TABLE IX

MOLECULAR CONTACTS LESS THAN 3.6 A

Atom 1 (in x, y, z)	Atom 2	Distance, A	Molecule position
C(1)	C(1)	3.422	$\bar{x}, \bar{y}+1, \bar{z}$
C(1)	C(7)	3.378	$\bar{x}, \bar{y}+1, \bar{z}$
C(2)	C(11)	3.534	$\bar{x}, \bar{y}, \bar{z}$
C(4)	C(8)	3.540	$\bar{x}, \bar{y}+1, \bar{z}$
C(5)	C(8)	3.592	$\bar{x}, \bar{y}+1, \bar{z}$
C(6)	C(7)	3.501	$\bar{x}, \bar{y}+1, \bar{z}$
C(8)	C(8)	3.579	$\bar{x}-1, \bar{y}, \bar{z}$
C(14)	C(7)	3.569	$x, y, z+1$
C(14)	C(15)	3.438	$\bar{x}, \bar{y}, \bar{z}+1$
N(1)	C(5)	3.519	$\bar{x}, \bar{y}+1, \bar{z}$
N(1)	C(6)	3.510	$\bar{x}, \bar{y}+1, \bar{z}$
N(1)	O(2)	3.342	$\bar{x}, \bar{y}, \bar{z}$
O(1)	C(10)	3.358	$\bar{x}, \bar{y}, \bar{z}$
O(1)	C(11)	3.066	$\bar{x}, \bar{y}, \bar{z}$
O(1)	O(2)	3.020	$\bar{x}, \bar{y}, \bar{z}$
O(2)	N(2)	3.598	$\bar{x}, \bar{y}, \bar{z}$
Zn	C(10)	3.051	$\bar{x}, \bar{y}, \bar{z}$
Zn	C(11)	3.537	$\bar{x}, \bar{y}, \bar{z}$

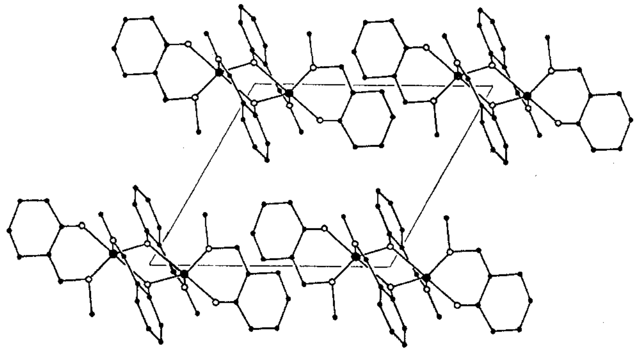

Figure 3.—The crystal structure of bis(N-methylsalicylaldiminato)zinc(II) viewed down the c axis.

ported by other authors.[9–11] On the basis of the isomorphism with the zinc(II) complex, bis(N-methylsalicylaldiminato)cobalt(II) and -manganese(II) very likely contain high-spin five-coordinated cobalt(II) and manganese(II).

It has been reported[12] that bis(N-β-diethylamineethyl-5-chlorosalicylaldimine)cobalt(II) is isomorphous with the nickel(II) analog, which has been shown by three-dimensional X-ray analysis to contain high-spin five-coordinated nickel(II).

More recently[13] Pauling, *et al.*, have reported preliminary X-ray results on the high-spin five-coordinated cobalt(II) complex with diphenylmethylarsine oxide. No structure has been so far described for five-coordinated Mn(II) complexes.

It might have been expected that the dimeric arrangement would afford a good electronic framework for a superexchange process between the metal atoms *via* the bridging oxygens.

Magnetic measurements on the Co(II) and Mn(II) complexes have shown no anomalous behavior in the magnetic properties of these complexes.[4] The same behavior has been found in the trimeric bis(acetylacetonato)nickel(II), where the magnetic susceptibility follows the Curie–Weiss law.[14]

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(11) (a) M. Bonamico, G. Dessy, G. Mazzone, A. Mugnoli, A. Vaciago, and L. Zambonelli, *Rend. Accad. Nazl. Lincei*, **35**, 538, 338 (1963); (b) D. E. Corbridge and E. G. Cox, *J. Chem. Soc.*, 594 (1956).

(12) L. Sacconi, P. L. Orioli, and M. Di Vaira, *J. Am. Chem. Soc.*, **87**, 2059 (1965).

(13) P. Pauling, G. B. Robertson, and G. A. Rodley, *Nature*, **207**, 73 (1965).

