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The Structure of a Metal–Cyclobutenyl Complex, $[(CH_3)_4C_4C_5H_5]NiC_5H_5$[1]

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The structural determination of the Criegee–Ludwig–King compound of composition $C_{13}H_{17}NiC_5H_5$ has revealed the first proven example of a cyclobutenyl–metal complex. The crystals contain four formula units in an orthorhombic unit cell of symmetry $P2_12_12_1$ (D_2^4) and dimensions $a = 11.66 \pm 0.03$ Å., $b = 11.77 \pm 0.03$ Å., $c = 11.41 \pm 0.03$ Å. The final three-dimensional isotropic least-squares refinement has yielded discrepancy factors of $R_1 = 7.8\%$ and $R_2 = 10.2\%$ for 970 observed reflections. The structure consists of discrete molecules of approximately C_s-m symmetry in which each nickel(II) is covalently bonded to a π-cyclopentadienyl anion and a nonplanar 1,2,3,4-tetramethyl-1-*exo*-cyclopenta-1′,3′-dienecyclobutenyl anion. The latter is symmetrically coordinated to the nickel(II) *via* the allylic fragment of the cyclobutenyl ring system. The planes of the allylic carbons and the cyclopentadienyl ring carbons are essentially parallel with the nickel(II) sandwiched between them. The detailed geometries of the rings and resulting stereochemistry are discussed.

Introduction

The reaction of sodium cyclopentadienide with tetramethylcyclobutadienenickel dichloride[4,5] was first carried out by Criegee and Ludwig,[6] who obtained a diamagnetic, red, volatile solid of composition $C_{13}H_{17}NiC_5H_5$. From degradation studies with *p*-toluenesulfonic acid in benzene and from hydrogenation experiments, Criegee and Ludwig[6] proposed a 4,5,6,7-tetramethyl-8,9-dihydroindenyl residue symmetrically bonded to the nickel atom *via* a π-allylic group in the five-membered ring. An independent investigation of this complex was made by King,[7] who from the compound's n.m.r. spectrum suggested a different type of interaction of the same dihydroindenyl system with the nickel atom. King's postulated model involved the coordination of the nickel both to one of the two double bonds in the six-membered ring *via* a μ-type bond and to a carbon atom in the five-membered ring *via* a σ-type bond. In order to elucidate the structure and nature of bonding of this complex, a three-dimensional X-ray analysis was performed. The subsequent results showed both proposed configurations to be incorrect and instead revealed the first proven example of a cyclobutenyl–metal complex.

Experimental

A sample of the compound was kindly made available to us by Dr. R. B. King of the Mellon Institute. Suitable single crystals were obtained by sublimation *in vacuo* (0.01 mm., 70°). A crystal of an average width of 0.03 cm. was used for obtaining intensity data. The value of 0.2 for μR of this crystal is sufficiently small that absorption corrections were neglected. The crystal density was measured by the flotation method in mixtures of nitromethane and carbon tetrachloride.

The unit cell dimensions were obtained from precession photographs taken on a camera calibrated with a sodium chloride crystal.

Multiple-film equi-inclination photographs were taken for 13 reciprocal levels (*hk*0 through *hk*12) with Zr-filtered Mo Kα radiation. The intensity data which consist of 970 independent reflections were visually estimated with the aid of a calibrated standard and then corrected for Lorentz-polarization effects. Corrected intensities from precession photographs of 0*kl* and 1*kl* data were obtained and used to place the Weissenberg intensities on an initial common scale. The final scale-factor adjustment of the resulting structure factor amplitudes (*i.e.*, $|F_o| \sim I_0^{1/2}$) for different Weissenberg levels was made by least-squares refinement.

Crystal Data

Crystals of $[(CH_3)_4C_4C_5H_5]NiC_5H_5$ are orthorhombic and belong to the space group $P2_12_12_1$ (D_2^4).[8] The systematic absences are $h00$ for h odd, $0k0$ for k odd, $00l$ for l odd. The unit cell dimensions are $a = 11.66 \pm 0.03$ Å., $b = 11.77 \pm 0.03$ Å., $c = 11.40 \pm 0.03$ Å.; volume of unit cell = 1565 Å.^{3}; $\rho_{\mathrm{obsd}} = 1.33$ g. cm.$^{-3}$ *vs.* $\rho_{\mathrm{caicd}} = 1.28$ g. cm.$^{-3}$ for four molecules per unit cell. The total number of electrons per unit cell, $F(000) = 632$. The linear absorption coefficient for Mo Kα radiation (λ 0.7107 Å.) is 13 cm.$^{-1}$. All atoms occupy the general fourfold set of positions (4a): $x, y, z;\ {}^1/_2 - x, -y, {}^1/_2 + z;\ {}^1/_2 + x, {}^1/_2 - y, -z;\ -x, {}^1/_2 + y, {}^1/_2 - z$. The asymmetric unit consists of one molecule comprised of one nickel, eighteen carbon, and twenty-two hydrogen atoms.

Determination of the Structure

A trial set of coordinates for the asymmetric nickel was obtained from a three-dimensional Patterson map computed with the Sly–Shoemaker program.[9] A complication arose immediately in that the determined z-coordinate of approximately ${}^3/_4$ meant that the four nickel atoms in the unit cell were related to one another by a higher symmetry (*i.e.*, if the present origin is shifted by ${}^1/_4$, 0, 0, the nickel atoms are in set 4c of Pbnm (D_{2h}^{16})[8]) than the actual crystallographic symmetry of $P2_12_12_1$ imposed on the molecules in the unit cell. When only these nickel coordinates were

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[8] "International Tables for X-Ray Crystallography," Vol. I, The Kynoch Press, Birmingham, England, 1952.

[9] W. G. Sly and D. P. Shoemaker, "Two- and Three-Dimensional Crystallographic Fourier Summation Program for the IBM 704 Computer," MIFR1 (1960).

used to determine the phases of the observed structure amplitudes from which the first approximation to a three-dimensional electron density map was calculated, the peaks obtained conformed to the higher space group symmetry Pbnm. The result of this pseudo-symmetry was that besides the approximately correct peaks, mirror images were observed, and the assignment of atoms to these peaks thus was somewhat difficult. The first calculated Fourier map yielded about 70 peaks in the asymmetric unit cell, only 19 of which could possibly represent actual atomic positions. The interpretation of the Fourier maps was further complicated by our initial assumption that the basic dihydroindenyl system proposed both by Criegee and Ludwig[6] and King[7] was essentially correct. Attempts to find an indenyl ring system in the first and subsequent Fourier maps failed. From the first map phased only on the nickel atoms the coordinates of five peaks, which seemed to represent a five-membered carbon ring, were eventually obtained. At this point the Patterson map was re-examined; a careful plotting of the contours of the nickel peaks revealed the possibility that the z-coordinate of the asymmetric nickel atom might be slightly different from $^3/_4$. Even a small shift in the z-coordinate would help to reduce the unwanted effect of false carbon peaks due to the previously mentioned pseudo-symmetry. An assumed noncentrosymmetric z-coordinate (of value 0.752) for the nickel was used together with the coordinates of the five ring carbons to obtain a new set of phases from which a better approximation of the electron density map was obtained. This successive Fourier technique at first gave several false structures due to the assignment of wrong peaks as atoms, but finally all the nonhydrogen atoms in the asymmetric unit were unambiguously located. The nickel and 18 carbon positions obtained from the last electron density map yielded an unweighted discrepancy value of $R_1 = [\Sigma||F_o| - |F_c||/\Sigma|F_o|] \times 100 = 14.9\%$.

An isotropic least-squares refinement of the structure was performed by the application of five cycles of a block diagonal program.[10] The discrepancy value calculated for the fifth cycle was $R_1 = 8.1\%$. The final refinement was achieved by the calculation of three cycles with the full-matrix least-squares Busing–Levy program.[11] This final refinement of all the nonhydrogen atomic positions with isotropic thermal parameters for each atom and different scale factors for each reciprocal layer of data resulted in discrepancy values of $R_1 = 7.8$ and $R_2 = [(\Sigma w||F_o| - |F_c||^2)^{1/2}/(\Sigma w|F_o|^2)^{1/2}] \times 100 = 10.2\%$. The weights ($w$) for the individual reflections were assigned as

$$\sqrt{w} = 20/F_o \qquad \text{if } I_0 \geq \sqrt{10}I(\text{min.})_0$$

$$\sqrt{w} = 2I_0{}^2/F_oI(\text{min.})_0{}^2 \qquad \text{if } I_0 < \sqrt{10}I(\text{min.})_0$$

The refined structure was confirmed by a calculation of a three-dimensional difference synthesis[9] which revealed no residual peak heights greater then 0.5 electron/Å.^{3}. For the calculation of structure factors the atomic scattering factors of Freeman and Watson[12] for nickel and of Freeman[13] for carbon were used. Table I shows the positional and isotropic thermal parameters together with their standard deviations obtained from the final least-squares cycle. The observed and calculated structure factors from the last cycle of the least-squares refinement are listed in Table II. The intramolecular bond lengths and angles along with their standard deviations were calculated with the Busing–Levy function and error program[14] and are listed in Tables III and IV.

All intermolecular distances less than 4.0 Å. were calculated[14] and are given in Table V. The shortest of these distances is 3.57 Å., which suggests the absence of any interactions between molecules other than those of the van der Waals type. Table VI lists the equations of the "best" molecular planes defined by a given number of atoms and the perpendicular distances of these and other atoms from the planes.[15] Some of the more important dihedral angles between planes are presented in Table VII.

Discussion

The structure of $[(CH_3)_4C_4C_5H_5]NiC_5H_5$ represents a new type of π-allylic complex whose configuration is defined by the parameters in Table I. The molecular configuration can be described as a sandwich-type complex in which a nickel(II) lies between a π-cyclopentadienyl anion and a substituted cyclobutenyl anion. The resulting compound, π-cyclopentadienyl-1,2,3,4-tetramethyl-1-*exo*-cyclopenta-1′,3′-dienecyclobutenyl-nickel(II), conforms to the "inert gas configuration" for the nickel atom (*i.e.*, only the bonding MO's are occupied) in agreement with its observed diamagnetism. The molecular configuration of this complex projected down the [010] direction is shown in Figure 1.

