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The Structure of Chlorocarbonyl(sulfur dioxide)bis(triphenylphosphine)rhodium, $RhCl(CO)(SO_2)(P(C_6H_5)_3)_2$

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The structure of chlorocarbonyl(sulfur dioxide)bis(triphenylphosphine)rhodium, $RhCl(CO)(SO_2)(P(C_6H_5)_3)_2$, has been determined by single-crystal X-ray analysis. The compound crystallizes in the space group C_{2h}^5-$P2_1/c$ of the monoclinic system, with four monomeric molecules in a cell of dimensions $a = 12.192$ (3) Å, $b = 17.020$ (4) Å, $c = 16.724$ (5) Å, and $\beta = 104.03$ (2)°. The structure has been refined by least-squares methods to a conventional R factor of 5.0%, over 3716 counter-diffractometer data. The compound is isostructural with the analogous iridium compound. The coordination around the rhodium atom is that of a tetragonal pyramid, with CO, Cl, and *trans* P atoms in the basal plane and the S of the SO_2 group at the apex. The basal interatomic distances are normal. The Rh–S distance of 2.450 (2) Å is long. The bond angles about S are all within 5° of the tetrahedral angle, and the Rh–S vector makes an angle of 30.3 (3)° with the normal to the SO_2 plane. These results may be rationalized in terms of the formation of a Rh–S σ bond through the donation of a pair of electrons from the Rh to the weak Lewis acid SO_2. The bonding of SO_2 to the metal here is contrasted with that in $[RuCl(NH_3)_4(SO_2)]Cl$, where the Ru–S bond is much shorter and the Ru lies in the SO_2 plane.

Introduction

In a previous study we called attention to the great difference between the coordination of SO_2 to Ir in $IrCl(CO)(SO_2)(P(C_6H_5)_3)_2$[1] compared with its coordination to Ru in $[RuCl(NH_3)_4(SO_2)]Cl$.[2] In the Ir complex the Ir–S bond length is 2.488 (10) Å and the Ir–S vector makes an angle of 31.6 (15)° with the normal to the SO_2 plane. In the Ru complex the Ru–S distance is only 2.072 (3) Å and the Ru–SO_2 fragment is planar. The differences in these bonding arrangements of SO_2 to transition metals were not understood.

Recently we have prepared and carried out determinations of the structures of the new nitrosyl complexes $[IrX(CO)(NO)(P(C_6H_5)_3)_2][BF_4]$, (X = Cl,[3,4] I[5]). We find that the structures of these NO complexes bear a striking resemblance to the SO_2 complex of Ir. Thus, in all three complexes the Ir coordination polyhedron is a tetragonal pyramid, with basal *trans*-phosphine groups and with either SO_2 or NO at the apex. The Ir–N bond length of 1.972 (11) Å in the chloro complex is very long, and in addition the Ir–N–O fragment is not linear, but rather the Ir–N–O angle is 124.1 (9)°. These results on the NO complexes were rationalized by describing the NO groups as being capable of acting either as a Lewis acid or as a Lewis base.[3] In the more common linear metal–N–O arrangement, the NO group may be thought of as a weak Lewis base, donating a pair of electrons to the metal, with subsequent back-donation from the metal to an empty ligand antibonding orbital. This leads to a short, multiple metal–N bond and to the linear arrangement. However, under circumstances that cannot be generally delineated at this time, the NO group can also act as a Lewis acid, receiving a pair of electrons from the metal. This leads to a metal–N σ bond which is longer than in the linear arrangement and to a M–N–O angle consistent with sp^2 hybridization at N.

The SO_2 ligand also appears to exhibit this amphoteric nature. Thus we would describe the Ir–SO_2 complex as one in which the SO_2 ligand has acted as a Lewis acid. The Ir–S bond is mainly σ in nature, and the Ir–SO_2 geometry is that of a shallow pyramid with S at the apex. In the Ru–SO_2 complex the SO_2 ligand has acted as a Lewis base, with subsequent multiple bonding between Ru and S resulting in a much shorter metal–S bond and in a planar Ru–SO_2 arrangement.

As a further test of this conclusion that certain ligands, notably NO and SO_2, can act either as Lewis acids or Lewis bases, we report here the determination of the structure of the analogous Rh–SO_2 complex, $RhCl(CO)(SO_2)(P(C_6H_5)_3)_2$, chlorocarbonyl(sulfur dioxide)bis(triphenylphosphine)rhodium. Although we anticipated, on the basis of the σ-bonding scheme, that there would be little difference between the Ir and Rh structures, we believed that it would be possible to obtain more precise structural information on the Rh complex, both because Rh does not dominate the scattering as much as Ir and because diffractometric data could be obtained for the Rh complex whereas film data were used for the Ir complex. More meaningful comparisons between the geometries of bound and free SO_2 would thus be possible.

In addition, this investigation represents one of an extended series of studies from this laboratory on closely related five-coordinate transition metal complexes.

Preparation of the Compound

A sample of $RhCl(CO)(P(C_6H_5)_3)_2$ was prepared.[6] The compound was dissolved in benzene, which had previously been refluxed under dry nitrogen for 20 min, to give a saturated solution at room temperature. SO_2 gas was passed into the solution at about 30° for 1.5 hr. The solution was then left overnight, at room temperature under an SO_2 atmosphere, and green, well-formed

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[3] D. J. Hodgson, N. C. Payne, J. A. McGinnety, R. G. Pearson, and J. A. Ibers, *J. Am. Chem. Soc.*, **90**, 4486 (1968).

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[5] D. J. Hodgson and J. A. Ibers, *ibid.*, **8**, 1282 (1969).

[6] J. A. McCleverty and G. Wilkinson, *Inorg. Syn.*, **8**, 211 (1966).

crystals separated out. These were filtered off, washed with ether, and dried in a stream of dry nitrogen gas.

The compound shows an infrared absorption band at 2035 cm^{-1} which may be ascribed to the CO stretching mode. (The parent Rh complex shows a CO stretching band at 1970 cm^{-1}.) Absorptions associated with the formation of the SO_2 complex occur at 1053 and 1208 cm^{-1}.

The preparation was carried out by Dr. N. C. Payne.

Collection and Reduction of the X-Ray Data

Preliminary optical and X-ray examination indicated that the crystals belong to the monoclinic system. From precession photographs of the reciprocal lattice layers 0*kl* and *h*0*l* through *h*2*l* the systematic absences were found to be *h*0*l* when *l* is odd and 0*k*0 when *k* is odd. These absences are consistent only with the space group C_{2h}^5-$P2_1/c$, and this determination has been confirmed by a successful structure analysis. The unit cell dimensions at 22°, obtained by a procedure described below, are a = 12.192 (3) Å, b = 17.020 (4) Å, c = 16.724 (5) Å, β = 104.03 (2)°, based on a value of 0.70930 Å for the wavelength of Mo Kα_1 radiation. For the analogous Ir complex, which also crystallizes in $P2_1/c$, the corresponding cell dimensions are a = 12.11 (2) Å, b = 16.79 (2) Å, c = 17.09 (2) Å, and β = 103.0 (5)°. Thus the two compounds are nearly isomorphous. The density of 1.51 (1) g/cm^3 observed for the Rh complex, by flotation in $CHCl_2CHCl_2$–C_2H_5Br, is in good agreement with the value of 1.489 g/cm^3 calculated for four molecules in the unit cell. Thus no symmetry conditions are imposed on the molecule by the space group.