(14) G. J. Bullen, R. Mason, and P. Pauling, *Inorg. Chem.*, **4**, 456 (1965)

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Structure of Chlorocarbonyl(sulfur dioxide)bis(triphenylphosphine)iridium[1]

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The crystal and molecular structure of chlorocarbonyl(sulfur dioxide)bis(triphenylphosphine)iridium, $IrCl(CO)(SO_2)(P(C_6H_5)_3)_2$, has been determined from three-dimensional X-ray data. The material crystallizes in space group C_{2h}^5-$P2_1/c$ of the monoclinic system, with four molecules in a cell of dimensions $a = 12.11$, $b = 16.79$, $c = 17.09$ A, $\beta = 103.0°$. The individual monomeric units are well separated, the closest Ir–Ir distance being greater than 8 A. The coordination geometry around the Ir is that of a tetragonal pyramid, with CO, Cl, and *trans* P atoms in the base and the S of the SO_2 group at the apex. The O (of the CO), Cl, and two P atoms are coplanar; the Ir lies 0.21 A above this plane toward the S. The basal interatomic distances are normal. However, the Ir–S bond length of 2.49 A is very long and the Ir, S, and two O atoms of the SO_2 group are not coplanar. Rather the Ir–S vector makes an angle of 32° with the normal to the SO_2 plane. The dimensions of the SO_2 group are not significantly different from those found in solid SO_2. The basic geometry of the SO_2 complex differs markedly from that of the analogous O_2 complex, $Ir(O_2)Cl(CO)(P(C_6H_5)_3)_2$, in which the Ir is in a trigonal bipyramidal configuration with *trans* P atoms at the apices.

Introduction

Vaska has found that several molecular species interact *reversibly* in benzene solution with $IrCl(CO)(P(C_6H_5)_3)_2$ to form stable adducts that can be crystallized. Among these species are molecular oxygen[3] and molecular sulfur dioxide.[4] A complete structure determina-

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(3) L. Vaska, *Science*, **140**, 809 (1963).

(4) L. Vaska, unpublished results.

tion on the O_2 adduct was undertaken because of an interest in the mode of attachment of molecular oxygen to the transition metal in the adduct of a synthetic molecular oxygen carrier. It was found[5,6] that in the compound $Ir(O_2)Cl(CO)(P(C_6H_5)_3)_2$ the O_2 group, Cl, CO, and Ir are coplanar, with *trans* P atoms being above and below this plane. If one counts the O_2 group as a bidentate ligand (the Ir–O distances are equal) then the arrangement around Ir is that of a distorted octahedron; if one considers the O_2 group to be unidentate, then the arrangement is that of a trigonal bipyramid. The present study of the structure of the SO_2 adduct, $IrCl(CO)(SO)_2(P(C_6H_5)_3)_2$, was undertaken for two principal reasons. The first is that since SO_2 can presumably function as a unidentate or bidentate ligand a comparison of the structures of the O_2 and SO_2 adducts, which we anticipated would be closely related, should provide a better understanding of the bonding in each. It turns out, in fact, that the two structures are very different. A second reason for the present study was to obtain information on the mode of attachment of SO_2 to a transition metal. Sulfur dioxide is, as yet, a rare ligand in transition metal chemistry, and the only other well-characterized SO_2 complexes are the ruthenium amines.[7,8] Fortunately, an X-ray study[9] of the structure of $(RuCl(NH_3)_4(SO_2))Cl$ has recently been completed and so a comparison of the SO_2–metal geometries in the two compounds can be made. Although in both cases the linkage of the SO_2 group to the metal is through the sulfur, the geometries are different.

Collection and Reduction of the X-Ray Data

The sample of $IrCl(CO)(SO_2)(P(C_6H_5)_3)_2$, kindly supplied by L. Vaska, contained many beautifully formed, green crystals. On the basis of optical goniometry and precession photography we established that these crystals belong to the monoclinic system and crystallize in a cell of dimensions $a = 12.11 \pm 0.02$, $b = 16.79 \pm 0.02$, $c = 17.09 \pm 0.02$ A, $\beta = 103.0 \pm 0.5°$; $V = 3386$ A^3. The observed extinctions are $0k0$ for k odd and $h0l$ for l odd, and the space group is very probably C_{2h}^5-$P2_1/c$. A density of 1.632 g/cm^3 calculated for four molecules in the unit cell agrees satisfactorily with that of 1.54 ± 0.05 g/cm^3 measured by flotation in zinc chloride solutions. Thus no crystallographic symmetry conditions need be imposed on the molecules.