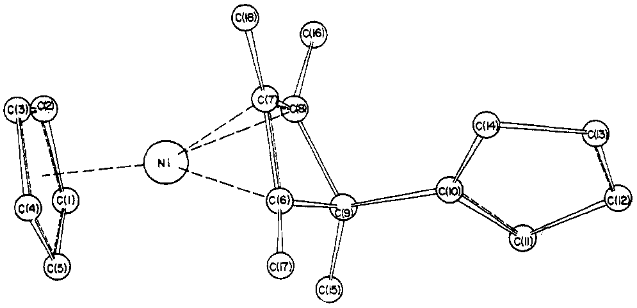

Figure 1.—Molecular configuration of $[(CH_3)_4C_4C_5H_5$ NiC_5H_5 projected down the [010] direction.

The molecular parameters given in Figure 2 indicate that the molecule in the solid state has approximately Cs-m symmetry. The mirror plane contains the

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Table I

Final Atomic Parameters with Standard Deviations

	x	y	z	B, Å.^{2}	$10^4\sigma_x$	$10^4\sigma_y$	$10^4\sigma_z$	σ_B
Ni	0.3351	0.2068	0.7557	3.15	1.2	1.2	1.6	0.04
C_1	0.4538	0.0765	0.7090	5.29	15	16	16	0.36
C_2	0.4781	0.1132	0.8242	5.07	16	16	15	0.38
C_3	0.5083	0.2278	0.8211	5.13	14	17	14	0.37
C_4	0.4971	0.2654	0.7037	4.44	14	14	14	0.34
C_5	0.4677	0.1708	0.6348	4.38	12	14	14	0.33
C_6	0.1996	0.2980	0.7043	3.05	11	14	11	0.24
C_7	0.2133	0.2854	0.8294	3.26	11	14	11	0.26
C_8	0.1818	0.1678	0.8176	2.72	10	11	10	0.24
C_9	0.1255	0.1894	0.6931	2.80	10	11	11	0.22
C_{10}	−0.0041	0.2156	0.7124	3.41	11	13	10	0.24
C_{11}	−0.0866	0.1628	0.6515	4.71	13	14	15	0.33
C_{12}	−0.2037	0.2066	0.6959	5.59	16	18	16	0.33
C_{13}	−0.1761	0.2942	0.7755	7.02	16	17	25	0.60
C_{14}	−0.0487	0.2996	0.7882	4.90	13	15	14	0.33
C_{15}	0.1462	0.1070	0.5947	3.31	11	13	12	0.28
C_{16}	0.1518	0.0769	0.9055	4.72	14	16	15	0.36
C_{17}	0.2010	0.4018	0.6257	4.99	15	15	15	0.37
C_{18}	0.2347	0.3614	0.9318	4.61	13	14	15	0.34

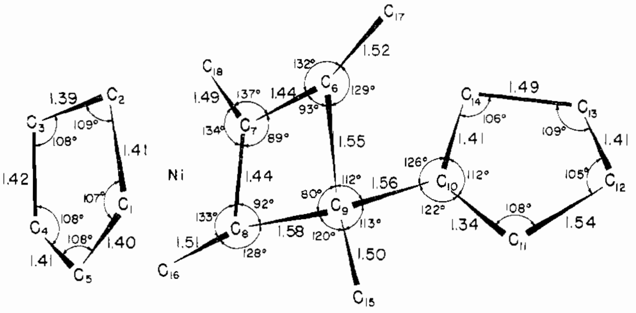

Figure 2.—Schematic drawing of $[(CH_3)_4C_4C_5H_5]NiC_5H_5$ with molecular parameters.

cyclopentadiene ring carbons (C_{10}–C_{14}), the nickel atom, two methyl carbons (C_{15}, C_{18}), and symmetrically cuts the cyclopentadienyl anion at C_3 and the midpoint of C_1–C_5 and the cyclobutenyl anion at C_7 and C_9. The eleven atoms defining the "mean" plane (Table VI, a) all show deviations from this noncrystallographic mirror plane of less than 0.18 Å., and furthermore the perpendicular distances of the symmetry related pairs of atoms from this plane all agree within 0.08 Å.

The π-cyclopentadienyl ring is symmetrically bonded to the nickel and is planar within the accuracy of our data (Table VI, b). The perpendicular distances of these ring carbons from the "mean" plane vary between 0.002 and 0.022 Å. and consequently are all within 2 e.s.d. of each of the atomic coordinates. The perpendicular distance of the nickel atom from this "best" plane is 1.76 Å., which compares well with the corresponding perpendicular distance found in $C_5H_5NiC_5H_5C_2(CO_2CH_3)_2$ (1.75 Å.)[16] and as expected is somewhat longer than the corresponding distances found in ferrocene (1.66 Å.)[17] and $C_5H_5Co(CH_3C_2CH_3)_2CO$ (1.67 Å.).[18] Although the distances from the nickel to the carbons of the cyclopentadienyl ring in $[(CH_3)_4C_4C_5H_5]NiC_5H_5$ vary from 2.10 to 2.17 Å. (Table III), the deviations appear not to be statistically significant.

The average Ni–C_5H_5 distance of 2.13 Å. (individual e.s.d. 0.012–0.019 Å.) is in agreement with the average Ni–C_5H_5 distance of 2.13 Å. (individual e.s.d. 0.012–0.016 Å.) found in $C_5H_5NiC_5H_5C_2(CO_2CH_3)_2$.[16] The five cyclopentadienyl C–C bond lengths are all within 1.39–1.42 Å. (individual e.s.d. 0.023–0.026 Å.). The average C–C ring distance of 1.406 Å. compares well with the corresponding average distances obtained by X-ray diffraction in $(C_5H_5)_2Fe$ (1.40 Å.),[17] $(C_5H_5)_2Ru$ (1.43 Å.),[19] $[C_5H_5Fe(CO)_2]_2$ (1.41 Å.),[20] $[C_5H_5Mo(CO)_3]_2$ (1.42 Å.),[21] $(C_5H_5)_2MoH_2$ (1.43 Å.),[22] $C_5H_5Mo(CO)_3C_2H_5$ (1.43 Å.),[23] $C_5H_5Mn(CO)_3$ (1.42 Å.),[24] $C_5H_5RhC_6(CF_3)_6$ (1.39 Å.),[25] $C_5H_5Co(CF_3C_2CF_3)_2CO$ (1.44 Å.),[26] $C_5H_5Co(CH_3C_2CH_3)_2CO$ (1.42 Å.),[18] and $C_5H_5NiC_5H_5C_2(CO_2CH_3)_2$ (1.43 Å.).[16] The observed equality of the cyclopentadienyl C–C bond lengths in $[(CH_3)_4C_4C_5H_5]NiC_5H_5$ together with the unusually small deviations (Table IV) of the bond angles (all of which are within 1.0° of 108°) from those of a regular pentagon demonstrate the C_{5v} localized symmetry of the ring carbons and provide no indication of any localized interaction between the nickel and the cyclopentadienyl ring. Of note is the considerable variation (in some cases not statistically significant) of the C–C bond lengths and angles generally found in the above and other cyclopentadienyl complexes which for several complexes has been attributed to a small localized metal–cyclopentadienyl interaction.[16,27]

The most significant feature of this complex is the cyclobutenyl portion of the molecule which contains an allylic fragment symmetrically bonded to the nickel. The nickel to carbon distances of 2.00 Å. (C_6), 1.89 Å.

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(C_7), 1.98 Å. (C_8), and 2.55 Å. (C_9) conclusively show that only three (C_6, C_7, and C_8) of the four cyclobutenyl ring carbons take part in the bonding to the nickel. Although the central carbon C_7 of this allylic fragment is closer than the two terminal carbons C_6 and C_8 to the nickel [1.89 ± 0.014 *vs.* 1.99 ± 0.010 (av.) Å.], the possible significance of this difference may be questioned in light of the rather large previously mentioned variations (2.10–2.17 Å.) in the five Ni–C_5H_5 distances. In any event these three allylic carbon to nickel distances are considerably shorter than the cyclopentadienyl carbon to nickel distances and compare much better with the olefinic carbon to nickel distances [1.97 Å. (av.)] observed in $C_5H_5NiC_5H_5C_2(CO_2CH_3)_2$[16] and the cyclobutadiene carbon to nickel distances [2.02 Å. (av.)] found in 1,2,3,4-tetramethylcyclobutadienenickel dichloride.[5] The allylic character of the ring carbon atoms C_6, C_7, and C_8 also is clearly shown by the equivalence of the two bond lengths C_6–C_7 and C_7–C_8, both of which are 1.44 Å. The two bond lengths joining the terminal carbons of the allylic fragment with the fourth tetrahedral-type ring carbon atom C_9 are 1.55 Å. (C_6–C_7) and 1.58 Å. (C_8–C_9). The four inner bond angles in the cyclobutenyl ring of 88.7° (C_7–C_8–C_9), 93.4° (C_7–C_6–C_9), 92.0° (C_7–C_8–C_9), and 80.1° (C_6–C_9–C_8) are all within $19 \pm 3°$ below the strain-free *idealized* values for three assumed trigonal and one assumed tetrahedrally hybridized carbon atoms, respectively. The nonplanarity of the four-membered cyclobutenyl ring is shown by the perpendicular distance of 0.50 Å. of the tetrahedral ring carbon C_9 from the plane defined by the allylic carbon atoms (Table VI, c). This large distortion results in a dihedral angle of 25° (Table VII) between the planes defined by atoms C_6–C_7–C_8 and C_6–C_9–C_8.

Attached to each of the four cyclobutenyl carbon atoms is a methyl group and in addition to the fourth (tetrahedral) carbon C_9 a cyclopentadiene group which is in the *exo* position with respect to the nickel.

Of interest is the relative displacement of each of the three allylic carbons from the plane defined by its three attached carbon neighbors. The central allylic carbon C_7 is displaced 0.05 Å., whereas the terminal two carbons C_6 and C_8 are displaced 0.21 and 0.23 Å., respectively, out of the corresponding planes of bonded carbon atoms. Hence, the terminal allylic carbons show considerably more distortion from an ideally trigonal character than is observed for the central carbons. It is also found that the three methyl carbons C_{16}, C_{17}, and C_{18} are deformed by 0.13–0.21 Å. away from the nickel out of the plane defined by the allylic fragment. This deformation of the σ-framework of the nickel-coordinated olefinic carbons is no doubt partly due to the unsymmetrical charge distribution arising from the partial donation of the π-electrons to the nickel(II), which relaxes to some extent the geometrical restrictions which the olefinic bonds place upon attached groups. A similar effect was observed by Dunitz, *et al.*,[5] in 1,2,3,4-tetramethylcyclobutadienenickel(II) chloride. In this organonickel complex the four methyl groups bonded to the cyclobutadiene ring are displaced out of the mean plane of the four cyclobutadiene carbons away from the nickel(II) by essentially the same amount (0.12–0.19 Å.). Although Dunitz, *et al.*,[5] suggested that this distortion may be attributed to steric interference due to the chlorine atoms, we feel that the deformations may be mainly rationalized on the basis of the arguments stated above. For $[(CH_3)_4C_4C_5H_5]NiC_5H_5$ the three methyl carbons attached to the allylic fragment all show bond lengths of 1.505 ± 0.010 Å., which is normal[28] for a carbon–carbon single bond between aliphatic and olefinic carbon atoms. The tetrahedral nature of the fourth ring carbon C_9 is easily recognized from the location of the attached carbon substituents. The two planes defined by carbons C_6, C_9, C_8 and C_{15}, C_9, C_{18} form a dihedral angle of 91.8°. The six bond angles which have C_9 as vertex are all within $114.5 \pm 7°$ (Table IV) except for the previously mentioned inner cyclobutenyl ring angle (C_6–C_9–C_8) of 80.1°.