For intensity measurements a needlelike crystal of roughly hexagonal cross section, 0.42 mm long and 0.25 mm in diameter, was cut from a larger crystal. It was mounted in air on a Picker four-circle automatic diffractometer with c^* (the long axis) nearly coincident with the ϕ axis. The mosaic spread of the crystal, as judged by narrow-source, open counter ω scans through a number of strong reflections, was small.[7] The mean half-width of the ω scans was 0.11°. Intensity measurements were made with the θ–2θ technique, following procedures which have already been described.[8] Fourteen reflections were accurately centered through a narrow vertical slit at a takeoff angle of 0.5°. These observations were used to determine the crystal orientation and cell dimensions by the method of least squares.[9] Each reflection was scanned from −0.8° to +0.8° in 2θ from the peak center at a takeoff angle of 2° and a scan rate of 1°/min. The background was counted for 10 sec at each end of the scan range. Molybdenum radiation was used in conjunction with a 3-mil Zr β filter. The pulse-height analyzer was set for approximately a 90% window centered on the Mo Kα_1 peak. Coincidence losses were minimized by insertion of Cu-foil attenuators until the maximum counting rate was less than 7000 counts/sec. The crystal-source distance was 21 cm and the crystal-detector distance was 30 cm. The counter aperture was 4 × 4 mm. A total of 4152 independent intensities were measured within the sphere 2θ(Mo Kα_1) $\leq$ 44°. Past this point an appreciable fraction of the reflections were still significantly above background. Since these reflections come mainly from the Rh scattering, we did not feel that their collection would allow us to determine the positions of the lighter atoms with much greater accuracy.

The intensities of four strong reflections were measured periodically throughout the experiment to check on crystal and electronic stability. No systematic variation on these standards was observed. One standard fluctuated by as much as 6% of its mean value; the other three varied by less than 2%. At the end of the experiment eleven strong reflections in the range 34° < 2θ < 40° were accurately centered. These were used for the determination of the final lattice constants. The crystal orientation derived from these reflections did not differ significantly from that derived initially.

The intensities were corrected for background and values of $\sigma(I)$ were derived, as previously described,[8] using a value of p of 0.06. The data were then corrected for Lorentz–polarization effects and for absorption. For the absorption correction the eight faces of the crystal were identified by optical goniometry and this identification was checked on the diffractometer. All members of the forms $\{010\}$, $\{001\}$, and $\{110\}$ were exhibited. The dimensions of the crystal were measured with a calibrated micrometer eyepiece. The resultant transmission factors ranged from 0.81 to 0.88 based on a linear absorption coefficient of 7.7 cm^{-1}. A total of 3716 independent reflections had intensities greater than their estimated standard deviations. Only these reflections were used in the analysis.

Structure Analysis

On the assumption that $RhCl(CO)(SO_2)(P(C_6H_5)_3)_2$ is nearly isostructural with its Ir analog[1] the final parameters from the Ir structure were taken as starting values for a full-matrix least-squares refinement of the structure of the Rh complex. The function minimized was $\Sigma w\Delta^2$, where $\Delta = |F_o| - |F_c|$, with $|F_o|$ and $|F_c|$ the observed and calculated structure amplitudes, respectively, and where $w = 4F_o^2/\sigma(F_o^2)$. The atomic scattering factors used throughout the analysis were taken from ref 10, with the exceptions of those for Rh[11] and H.[12] The anomalous dispersion corrections of Cromer[13] for Rh, Cl, S, and P were applied to the calculated structure factors.[14] In all refinements

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(9) The FORTRAN program PICK for the CDC 6400 was used. In addition to the other local programs used in this work, local modifications of Hamilton's GONO absorption correction program, Busing and Levy's ORFFE function and error program, Johnson's ORTEP thermal ellipsoid plotting program, and Zalkin's FORDAP Fourier program were employed.

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TABLE I

POSITIONAL, THERMAL, AND GROUP PARAMETERS FOR $RhCl(CO)(SO_2)(P(C_6H_5)_3)_2$

Atom	x	y	z	β_{11}[a]	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Rh	0.21386 (4)[b]	0.27063 (3)	0.26266 (3)	468 (4)	217 (2)	286 (2)	−10 (2)	84 (2)	0 (2)
S	0.27118 (13)	0.33610 (10)	0.39680 (9)	601 (13)	305 (7)	313 (7)	26 (8)	63 (8)	−30 (5)
Cl	0.27011 (13)	0.14131 (9)	0.30317 (10)	757 (14)	217 (6)	487 (8)	25 (7)	179 (9)	37 (6)
P(1)	0.39391 (12)	0.28594 (9)	0.23411 (9)	464 (12)	275 (7)	289 (7)	0 (7)	103 (7)	−5 (5)
P(2)	0.02639 (13)	0.23741 (9)	0.26577 (10)	473 (12)	237 (6)	319 (7)	−17 (7)	102 (7)	−7 (5)
O(1)	0.32220 (36)	0.40933 (25)	0.38095 (28)	888 (42)	302 (19)	504 (23)	−122 (23)	160 (25)	−101 (17)
O(2)	0.16918 (36)	0.34596 (30)	0.42642 (27)	769 (41)	579 (25)	419 (21)	−48 (25)	241 (24)	−136 (19)
O (of CO)	0.13552 (39)	0.42434 (29)	0.18509 (29)	941 (45)	340 (21)	551 (25)	122 (25)	109 (26)	157 (20)
C (of CO)	0.16519 (49)	0.36595 (40)	0.21404 (38)	565 (51)	308 (28)	335 (28)	−16 (31)	103 (30)	1 (24)

Group	x_c[c]	y_c	z_c	δ	ϵ	η
P(1)R(1)[d]	0.59457 (23)	0.30996 (17)	0.39698 (17)	2.5879 (33)	0.6168 (24)	0.9986 (33)
P(1)R(2)	0.46918 (24)	0.13596 (18)	0.14329 (17)	4.9163 (25)	0.2047 (27)	3.7144 (28)
P(1)R(3)	0.39544 (22)	0.43314 (19)	0.11426 (18)	3.0295 (44)	5.3865 (24)	4.5836 (42)
P(2)R(1)	−0.04938 (21)	0.10973 (16)	0.12176 (17)	5.5448 (38)	5.5129 (21)	4.4679 (37)
P(2)R(2)	−0.15827 (22)	0.37581 (17)	0.21495 (16)	5.5175 (27)	0.6805 (27)	6.1699 (31)
P(2)R(3)	−0.03176 (28)	0.15767 (20)	0.42528 (20)	4.3554 (32)	0.0565 (28)	2.1020 (31)

[a] The β_{ij} have been multiplied by 10^5; the form of the anisotropic temperature factor 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] Throughout this paper limits of error are estimated standard deviations and they are in units of the least significant digits of the quantities to which they refer. [c] x_c, y_c, and z_c are the fractional coordinates of the phenyl ring centroids; the angles δ, ϵ, and η (in radians) have been defined previously.[15] [d] P(1)R(1): phenyl ring 1 bonded to phosphorus atom P(1).

the phenyl rings were refined as groups,[15] with the rings constrained to D_{6h} symmetry and a C–C distance of 1.392 Å assumed. The initial refinement, in which all nongroup atoms were constrained to isotropic vibration and each atom of a given group was assigned an individual isotropic thermal parameter, converged after four cycles to values of R_1 and R_2 of 0.066 and 0.094, where the reliability indices are $R_1 = \Sigma |\Delta|/\Sigma|F_o|$ and $R_2 = (\Sigma w\Delta^2/\Sigma wF_o^2)^{1/2}$.

Fixed contributions for the scattering of the group hydrogen atoms were now added to the structure factors. The C–H distance was assumed to be 1.0 Å and all hydrogen atoms were assigned an isotropic thermal parameter of 5.5 Å^2. Further refinement resulted in values of R_1 and R_2 of 0.061 and 0.084. Additional calculations, in which anisotropic vibrational parameters were refined for the atoms Rh, Cl, S, P(1), and P(2), produced a significant drop in both reliability indices ($R_1 = 0.052$, $R_2 = 0.074$).