Intensity data were collected at room temperature by the equiinclination Weissenberg method, using Zr-filtered Mo Kα radiation and a Nonius integrating Weissenberg camera. The crystal selected for the photography was mounted with a as the rotation axis, and in successive 96-hr exposures the layers $0kl$ through $9kl$ were recorded on Ilford Industrial G X-ray film. The intensities of 1365 independent reflections accessible within the angular range $\theta_{Mo} \leq 20°$ were estimated visually. This represents approximately 50% of the reflections that can occur within this range. A larger fraction of these reflections might have been recorded had a larger crystal been used. However, since the use of a larger crystal would have resulted in a larger absorption correction it is doubtful if increased precision in the final atomic parameters would have resulted. After the usual Lorentz-polarization corrections had been applied, the resultant F_o^2 values, where F_o is the observed structure amplitude, were corrected for absorption. The ten faces of the crystal were identified by optical means and were carefully measured, in order that the path lengths of the diffracted beams through the crystal could be calculated and the absorption correction made. Even though the calculated volume of the crystal is only 0.0026 mm^3 and the calculated weight 4.2 μg, the resultant transmission factors for a linear absorption coefficient of 44.47 cm^{-1} range from 0.43 to 0.63.[10] Thus the absorption correction is a significant and important one, even though the "average" value of μR of 0.6 is in the range that is often thought to be sufficiently small so that absorption corrections are of no consequence. The F_o values were subsequently brought to an approximate common scale through a modification of Wilson's procedure.

Solution and Refinement of the Structure

The positions of the Ir, P, S, and Cl atoms were determined by inspection of the three-dimensional sharpened, origin-removed Patterson function. A refinement of these positions, along with individual isotropic thermal parameters and separate scale factors for the separate layers, led to a conventional R factor ($R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$) of 0.19. The remaining light atoms were readily located in a difference Fourier based on the phases from these heavy atoms.

The structure was refined by the least-squares method. The function minimized was $\Sigma\, w(F_o - F_c)^2$, where the weights w were assigned in the following way: $I \leq 16$, w proportional to $(I/F)^2$; $I > 16$, w proportional to $(16/F)^2$, where I is the raw intensity value for the particular reflection. The atomic scattering factor for Ir was from the Dirac–Slater calculation of Cromer and Waber[11]; scattering factors for the other atoms were taken from the tabulation by Ibers.[12] The anomalous parts of the Ir, Cl, S, and P scattering factors given by Cromer[13] were included in the calculated structure factors.[14] For both practical and theoretically sound reasons[15–17] in the least-squares refinement the phenyl rings were treated as rigid groups and were restricted to their well-known geometry (D_{6h} symmetry, C–C =

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[5] J. A. Ibers and S. J. La Placa, *Science*, **145**, 920 (1964).

[6] S. J. La Placa and J. A. Ibers, *J. Am. Chem. Soc.*, **87**, 2581 (1965).

[7] K. Gleu and K. Rehm, *Z. Anorg. Allgem. Chem.*, **227**, 237 (1936).

[8] K. Gleu, W. Breuel, and K. Rehm, *ibid.*, **235**, 201, 211 (1938).

[9] L. H. Vogt, Jr., J. L. Katz, and S. E. Wiberley, *Inorg. Chem.*, **4**, 1157 (1965).

[10] Programs for the IBM 7094 used in this work, in addition to those of local origin, were local modifications of Burnham's GNABS absorption program, Zalkin's FORDAP Fourier program, and the Busing–Levy ORFLS least-squares program and ORFFE error function program.

[11] D. T. Cromer and J. T. Waber, *Acta Cryst.*, **18**, 104 (1965).

[12] J. A. Ibers in "International Tables for X-ray Crystallography," Kynoch Press, Birmingham, England, 1962, Vol. 3, Table 3.3.1.

[13] D. T. Cromer, *Acta Cryst.*, **18**, 17 (1965).

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

[15] S. J. La Placa and J. A. Ibers, *J. Am. Chem. Soc.*, **85**, 3501 (1963).

[16] S. J. La Placa and J. A. Ibers, *Acta Cryst.*, **18**, 511 (1965).

[17] R. Eisenberg and J. A. Ibers, *Inorg. Chem.*, **4**, 773 (1965).

TABLE I

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

Atom	x	y	z	B, A^2
Ir	0.21335 (13)[a]	0.27084 (9)	0.26122 (11)	2.1[b]
S	0.2683 (7)	0.3352 (6)	0.3955 (5)	2.8 (2)
Cl	0.2689 (8)	0.1393 (6)	0.3029 (5)	3.5 (2)
P_1	0.3959 (7)	0.2879 (6)	0.2366 (6)	2.8 (3)
P_2	0.0276 (6)	0.2388 (6)	0.2648 (5)	2.6 (2)
O_1	0.3232 (18)	0.4060 (14)	0.3811 (13)	4.1 (6)
O_2	0.1654 (20)	0.3434 (14)	0.4266 (13)	4.6 (6)
O (of CO)	0.1321 (20)	0.4267 (17)	0.1835 (15)	4.7 (6)
C (of CO)	0.1604 (30)	0.3741 (25)	0.2132 (21)	3.2 (9)