The planarity of the cyclopentadiene ring attached to C_9 is easily verified by a "best" plane calculation (Table VI, d) which shows no deviations of ring carbons by more than 0.032 Å. from this plane. This C_5H_5 ring contains two localized double bonds, which from the observed bond lengths can be ascertained as occurring between carbon atoms C_{10}–C_{11} and C_{12}–C_{13}. The cyclopentadiene ring is approximately perpendicular to both the allylic fragment and the coplanar cyclopentadienyl group.

A reinterpretation of the high resolution n.m.r. spectrum of $[(CH_3)_4C_4C_5H_5]NiC_5H_5$ as measured by King[7] is found to be compatible with the correct molecular configuration. The spectrum shows a sharp, strong peak at τ 4.94 which can be assigned to the five identical π-cyclopentadienyl protons. The peaks due to the four methyl hydrogen groups are centered at τ values of 7.66, 8.46, 9.05, and 9.09. The relative location of these methyl hydrogen resonances enables an assignment of the 9.05 and 9.09 values to the methyl groups attached to the two terminal carbons of the π-allylic fragment. The closeness of these two τ values indicates the nearly identical surroundings of these methyl groups which for the *idealized* C_s-m molecular symmetry are equivalent. The peaks centered at 8.46 and 7.66 then are assigned to the methyl groups attached to the tetrahedral-type cyclobutenyl carbon C_9 and to the central allylic carbon C_7, respectively. The resonances due to the hydrogens of the cyclopentadiene ring are found at τ 3.79 (singlet), 3.83 (doublet), 4.25 (doublet), 7.25 (singlet), and 7.45 (singlet); the peaks at 7.25 and 7.45 presumably represent the two hydrogens located on the aliphatic cyclopentadiene ring carbon C_{14}. These conclusions are in agreement with those made by King[29] based on these X-ray results.

From the molecular configuration one can speculate

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Table II
Comparison of Observed and Calculated Structure Factors

