to describe these structures and their differences.

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