Group	x_c[c]	y_c	z_c	δ	ϵ	η	B, A^2
P_1R_1[d]	0.596 (1)	0.310 (1)	0.398 (1)	2.57 (2)	0.63 (1)	1.01 (2)	4.1 (4)
P_1R_2	0.473 (1)	0.137 (1)	0.143 (1)	4.92 (1)	0.25 (1)	3.74 (1)	3.6 (5)
P_1R_3	0.397 (2)	0.434 (1)	0.116 (1)	3.09 (2)	5.38 (2)	4.66 (2)	4.7 (5)
P_2R_1	−0.051 (1)	0.108 (1)	0.125 (1)	5.50 (2)	5.49 (1)	4.46 (2)	3.5 (4)
P_2R_2	−0.158 (1)	0.374 (1)	0.214 (1)	5.52 (2)	0.70 (1)	6.11 (2)	3.5 (4)
P_2R_3	−0.031 (2)	0.158 (1)	0.427 (1)	4.40 (2)	0.10 (2)	2.09 (2)	5.0 (5)

[a] Numbers in parentheses here and in succeeding tables are standard deviations in the least significant digits. [b] From the isotropic refinement. Ir was refined anisotropically, the form of the anisotropic thermal ellipsoid being $\exp(-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl))$. The resultant parameters for Ir are: 0.00392 (9), 0.00096 (5), 0.00297 (6), −0.00012 (12), 0.00101 (5), and −0.00011 (10). These lead to root-mean-square amplitudes of vibration for Ir of 0.116 (3), 0.163 (2), and 0.205 (2) A. [c] x_c, y_c, and z_c are the fractional coordinates of the ring centers. The angles δ, ϵ, and η (in radians) which bring about alignment (except for translation) of an internal coordinate system within the ring with a fixed external coordinate system have been defined in previous papers.[5,6,17] [d] P_1R_1 is phosphorus 1, ring 1, etc.

1.392, C–H = 1.08 A). The variable parameters for each phenyl ring include an over-all isotropic thermal parameter, the positions of the center of the ring, and three rotation angles that have been defined previously.[5,6,17] In the initial calculation the nongroup atoms were restricted to isotropic vibration and this refinement of 88 parameters (including scale factors) converged to an R factor of 0.089 and to a weighted R factor R' ($R' = (\Sigma w(F_o - F_c)^2/\Sigma wF_o^2)^{1/2}$ of 0.087. A difference Fourier calculated at this point provided a clear indication of significant anisotropy in the vicinity of the Ir atom. In a final round of calculations the contributions of the hydrogen atom from the phenyl rings were included and the iridium atom was allowed to vibrate anisotropically. This refinement converged to values of R of 0.070 and of R' of 0.070 and of the error of fit function $(\Sigma w(F_o - F_c)^2/(n - m))^{1/2}$ (where n is the number of observations and m the number of variable parameters) of 0.66. This latter value is sufficiently close to the expected value of unity to support both the reasonableness of the weighting scheme and the standard deviations of the parameters as derived from the inverse matrix. The highest peak on a final difference Fourier is 1.5 e/A^3, about 30% of the height of a light atom in this structure.

In Table I the final parameters, together with their standard deviations, are listed. The group parameters of Table I lead to the positional parameters for the phenyl carbon atoms given in Table II. The standard deviations given in Table II are for use in error analyses of functions not involved in the same ring; the intraring distances are, of course, fixed. The tabulation of observed and calculated structure amplitudes (in electrons) given in Table III includes only observed reflections. None of the unobserved reflections accessible on the films has a calculated intensity that exceeds our estimate of the minimum observable.

TABLE II

DERIVED PARAMETERS FOR GROUP CARBON ATOMS[a]