H	K	L	FO	FC	AC	BC
0	14	0	14.7	13.3	13.3	.0
	12		25.4	25.5	-25.5	.0
	10		49.7	50.5	50.5	.0
	8		44.9	47.3	-47.3	.0
	4		24.8	24.4	24.4	.0
1	10	0	7.8	7.6	.0	-7.6
	9		8.9	10.6	.0	10.6
	8		23.8	24.9	.0	24.9
	7		41.3	44.4	.0	-44.4
	6		30.9	32.1	.0	-32.1
	5		58.0	50.5	.0	50.5
	4		31.3	30.1	.0	30.1
	3		47.3	44.9	.0	-44.9
2	13	0	15.7	16.7	-16.7	.0
	12		13.5	14.4	14.4	.0
	11		17.9	19.3	19.3	.0
	10		17.0	20.1	-20.1	.0
	9		18.7	19.0	-19.0	.0
	8		16.4	17.3	17.3	.0
	7		21.3	22.3	22.3	.0
	6		12.5	13.6	-13.6	.0
	5		12.0	12.5	12.5	.0
	3		93.0	79.5	-79.5	.0
	2		19.7	22.9	22.9	.0
3	10	0	25.6	27.6	.0	27.6
	9		9.4	11.3	.0	11.3
	8		45.5	45.4	.0	-45.4
	7		19.9	21.2	.0	-21.2
	6		76.6	72.5	.0	72.5
	5		9.3	6.9	.0	6.9
	4		80.3	76.3	.0	-76.3
	3		45.1	42.2	.0	-42.2
	2		6.3	6.2	.0	-6.2
	1		68.1	54.7	.0	54.7
4	13	0	12.9	15.2	15.2	.0
	11		19.3	20.8	-20.8	.0
	10		11.1	15.5	-15.5	.0
	9		9.3	11.9	11.9	.0
	8		21.9	22.4	22.4	.0
	7		11.2	9.2	-9.2	.0
	6		13.3	12.7	-12.7	.0
	5		26.8	25.5	-25.5	.0
	3		83.2	75.2	75.2	.0
	2		13.6	9.3	-9.3	.0
	1		7.1	5.5	5.5	.0
	0		19.9	12.5	12.5	.0
5	9	0	20.7	21.4	.0	-21.4
	8		18.1	19.8	.0	19.8
	7		34.9	37.6	.0	37.6
	6		19.8	21.5	.0	-21.5
	5		52.3	50.8	.0	-50.8
	4		35.1	34.9	.0	34.9
	3		58.2	61.9	.0	61.9
	2		58.0	55.3	.0	-55.3
	1		29.8	33.2	.0	-33.2
6	12	0	15.1	16.3	-16.3	.0
	10		26.1	28.4	28.4	.0
	8		18.3	19.7	-19.7	.0
	4		35.8	36.4	36.4	.0
	3		14.5	11.4	11.4	.0
	2		83.7	77.1	-77.1	.0
	1		15.0	12.0	12.0	.0
	0		118.7	115.4	115.4	.0
7	7	0	21.1	19.4	.0	-19.4
	6		12.0	11.9	.0	-11.9
	5		29.5	31.0	.0	31.0
	4		18.2	21.9	.0	21.9
	3		46.7	48.0	.0	-48.0
	1		35.2	32.1	.0	32.1
8	13	0	10.3	12.2	-12.2	.0
	11		17.9	18.3	18.3	.0
	9		19.2	17.8	-17.8	.0
	8		13.9	15.4	15.4	.0
	7		8.0	9.8	9.8	.0
	3		27.7	33.0	-33.0	.0
	2		14.0	13.8	13.8	.0
	1		52.2	54.8	54.8	.0
	0		25.0	21.0	-21.0	.0
9	8	0	19.9	20.7	.0	-20.7
	7		8.4	11.1	.0	-11.1
	6		36.5	38.3	.0	38.3
	4		35.3	37.3	.0	-37.3
	3		19.5	16.7	.0	-16.7
	2		20.3	17.4	.0	17.4
	1		18.2	18.5	.0	18.5
10	11	0	12.4	12.4	-12.4	.0
	3		22.1	22.1	22.1	.0
	1		26.6	30.0	-30.0	.0
11	9	0	11.4	14.3	.0	-14.3
	7		22.9	25.3	.0	25.3
	5		22.8	22.2	.0	-22.2
	3		20.3	18.5	.0	18.5
	1		8.3	10.2	.0	-10.2
12	4	0	11.1	9.7	9.7	.0
	2		18.1	17.2	-17.2	.0
	0		18.4	17.7	17.7	.0
13	5	0	11.9	13.0	.0	13.0
	3		11.4	11.4	.0	-11.4
14	3	0	12.1	10.8	-10.8	.0
	1		14.5	16.8	16.8	.0
0	8	1	30.7	30.9	-30.9	.0
	6		56.9	56.5	56.5	.0
	4		72.6	72.2	-72.2	.0
1	13	1	12.5	12.7	2.0	-12.6
	11		26.8	25.1	3.8	24.8
	9		37.2	35.6	-10.6	-34.0
	7		15.2	14.4	3.0	14.1
	6		24.1	24.5	-11.2	-21.8
	5		13.8	11.3	-9.2	6.5
	4		21.1	18.7	-3.7	18.3
	3		24.9	30.9	20.3	-23.3
2	9	1	24.8	24.5	-24.3	-3.5
	7		46.1	44.1	42.8	-10.4
	6		23.9	25.1	-24.2	6.4
	5		54.9	54.3	-53.2	10.8
	4		30.8	24.6	24.5	1.7
	3		51.0	49.0	48.7	4.9
	2		35.3	33.2	33.2	-.6
3	14	1	9.8	13.3	-.0	-13.3
	12		22.7	23.6	4.4	23.2
	10		20.6	21.3	-3.2	-21.1
	8		18.3	18.6	-4.7	18.0
	6		12.1	11.8	4.4	-11.0
	5		11.3	10.3	6.9	7.7
	4		41.6	43.2	4.9	-42.9
	3		19.0	18.0	-8.0	16.1
	2		26.4	26.6	-4.8	26.1
	1		17.6	16.1	-6.4	-14.8
	0		65.7	54.9	.0	54.9
4	11	1	7.9	8.7	-7.8	3.8
	9		32.5	33.6	33.2	4.7
	8		14.5	15.9	15.9	.0
	7		51.1	52.4	-52.2	-4.7
	6		30.6	29.3	-29.3	-.8
	5		74.1	70.4	69.3	-12.4
	4		40.6	38.7	38.3	-5.7
	3		47.8	44.3	-44.0	4.7
	2		39.3	34.2	-34.2	.7
	1		14.3	12.5	.2	12.5
	0		10.1	8.1	.0	8.1
5	13	1	9.6	10.3	-1.0	10.2
	11		19.9	22.1	6.9	-21.0
	9		23.7	27.3	-8.3	26.1
	7		17.0	19.0	5.3	-18.2
	5		7.4	9.1	-4.8	-7.7
	3		52.4	49.1	-3.1	49.0
	2		15.8	15.8	9.1	-13.0
	1		73.4	71.4	6.5	-71.1
	0		17.2	14.9	.0	14.9
6	10	1	9.7	11.6	11.5	-.7
	8		30.5	31.0	-31.0	-.8
	7		10.5	11.9	10.8	4.9
	6		42.2	43.8	43.3	6.7
	4		50.7	50.5	-50.5	-.3
	3		16.4	17.3	17.3	-.5
	2		44.3	48.3	46.8	-11.8
	1		26.4	26.6	-26.6	.0
	0		14.1	13.7	.0	13.7
7	12	1	9.6	10.0	-.6	-9.9
	11		9.2	9.2	-1.7	9.1
	10		9.7	10.9	-1.4	10.8
	9		16.9	16.7	-6.0	-15.6
	7		9.9	9.0	2.7	8.5
	4		20.9	20.3	2.6	20.1
	3		6.9	10.5	1.1	-10.4
	2		53.4	49.4	-9.6	-48.4
	1		46.8	48.7	-2.1	48.6
8	9	1	9.3	8.6	-8.5	1.5
	7		18.1	17.7	17.5	-2.8
	5		19.6	22.1	-22.1	-.4
	3		14.2	16.4	15.2	6.0
	2		6.4	5.5	-2.0	5.1
9	12	1	12.4	14.4	2.0	14.3
	10		17.0	18.2	-1.3	-18.1
	8		16.6	16.5	1.5	16.4
	4		13.8	16.7	-6.8	-15.3
	3		6.9	8.0	5.5	5.9
	2		30.7	34.5	11.9	32.4
	1		9.9	9.4	-4.8	8.1
	0		39.2	41.7	.0	-41.7
10	8	1	9.1	13.2	13.2	.8
	7		15.5	16.4	-16.3	-1.1
	6		9.4	12.6	-12.6	-.6
	5		20.1	20.7	20.7	-1.0
	3		11.4	12.9	-12.9	.1
	2		11.2	13.3	-13.0	-2.8
11	4	1	9.1	8.5	-2.7	8.0
	3		13.5	13.6	-2.6	13.4
	2		8.8	10.5	-1.4	-10.4
	1		16.9	16.2	1.8	-16.1
12	4	1	19.8	20.2	-20.2	.3
	2		11.9	13.1	13.0	-1.8
13	2	1	15.7	14.4	-2.1	-14.2
	0		14.2	13.2	.0	13.2
14	5	1	11.3	12.3	-12.2	1.2
	3		12.3	11.8	11.8	-1.0
15	2	1	9.5	11.6	.4	11.6
	0		13.1	15.8	.0	-15.8
0	14	2	11.1	13.4	-13.4	.0
	12		23.7	26.5	26.5	.0
	10		39.7	42.6	-42.6	.0
	8		44.5	45.4	45.4	.0
	5		29.2	27.6	.0	27.6
	4		93.9	78.7	-78.7	.0
	3		49.0	43.5	.0	-43.5
1	10	2	9.2	9.9	-8.2	5.4
	9		13.4	13.0	-.1	-13.0
	8		26.5	26.4	-2.9	-26.3
	7		33.1	33.4	9.8	31.9
	6		28.4	30.5	11.1	28.4
	5		60.9	57.8	5.4	-57.5
	3		72.3	65.2	.4	65.2
2	13	2	13.4	14.7	14.7	.1
	12		9.8	11.5	-10.9	-3.5
	11		22.3	24.5	-22.2	10.5
	10		19.6	20.0	17.2	-10.1
	9		27.1	29.3	25.4	-14.6
	8		22.3	22.6	-21.6	6.5
	6		19.4	19.5	18.7	5.5
	5		21.4	20.1	-19.9	2.9
	4		25.8	21.9	21.6	-3.7
	3		29.9	35.1	34.4	-6.7
	2		47.6	42.4	-33.3	26.2
3	10	2	18.7	20.5	-1.7	-20.4
	9		6.5	8.6	-7.3	-4.7
	8		44.9	46.5	3.0	46.4
	7		20.3	19.5	2.2	19.3
	6		72.7	67.4	-4.5	-67.2
	5		20.3	18.8	-5.1	-18.1
	4		68.3	65.6	-6.2	65.3
	3		9.5	12.6	1.2	12.5
	2		41.1	38.7	21.6	-32.1
	1		16.5	15.2	11.1	-10.3
	0		27.7	26.9	-26.9	.0
4	13	2	12.1	12.6	-12.1	3.6
	12		11.5	7.8	-7.5	-2.2
	11		18.4	19.5	19.3	-2.5
	10		9.8	9.9	9.6	2.5
	9		14.8	17.1	-16.0	-6.1
	8		16.4	15.6	-15.4	2.7
	6		21.4	22.3	22.0	3.6
	5		13.6	15.9	13.9	7.8
	4		14.5	13.0	-.8	-12.9
	3		42.6	42.3	-42.2	2.4
	2		16.0	14.9	-14.9	.7
	1		50.2	43.7	43.7	-2.0
5	9	2	15.9	16.4	3.7	15.9
	8		16.8	19.9	11.1	-16.5
	7		37.1	37.4	13.0	-35.1
	6		24.3	25.4	.6	25.4
	5		65.5	65.5	-13.6	64.1
	4		29.7	28.9	-9.6	-27.2
	3		43.5	44.7	-4.9	-44.4
	2		23.9	22.4	-.7	22.4
	1		9.2	7.2	7.0	1.4
6	12	2	16.6	18.6	17.6	6.0
	10		21.1	21.8	-21.0	-5.8
	8		16.1	16.3	16.1	-2.7
	4		35.0	36.4	-34.1	-12.8
	3		16.9	17.3	-4.8	16.6
	2		79.0	79.8	77.0	20.8
	1		19.3	18.3	-8.1	-16.4
	0		91.5	92.5	-92.5	.0
7	9	2	9.2	9.8	-.0	-9.8
	8		8.1	6.8	-1.3	-6.6
	7		23.8	25.3	3.0	25.1
	6		8.7	6.5	-.5	6.5
	5		29.2	31.2	.8	-31.2
	4		13.2	11.8	3.3	-11.4
	3		32.3	32.3	6.0	31.7
	2		14.7	14.9	1.5	14.8
	1		20.5	19.7	-9.4	-17.3
8	11	2	17.3	17.4	-17.0	3.5
	9		20.1	20.2	20.2	-1.5
	8		10.8	10.8	-10.5	2.5
	5		9.2	12.2	-12.2	-.1
	3		25.0	26.1	24.9	-7.7
	2		14.2	13.8	-13.7	-1.6
	1		46.4	49.5	-49.2	5.3
	0		24.5	26.2	26.2	.0
9	8	2	22.2	22.4	3.6	22.1
	6		33.4	33.7	-8.3	-32.6
	4		32.1	32.8	-.8	32.8
	2		27.6	29.2	10.0	-27.4
	0		12.3	9.3	-9.3	.0
10	11	2	10.2	10.8	10.7	-1.7
	9		12.2	12.4	-12.3	-1.8
	3		23.5	22.0	-21.6	4.0
	1		27.2	25.7	25.2	-5.2
11	7	2	20.1	18.8	-.6	-18.7
	5		25.7	25.2	-1.4	25.1
	3		19.0	19.3	1.4	-19.3
12	4	2	9.6	11.8	-10.2	-5.9
	2		18.7	18.6	17.5	6.4
	0		18.9	17.6	-17.6	.0
13	5	2	11.3	10.9	2.0	-10.7
	4		8.3	8.1	-4.5	-6.7
	3		11.8	11.0	.7	11.0
0	10	3	15.0	14.7	-14.7	.0
	8		30.8	30.9	30.9	.0
	6		50.3	49.5	-49.5	.0
	4		66.2	59.5	59.5	.0
1	13	3	12.1	13.1	-1.6	13.0
	11		20.4	20.4	-6.3	-19.4
	10		10.2	9.9	-2.3	-9.7
	9		29.8	29.0	16.6	23.8
	7		34.5	30.8	-14.9	-27.0
	6		22.9	21.7	4.2	21.3
	5		29.7	29.1	26.2	-12.7
	4		24.6	19.6	-19.6	-1.0
	3		107.1	82.0	-35.8	73.7
2	10	3	12.0	12.8	5.0	11.8
	9		22.7	24.9	24.9	-.3
	7		50.6	48.7	-47.1	12.4
	6		17.2	17.3	16.3	-5.9
	5		34.0	32.4	32.3	.7
	4		41.2	42.6	-42.2	5.5
	3		32.3	36.1	-32.6	-15.5
	2		37.0	30.8	30.4	-4.7
3	12	3	18.0	18.4	-3.1	-18.1
	10		26.9	28.2	4.6	27.8
	8		17.5	19.0	1.1	-19.0
	5		10.9	10.9	-10.0	4.4
	4		7.7	8.6	-.6	8.6
	3		12.0	10.8	-4.4	-9.9
	2		42.0	43.7	-11.0	-42.3
	1		15.1	12.7	9.5	-8.5
	0		104.4	88.0	.0	88.0
4	9	3	16.4	18.4	-18.4	.3
	7		39.5	39.4	39.4	.5
	6		35.9	35.2	35.0	2.8
	5		60.2	57.0	-56.7	5.8
	4		44.8	42.7	-42.4	4.8
	3		53.5	49.3	49.2	-2.8
	2		8.6	6.8	-6.0	-3.3
	1		20.3	17.3	-17.2	-1.3
	0		11.9	12.6	.0	-12.6
5	11	3	19.3	21.0	-10.9	18.0
	9		19.9	24.1	18.2	-15.7
	7		24.9	27.6	-16.3	22.2
	6		9.2	10.8	-8.2	7.1
	5		10.1	8.4	7.9	-2.8
	3		54.0	56.9	5.5	-56.6
	2		11.9	9.7	-1.6	9.5
	1		62.6	60.2	-7.4	59.8
	0		19.5	21.1	.0	-21.1
6	10	3	9.6	9.1	-9.1	.7
	8		22.5	24.2	23.0	7.4
	6		43.0	44.4	-44.0	-5.5
	4		52.8	50.2	49.6	-7.6
	3		10.4	9.4	7.8	-5.2
	2		24.7	22.9	-17.3	15.0
	1		15.8	15.7	-10.0	-12.1
	0		14.7	16.6	.0	-16.6
7	11	3	11.9	11.5	.3	-11.5
	10		12.0	12.8	.9	-12.8
	9		11.9	11.7	5.8	10.2
	6		10.4	10.0	8.3	5.6
	4		20.7	18.8	-12.8	-13.8
	3		19.1	21.4	-6.2	20.4
	2		29.4	27.7	11.3	25.3
	1		28.8	33.1	7.6	-32.2
	0		36.5	36.8	.0	-36.8
8	9	3	13.0	13.5	13.4	-1.2
	7		22.2	22.9	-21.9	6.5
	5		15.1	14.5	14.2	-3.1
	3		24.6	25.5	-23.6	-9.8
	2		11.8	10.5	6.9	-7.9
	1		19.9	22.6	20.6	9.4
9	10	3	15.6	17.5	5.7	16.5
	8		14.4	14.7	-2.6	-14.5
	4		17.4	18.2	11.1	14.5
	2		27.6	28.3	-11.8	-25.7
	0		34.4	36.7	.0	36.7
10	7	3	13.8	13.5	13.4	1.0
	6		13.4	14.1	13.0	5.3
	5		18.4	19.6	-19.5	1.8
	4		14.6	17.6	-15.1	-8.9
	3		18.7	18.6	17.8	-5.4
	1		11.0	9.6	-7.0	6.5
11	6	3	10.3	5.2	-4.5	-2.6
	3		15.1	16.3	1.5	-16.2
	2		10.0	10.3	-.7	10.3
	1		19.5	18.3	.5	18.3
12	6	3	14.1	16.4	-16.0	-3.7
	4		17.5	19.3	19.3	.1
	2		10.4	10.0	-9.4	3.3
13	2	3	12.7	12.1	4.8	11.1
	1		12.3	12.1	2.9	-11.8
	0		16.5	17.5	.0	-17.5
0	12	4	23.4	25.4	-25.4	.0
	10		25.4	27.9	27.9	.0
	8		27.6	27.5	-27.5	.0
	7		19.5	18.4	.0	18.4
	5		17.0	18.3	.0	-18.3
	4		60.8	68.3	68.3	.0
1	9	4	21.2	20.5	-3.1	20.3
	8		15.4	16.5	-1.4	16.4
	7		41.8	39.2	1.5	-39.2
	6		25.7	25.3	-1.4	-25.2
	5		53.8	55.5	-3.0	55.4
	4		19.7	20.9	-6.0	20.0
	3		54.8	54.0	-8.5	-53.3
2	13	4	11.4	12.5	-12.4	1.3
	12		10.7	7.6	7.6	.3
	11		20.3	23.4	22.9	-4.5
	9		28.5	29.6	-27.7	10.4
	8		15.1	14.1	13.1	-5.3
	6		20.9	19.3	-18.3	6.3
	5		24.1	22.9	22.5	-3.8
	4		14.8	14.4	-12.4	7.3
	3		30.1	32.4	-28.0	16.4
	2		43.9	40.5	36.9	-16.7
3	10	4	11.6	12.7	4.8	11.7
	9		10.0	10.4	9.9	-3.4
	8		33.9	35.2	-11.6	-33.2
	6		59.9	54.3	-3.7	54.2
	5		15.2	13.5	-8.4	10.6
	4		67.9	67.8	17.1	-65.6
	3		8.6	8.2	7.5	-3.3
	2		54.2	55.5	-12.4	54.1
	1		8.4	8.5	-7.8	-3.5
	0		14.3	13.3	13.3	.0
4	12	4	11.3	9.2	8.7	3.2
	11		16.3	16.0	-16.0	-.1
	10		11.8	10.8	-10.8	.0
	9		19.9	20.2	20.0	-3.1
	8		11.6	12.1	10.5	6.0
	7		9.6	11.3	-9.4	6.2
	6		10.7	12.6	-8.4	-9.3
	4		14.3	14.4	-12.7	-6.8
	3		30.0	27.1	25.8	-8.5
	2		33.3	30.4	30.1	4.4
	1		78.8	76.0	-75.4	9.1
	0		32.6	26.0	-26.0	.0
5	9	4	13.3	13.2	-2.0	-13.0
	7		26.8	27.2	-7.5	26.1
	6		18.7	19.9	1.4	-19.8
	5		50.0	50.0	6.0	-49.6
	4		16.7	17.5	-4.5	16.9
	3		40.6	36.6	-.6	36.6
	0		17.5	16.1	16.1	.0
6	12	4	15.4	15.9	-15.8	-1.8
	10		18.3	18.4	17.2	6.6
	8		15.1	16.5	-16.5	.4
	6		12.2	16.4	7.0	-14.9
	4		30.1	34.6	29.9	17.5
	3		14.1	14.0	-.6	-14.0
	2		58.6	59.6	-56.8	-18.0
	0		56.1	55.6	55.6	.0
7	9	4	14.4	16.3	-6.4	15.0
	8		14.2	15.0	-1.2	15.0
	7		24.8	26.9	2.7	-26.8
	6		13.2	13.9	-7.1	-12.0
	5		28.2	27.6	7.0	26.6
	4		11.0	10.6	6.6	8.3
	3		19.9	20.0	-5.5	-19.2
	2		17.5	16.9	5.3	-16.1
	0		8.6	8.1	-8.1	.0
8	11	4	13.5	13.0	12.2	-4.6
	9		16.1	15.7	-14.8	5.2
	8		9.9	6.5	6.4	.9
	4		7.8	6.6	-6.2	-2.3
	3		21.0	20.8	-20.4	4.2
	2		13.8	13.6	12.9	4.5
	1		36.4	37.7	37.7	2.0
	0		17.5	17.4	-17.4	.0
9	8	4	20.9	22.2	-4.8	-21.7
	6		29.4	29.0	5.5	28.5
	4		27.8	27.5	.6	-27.5
	2		25.8	25.7	-6.4	24.8
	0		10.0	10.6	10.6	.0
10	3	4	14.8	14.4	14.3	1.8
	2		12.6	12.7	12.0	4.2
	1		24.0	22.2	-22.2	1.2
	0		15.1	14.1	-14.1	.0
11	5	4	21.5	22.1	4.6	-21.6
	4		11.3	11.3	2.1	11.1
	3		15.9	16.9	-1.8	16.8
12	2	4	17.4	17.0	-17.0	-.6

