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Alkoxy- and aryloxycarbonylcobalt carbonyls

IV *. Preparation and structure of derivatives with tertiary pnicogen ligands

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Abstract

The (alkoxycarbonyl)cobalt tetracarbonyl $^nBuOC(O)Co(CO)_4$ (Ia) was treated with the ligands ER_3 (E = P, As, Sb; R = alkyl, aryl, alkoxy, dialkylamino) to give 37 monosubstituted products (IIa). Disubstituted derivatives (IIIa) containing PR_3 (R = Et, OMe) ligands were also made from Ia. The IR spectra of compounds IIa containing various PR_3 ligands were correlated with the electronic and steric parameters of the P-ligands. The crystal structure of $^nBuOC(O)Co(CO)_3PPh_3$ (IIa1) was determined by an X-ray diffraction study.

Introduction

(Alkoxycarbonyl)cobalt tetracarbonyls, $ROC(O)Co(CO)_4$ (I), are the most studied transition metal carbonyl derivatives of carbonic acid. These complexes were assumed or proved to be intermediates or (side) products in important catalytic reactions [1b,2–5]. Some recent reports on such complexes deal with (i) their formation from $R^1C(O)Co(CO)_3L$ (L = CO or PPh_2Me) type acylcobalt carbonyls [6***,7***], (ii) decarboxylation [1a,c], and (iii) their formation in the reaction of cobalt alcoholates with synthesis-gas under unusually mild conditions [8].

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* For Parts I–III see refs. 1a–c.

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*** Reference number with asterisk indicates a note in the list of references.

Since both the related homologation of alcohols [5e,9] and decarboxylation reactions [1c] are promoted by tertiary pnicogen (Group 15) ligands, the chemistry of complexes I containing such Lewis bases is of interest. Some monotertiary phosphine and phosphite derivatives of a single representative of this class of compound, Ia have been prepared by a one-pot synthesis [10a] or by direct substitution of the parent tetracarbonyl Ia, but no systematic investigation has been reported until now. We describe here some preparative, spectroscopic, and structural observations on such species.

Results and discussion

Compound Ia was treated with several tertiary phosphine ligands and also with triphenyl-arsine and -stilbine. The formation of the monosubstituted derivatives, ^{n}BuOC(O)Co(CO)$_3$L (IIa), was generally under mild conditions when equimolar amounts of the ligand were used. Use of an excess (up to 5-fold) of the ligand L yielded disubstituted products, ^{n}BuOC(O)Co(CO)$_2$L$_2$ (IIIa) in the case of ligands with either strong donor (PEt$_3$) (IIIa1) or marked π-acceptor (P(OMe)$_3$) (IIIa2) character. However, with ligands intermediate in nature (e.g. PPh$_3$) or with very bulky ones (P(t-Bu)$_3$) only monosubstitution products were obtained.

Tertiary amines (NEt$_3$ and NPh$_3$) react with complex Ia, but the (probably ionic) products have not yet been identified. Tertiary arsines and stilbines were found to yield monosubstitution products.

The infrared and ^{1}H NMR spectra of the monosubstituted derivatives IIa are similar to those of MeOC(O)Co(CO)$_3$PPh$_3$ (IIb1) [3a] and IIa1 (see below), the structures of which were determined by an X-ray diffraction study. Thus it seems reasonable to assume that all the complexes of type IIa reported here have trigonal bipyramidal geometry, with the R^{1}OC(O) and L groups in the axial (*trans*) positions. Such a geometry was established previously for the two RC(O)Co(CO)$_3$L type acylcobalt carbonyls, 2,6-Cl$_2$C$_6$H$_3$CH$_2$C(O)Co(CO)$_3$PPh$_3$ [6b*], and ClCH$_2$C(O)Co(CO)$_3$PPh$_3$ [11].

The spectra do not give conclusive indications of the relative positions of the acyl, CO, and L substituents in the disubstituted compounds IIIa, but on the basis of steric considerations and the geometry of compounds IIa, it can reasonably be assumed that their overall geometry is trigonal bipyramidal, with the acyl group occupying an axial position and one of the ligands the other axial site. The relatively small difference between the ν(C–O)$_t$ absorptions of compound IIIa2 would be compatible also with a bis-equatorial distribution of the P-ligands [13d], but the almost identical intensity patterns exclude this possibility.

The large number of complexes of type IIa prepared in the course of this work allows a correlation analysis to be made on the influence of the substitution of one CO ligand on the rest of the molecule. This was done by seeking correlations between the characteristic ν(C–O) frequencies (the 'totally symmetric (A_1)' [12], the E_{av} and the 'acyl' stretching band) and the $^{FT}\chi$ [13] and θ [14] parameters of the ligands in ^{n}BuOC(O)Co(CO)$_3$L IIa1–IIa37 derivatives (see Table 1). The three dimensional correlation surfaces are shown in Figs. 1a–c.

It is of interest that while the ν(C–O)$_t$ frequencies (Fig. 1a,b) are independent of θ, the ν(C–O)$_{acyl}$ absorptions vary with this parameter. This shows clearly how much the 'steric' influence of the PR$_3$ ligand expresses itself apparently as a

σ-'electronic' effect. If θ reflected only 'steric' characteristics, the coordinated carbonyls (*cis* to the PR_3 ligand) would be expected to be affected more than the *trans*-acyl group.