Group atom	x	y	z
$P_1R_1C_1$	0.511 (2)	0.300 (2)	0.329 (1)
$P_1R_1C_2$	0.509 (2)	0.256 (1)	0.397 (2)
$P_1R_1C_3$	0.593 (2)	0.267 (2)	0.467 (1)
$P_1R_1C_4$	0.681 (2)	0.321 (2)	0.467 (1)
$P_1R_1C_5$	0.683 (2)	0.364 (1)	0.389 (2)
$P_1R_1C_6$	0.598 (2)	0.354 (1)	0.329 (1)
$P_1R_2C_1$	0.437 (2)	0.202 (1)	0.182 (1)
$P_1R_2C_2$	0.552 (2)	0.184 (1)	0.195 (1)
$P_1R_2C_3$	0.588 (1)	0.119 (2)	0.157 (1)
$P_1R_2C_4$	0.509 (2)	0.072 (1)	0.105 (1)
$P_1R_2C_5$	0.394 (2)	0.091 (1)	0.091 (1)
$P_1R_2C_6$	0.358 (1)	0.156 (2)	0.130 (1)
$P_1R_3C_1$	0.399 (2)	0.368 (2)	0.167 (2)
$P_1R_3C_2$	0.394 (1)	0.357 (1)	0.086 (2)
$P_1R_3C_3$	0.393 (2)	0.422 (2)	0.035 (1)
$P_1R_3C_4$	0.395 (2)	0.499 (2)	0.066 (2)
$P_1R_3C_5$	0.399 (2)	0.511 (1)	0.147 (2)
$P_1R_3C_6$	0.401 (2)	0.445 (2)	0.198 (1)
$P_2R_1C_1$	−0.015 (2)	0.163 (1)	0.186 (1)
$P_2R_1C_2$	0.017 (2)	0.171 (1)	0.113 (2)
$P_2R_1C_3$	−0.019 (2)	0.116 (2)	0.052 (1)
$P_2R_1C_4$	−0.088 (2)	0.053 (1)	0.064 (1)
$P_2R_1C_5$	−0.120 (2)	0.045 (1)	0.136 (2)
$P_2R_1C_6$	−0.083 (2)	0.100 (2)	0.197 (1)
$P_2R_2C_1$	−0.083 (2)	0.311 (1)	0.236 (1)
$P_2R_2C_2$	−0.066 (2)	0.382 (2)	0.279 (1)
$P_2R_2C_3$	−0.141 (2)	0.445 (1)	0.257 (1)
$P_2R_2C_4$	−0.233 (2)	0.437 (1)	0.191 (2)
$P_2R_2C_5$	−0.249 (2)	0.366 (2)	0.149 (1)
$P_2R_2C_6$	−0.174 (2)	0.303 (1)	0.171 (1)
$P_2R_3C_1$	−0.004 (2)	0.195 (2)	0.361 (1)
$P_2R_3C_2$	0.079 (2)	0.155 (2)	0.416 (2)
$P_2R_3C_3$	0.052 (2)	0.118 (2)	0.482 (1)
$P_2R_3C_4$	−0.059 (2)	0.121 (2)	0.493 (1)
$P_2R_3C_5$	−0.142 (2)	0.161 (2)	0.437 (2)
$P_2R_3C_6$	−0.114 (2)	0.198 (1)	0.371 (1)

[a] C_1 is attached to P; other C atoms are numbered in succession so that C_4 is *para* to C_1.