TABLE II (*Continued*)

H	K	L	FO	FC	AC	BC
	0		20.9	19.7	19.7	.0
0	10	5	14.3	14.6	14.6	.0
	8		42.6	43.0	-43.0	.0
	6		52.5	50.5	50.5	.0
	4		24.6	23.9	-23.9	.0
1	11	5	16.2	15.9	3.7	15.5
	9		18.1	17.7	-10.7	-14.1
	8		13.1	12.4	2.4	-12.1
	7		21.6	21.3	18.7	10.4
	6		9.6	9.8	-8.8	4.3
	5		28.8	30.0	-29.7	4.3
	4		34.4	34.4	32.6	11.1
	3		40.7	42.2	30.7	-29.0
2	10	5	8.9	8.4	-5.4	-6.4
	9		14.4	14.8	-14.7	.9
	8		22.8	23.0	19.1	12.9
	7		29.9	31.7	31.3	4.9
	6		25.9	25.4	-24.6	-6.5
	5		44.5	44.6	-43.1	-11.2
	4		29.0	31.0	28.2	-13.0
	3		27.4	28.7	28.5	2.5
	2		32.2	33.7	-27.7	19.1
3	12	5	13.1	15.6	-.4	15.6
	10		23.5	24.0	-4.1	-23.7
	8		21.4	20.5	2.1	20.4
	7		11.6	10.1	-10.1	-.1
	4		25.3	24.0	-4.1	-23.6
	3		11.5	12.2	12.0	-2.3
	2		65.6	67.9	6.5	67.6
	0		89.9	91.7	.0	-91.7
4	8	5	13.3	13.0	12.0	-4.9
	7		17.8	18.6	-17.7	5.8
	6		16.0	16.3	-14.9	-6.6
	5		42.7	41.8	41.6	-3.9
	4		23.7	23.9	21.6	10.3
	3		44.0	45.4	-44.7	7.9
	2		21.2	22.2	-22.1	1.4
	1		20.1	18.4	16.2	-8.8
5	11	5	17.7	18.6	6.5	-17.4
	9		20.4	23.9	-14.2	19.2
	8		8.5	9.2	-5.3	-7.5
	7		13.6	15.7	13.4	-8.1
	5		11.0	11.2	-4.1	-10.5
	4		12.6	12.0	1.5	11.9
	3		31.0	31.3	5.9	30.7
	2		13.9	13.0	.8	-12.9
	1		43.8	45.9	-6.2	-45.5
	0		14.3	13.8	.0	13.8
6	8	5	19.6	19.8	-18.9	-5.8
	7		7.7	6.5	-6.3	1.5
	6		30.1	29.6	29.3	-3.7
	5		11.7	12.5	6.8	-10.5
	4		34.7	34.5	-34.3	4.3
	3		10.1	10.4	-9.0	5.3
	2		24.4	26.3	26.2	-1.4
	1		10.1	10.5	4.9	9.3
7	9	5	11.8	13.0	-.1	-13.0
	7		10.8	9.4	8.7	3.7
	6		13.6	13.3	-12.6	4.1
	5		17.5	18.9	-11.3	15.1
	4		26.8	26.1	24.5	9.2
	3		24.7	25.4	8.2	-24.1
	2		18.3	18.9	-12.7	-14.0
	1		17.9	20.1	-5.2	19.5
	0		11.1	9.1	.0	9.1
8	9	5	14.2	11.1	-10.9	2.0
	7		25.6	23.4	22.8	-5.3
	5		28.4	28.2	-28.2	1.9
	4		8.1	8.0	6.9	-4.0
	3		22.4	22.9	21.3	8.7
	2		10.1	10.8	-8.5	6.7
	1		16.1	15.9	-7.5	-14.0
	0		9.9	9.1	.0	-9.1
9	4	5	13.5	12.1	-6.5	-10.2
	2		23.6	23.5	.4	23.5
	0		29.9	29.8	.0	-29.8
10	7	5	12.8	13.4	-13.4	-1.0
	6		12.5	12.7	-10.3	-6.5
	5		14.4	16.5	16.5	-.9
	4		13.2	12.6	10.6	6.9
	3		19.9	18.5	-14.8	11.0
	1		14.4	11.5	6.2	-9.6
11	1	5	22.5	23.8	-1.1	-23.7
	0		11.8	11.2	.0	11.2
12	4	5	13.5	13.2	-13.1	1.3
13	1	5	12.2	11.6	-.5	11.6
0	12	6	16.3	16.6	16.6	.0
	10		21.2	21.0	-21.0	.0
	8		12.3	12.9	12.9	.0
	6		11.0	9.0	9.0	.0
	5		8.6	10.0	.0	-10.0
1	9	6	22.1	23.9	4.6	-23.5
	7		45.8	44.5	-7.1	43.9
	6		25.0	24.8	-1.8	24.8
	5		40.7	40.9	3.2	-40.8
	4		35.5	34.7	-7.1	-33.9
	3		35.6	37.3	12.8	35.1
2	13	6	12.2	11.3	11.1	-2.2
	11		16.5	16.9	-16.9	1.1
	9		19.2	19.3	19.3	.9
	7		21.3	21.2	-18.6	-10.1
	5		13.3	13.8	-9.3	10.3
	3		48.8	52.2	52.1	1.5
	2		18.7	20.9	-20.3	-5.2
3	8	6	20.1	18.9	3.4	18.6
	7		10.3	9.2	5.6	-7.4
	6		41.2	40.9	.6	-40.9
	5		10.4	13.2	11.4	6.5
	4		61.6	59.1	4.2	58.9
	3		16.7	15.4	-15.0	3.5
	2		30.9	35.0	3.6	-34.8
	1		10.6	11.1	9.4	-6.0
	0		20.2	21.7	-21.7	.0
4	11	6	13.5	13.1	12.9	-2.5
	10		12.8	14.0	13.9	2.2
	9		17.8	16.4	-15.7	4.6
	8		10.9	10.4	-5.3	-8.9
	7		13.5	16.0	15.9	-2.3
	6		10.0	12.3	-12.2	1.6
	4		17.8	18.2	13.3	12.4
	3		35.1	35.3	-35.2	-2.6
	2		25.8	24.4	-24.4	.9
	1		55.3	54.3	54.1	4.1
	0		44.3	42.9	42.9	.0
5	9	6	16.7	16.6	4.0	16.1
	7		23.6	23.9	-4.9	-23.4
	6		12.7	11.2	4.5	10.2
	5		19.3	18.2	-.8	18.2
	4		13.0	12.4	-4.3	-11.7
	3		31.6	30.0	10.8	-28.0
	1		24.6	23.1	-9.0	21.3
6	10	6	17.8	18.0	-17.9	-2.0
	8		15.8	16.2	15.5	-4.8
	6		15.3	15.9	1.6	15.8
	4		18.3	20.3	-16.1	-12.3
	3		9.7	9.4	-.0	9.4
	2		29.7	30.4	29.8	5.8
	0		42.8	40.9	-40.9	.0
7	9	6	12.8	13.6	4.2	-12.9
	8		12.6	9.8	-2.7	-9.5
	7		22.2	23.1	-2.8	23.0
	6		22.6	22.4	6.5	21.4
	5		25.0	24.7	1.4	-24.6
	4		20.3	20.4	-2.4	-20.3
	3		18.8	18.5	-1.9	18.4
	1		12.9	13.1	-10.8	-7.4
	0		8.9	8.4	8.4	.0
8	9	6	10.5	8.1	7.8	-2.3
	7		11.0	10.7	-10.7	-.0
	5		10.1	9.6	-1.2	9.5
	4		10.3	13.0	10.7	7.3
	3		24.3	24.5	23.2	-7.8
	2		12.6	12.0	-12.0	.2
	1		26.2	25.0	-25.0	.1
	0		10.5	9.5	9.5	.0
9	8	6	14.4	14.6	1.2	14.5
	6		24.5	23.9	2.9	-23.7
	4		26.2	25.4	-.9	25.3
	2		13.0	13.0	-2.3	-12.8
10	3	6	7.6	7.0	-7.0	-.2
	2		16.1	15.1	-14.8	-3.1
	1		19.7	18.1	18.1	-.6
	0		27.6	26.3	26.3	.0
11	3	6	13.5	12.2	.4	-12.2
12	2	6	15.2	14.6	14.6	.5
	0		18.2	18.5	-18.5	.0
0	10	7	10.3	12.0	-12.0	.0
	8		27.1	27.8	27.8	.0
	6		38.1	36.5	-36.5	.0
	5		8.2	15.6	.0	15.6
	4		26.7	29.1	29.1	.0
	3		7.9	5.6	.0	-5.6
1	11	7	16.6	14.1	-1.6	-14.0
	9		19.2	17.0	8.3	14.8
	8		17.9	19.7	-10.5	16.7
	6		27.0	29.3	23.8	-17.1
	5		22.7	23.4	20.1	-11.9
	4		25.0	23.1	-19.4	-12.5
	3		19.2	22.7	-18.9	12.6
	2		25.0	28.0	.9	28.0
2	10	7	11.7	12.1	9.4	7.7
	8		18.3	19.4	-17.9	-7.5
	7		21.4	23.0	-20.7	-10.0
	6		20.7	20.8	18.2	10.1
	5		41.6	41.9	41.0	8.4
	4		19.7	17.3	-16.2	6.1
	3		31.1	31.9	-31.6	4.0
	2		28.8	29.9	16.5	-24.9
3	12	7	15.2	14.0	-1.1	-14.0
	10		17.0	16.7	1.9	16.6
	8		15.8	16.9	2.2	-16.7
	6		12.3	10.1	-5.8	8.3
	4		26.5	28.0	2.5	27.9
	2		55.8	60.1	-1.9	-60.0
	1		9.4	8.8	-5.4	-6.9
	0		58.9	64.3	.0	64.3
4	8	7	18.4	16.0	-15.8	2.8
	7		13.4	13.1	13.0	-1.3
	6		10.9	11.4	9.5	6.3
	5		25.9	25.2	-21.7	12.8
	4		11.5	11.6	-5.1	-10.4
	3		26.8	27.6	24.1	-13.5
	2		18.1	17.6	16.4	6.3
	1		15.3	15.7	-10.8	11.3
5	9	7	14.6	13.5	3.3	-13.1
	8		10.6	10.3	2.4	10.0
	5		12.0	11.6	4.8	10.5
	4		11.1	9.4	-1.9	-9.2
	3		15.5	15.5	-10.2	-11.7
	2		18.3	19.6	-6.1	18.7
	1		33.3	34.5	6.5	33.8
	0		16.4	17.1	.0	-17.1
6	8	7	19.0	18.0	17.8	-3.0
	6		24.7	24.6	-24.2	4.5
	5		11.6	11.7	-11.4	-2.7
	4		21.2	21.8	21.0	6.0
	2		17.2	17.4	-16.3	-6.0
7	9	7	11.2	12.0	4.1	11.3
	6		13.4	12.1	10.7	-5.7
	5		14.4	14.0	11.7	-7.8
	4		20.8	21.1	-20.4	-5.7
	3		20.8	20.4	-10.0	17.8
	2		16.2	15.2	13.0	8.0
	1		23.6	24.3	3.3	-24.1
8	7	7	17.1	16.8	-16.8	.4
	6		13.4	12.7	12.5	2.3
	5		33.0	31.2	31.1	1.7
	4		9.7	11.7	-11.6	-.3
	3		22.9	22.6	-21.4	-7.2
	1		12.0	10.8	3.0	10.4
9	4	7	10.0	9.4	1.3	9.3
	2		21.1	19.4	-1.2	-19.4
	0		22.8	21.1	.0	21.1
10	4	7	12.1	7.6	-7.5	-1.2
	3		19.1	16.4	12.2	-10.9
	2		13.4	11.9	11.6	2.8
	1		13.6	12.6	-6.1	11.0
11	1	7	19.3	18.6	-1.1	18.6
0	10	8	15.0	12.8	12.8	.0
	8		11.9	10.2	-10.2	.0
	5		13.4	12.9	.0	12.9