At this stage an error analysis made it apparent that the strong reflections had been excessively downweighted. New weights were calculated with a value of p of 0.038. In addition, a difference synthesis indicated that the oxygen atoms of the SO_2 ligand were undergoing appreciable anisotropic motion. Accordingly, in a final round of calculations, the new weighting scheme was applied and anisotropic thermal parameters were refined for all the nongroup atoms. The refinement converged to values of R_1 of 0.050 and R_2 of 0.062. In the final cycle the maximum value of the ratio (shift/standard deviation) was 0.3 for a nongroup positional parameter, 0.8 for a vibrational parameter, and 1.0 for a group positional parameter. The standard deviation of an observation of unit weight was 2.2, suggesting that the standard deviations of the intensities had been somewhat underestimated. The relative correctness of the weighting scheme, as judged by the variation of mean $w\Delta^2$ with $\lambda^{-1} \sin \theta$ and $|F_o|$, was satisfactory. Calculation of the structure factors for the 436 weak reflections omitted from the analysis revealed none which failed to meet one of the conditions $|\Delta|/\sigma(F_o) < 4$ or $F_c^2/\sigma(F_o^2) < 3$. Careful inspection of the low-angle data did not suggest that an extinction correction was necessary.

The values in a final difference synthesis ranged from 1.1 to −0.6 e$^-$/Å^3. All regions in which the electron density was greater than 0.3 e$^-$/Å^3 were close to the positions of the ring carbon atoms and presumably result from our failure to correct for the effects of anisotropic thermal motion of these atoms.

The final structure parameters are listed in Table I and the derived group carbon atom parameters are given in Table II. In Table III the final values of $|F_o|$ and $|F_c|$ (in electrons × 10) for the reflections used in the refinement are presented. In Table IV the root-mean-square amplitudes of vibration of the nongroup atoms are presented. They show no unusual features and, in particular, do not suggest that there is any disorder between the chlorine atom and the carbonyl group, such as occurs in the related molecular oxygen complexes.[16,17] No corrections have been made to the bond lengths (Table V) for the shortening due to the thermal motion, partly because the validity of such corrections is difficult to assess and partly because the corrections appear to be small and do not affect the conclusions drawn from the analysis.

Description of the Structure

Within the limits of experimental error $RhCl(CO)(SO_2)(P(C_6H_5)_3)_2$ is isostructural with the analogous Ir complex.[1] Crystals of both compounds contain discrete monomeric molecular species. Intermolecular distances are not presented here for the Rh complex since, without exception, they appear to represent normal van der Waals contacts. Perspective views of the entire molecule and of the coordination about the Rh atom are shown in Figures 1 and 2, respectively. The coordination polyhedron is a distorted tetragonal pyramid, with the S atom of the SO_2 ligand at the apex,

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TABLE II

DERIVED PARAMETERS FOR GROUP CARBON ATOMS[a]

Atom	*x*	*y*	*z*	*B*, Å^2
P(1)R(1)C(1)	0.5103 (3)	0.2994 (3)	0.3250 (2)	3.3 (1)
P(1)R(1)C(2)	0.5087 (4)	0.2555 (3)	0.3950 (3)	4.0 (1)
P(1)R(1)C(3)	0.5930 (4)	0.2661 (2)	0.4669 (2)	5.2 (2)
P(1)R(1)C(4)	0.6789 (3)	0.3205 (4)	0.4690 (2)	5.2 (2)
P(1)R(1)C(5)	0.6804 (4)	0.3644 (3)	0.3990 (3)	5.1 (2)
P(1)R(1)C(6)	0.5961 (3)	0.3538 (2)	0.3270 (2)	4.3 (1)
P(1)R(2)C(1)	0.4365 (4)	0.2015 (2)	0.1817 (2)	3.3 (1)
P(1)R(2)C(2)	0.5506 (3)	0.1828 (2)	0.1944 (2)	4.4 (1)
P(1)R(2)C(3)	0.5833 (3)	0.1173 (3)	0.1560 (3)	5.6 (2)
P(1)R(2)C(4)	0.5019 (4)	0.0705 (2)	0.1049 (3)	5.4 (2)
P(1)R(2)C(5)	0.3878 (3)	0.0892 (2)	0.0922 (3)	5.1 (2)
P(1)R(2)C(6)	0.3551 (2)	0.1547 (3)	0.1306 (3)	4.3 (1)
P(1)R(3)C(1)	0.4003 (7)	0.3690 (2)	0.1666 (2)	3.2 (1)
P(1)R(3)C(2)	0.3907 (6)	0.3571 (2)	0.0829 (2)	4.2 (1)
P(1)R(3)C(3)	0.3859 (4)	0.4213 (3)	0.0305 (2)	5.6 (2)
P(1)R(3)C(4)	0.3906 (7)	0.4973 (2)	0.0619 (3)	6.1 (2)
P(1)R(3)C(5)	0.4001 (6)	0.5092 (2)	0.1457 (3)	5.9 (2)
P(1)R(3)C(6)	0.4050 (3)	0.4450 (3)	0.1980 (2)	4.6 (1)
P(2)R(1)C(1)	−0.0169 (5)	0.1639 (3)	0.1855 (2)	3.0 (1)
P(2)R(1)C(2)	0.0161 (4)	0.1744 (3)	0.1121 (2)	4.0 (1)
P(2)R(1)C(3)	−0.0164 (3)	0.1202 (2)	0.0484 (2)	4.8 (1)
P(2)R(1)C(4)	−0.0818 (5)	0.0555 (3)	0.0581 (2)	4.8 (1)
P(2)R(1)C(5)	−0.1149 (5)	0.0450 (3)	0.1314 (3)	4.7 (1)
P(2)R(1)C(6)	−0.0824 (3)	0.0992 (2)	0.1951 (2)	4.1 (1)
P(2)R(2)C(1)	−0.0798 (4)	0.3153 (2)	0.2361 (2)	3.1 (1)
P(2)R(2)C(2)	−0.0641 (3)	0.3852 (3)	0.2806 (2)	3.8 (1)
P(2)R(2)C(3)	−0.1426 (4)	0.4458 (2)	0.2594 (2)	4.9 (2)
P(2)R(2)C(4)	−0.2368 (4)	0.4363 (3)	0.1938 (2)	4.7 (1)
P(2)R(2)C(5)	−0.2524 (3)	0.3664 (3)	0.1493 (2)	4.8 (1)
P(2)R(2)C(6)	−0.1739 (4)	0.3059 (2)	0.1705 (2)	4.3 (1)
P(2)R(3)C(1)	−0.0056 (4)	0.1951 (3)	0.3583 (2)	3.6 (1)
P(2)R(3)C(2)	0.0767 (3)	0.1517 (3)	0.4127 (3)	5.6 (2)
P(2)R(3)C(3)	0.0505 (4)	0.1142 (3)	0.4797 (3)	7.2 (2)
P(2)R(3)C(4)	−0.0580 (5)	0.1202 (3)	0.4923 (3)	6.3 (2)
P(2)R(3)C(5)	−0.1402 (3)	0.1637 (3)	0.4379 (3)	6.4 (2)
P(2)R(3)C(6)	−0.1140 (3)	0.2011 (3)	0.3709 (3)	5.6 (2)

[a] P(1)R(1)C(1) is attached to phosphorus atom P(1); other ring carbon atoms are numbered successively so that, *e.g.*, P(1)R(1)C(4) is *para* to P(1)R(1)C(1).

and with *trans* phosphines, CO, and Cl ligands in the basal plane. The next closest approach to the Rh atom is made by the H atom bonded to P(2)R(1)C(2). On the assumption of a normal phenyl-ring geometry, this atom is 2.94 Å from the metal. Much closer intramolecular nonbonded metal–hydrogen interactions have been observed; in $RuCl_2(P(C_6H_5)_3)_3$[18] a Ru···H contact of 2.59 Å was found. The Rh···H contact found here is probably the result of efficient molecular packing in the solid state, rather than of bonding forces. Of the atoms in the basal plane of the coordination polyhedron, no set of four is strictly coplanar. The best least-squares plane[19] which can be defined is that through the atoms Cl, P(1), P(2), and O. The equation of this plane, in terms of monoclinic coordinates, is $0.407X + 6.594Y + 14.813Z = 5.522$; the deviations of the atoms from this plane are: Cl, 0.011 (2) Å; P(1), −0.008 (2) Å; P(2), −0.009 (2) Å; O, 0.073 (5) Å. The Rh atom is 0.24 Å and the C atom of the CO group is 0.13 Å above this plane toward the SO_2 ligand.