TABLE III

OBSERVED AND CALCULATED STRUCTURE AMPLITUDES (IN ELECTRONS) FOR $IrCl(CO)(SO_2)(P(C_6H_5)_3)_2$

K	L	OBS	CALC
******H=0******			
0	0		1659
0	4	194	191
0	6	249	261
0	8	157	160
0	10	103	97
0	12	114	103
0	14	115	107
0	16	56	51
1	4	59	47
1	5	140	140
1	6	72	74
1	8	140	143
1	10	133	138
1	12	81	79
1	14	103	97
2	3	108	107
2	4	260	274
2	5	85	87
2	6	258	264
2	7	100	109
2	8	201	217
2	10	135	133
2	12	116	111
2	14	90	93
3	2	173	163
3	3	55	59
3	4	72	55
3	6	118	107
3	8	77	75
3	10	97	87
3	12	107	99
3	14	105	83
4	1	115	108
4	2	299	278
4	3	61	56
4	4	302	294
4	5	175	169
4	6	239	226
4	7	151	146
4	8	199	205
4	9	103	94
4	10	182	193
4	11	66	86
4	12	84	98
4	13	72	70
4	14	53	56
5	1	33	19
5	2	75	65
5	4	98	90
5	5	114	119
5	10	120	118
5	12	140	127
5	14	76	96
6	0	131	123
6	1	207	205
6	2	216	211
6	3	280	256
6	4	261	260
6	5	216	212
6	6	143	142
6	7	72	75
6	8	155	143
6	9	100	94
6	10	114	107
6	12	51	60
6	13	75	72
7	4	107	93
7	6	73	82
7	7	87	73
7	8	100	80
7	10	96	93
7	12	74	64
8	0	127	124
8	1	212	220
8	2	104	105
8	3	221	222
8	4	129	135
8	5	151	167
8	6	89	86
8	7	112	110
8	8	81	73
8	9	97	129
8	11	116	81
9	4	79	58
9	5	103	89
9	6	124	110
9	7	83	77
9	8	85	91
10	0	117	98
10	1	165	186
10	2	68	50
10	3	172	189
10	5	161	162
10	6	70	73
10	7	142	161
10	9	118	112
10	11	96	96
12	1	175	187
12	3	140	149
12	5	131	140
12	7	110	119
12	9	91	102
13	9	84	93
14	0	81	67
14	1	57	131
14	2	115	65
14	3	81	94
14	5	101	119
14	7	103	106
15	3	60	66
15	5	61	44
16	0	88	62
16	2	88	59
******H=1******			
0	4	38	46
0	6	57	25
0	8	76	75
0	10	43	39
0	12	68	49
0	14	74	77
0	-4	266	292
0	-6	129	139
0	-8	190	206
0	-10	132	138
0	-12	93	82
0	-14	51	53
0	-16	79	97
1	4	241	246
1	5	53	47
1	6	302	315
1	7	62	79
1	8	200	224
1	10	122	124
1	12	152	155
1	14	91	123
1	-4	195	203
1	-6	252	247
1	-8	122	111
2	3	122	121
2	4	40	48
2	5	113	121
2	14	92	86
2	-4	97	105
2	-5	151	155
2	-6	177	182
2	-8	180	190
2	-10	127	124
2	-12	105	105
2	-14	89	94
3	2	310	286
3	3	40	27
3	4	343	328
3	5	122	116
3	6	263	264
3	7	175	184
3	8	191	216
3	9	42	71
3	10	178	184
3	12	147	159
3	-2	242	290
3	-3	119	116
3	-4	170	162
3	-5	153	147
3	-6	163	165
3	-7	95	97
3	-8	138	140
3	-10	114	109
4	1	112	107
4	2	154	146
4	-2	91	90
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7	5	104	110
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11	3	140	147
11	5	114	110
11	-1	164	167
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1	-8	98	96
1	-10	119	115
1	-12	78	87
1	-14	87	75
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2	3	86	94
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3	-10	80	59
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6	-6	111	110
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7	-11	62	43
8	0	94	80
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8	-4	101	94
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10	3	124	130
10	5	112	112
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12	-5	116	113
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2	-12	110	108
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11	-1	128	132
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11	-5	114	116
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2	-6	87	93
2	-8	75	49
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3	-5	81	78
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4	2	125	115
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8	3	66	65
8	-1	63	69
8	-2	64	58
8	-5	95	86
8	-6	82	79
8	-7	82	75
9	-1	106	103
9	-3	97	89
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10	-4	74	67
10	-5	76	70

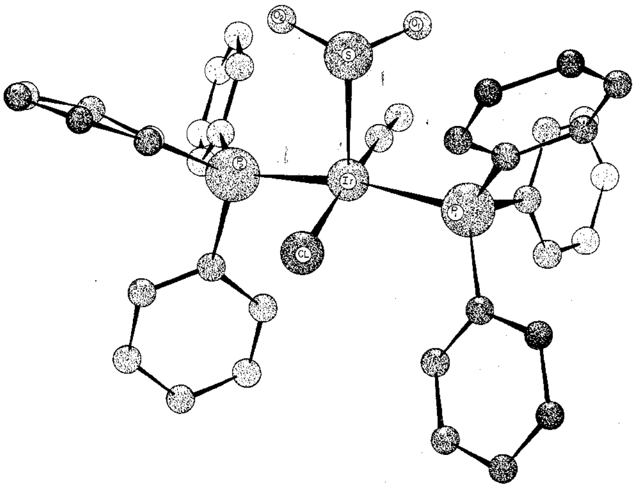

Figure 1.—A perspective drawing of the $IrCl(CO)(SO_2)(P(C_6H_5)_3)_2$ molecule. Phenyl hydrogens are not shown.

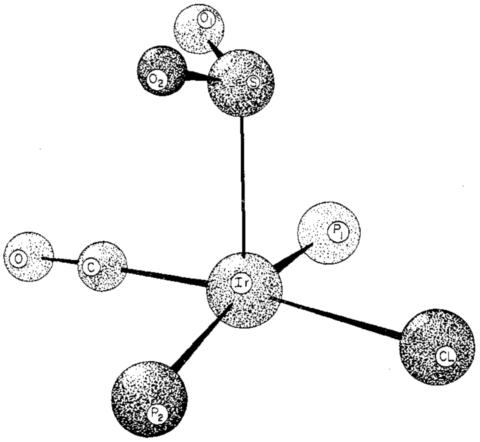

Figure 2.—A perspective drawing of the coordination around Ir in $IrCl(CO)(SO_2)(P(C_6H_5)_3)_2$.