	4		11.8	10.7	10.7	.0
1	9	8	16.8	17.0	-2.9	16.7
	7		25.7	25.7	2.8	-25.5
	6		19.0	19.4	2.0	-19.3
	5		32.3	34.6	-2.4	34.5
	4		24.4	25.6	-3.5	25.3
	3		24.6	28.0	-7.8	-26.9
2	11	8	13.4	11.8	11.7	1.5
	9		16.7	17.3	-15.6	-7.4
	7		22.6	22.3	16.8	14.7
	6		12.5	13.7	13.6	-1.8
	5		13.3	8.8	-.2	-8.8
	4		14.4	15.1	-11.9	-9.3
	3		29.7	31.5	-31.0	5.9
	2		11.2	12.8	11.3	6.0
3	8	8	20.1	18.6	.5	-18.6
	6		26.4	27.2	1.2	27.2
	4		31.0	31.7	-6.7	-30.9
	3		10.5	11.6	8.8	7.6
	2		25.7	29.2	1.9	29.2
	1		17.3	21.7	-21.2	-4.5
4	11	8	12.0	11.2	-11.1	1.6
	9		11.5	12.4	12.4	-.5
	7		11.2	10.9	-9.6	5.1
	5		9.8	5.3	-3.6	-3.9
	4		10.2	11.7	-11.6	-1.3
	3		22.3	23.1	22.7	3.8
	2		21.2	23.0	22.8	-3.0
	1		35.1	37.2	-36.9	-4.4
	0		30.7	30.9	-30.9	.0
5	9	8	13.2	13.2	-4.9	-12.3
	7		23.1	21.4	6.7	20.3
	6		12.6	9.3	-2.8	-8.8
	5		18.6	17.1	-1.6	-17.0
	4		12.9	12.2	5.7	10.8
	3		14.7	14.1	-8.2	11.5
	2		11.4	10.7	-5.3	-9.4
	1		13.4	13.0	11.7	-5.6
6	10	8	14.2	12.3	12.0	-2.4
	4		11.3	10.5	8.6	6.1
	2		18.4	20.7	-18.8	-8.8
	0		24.1	23.9	23.9	.0
7	7	8	18.7	17.9	1.2	-17.8
	6		18.6	16.3	-1.8	-16.2
	5		26.9	25.2	-4.2	24.8
	4		21.1	19.0	-2.8	18.8
	3		16.6	15.8	1.4	-15.7
	2		11.1	11.1	4.3	-10.2
8	3	8	16.3	15.1	-14.1	5.3
	2		9.7	10.2	10.0	1.9
	1		20.5	19.4	19.3	-1.9
	0		15.1	14.2	-14.2	.0
9	6	8	13.3	13.8	-3.2	13.4
	4		17.8	17.7	-2.4	-17.5
	2		13.9	12.6	4.6	11.8
10	2	8	18.1	15.4	15.2	-2.8
	1		15.0	11.3	-11.2	1.5
	0		17.2	15.4	-15.4	.0
12	0	8	14.6	13.0	13.0	.0
0	6	9	28.4	26.1	26.1	.0
	4		32.4	34.8	-34.8	.0
1	11	9	11.7	10.5	1.2	10.4
	10		12.6	12.2	-5.0	11.2
	9		10.3	9.5	-3.8	-8.8
	8		17.4	16.7	11.0	-12.5
	6		14.9	15.9	-13.8	7.8
	5		14.0	15.0	-11.2	10.0
	4		13.8	13.3	12.2	5.3
	3		20.2	22.5	5.1	-21.9
	2		19.5	22.3	-9.9	-20.0
	1		12.2	17.9	2.9	17.6
2	10	9	9.7	9.0	-6.8	-5.9
	9		8.3	6.4	-6.3	1.0
	8		11.6	11.5	10.9	3.7
	7		20.8	17.7	17.4	3.3
	6		12.7	13.1	-12.5	-4.0
	5		25.1	24.5	-23.3	-7.9
	4		11.1	10.3	9.8	-3.1
	3		28.9	29.9	29.6	4.5
	2		16.3	17.5	-4.9	16.8
	1		14.2	17.5	-17.0	-4.1
	0		18.4	21.4	.0	-21.4
3	10	9	16.2	14.9	1.3	-14.9
	8		13.5	12.4	-1.6	12.3
	4		12.9	13.4	-.8	-13.4
	3		9.6	9.2	-7.4	-5.4
	2		30.8	35.4	8.6	34.4
	0		43.1	52.3	.0	-52.3
4	10	9	10.0	7.7	-5.0	5.8
	8		9.8	8.7	8.0	-3.3
	7		14.9	14.1	-14.1	.3
	6		13.6	11.1	-11.0	-.9
	5		10.8	9.7	8.9	-3.9
	4		10.9	8.9	8.8	1.2
	3		15.6	14.1	-11.7	7.8
	2		13.3	11.0	-.9	-10.9
	1		20.0	22.3	10.2	-19.8
	0		21.8	21.3	.0	21.3
5	8	9	10.7	9.0	-3.6	-8.3
	3		15.7	15.6	3.2	15.3
	2		15.8	15.9	2.9	-15.7
	1		15.7	16.6	1.3	-16.5
	0		15.7	17.9	.0	17.9
6	6	9	22.0	20.4	20.3	-1.8
	4		20.4	18.4	-18.1	-3.2
7	9	9	11.6	9.0	-5.0	-7.5
	4		9.3	7.1	7.0	-.7
	3		18.5	16.7	8.0	-14.6
	1		22.6	21.4	-4.4	20.9
	0		15.8	14.4	.0	14.4
8	7	9	15.7	13.5	13.4	1.9
	6		11.7	10.2	-10.2	-1.1
	5		20.9	17.3	-17.2	-2.0
	4		12.2	10.9	10.3	-3.5
	3		20.0	17.6	16.9	5.0
	1		11.2	9.9	-7.9	-6.0
9	7	9	10.2	5.7	-3.2	4.8
	5		11.8	6.9	6.7	-1.7
	3		11.8	10.3	-8.3	-6.0
	2		15.9	13.7	1.0	13.7
	0		20.3	18.1	.0	-18.1
10	3	9	13.4	10.6	-8.0	7.0
11	3	9	12.6	10.6	2.9	10.2
	1		12.5	11.0	-1.6	-10.8
0	4	10	8.0	7.4	-7.4	.0
	3		5.9	4.0	.0	4.0
	2		12.1	15.1	15.1	.0
1	9	10	13.9	9.8	1.5	-9.7
	8		11.8	9.9	-1.4	-9.8
	7		17.7	17.2	-1.8	17.1
	6		13.2	12.6	-1.0	12.6
	5		25.9	24.4	-1.5	-24.3
	4		15.9	15.5	6.2	-14.3
	3		12.8	13.8	3.9	13.3
	2		11.4	11.2	-1.4	11.1
2	9	10	16.0	14.9	12.7	7.8
	7		11.7	11.5	-7.8	-8.4
	4		12.7	11.4	10.1	5.2
	3		18.7	17.8	12.8	-12.3
	2		12.4	12.8	-12.8	.4
	1		28.7	34.5	-33.1	9.6
	0		12.1	14.7	14.7	.0
3	8	10	15.8	13.2	.5	13.2
	6		17.6	17.2	.3	-17.2
	4		14.3	17.1	.1	17.1
	2		20.6	21.1	-4.2	-20.6
	1		18.3	19.7	19.1	4.8
4	9	10	13.3	11.9	-11.6	2.7
	4		16.1	14.6	12.6	-7.4
	3		12.9	12.6	-11.1	-5.9
	2		15.8	17.3	-16.3	5.8
	1		21.0	24.2	24.0	2.7
	0		11.0	12.9	12.9	.0
5	7	10	15.2	12.5	-3.1	-12.2
	6		11.5	7.8	-.6	7.8
	5		21.2	17.3	1.0	17.3
	3		14.3	12.0	3.0	-11.6
	2		12.2	11.2	7.9	7.9
	1		9.0	9.4	-9.1	2.5
	0		14.0	14.6	-14.6	.0
6	4	10	11.1	9.1	-9.1	-.9
	2		15.3	13.7	12.4	5.8
	1		9.3	6.7	6.5	1.6
	0		7.8	8.9	-8.9	.0
7	8	10	13.8	8.7	1.4	-8.6
	6		14.3	11.0	-2.1	10.8
	5		19.6	16.8	-1.5	-16.7
	4		14.1	11.7	4.5	-10.9
	3		15.8	14.6	2.4	14.4
	2		13.9	13.0	-2.0	12.8
8	2	10	9.3	8.0	-7.6	-2.6
	1		18.2	15.3	-15.3	-.4
9	2	10	10.9	7.0	-3.3	-6.2
10	2	10	13.6	13.0	-10.9	7.0
0	8	11	12.0	10.6	10.6	.0
	6		17.2	16.5	-16.5	.0
	4		18.8	18.7	18.7	.0
	3		7.9	7.6	.0	7.6
	2		7.0	9.5	-9.5	.0
1	5	11	10.1	6.8	5.8	-3.5
	4		11.3	9.3	-7.3	-5.7
	3		14.1	14.8	-.8	14.8
	2		12.4	14.6	5.8	13.4
	1		16.9	18.2	-1.6	-18.2
2	8	11	11.6	7.8	-6.6	-4.1
	7		15.5	11.5	-11.5	-.4
	6		11.7	9.5	9.5	-.3
	5		19.6	17.7	17.6	1.0
	3		17.3	17.7	-17.2	-4.0
	2		8.2	8.6	3.6	-7.7
	1		8.3	10.3	6.9	7.7
	0		9.6	9.1	.0	9.1
3	9	11	13.2	9.2	1.1	-9.1
	5		9.8	7.7	-7.4	-2.0
	3		8.3	7.8	7.6	1.5
	2		16.9	18.8	.8	-18.8
	0		23.5	26.8	.0	26.8
4	6	11	11.5	8.0	7.4	-2.8
	5		11.6	10.1	-10.1	.4
	4		11.7	9.0	-9.0	-.8
	3		10.9	9.2	8.0	-4.7
	2		13.8	11.2	5.8	9.6
	1		14.7	13.3	-4.0	12.7
	0		17.5	17.5	.0	-17.5
5	4	11	10.1	6.1	5.4	-2.8
	3		12.8	9.9	-2.9	-9.5
	2		11.4	10.3	-5.8	8.5
	1		12.8	11.8	-.0	11.8
	0		11.0	12.1	.0	-12.1
6	6	11	13.1	11.9	-11.9	.6
	4		14.7	12.6	12.6	.6
	2		12.0	9.6	-8.7	-4.1
	1		9.8	4.4	-2.9	-3.3
	0		9.7	5.6	.0	5.6
7	3	11	13.9	10.3	-.3	10.3
	1		15.6	12.5	.1	-12.5
	0		16.0	11.6	.0	-11.6
8	5	11	13.9	10.4	9.8	3.7
9	2	11	13.7	10.3	.6	-10.3
0	2	12	8.9	10.0	-10.0	.0
1	7	12	13.0	10.8	1.3	-10.7
	6		12.4	8.9	-.4	-8.9
	5		12.2	10.1	1.2	10.0
	4		13.0	9.5	-1.0	9.4
	3		12.2	11.5	-2.5	-11.3
	2		6.5	5.8	5.4	-1.9
2	3	12	12.2	12.1	-11.6	3.7
	2		12.2	11.4	11.3	1.1
	1		12.0	13.2	13.1	-1.5
	0		11.6	14.5	-14.5	.0
3	6	12	18.0	13.0	-1.3	13.0
	4		14.6	13.8	-1.0	-13.7
	1		8.6	7.4	-7.3	-1.6
4	4	12	11.4	9.7	-4.1	8.8
	3		14.6	11.6	9.0	7.2
	2		13.1	11.8	8.6	-8.0
	1		14.6	14.5	-14.0	-3.8
	0		14.6	13.6	-13.6	.0
5	7	12	16.3	10.1	2.0	9.9
	5		12.3	10.3	.5	-10.3
	3		15.4	12.0	-2.6	11.8
	1		10.9	8.0	3.0	-7.4
6	2	12	11.7	8.0	-7.6	2.6
	0		15.9	11.9	11.9	.0
7	6	12	14.7	8.5	3.4	-7.8
	4		14.0	9.4	-4.5	8.3