The agreement between the intramolecular distances and angles given in Table V and the corresponding ones for the Ir complex is extremely good. Differences in comparable bond distances are, in most cases, covered by the estimated standard deviations, while comparable bond angles all agree to within 4° or less. However, as expected, the standard deviations assigned to the bond distances and angles for the Rh complex are four to five times smaller than those assigned to the Ir complex. The Rh–P distances of 2.371 (2) and 2.367 (2) Å are equal within experimental error and are close to the values of 2.33 (1) and 2.36 (1) Å found in the Ir complex. Literature values for Rh–P bond lengths appear to be in the surprisingly small range from 2.32 to 2.36 Å.[15,20–24] The Rh–Cl bond length of 2.355 (2) Å is comparable to the value of 2.37 (1) Å found in the Ir complex. The Rh–C–O geometry found in this analysis agrees well with that found in $RhH(CO)(P(C_6H_5)_3)_3$.[15] This confirms the earlier contention[1] that the anomalously short C–O bond length found in the Ir complex of SO_2 is due to an underestimate of its standard deviation.

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TABLE III

FINAL CALCULATED AND OBSERVED STRUCTURE AMPLITUDES (×10) IN ELECTRONS

K	L	FO	FC
***** H = 0 *****			
0	0		15331
0	2	3458	3354
0	4	768	851
0	6	1505	1510
0	8	731	759
0	10	232	247
0	12	468	466
0	14	669	636
0	16	101	173
1	1	335	317
1	2	697	683
1	3	225	233
1	4	756	690
1	5	1421	1380
1	6	324	337
1	7	59	2
1	8	959	977
1	9	406	385
1	10	842	832
1	11	158	68
1	12	324	346
1	14	559	542
1	15	194	194
1	16	404	404
1	17	131	141
2	0	3386	3477
2	1	995	979
2	2	2503	2521
2	3	799	760
2	4	1652	1615
2	5	627	613
2	6	1606	1621
2	7	752	788
2	8	1241	1254
2	9	242	235
2	10	655	664
2	11	314	285
2	12	608	621
2	13	409	429
2	14	478	497
2	15	67	35
2	16	67	60
2	17	205	240
3	1	712	660
3	2	1508	1434
3	3	330	367
3	4	332	349
3	5	370	375
3	6	749	711
3	7	89	78
3	8	294	287
3	10	461	462
3	11	206	235
3	12	510	498
3	13	262	273
3	14	446	399
3	15	225	241
3	16	411	366
4	0	961	900
4	1	394	385
4	2	1684	1726
4	3	115	46
4	4	1945	1950
4	5	1207	1172
4	6	1435	1381
4	7	976	939
4	8	1317	1353
4	9	485	513
4	10	1249	1243
4	11	513	518
4	12	420	422
4	13	449	438
4	14	226	212
4	16	173	164
5	2	659	678
5	3	254	264
5	4	665	691
5	5	905	903
5	7	86	107
5	9	89	81
5	10	759	758
5	11	310	299
5	12	877	867
5	13	125	153
5	14	515	562
5	15	148	139
5	16	402	414
6	0	389	404
6	1	1140	1126
6	2	1203	1242
6	3	1835	1772
6	4	1742	1766
6	5	1363	1346
6	6	791	736
6	7	113	136
6	8	915	924
6	9	448	416
6	10	618	608
6	11	201	224
6	12	208	211
6	13	291	321
6	14	209	170
6	15	211	217
6	16	85	64
7	1	256	230
7	2	141	115
7	3	150	159
7	4	681	670
7	5	237	257
7	6	566	566
7	7	363	394
7	8	608	597
7	9	119	84
7	10	671	652
7	11	83	129
7	12	352	353
7	13	214	190
7	14	228	244
8	0	566	647
8	1	1168	1186
8	2	475	510
8	3	1289	1243
8	4	739	785
8	5	688	748
8	6	491	476
8	7	354	326
8	8	397	375
8	9	643	622
8	10	293	292
8	11	300	266
8	12	198	206
8	14	131	99
8	15	198	222
9	1	433	386
9	2	498	502
9	3	130	158
9	4	524	499
9	5	715	629
9	6	841	869
9	7	425	422
9	8	729	713
9	10	145	167
9	11	219	202
9	13	198	179
9	14	274	261
10	0	746	766
10	1	792	793
10	2	317	294
10	3	803	834
10	4	134	129
10	5	708	690
10	6	530	548
10	7	701	728
10	9	484	440
10	10	175	182
10	11	474	463
10	13	148	163
11	1	92	125
11	2	195	247
11	3	317	332
11	4	95	61
11	5	89	80
11	6	193	190
11	7	82	39
11	8	394	384
11	10	78	93
11	11	495	484
11	12	185	153
11	13	390	388
12	1	809	798
12	2	376	376
12	3	494	505
12	4	356	349
12	5	531	500
12	6	287	306
12	7	487	472
12	8	108	70
12	9	397	398
12	10	159	213
12	11	323	287
13	2	217	211
13	3	57	36
13	4	205	211
13	5	170	200
13	6	78	64
13	8	96	101
13	9	423	410
13	10	177	172
13	11	238	231
14	0	528	525
14	1	364	405
14	2	399	434
14	4	175	150
14	5	386	403
14	7	448	441
14	9	322	342
15	1	423	416
15	2	209	211
15	3	507	486
15	4	95	140
15	5	194	198
15	7	257	258
15	8	98	25
15	9	344	350
16	0	218	217
16	1	363	340
16	2	202	201
16	3	261	313
16	4	145	115
16	5	267	285
16	6	377	351
16	7	303	307
17	1	85	126
17	3	120	106
17	4	83	78
17	5	148	149
***** H = 1 *****			
0	-16	507	512
0	-14	130	109
0	-12	255	221
0	-10	725	762
0	-8	1444	1419
0	-6	761	755
0	-4	2356	2270
0	-2	1303	1301
0	0	512	444
0	2	280	282
0	4	506	477
0	6	438	400
0	8	469	485
0	10	69	77
0	12	214	222
0	14	460	450
0	16	194	185
1	-17	86	62
1	-15	102	118
1	-14	135	146
1	-12	259	298
1	-11	149	148
1	-10	337	337
1	-9	386	369
1	-8	351	357
1	-7	145	110
1	-6	1544	1557
1	-5	56	67
1	-4	949	932
1	-3	615	598
1	-2	1716	1706
1	-1	473	432
1	0	2507	2440
1	1	385	376
1	2	2368	2330
1	3	761	702
1	4	1378	1372
1	5	436	410
1	6	2117	2126
1	7	591	578
1	8	1303	1307
1	10	522	549
1	11	296	323
1	12	984	1020
1	14	691	725
1	16	209	202
2	-17	177	166
2	-16	394	394
2	-15	132	94
2	-14	409	435
2	-13	58	90
2	-12	516	518
2	-11	204	218
2	-10	625	665
2	-9	130	135
2	-8	1257	1244
2	-7	112	162
2	-6	1212	1216
2	-5	1684	1673
2	-4	481	484
2	-3	884	827
2	-2	727	749
2	-1	316	292
2	0	506	475
2	1	564	547
2	2	70	38
2	3	1196	1154
2	4	475	469
2	5	1224	1214
2	6	41	35
2	7	612	535
2	8	288	327
2	9	441	397
2	11	70	75
2	12	296	282
2	13	261	250
2	14	525	553
2	15	214	243
2	16	350	351
3	-17	193	157
3	-16	145	99
3	-14	89	110
3	-13	224	226
3	-11	246	290
3	-10	514	478
3	-8	651	696
3	-7	622	615
3	-6	772	774
3	-5	1172	1166
3	-4	718	754
3	-3	771	743
3	-2	1935	1936
3	-1	1309	1285
3	0	1066	1039
3	1	818	737
3	2	1790	1787
3	3	239	245
3	4	2283	2251
3	5	749	754
3	6	1691	1682
3	7	1409	1363
3	8	1282	1261
3	9	298	296
3	10	1120	1136
3	11	235	231
3	12	989	956
3	13	279	275
3	14	221	239
3	15	111	115
3	16	348	327
4	-17	298	311
4	-16	323	356
4	-15	297	267
4	-14	606	584
4	-13	80	27
4	-12	797	786
4	-11	124	142
4	-10	745	777
4	-9	179	172
4	-8	799	815
4	-7	198	155
4	-6	629	596
4	-5	76	96
4	-4	147	126
4	-3	816	850
4	-2	480	478
4	-1	53	6
4	0	374	349
4	1	1110	1139
4	2	1326	1345
4	4	466	458
4	5	368	349
4	6	75	78
4	7	473	445
4	8	94	88
4	9	259	263
4	10	221	202
4	11	217	225
4	12	354	362
4	13	329	355
4	14	404	392
4	15	154	200
4	16	330	332
5	-16	261	242
5	-12	245	238
5	-11	254	250
5	-10	466	473
5	-9	69	21
5	-8	313	297
5	-7	1040	1028
5	-5	1408	1360
5	-4	696	699
5	-3	963	963
5	-2	1238	1255
5	-1	958	954
5	0	197	203
5	1	1042	1050
5	2	662	656
5	3	369	326
5	4	1936	1968
5	5	436	530
5	6	976	961
5	7	868	855
5	8	1167	1190
5	9	657	633
5	10	1230	1201
5	11	344	327
5	12	529	538
5	13	292	277
5	14	374	367
5	15	89	122
5	16	394	365
6	-16	301	264
6	-15	265	276
6	-14	201	197
6	-13	384	394
6	-12	750	757
6	-11	68	75
6	-10	797	770
6	-8	58	16
6	-7	300	298
6	-6	121	134
6	-5	718	749
6	-4	859	862
6	-3	692	669
6	-2	695	670
6	-1	118	100
6	0	295	280
6	1	391	407
6	2	923	930
6	3	940	952
6	4	448	464
6	5	719	647
6	6	186	229
6	7	679	672
6	8	71	36
6	9	443	433
6	10	237	249
6	11	95	47
6	12	485	489