Description of the Structure

The structure described by the cell dimensions, symmetry operations of the space group, and parameters of Table I consists of the packing of discrete, monomeric molecules (shortest Ir–Ir distance is greater than 8.5 A). The molecular structure of the monomer is shown in perspective in Figure 1, and the inner coordination geometry is displayed in Figure 2. The Ir is five-coordinated; the coordination polyhedron is a tetragonal pyramid, with *trans* P, Cl, and CO in the base and the S of the SO_2 group at the apex.[18] The best least-squares plane[20] through Cl, P_1, P_2, and O (of the CO) has the equation $0.2985X + 6.513Y + 15.248Z = 5.604$ (monoclinic coordinates) and the deviations of these atoms from this plane are insignificant (0.002 (9), −0.003 (10), −0.002 (9), and 0.013 (24) A, respectively). The Ir atom lies about 0.21 A above this plane toward the SO_2 group. Atoms Cl, P_1, P_2, and C (of the CO) deviate significantly from planarity.

Table IV gives a selection of intramolecular distances and angles. (The intermolecular distances are not tabulated, since for the most part they are normal and uninteresting. The volume per triphenylphosphine group is only 15% greater than in triphenylphosphine itself[21] and so most of the short intermolecular contacts are between triphenylphosphine ligands.)

TABLE IV

SELECTED INTRAMOLECULAR DISTANCES AND ANGLES

Intramolecular distance, A		Angle, deg	
Ir–S	2.488 (10)	S–Ir–P_1	92.6 (4)
Ir–Cl	2.371 (10)	S–Ir–Cl	97.4 (3)
Ir–P_1	2.359 (9)	S–Ir–P_2	97.8 (4)
Ir–P_2	2.328 (8)	S–Ir–C	89.8 (1.1)
Ir–O_1	3.15 (2)	S–Ir–O	91.3 (5)
Ir–O_2	3.25 (2)	P_1–Ir–Cl	87.3 (4)
Ir–C	1.96 (4)	P_1–Ir–P_2	169.5 (4)
Ir–O	3.00 (3)	P_1–Ir–C	92.8 (1.0)
S–O_1	1.41 (2)	P_1–Ir–O	92.4 (5)
S–O_2	1.47 (2)	Cl-Ir–P_2	89.3 (3)
S–P_1	3.50 (1)	Cl-Ir–C	172.8 (1.0)
S–P_2	3.63 (2)	Cl-Ir–O	171.3 (5)
S–Cl	3.65 (1)	P_2–Ir–C	89.4 (1.0)
S–C	3.16 (4)	P_2–Ir–O	89.5 (5)
P_1–Cl	3.26 (1)	Ir–C–O	175.6 (3.5)
P_1–P_2	4.67 (1)	Ir–S–O_1	104.2 (1.5)
P_1–C	3.14 (4)	Ir–S–O_2	107.6 (1.5)
P_1–O	3.89 (3)	O_1–S–O_2	117.1 (1.5)
Cl–P_2	3.30 (1)	P_1–Cl–P_2	90.6 (3)
Cl–C	4.33 (5)	Cl–P_2–C	86.1 (8)
P_2–C	3.03 (4)	P_2–C–P_1	98.3 (1.2)
P_2–O	3.78 (3)	C–P_1–Cl	84.9 (8)
P–C (av of 6)	1.84	C–P–C (av of 6)	104.9

The Ir–P distances of 2.33 and 2.36 A and the Ir–Cl distance of 2.37 A are in the range found between second- and third-row transition metals and P or Cl in a variety of compounds[16,17,19] and in particular may be compared with Ir–P distances of 2.36 and 2.37 A and an Ir–Cl distance of approximately 2.40 A in the analogous oxygen adduct.[5,6] The CO distance of 1.04 ± 0.04 A is surely anomalous, being about three standard deviations away from the expected value of 1.12 A. It seems more likely that the estimate of the standard deviation is optimistic, rather than that the CO bond is extremely short or that the 0.2% probability of a deviation of three standard deviations has occurred. A difference Fourier based on F_c values from which the contributions of CO and Cl have been subtracted shows no unusual features; in the analogous oxygen adduct the Cl and CO positions are disordered.

The bonding of Ir to SO_2 is a very interesting feature of the structure. Although there are few direct comparisons that can be made, the Ir–S bond length of 2.49 ± 0.01 A seems long by any standards. The Ir–SO_2 portion of the molecule is not planar; rather, the Ir–S vector makes an angle of 31.6 ± 1.5° with the normal to the SO_2 plane. Moreover, when the coordination polyhedron is a tetragonal pyramid it is

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[18] The hydrogen atom attached to $P_2R_1C_2$ makes the next closest approach to Ir. On the assumption of normal phenyl geometry this hydrogen is calculated to be 3.00 A from Ir. This is considerably greater than the distance of 2.69 A found between a phenyl hydrogen and Ru in the five-coordinated d^6 complex $RuCl_2(P(C_6H_5)_3)_3$[19] where the H effectively blocks the sixth coordination position of the Ru.