TABLE III

INTRAMOLECULAR DISTANCES WITH STANDARD DEVIATIONS

Bond	Length, Å.	Std. dev., Å.	Bond	Length, Å.	Std. dev., Å.
Ni–C_1	2.133	0.019	C_6–C_7	1.444	0.019
Ni–C_2	2.146	0.019	C_6–C_9	1.548	0.020
Ni–C_3	2.168	0.017	C_6–C_{17}	1.515	0.024
Ni–C_4	2.098	0.017	C_7–C_8	1.439	0.021
Ni–C_5	2.114	0.012	C_7–C_{18}	1.492	0.023
Ni–C_6	1.998	0.014	C_8–C_9	1.585	0.017
Ni–C_7	1.892	0.014	C_8–C_{16}	1.507	0.022
Ni–C_8	1.976	0.013	C_9–C_{10}	1.559	0.017
Ni–C_9	2.554	0.013	C_9–C_{15}	1.503	0.020
C_1–C_2	1.411	0.026	C_{10}–C_{11}	1.340	0.020
C_2–C_3	1.394	0.026	C_{10}–C_{14}	1.412	0.020
C_3–C_4	1.416	0.024	C_{11}–C_{12}	1.545	0.022
C_4–C_5	1.405	0.023	C_{12}–C_{13}	1.411	0.027
C_5–C_1	1.404	0.025	C_{13}–C_{14}	1.495	0.020