6	14	213	204
6	15	115	90
7	-16	83	80
7	-15	132	98
7	-14	277	245
7	-11	101	87
7	-10	245	263
7	-9	249	242
7	-8	293	317
7	-7	344	353
7	-6	233	225
7	-5	402	429
7	-4	633	666
7	-3	1832	1818
7	-2	824	828
7	-1	1751	1761
7	0	887	887
7	1	1036	1103
7	2	956	896
7	3	873	919
7	4	1184	1195
7	5	632	608
7	6	472	511
7	7	521	563
7	8	543	504
7	9	786	778
7	10	727	736
7	11	393	386
7	12	364	378
7	13	238	228
7	14	400	398
7	15	243	242
8	-15	143	163
8	-14	205	189
8	-13	332	346
8	-12	218	243
8	-11	304	297
8	-10	202	208
8	-8	267	254
8	-7	286	247
8	-6	625	643
8	-5	333	352
8	-4	1298	1266
8	-3	89	93
8	-2	302	326
8	-1	99	105
8	0	132	184
8	2	296	234
8	3	686	714
8	4	437	453
8	5	815	776
8	6	271	238
8	7	400	407
8	9	525	557
8	10	379	361
8	11	204	221
8	12	178	200
8	13	111	104
9	-15	68	37
9	-14	110	147
9	-13	76	35
9	-12	98	101
9	-11	308	307
9	-9	642	608
9	-8	176	176
9	-7	297	284
9	-6	105	140
9	-5	719	707
9	-4	428	429
9	-3	1274	1286
9	-2	799	767
9	-1	1161	1142
9	0	644	655
9	1	948	946
9	2	634	651
9	3	1430	1440
9	4	684	606
9	5	782	747
9	6	416	442
9	7	720	744
9	8	69	47
9	9	749	766
9	10	89	59
9	11	631	622
9	12	173	180
9	13	282	280
9	14	166	178
10	-14	117	120
10	-13	268	263
10	-12	226	208
10	-11	357	339
10	-10	299	331
10	-8	415	370
10	-6	565	580
10	-5	251	234
10	-4	394	408
10	-3	246	236
10	-2	639	646
10	-1	464	461
10	0	336	314
10	1	116	61
10	2	95	51
10	3	57	79
10	4	199	199
10	5	549	594
10	6	77	110
10	7	163	84
10	8	232	282
10	9	110	131
10	11	432	437
10	12	92	83
10	13	451	419
11	-13	174	137
11	-12	73	79
11	-11	467	452
11	-10	175	150
11	-9	571	589
11	-7	553	559
11	-6	83	85
11	-5	814	817
11	-3	632	687
11	-2	204	197
11	-1	407	413
11	0	565	577
11	1	647	640
11	2	73	66
11	3	1030	1051
11	4	461	480
11	5	867	904
11	6	111	112
11	7	735	725
11	8	145	151
11	9	529	578
11	10	190	181
11	11	536	519
11	13	273	296
12	-13	295	294
12	-12	90	160
12	-11	315	310
12	-10	232	197
12	-9	338	344
12	-8	220	239
12	-7	118	142
12	-5	101	100
12	-4	225	197
12	-3	198	191
12	-1	227	233
12	0	145	155
12	1	55	91
12	2	384	397
12	3	66	35
12	4	330	288
12	5	90	130
12	6	109	150
12	7	139	102
12	8	424	431
12	9	250	231
12	11	454	450
12	12	198	218
13	-11	309	343
13	-9	474	484
13	-8	240	252
13	-7	698	689
13	-5	510	518
13	-4	327	392
13	-3	462	458
13	-2	242	221
13	-1	691	715
13	0	172	196
13	1	747	737
13	2	581	581
13	3	509	512
13	4	537	539
13	5	791	806
13	6	153	132
13	7	504	500
13	8	88	95
13	9	287	275
13	10	194	101
13	11	286	254
14	-11	341	367
14	-10	106	87
14	-9	565	554
14	-8	107	86
14	-7	342	308
14	-6	75	59
14	-5	153	133
14	-3	84	108
14	-2	265	267
14	-1	165	183
14	0	442	428
14	1	336	353
14	2	168	167
14	3	392	384
14	4	246	261
14	6	247	254
14	7	349	379
14	8	86	111
14	9	398	372
14	10	77	83
15	-9	155	155
15	-7	483	477
15	-6	275	253
15	-5	241	249
15	-4	434	464
15	-3	247	221
15	-2	345	317
15	-1	742	758
15	0	712	733
15	1	704	707
15	2	422	406
15	3	571	570
15	5	410	403
15	6	213	215
15	7	288	316
15	8	243	249
15	9	69	69
16	-7	435	439
16	-6	99	98
16	-5	279	225
16	-4	105	143
16	-3	278	294
16	-2	72	92
16	0	111	98
16	1	195	187
16	2	206	208
16	3	148	169
16	4	113	110
16	5	217	223
16	6	130	134
16	7	320	323
17	-5	281	260
17	-4	115	83
17	-3	201	215
17	-2	242	221
17	-1	334	361
17	0	341	354
17	1	458	462
17	2	159	161
17	3	367	400
17	4	162	138
17	5	103	115
***** H = 2 *****			
0	-16	292	290
0	-14	404	393
0	-12	380	377
0	-10	120	145
0	-8	314	334
0	-6	101	135
0	-4	926	865
0	-2	518	483
0	0	44	125
0	2	2705	2559
0	4	85	81
0	6	1716	1692
0	8	644	653
0	10	287	300
0	12	596	592
0	14	670	659
0	16	334	341
1	-17	110	145
1	-16	338	335
1	-15	243	278
1	-14	234	251
1	-13	162	151
1	-12	188	195
1	-11	78	68
1	-10	497	484
1	-9	116	124
1	-8	1071	1087
1	-7	523	537
1	-6	924	927
1	-5	907	929
1	-4	779	770
1	-3	1195	1173
1	-2	843	851
1	-1	133	115
1	0	513	479
1	1	159	166
1	2	963	923
1	3	562	553
1	4	535	517
1	5	622	594
1	6	412	395
1	7	91	75
1	8	819	791
1	9	528	532
1	10	153	154
1	11	188	205
1	12	119	118
1	13	235	277
1	14	112	110
1	15	115	120
1	16	356	373
2	-17	167	174
2	-16	384	413
2	-15	113	69
2	-14	402	453
2	-13	82	5
2	-12	154	142
2	-11	119	78
2	-10	84	67
2	-9	574	547
2	-7	572	578
2	-6	216	208
2	-5	278	277
2	-4	125	130
2	-3	1097	1077
2	-2	397	371
2	-1	907	873
2	0	515	573
2	1	1796	1642
2	2	164	191
2	3	1311	1242
2	4	1380	1370
2	5	513	488
2	6	1419	1397
2	7	692	713
2	8	883	918
2	9	60	40
2	10	718	729
2	12	578	582
2	13	451	468
2	14	593	603
2	15	231	230
2	16	395	404
3	-17	262	273
3	-16	226	264
3	-15	480	469
3	-14	535	514
3	-13	271	263
3	-12	416	403
3	-11	263	285
3	-10	541	536
3	-9	795	747
3	-8	541	602
3	-7	339	287
3	-6	1206	1226
3	-5	934	927
3	-4	1265	1292
3	-3	1197	1146
3	-2	761	720
3	-1	716	706
3	0	1402	1311
3	1	66	20
3	2	707	689
3	3	578	558
3	4	151	149
3	5	1090	1045
3	6	57	64
3	7	377	362
3	8	125	105
3	9	614	621
3	10	185	203
3	11	313	302
3	12	421	434
3	13	455	481
3	14	236	248
3	15	303	298
3	16	175	118
4	-17	269	293
4	-16	176	164
4	-15	133	131
4	-14	108	108
4	-12	103	97
4	-11	159	202
4	-9	103	129
4	-8	167	153
4	-7	205	214
4	-6	350	291
4	-5	169	148
4	-4	671	662
4	-3	445	415
4	-2	160	203
4	-1	277	238
4	0	40	52
4	1	1786	1759
4	2	547	529
4	3	826	775
4	4	1737	1720
4	5	572	595
4	6	733	729
4	7	978	982
4	8	686	673
4	9	391	409
4	10	1117	1118
4	11	382	413
4	12	713	718
4	13	461	471
4	14	269	267
4	15	248	212
5	-16	198	155
5	-15	345	323
5	-14	450	487
5	-13	485	445
5	-12	785	821
5	-11	553	610
5	-10	531	536
5	-9	896	914
5	-8	70	102
5	-7	542	542
5	-5	45	39
5	-4	356	407
5	-3	54	31
5	-2	334	335
5	-1	55	86
5	1	485	435
5	2	1167	1107
5	3	619	625
5	4	273	309
5	5	342	334
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5	7	589	586
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10	4	177	169
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1	-14	78	56
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1	-12	598	608
1	-11	171	199
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1	-9	330	317
1	-8	303	310
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5	7	157	183
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5	11	75	14
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8	4	100	120
8	5	273	295
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8	7	437	432
8	8	234	244
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9	-10	352	401
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9	-7	165	142
9	-6	119	87
9	-5	172	165
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9	3	152	156
9	4	317	345
9	6	315	310
9	7	79	45
9	8	136	93
9	9	261	251
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9	11	314	319
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10	-10	217	202
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10	3	651	671
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10	8	174	165
10	9	315	300
10	10	94	19
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TABLE III (*Continued*)