[19] S. J. La Placa and J. A. Ibers, *Inorg. Chem.*, **4**, 778 (1965).

[20] W. C. Hamilton, *Acta Cryst.*, **14**, 185 (1961).

[21] J. J. Daly, *J. Chem. Soc.*, 3799 (1964).

usual to find[22] the central metal atom some 0.4 to 0.5 A above the basal plane, whereas here the Ir is only 0.21 A above the basal plane. All of these facts—the long Ir–S bond, the nonplanarity of the $IrSO_2$ group, and the closeness of the Ir to the basal plane—strongly suggest that the attachment of SO_2 in this complex is very weak. The bonding of Ru to SO_2 in $(RuCl(NH_3)_4(SO_2))Cl$[9] is very different indeed. In this compound the Ru is at the center of a slightly distorted octahedron. The Ru–Cl distance is 2.42 A. The Ru–N distances average 2.13 A, but the Ru–S distance is only 2.072 ± 0.003 A. As might be expected in view of this short distance, the $Ru{-}SO_2$ portion of the molecule is planar. Clearly a difference of over 0.4 A in the metal to sulfur dioxide bond distance in these two compounds ought to be reflected in the SO_2 geometry. Table V provides a comparison of this SO_2 geometry in solid SO_2 and in these two compounds. One could argue, consistent with the weak Ir–S bond, that the SO_2 geometry in the iridium compound, which does not deviate significantly from that in solid SO_2, does in fact differ from the SO_2 geometry found in the ruthenium compound. In view of the standard deviations assigned to the S–O bond lengths and O–S–O bond angles, this argument is not a strong one.

Table V

Sulfur Dioxide Geometries

Compound	$S{-}O_1$	$S{-}O_2$	$O_1{-}S{-}O_2$
SO_2 solid (−130°)[a]	1.430 (15)	*b*	119.5 (1.5)
$IrCl(CO)(SO_2)(P(C_6H_5)_3)_2$	1.411 (23)	1.467 (25)[c]	117.1 (1.5)
$(RuCl(NH_3)_4(SO_2))Cl$[d]	1.462 (10)	1.394 (10)	113.8 (6)

[a] B. Post, R. S. Schwartz, and I. Fankuchen, *Acta Cryst.*, **5**, 372 (1952). [b] In solid SO_2, $S{-}O_1$ is equal to $S{-}O_2$ by symmetry. [c] In the iridium complex the difference between $S{-}O_1$ and $S{-}O_2$ of 0.056 ± 0.034 A is not significant. The mean S–O distance is therefore 1.439 ± 0.017 A. [d] Ref 9.

Since bond order *vs.* bond length curves are available for O_2 species, the O–O bond length of 1.30 A in the oxygen analog of the present compound provides an indication of the degree of electron transfer into the O_2 molecule on bonding to iridium. Such an indication cannot be obtained for the SO_2 molecule, since information on the geometries of such species as SO_2^-, SO_2^{-2}, etc., is lacking. The dithionite ion, $S_2O_4^{-2}$, studied by Dunitz,[23] may be thought of as two SO_2^- ions joined very weakly together through S–S bonding (S–S distance is 2.39 A). Dunitz finds S–O distances averaging 1.50 ± 0.02 A and an O–S–O angle of 108°. These dimensions are significantly different from those found here.

The triphenylphosphine geometry found in this present study resembles closely that found in other compounds[6,16,20,21] and again the dihedral angles between adjacent phenyl rings show, within limits dictated by H–H repulsions, no particular trends.

A surprising and perplexing aspect of the present study is the discovery of the great difference in coordination geometry around iridium which occurs upon substitution of sulfur dioxide for oxygen. We offer no explanation at this time, but we plan to pursue structural studies on related complexes, including the presumed square-planar parent $IrCl(CO)(P(C_6H_5)_3)_2$. It is hoped that out of such a study of closely related complexes at least a rudimentary understanding of the various bonding arrangements will come.

Acknowledgment.—It is once again a pleasure to acknowledge the close cooperation we have enjoyed with Professor L. Vaska and to thank him for the present sample. We also enjoyed a very helpful conversation with Professor J. D. Dunitz.

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(22) J. A. Ibers, *Ann. Rev. Phys. Chem.*, **16**, 375 (1965).

(23) J. D. Dunitz, *Acta Cryst.*, **9**, 579 (1956).