TABLE IV

BOND ANGLES WITH STANDARD DEVIATIONS

Bond	Angle, deg.	Std. dev., deg.	Bond	Angle, deg.	Std. dev., deg.
C_1–C_2–C_3	108.8	1.5	C_9–C_8–C_{16}	127.9	1.2
C_2–C_3–C_4	107.7	1.4	C_8–C_9–C_{10}	107.9	0.9
C_3–C_4–C_5	107.6	1.5	C_6–C_9–C_{15}	120.3	1.0
C_4–C_5–C_1	108.5	1.5	C_{10}–C_9–C_{15}	112.9	1.0
C_5–C_1–C_2	107.3	1.7	C_6–C_9–C_{10}	111.5	1.0
C_6–C_7–C_8	88.7	1.3	C_8–C_9–C_{15}	119.9	1.1
C_6–C_9–C_8	80.1	0.9	C_9–C_{10}–C_{11}	122.1	1.3
C_7–C_6–C_9	93.4	1.3	C_9–C_{10}–C_{14}	125.6	1.2
C_7–C_8–C_9	92.0	1.0	C_{10}–C_{11}–C_{12}	108.0	1.5
C_7–C_6–C_{17}	131.8	1.7	C_{11}–C_{12}–C_{13}	104.7	1.5
C_9–C_6–C_{17}	128.5	1.1	C_{12}–C_{13}–C_{14}	108.7	1.7
C_6–C_7–C_{18}	137.0	1.7	C_{13}–C_{14}–C_{10}	106.0	1.5
C_8–C_7–C_{18}	133.8	1.2	C_6–Ni–C_8	61.0	0.6
C_7–C_8–C_{16}	132.8	1.2			

TABLE V

INTERMOLECULAR DISTANCES LESS THAN 4.0 Å.[a]

Atoms	Distance, Å.	Atoms	Distance, Å.
$C_{12}\cdots C_3^{I}$	3.66	$C_{18}\cdots C_{17}^{II}$	3.64
$C_{12}\cdots C_4^{I}$	3.56	$C_{18}\cdots C_{13}^{III}$	3.95
$C_{12}\cdots C_5^{I}$	3.92	$C_{16}\cdots C_{15}^{IV}$	3.86
$C_{13}\cdots C_3^{I}$	3.80	$C_4\cdots C_1^{V}$	3.84
$C_{13}\cdots C_4^{I}$	3.91	$C_5\cdots C_{11}^{VI}$	3.86

[a] Superscripts refer to the following positions.

I	$-1 + x$	y	z
II	$^1/_2 - x$	$1 - y$	$^1/_2 + z$
III	$^1/_2 + x$	$^1/_2 - y$	$2 - z$
IV	$^1/_2 - x$	$-y$	$^1/_2 + z$
V	$1 - x$	$^1/_2 + y$	$^3/_2 - z$
VI	$^1/_2 + x$	$^1/_2 - y$	$1 - z$

that the mechanism of the reaction of tetramethylcyclobutadienenickel dichloride with sodium pentadienide[6,7] involves a nucleophilic attack of the second cyclopentadienyl ring on one of the carbons of the cyclobutadiene fragment with a concomitant migration of the hydrogen attached to the reacting cyclopentadienyl carbon to an adjacent carbon to give a cyclopentadiene moiety (structure I). The formation of two other cyclopentadiene isomers which differ in the relative location of the two double bonds is theoretically possible (structures II and III).

TABLE VI

EQUATIONS OF MOLECULAR PLANES AND DISTANCES (Å.) OF ATOMS FROM THESE PLANES[a]

(a) Plane through C_3, C_{15}, C_{18}, C_7, C_9, C_{10}, C_{11}, C_{12}, C_{13}, C_{14}, Ni

$$0.0986x + 0.7550y - 0.6483z + 3.3711 = 0$$

C_3	−0.092	C_{12}	−0.173	C_4	1.097
C_{15}	0.093	C_{13}	0.049	C_{16}	−2.467
C_{18}	−0.039	C_{14}	0.150	C_{17}	2.545
C_7	0.019	C_1	−0.670	C_8	−0.975
C_9	0.073	C_5	0.732	C_6	1.041
C_{10}	0.014	C_2	−1.168	Ni	0.060
C_{11}	−0.099				

(b) Plane through C_1, C_2, C_3, C_4, C_5

$$0.9628x - 0.2317y - 0.1390z - 3.7648 = 0$$

C_1	−0.002	C_6	−3.452	C_{17}	−3.595
C_2	−0.012	C_7	−3.462	C_{18}	−3.592
C_3	0.021	C_8	−3.476	C_{15}	−3.357
C_4	−0.022	C_{16}	−3.706	Ni	−1.764
C_5	0.015				

(c) Plane through C_6, C_7, C_8

$$0.9611x - 0.2421y - 0.1327z - 0.3230 = 0$$

C_{15}	0.111	C_{17}	−0.161	C_9	−0.505
C_{16}	−0.211	C_{18}	−0.132	Ni	1.700

(d) Plane through C_{10}, C_{11}, C_{12}, C_{13}, C_{14}

$$0.0310x + 0.6808y - 0.7318z + 4.1968 = 0$$

C_{10}	−0.023	C_{12}	−0.029	C_{14}	0.002
C_{11}	0.032	C_{13}	0.018		

(e) Plane through C_2, C_4, C_6, C_8, Ni

$$-0.0832x - 0.6160y - 0.7834z + 8.6520 = 0$$

Ni	0.065	C_4	−0.042	C_8	−0.045
C_2	0.004	C_6	0.006		

(f) Plane through midpoints (MP) of bonds C_1–C_2, C_4–C_5, C_6–C_7, C_7–C_8, and Ni

$$-0.4077x - 0.5285y - 0.7446z + 9.3195 = 0$$

Ni	0.022	MP(C_7–C_8)	−0.022	C_5	0.642
MP(C_4–C_5)	−0.015	C_1	0.664	C_6	0.536
MP(C_1–C_2)	0.004	C_2	−0.657	C_8	0.469
MP(C_6–C_7)	0.011	C_4	−0.671	C_7	−0.514

(g) Plane through C_7, C_9, C_{17}

$$0.8723x - 0.3958y - 0.2872z + 1.8756 = 0$$

C_6 0.212

(h) Plane through C_6, C_8, C_{18}

$$0.9732x - 0.2102y - 0.0929z - 0.7829 = 0$$

C_7 0.054

(i) Plane through C_9, C_{16}, C_7

$$0.8768x - 0.3667y - 0.3112z + 1.9944 = 0$$

C_8 0.228

(k) Plane through C_6, C_8, C_9

$$0.7640x - 0.4733y - 0.4385z + 3.4032 = 0$$

C_{15}	1.136	C_{10}	−1.398

[a] The *x*, *y*, *z* in the plane equations are not fractional coordinates of Table I but represent the coordinates of any point in the unit cell expressed in terms of the lengths, *a*, *b*, *c*.

Noteworthy is that a similar reaction occurs when dicyclopentadienylrhodium(III) cation reacts with sodium cyclopentadienide to yield (C_5H_5)(1-*exo*-$C_5H_5C_5H_5$)Rh.[30] From n.m.r. studies and comparison

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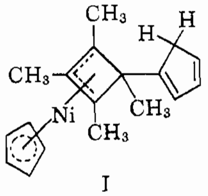
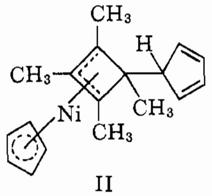
(30) R. J. Angelici and E. O. Fischer, *J. Am. Chem. Soc.*, **85**, 3733 (1963).



I



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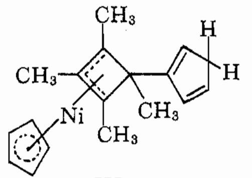


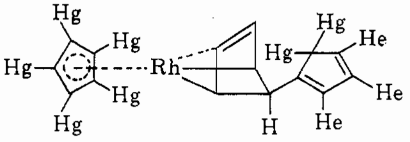
III

TABLE VII

DIHEDRAL ANGLES BETWEEN PLANES DEFINED IN TABLE VI

Planes	Angles, deg.
b, c	0.7
g, h	16.5
h, i	16.4
g, i	2.2
c, k	24.9

with the known X-ray structure[31] of (C_5H_5)(1-*exo*-$C_6H_5C_5H_5$)Co, structure IV was proposed, but a tentative assignment of the positions of the double bonds in the 1-*exo*-cyclopentadiene ring was not possible.[31] The n.m.r. spectrum of structure IV shows



IV

the typical resonances due to π-cyclopentadienyl (H_a) and cyclopentadiene (H_e, H_g) hydrogens as observed in $[(CH_3)_4C_4C_5H_5]NiC_5H_5$. For comparison these τ values are listed in Table VIII together with the corresponding values found in $[(CH_3)_4C_4C_5H_5]NiC_5H_5$. The close agreement of the observed τ values for the H_g and H_e hydrogens in the two complexes strongly supports the postulated configuration and suggests that the 1-*exo*-cyclopentadiene ring in (C_5H_5)(1-*exo*-$C_5H_5C_5H_5$)Rh is also bonded through the 2-position as in the case of $[(CH_3)_4C_4C_5H_5]NiC_5H_5$. However, before more definite conclusions can be drawn, the n.m.r. spectra of the two complexes should be measured and compared under identical conditions in the same solvent.

TABLE VIII

	(C_5H_5)(1-*exo*-$C_5H_5C_5H_5$)Rh[a]		$[(CH_3)_4C_4C_5H_5]NiC_5H_5$[b]	
H_e	3.69–4.35	(multiplet)	3.79–4.25	(multiplet)
H_a	4.96	(doublet)	4.94	(singlet)
H_g	7.46	(multiplet)	7.25 and 7.45	

[a] Measured in C_6D_6. [b] Measured in CS_2.

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Mass Spectrometric Studies of Chromium, Molybdenum, and Tungsten Hexacarbonyls[1]

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The appearance potentials of positive ions from chromium hexacarbonyl, molybdenum hexacarbonyl, and tungsten hexacarbonyl have been determined. The experimental data have been used to derive the heats of formation of various ionic species. The ionization potentials determined for the hexacarbonyls of chromium, molybdenum, and tungsten are 8.15 ± 0.17, 8.23 ± 0.12, and 8.56 ± 0.13 e.v., respectively. Comparisons of the energetics of the three compounds in the series are made along with their fragmentation schemes. From the determined energetic data, second ionization potentials have been calculated for a number of $M(CO)_x$ species.

Introduction

The increase in interest in the transition metal carbonyls over the past decade has arisen partly as a result of the discovery of many organometallic compounds in which the metal carbonyl system forms an integral part of the structure. The hexacarbonyls of chromium, molybdenum, and tungsten are well known. Infrared, Raman, electron diffraction, and X-ray measurements have shown that these compounds possess octahedral structures. Because an

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