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13	7	419	431
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14	-8	265	267
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15	3	214	222
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10	-7	120	80
10	-6	217	199
10	-5	244	232
10	-4	580	541
10	-3	279	282
10	-2	258	285
10	-1	334	324
10	1	423	417
10	3	236	245
10	4	82	110
11	-9	548	549
11	-8	244	205
11	-7	599	553
11	-5	594	575
11	-3	678	696
11	-2	223	247
11	-1	618	576
11	0	122	126
11	1	365	354
11	2	160	137
11	3	143	146
12	-5	105	83
12	-4	298	292
12	-3	376	384
12	-2	264	230
12	-1	501	468
12	0	83	68
12	1	398	394
***** H = 10 *****			
0	-14	594	664
0	-12	913	913
0	-10	1019	993
0	-8	656	667
0	-6	712	738
0	-4	622	590
0	-2	280	277
0	0	680	716
0	2	571	567
0	4	102	78
0	6	133	93
1	-14	125	92
1	-12	205	200
1	-11	113	86
1	-10	344	364
1	-8	565	574
1	-7	93	68
1	-6	376	378
1	-5	191	186
1	-4	500	494
1	-3	143	163
1	-2	644	653
1	-1	65	78
1	0	263	272
1	1	177	159
1	2	746	694
1	3	188	165
1	4	685	715
1	6	339	294
1	7	65	52
2	-13	132	108
2	-12	704	723
2	-11	199	197
2	-10	725	698
2	-9	151	176
2	-8	821	828
2	-7	154	151
2	-6	816	835
2	-5	467	481
2	-4	528	654
2	-3	330	354
2	-2	476	479
2	-1	82	89
2	0	584	502
2	1	241	233
2	2	559	568
2	4	197	198
2	5	131	116
2	7	115	139
3	-13	68	61
3	-12	236	235
3	-11	171	155
3	-10	142	127
3	-9	114	128
3	-8	225	226
3	-7	236	230
3	-6	355	338
3	-5	109	115
3	-4	482	499
3	-3	400	398
3	-2	424	395
3	-1	178	178
3	0	695	690
3	1	193	200
3	2	742	754
3	3	338	298
3	4	418	434
3	5	189	175
3	6	483	468
3	7	95	106
4	-13	312	294
4	-12	289	261
4	-11	324	312
4	-10	457	495
4	-9	131	138
4	-8	912	904
4	-7	215	233
4	-6	675	662
4	-5	513	519
4	-4	611	640
4	-3	509	502
4	-2	673	664
4	-1	376	382
4	0	562	568
4	1	552	557
4	2	119	128
4	3	261	233
4	4	149	171
4	5	102	96
4	6	105	74
5	-12	109	128
5	-11	121	139
5	-9	166	146
5	-6	396	381
5	-5	97	92
5	-4	295	290
5	-3	351	389
5	-2	356	400
5	-1	231	225
5	0	911	924
5	1	75	22
5	2	506	526
5	3	142	159
5	4	250	252
5	5	93	111
5	6	507	480
6	-12	207	196
6	-11	350	318
6	-10	428	429
6	-9	227	242
6	-8	657	681
6	-7	232	270
6	-6	438	436
6	-5	350	358
6	-4	254	248
6	-3	432	453
6	-2	623	605
6	-1	434	449
6	0	310	346
6	1	315	306
6	2	183	162
6	3	419	423
6	4	169	146
6	5	387	385
7	-11	106	116
7	-10	74	70
7	-9	142	131
7	-8	127	126
7	-7	357	350
7	-6	361	363
7	-5	230	248
7	-4	264	291
7	-2	324	335
7	-1	139	113
7	0	539	525
7	1	213	227
7	2	330	321
7	4	159	151
8	-10	362	348
8	-9	623	595
8	-8	197	195
8	-7	407	426
8	-6	265	258
8	-5	327	363
8	-4	137	99
8	-3	521	530
8	-2	270	267
8	-1	539	524
8	0	114	108
8	1	244	238
8	3	215	230
8	4	94	66
	-8	191	206
9	-7	220	237
9	-6	233	257
9	-5	134	149
9	-4	336	365
9	-2	164	125
9	-1	246	210
9	1	278	278
10	-8	68	71
10	-7	579	581
10	-5	491	492
10	-4	133	167
10	-3	508	500
10	-2	143	142
10	-1	510	505
10	0	67	64
10	1	346	346
11	-4	117	152
11	-3	112	112
11	-2	131	141
11	-1	127	153
***** H = 11 *****			
0	-10	73	38
0	-8	161	163
0	-4	320	276
0	-2	508	533
0	0	320	329
0	2	199	183
0	4	584	582
1	-12	532	523
1	-11	131	116
1	-10	659	676
1	-9	134	175
1	-8	581	584
1	-6	853	866
1	-5	111	106
1	-4	864	864
1	-3	122	111
1	-2	738	704
1	-1	107	110
1	0	622	645
1	1	253	250
1	2	639	647
1	3	65	47
1	4	529	531
2	-11	109	103
2	-10	107	113
2	-9	216	212
2	-7	258	267
2	-6	86	47
2	-4	325	356
2	-3	293	299
2	-2	283	251
2	-1	426	443
2	0	229	197
2	1	244	223
2	2	234	272
2	3	162	217
2	4	528	522
3	-12	263	237
3	-11	214	223
3	-10	443	446
3	-9	77	66
3	-8	644	664
3	-7	143	151
3	-6	815	805
3	-5	491	474
3	-4	859	847
3	-3	354	379
3	-2	745	781
3	-1	231	221
3	0	504	499
3	1	308	313
3	2	440	433
3	3	130	124
3	4	364	345
4	-10	126	112
4	-9	90	76
4	-7	82	86
4	-6	251	253
4	-5	143	114
4	-4	207	201
4	-3	276	284
4	-2	282	284
4	-1	174	163
4	0	514	522
4	1	115	112
4	2	479	488
4	3	139	144
4	4	398	363
5	-11	248	246
5	-10	359	355
5	-9	158	124
5	-8	462	464
5	-7	237	245
5	-6	520	534
5	-5	431	423
5	-4	562	563
5	-3	308	278
5	-2	690	695
5	-1	336	335
5	0	557	539
5	1	304	349
5	2	320	311
5	3	286	279
6	-10	311	302
6	-9	280	289
6	-8	72	15
6	-7	274	268
6	-6	155	172
6	-5	392	389
6	-3	284	292
6	-2	229	236
6	-1	208	172
6	0	585	604
6	1	243	225
6	2	385	387
6	3	125	112
7	-9	371	373
7	-8	431	460
7	-7	244	188
7	-6	161	194
7	-5	107	90
7	-4	208	198
7	-3	339	346
7	-2	477	475
7	-1	423	435
7	0	411	398
7	1	220	213
7	2	269	227
8	-7	322	302
8	-5	240	283
8	-4	98	72
8	-3	65	57
8	-1	222	225
8	0	209	202
9	-5	285	272
9	-3	387	385
9	-2	90	117
***** H = 12 *****			
0	-10	323	299
0	-8	247	253
0	-6	179	186
0	-4	409	445
0	-2	86	53
0	0	162	182
0	2	682	670
1	-10	81	40
1	-8	109	121
1	-7	91	79
1	-6	179	137
1	-3	63	32
1	-2	113	127
1	-1	121	151
1	1	79	6
1	2	196	179
2	-8	226	213
2	-7	176	149
2	-6	348	348
2	-5	296	283
2	-4	444	452
2	-3	63	21
2	-2	365	408
2	-1	108	106
2	0	349	364
2	1	133	149
3	-9	92	14
3	-8	152	131
3	-5	79	44
3	-4	122	111
3	-3	270	296
3	-2	214	222
3	-1	189	190
3	0	144	113
3	1	69	117
4	-8	304	318
4	-7	348	343
4	-6	447	460
4	-5	353	341
4	-4	455	440
4	-2	647	627
4	-1	67	52
4	0	516	495
5	-7	106	134
5	-6	75	83
5	-5	212	184
5	-4	82	64
5	-3	188	182
5	-2	67	59
5	-1	150	155
6	-6	315	287
6	-5	158	140
6	-4	356	345
6	-3	165	190
6	-2	473	484

TABLE IV

ROOT-MEAN-SQUARE AMPLITUDES OF VIBRATION (Å)

Atom	Min	Intermed	Max
Rh	0.177 (1)	0.184 (1)	0.196 (1)
S	0.196 (2)	0.202 (2)	0.228 (2)
Cl	0.176 (3)	0.228 (2)	0.257 (2)
P(1)	0.179 (2)	0.196 (2)	0.202 (2)
P(2)	0.179 (3)	0.189 (2)	0.207 (2)
O(1)	0.187 (7)	0.254 (6)	0.274 (6)
O(2)	0.197 (7)	0.238 (6)	0.308 (6)
O	0.184 (8)	0.269 (6)	0.295 (6)
C	0.199 (9)	0.212 (9)	0.214 (9)

The geometry of the Rh–SO_2 part of the molecule is the same as the Ir–SO_2 geometry in the Ir complex. However, this geometry is better defined in the present case. The Rh–S bond length of 2.450 (2) Å is shorter, but only slightly, than the comparable Ir–S distance of 2.488 (10) Å. The bond angles around the S atom are all within 5° of the tetrahedral angle: the O–S–O angle is 113.8 (3)° and the Rh–S–O angles are 105.3 (2) and 106.7 (2)°. The Rh–S vector makes an angle of 30.3 (3)° with the normal to the SO_2 plane. The comparable angle in the Ir complex is 31.6 (15)°. This angle is 35.3° for the regular tetrahedron. The two S–O distances are equal to within experimental error. Their mean value is 1.451 (4) Å. The extreme shortness of the Ru–S bond in $[\mathrm{RuCl(NH_3)_4(SO_2)}]\mathrm{Cl}$,[2] compared with the Rh–S bond in the present analysis, and the very different metal–SO_2 geometries might lead one to expect that there would be differences in the geometries of the bound SO_2 complexes in the two molecules. Unfortunately, the larger experimental errors in the analysis of the Ru complex prevent a discussion of possible differences. An electron diffraction study of gaseous SO_2 gave 1.431 (1) Å for the length of the S–O

Table V

Selected Intramolecular Distances and Angles

Atoms	Dist, Å	Atoms	Angle, deg
Rh–S	2.450 (2)	S–Rh–P(1)	93.6 (1)
Rh–Cl	2.355 (2)	S–Rh–Cl	99.4 (1)
Rh–P(1)	2.371 (2)	S–Rh–P(2)	98.7 (1)
Rh–P(2)	2.367 (2)	S–Rh–C	89.6 (2)
Rh–O(1)	3.156 (4)	S–Rh–O	89.4 (1)
Rh–O(2)	3.188 (4)	P(1)–Rh–Cl	86.6 (1)
Rh–C	1.847 (7)	P(1)–Rh–P(2)	167.6 (1)
Rh–O	2.973 (5)	P(1)–Rh–C	91.7 (2)
S–O(1)	1.446 (4)	P(1)–Rh–O	91.8 (1)
S–O(2)	1.456 (4)	Cl–Rh–P(2)	89.2 (1)
S–P(1)	3.514 (2)	Cl–Rh–C	170.9 (2)
S–P(2)	3.655 (2)	Cl–Rh–O	171.1 (1)
S–Cl	3.665 (2)	P(2)–Rh–C	90.6 (2)
S–C	3.059 (7)	P(2)–Rh–O	90.6 (1)
P(1)–Cl	3.243 (2)	Rh–C–O	179.4 (6)
P(1)–P(2)	4.710 (2)	Rh–S–O(1)	105.3 (2)
P(1)–C	3.048 (6)	Rh–S–O(2)	106.7 (2)
P(1)–O	3.859 (5)	O(1)–S–O(2)	113.8 (3)
Cl–P(2)	3.315 (2)	P(1)–Cl–P(2)	91.8 (1)
Cl–C	4.189 (7)	Cl–P(2)–C	82.7 (1)
P(2)–C	3.018 (7)	P(2)–C–P(1)	101.9 (2)
P(2)–O	3.819 (5)	C–P(1)–Cl	83.4 (1)
C–O	1.126 (7)	C′–P–C′ (av of 6)	104.7 (5)
P–C′[a] (av of 6)	1.826 (7)		

[a] C′ is a phenyl carbon atom bonded directly to a phosphorus atom.

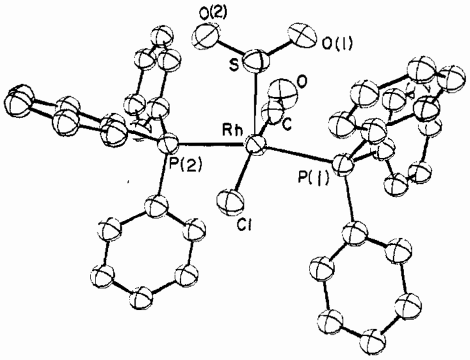

Figure 1.—A perspective view of the $RhCl(CO)(SO_2)(P(C_6H_5)_3)_2$ molecule. The hydrogen atoms have been omitted for clarity. Here and in Figure 2, 50% probability ellipsoids are shown.

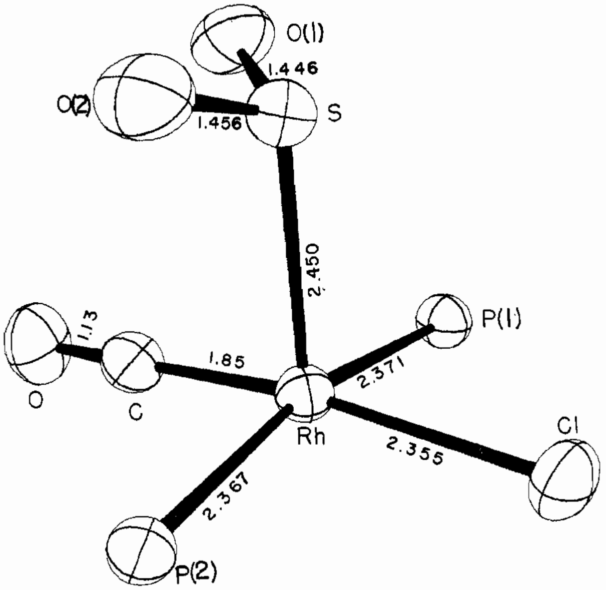

Figure 2.—A perspective view of the coordination polyhedron around the rhodium atom.

bond and 119.0 (5)° for the O–S–O angle.[25] Similar results have been obtained in microwave studies of the free molecule.[26] An X-ray study of the solid gave 1.430 (15) Å for the S–O bond and 119 (2)° for the O–S–O angle.[27] The S–O distance found here is thus slightly greater than that found in the free molecule and the O–S–O angle has closed a little. In the dithionite ion, $S_2O_4^{2-}$, which may be regarded as two SO_2^- ions joined together, the trend is continued since the S–O distance is 1.50 (2) Å and the bond angle is 108°.[28]

In the molecular oxygen complexes $[M(O_2)((C_6H_5)_2PCH_2CH_2P(C_6H_5)_2)][PF_6]$ a change of M from Ir[24,29] to Rh[24] leads to a reduction in the O–O distance of 0.24 Å and to an increase in the mean metal–O distance from 1.97 (2) to 2.026 (8) Å. These changes are believed to be due to the greater tendency of Ir to back-donate electrons from its filled d orbitals to a π* orbital of the bound oxygen molecule. The similarity between the $Rh–SO_2$ geometry found here and that found in the analogous Ir complex is strong evidence that the metal–sulfur bond in these complexes has little double-bond character. As indicated in the Introduction, we consider the bonding in the present complex to result from the donation of electrons from the Rh to the SO_2 ligand to form a σ bond. The following argument, although suggestive rather than conclusive, also indicates that

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[29] J. A. McGinnety and J. A. Ibers, *Chem. Commun.*, 235 (1968).

these bonds are single in character. In $RhI_2(CH_3)(P(C_6H_5)_3)_2$,[22] which has a tetragonal pyramidal configuration about Rh with CH_3 at the apex, the Rh–CH_3 distance is 2.081 (9) Å. If we take the normal covalent radius of C as 0.77 Å,[30] then a covalent radius of Rh of 1.31 Å may be derived. If one assumes a normal covalent radius of S of 1.04 Å,[30] then one predicts the length of a Rh–S single bond to be 2.35 Å, some 0.1 Å shorter than observed here. However, if one takes the radius of S in the SO_2^- ion to be half the S–S distance in the dithionite ion, namely, 1.20 Å, then one predicts a Rh–SO_2^- distance of 2.51 Å, closer to that observed here.

It would thus appear that the rationalization presented in the Introduction is a useful one in describing the varying geometries exhibited by NO and SO_2 in transition metal complexes. However, it is far from clear why NO and SO_2 may act either as Lewis acids or Lewis bases and why in their attachment to the $MX(CO)(P(C_6H_5)_3)_2$ systems (M = Ir or Rh, X = halogen) they should exhibit a Lewis acid character. This behavior must certainly be contrasted with the bonding of molecular oxygen,[16,17] tetracyanoethylene,[29] *trans*-1,2-dicyanoethylene,[31] and tetrafluoroethylene[32] in these systems, where the π-bonding scheme of Chatt and Dewar seems most applicable. Of even more interest, the contrast between the structures of $IrCl(CO)(NO)(P(C_6H_5)_3)_2^+$ and the formally isoelectronic $IrCl(CO)_2(P(C_6H_5)_3)_2$ molecule[33] is striking. As already indicated, in the NO complex the iridium coordination polyhedron is a tetragonal pyramid, with the apical NO group bonded to iridium through an Ir–N σ bond; in the bis-CO complex a trigonal-bipyramidal configuration is found, with *trans*-phosphine ligands and normal Ir–C–O geometries.

Acknowledgment.—We are indebted to Dr. N. C. Payne for the preparation of the crystals used in this study. This work was supported by the National Science Foundation.

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Nature of the Metal–Hydrogen Bond in Transition Metal–Hydrogen Complexes: Neutron and X-Ray Diffraction Studies[1] of β-Pentacarbonylmanganese Hydride

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An X-ray and neutron diffraction study of a new crystalline form of $HMn(CO)_5$, hereafter designated β-$HMn(CO)_5$, is described. The material crystallizes with eight molecules in space group C_{2h}^6-$C2/c$ of the monoclinic system in a cell (measured at −75°) of dimensions a = 12.16 (3) Å, b = 6.28 (2) Å, c = 19.34 (4) Å, and β = 91.2 (5)°. The structural details involving the nonhydrogen atoms derived from 596 visually estimated independent X-ray intensities collected at −75° and from 398 independent neutron diffraction counter data collected at −105° agree within the assigned limits of error. In addition, a precise position for the hydrogen atom has been derived from the neutron data. The β-$HMn(CO)_5$ molecule deviates only slightly from C_{4v} symmetry. The Mn–C_{ax} bond length is 1.882 (12) Å, while the average Mn–C_{eq} bond length is 1.853 (12) Å (ax = axial, *trans* to H; eq = equatorial, *cis* to H). The equatorial carbonyl groups are bent toward the hydrogen atom; the C_{ax}–Mn–C_{eq} bond angles range from 94.9 (5) to 98.2 (5)°. The Mn–C–O linkages do not deviate significantly from linearity. Thus the molecular structures of α- and β-$HMn(CO)_5$ are essentially identical, but the crystal structures differ markedly and these differences are dicussed. The Mn–H distance in β-$HMn(CO)_5$ is 1.601 (16) Å. This value, the first to be determined with such precision in a parent transition metal carbonyl hydride, is consistent with the usual covalent radii sums and with earlier, less accurate X-ray determinations of metal–hydrogen distances, but it is totally inconsistent with some theoretical studies and the various interpretations of the broad-line nmr spectra obtained from this and related compounds. From the present study it is concluded that the hydrogen atom is a stereochemically active ligand and that the metal–hydrogen distance is that of a normal covalent bond.

Introduction

The nature of the metal–hydrogen bond in transition metal hydride complexes has been of considerable interest for a number of years. A brief history of the structural aspects of the subject up to the end of 1964 is available.[5] As of that time it was clear from crystallographic studies on various stable hydride complexes[6]

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(1) Research carried out at Brookhaven National Laboratory under contract with the U. S. Atomic Energy Commission.

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