The ν(C–O) band pattern for compounds I and II can be analysed by comparison with those of other $RCo(CO)_3L$ (L = CO, PR_3) compounds with perfect C_{3v} symmetry by assuming that the two lowest frequency bands of I and II are derived from the splitting of the E band of the C_{3v} species [1a,6b*,11,15]. Thus the extent of splitting (ΔE) could be regarded as a 'measure of the asymmetry' in compounds II (either its absolute value or the difference from the splitting in the parent Ia: 12.5 cm^{-1} [1a]). The three-fold symmetry of the phosphine ligands in compounds II, especially in those of the type $PR_1R_2R_3$ ($R_1 = R_2 = R_3$) could be expected not to alter the ΔE value relative to that of Ia. In fact several phosphines increase and others decrease ΔE, irrespective of whether they are of C_{3v} ($R_1 = R_2 = R_3$) symmetry or not ($R_1 \neq R_2$ and $R_1 \neq R_2 \neq R_3$). The ΔE values observed for the phosphines listed in Table 1 do not show any correlation with ${}^{FT}\chi$, θ, A_1 or E_{av}, indicating that the factors governing the band splitting are more complex in nature, and could probably be interpreted only after several more X-ray structure determinations.

An increase extent of *cis*-stabilization [16] with increasing ${}^{FT}\chi$ could be expected to hinder the substitution of compounds IIa by the second phosphine. Apparently this effect is not decisive for these (alkoxycarbonyl)cobalt complexes, as shown by the ease of disubstitution both by a low ${}^{FT}\chi$ and by a high ${}^{FT}\chi$ ligand.

An X-ray diffraction study of only one monosubstituted I derivative, $MeOC(O)Co(CO)_3PPh_3$ (IIb1) [3a] has been reported previously. Because of the great changes in the reactivity of complexes $ROC(O)Co(CO)_4$ observed as a result of a systematic methyl-perturbation [13] of the σ-sp^3-C atom [1c] it seemed to us of interest to determine the molecular structure of another complex of type II with a mono-alkyl-substituted methyl group and the same phosphine. ${}^{n}BuOC(O)Co(CO)_3PPh_3$ (IIa1) fulfilled these requirements, and moreover yielded crystals which were suitable for an X-ray study. The results of this study are shown in Tables 2, 3 and Fig. 2. The most important structural parameters of compound IIa1 and IIb1 are compared in Table 4.

The structural parameters of compounds IIa1 and IIb1 appear to be fairly close to each other and show a general agreement with the structures of other X-$Co(CO)_3L$ type compounds. The similarity of the structural data for compounds IIa1 and IIb1 indicates that the difference in the reactivity in the decarboxylation [1a,c;19] should be attributed to difference(s) in the structure of the transition states rather than to those in the ground states of the starting compounds.

Experimental

General procedures

All reactions were carried out under deoxygenated CO or Ar in carefully dried (Na/K) solvents. The IR spectra were recorded by use of a CaF_2 cell on a Specord 75 (Carl Zeiss Jena, GDR), and the ^1H NMR spectra on a 80 MHz BS-487 (Tesla, Brno, CSFR) spectrometer. Starting materials were commercial products except for $Co_2(CO)_8$ [20] and some phosphines [21*] (see Table 1; L 6–8, 10, 11, 13–21, 23–32, 36).

Table 1

Infrared ν(C–O) spectra of $^{n}BuOC(O)Co(CO)_3L$ (IIa) complexes in n-heptane

No.	Ligand	$^{FT}\chi$ (cm^{-1})	θ (deg)	IR ν(C–O) absorption maxima (intensity) [a] (cm^{-1})				
				A_1	E		E_{av}	$\nu(C–O)_{acyl}$
1	PPh_3	13.25	145	2059.8(1.0)	1994.6(10.0)	1982.4(10.0)	1988.55	1666.8(2.8)
2	$AsPh_3$	–	–	2059.5(1.4)	1994.1(10.0)	1983.0(10.0)	–	1670.1(3.0)
3	$SbPh_3$	–	–	2059.5(1.9)	1994.1(10.0)	1983.7(9.2)	–	1674.5(3.1)
4	$P(^{t}Bu)_3$	0	182	2048.4(2.7) 2053.0(sh)	1978.1(10.0)	1962.2(9.9)	1970.15	1668.7(3.1)
5	$P(^{c}Hex)_3$	1.40	170	2051.6(1.8)	1981.8(10.0)	1968.0(9.7)	1974.90	1664.1(3.2)
6	$P(^{c}Hex)(o\text{-}OMe–Ph)_2$	1.60	153	2055.7(2.0)	1985.5(9.9)	1967.4(10.0)	1976.45	1663.5(3.2)
7	$P(NEt_2)_3$	3.10	170	2051.6(1.4)	1982.3(10.0)	1969.5(9.7)	1975.90	1663.9(3.2)
8	$P(^{i}Pr)_3$	3.45	160	2053.2(1.2)	1984.8(10.0)	1970.0(9.5)	1977.40	1665.2(2.5)
9	$P(^{n}Bu)_3$	5.25	132	2055.1(1.6)	1985.4(10.0)	1975.0(9.8)	1980.20	1665.1(3.2)
10	$PPh(^{c}Hex)_2$	5.40	162	2054.4(1.9)	1986.8(10.0)	1972.7(9.4)	1979.75	1664.6(3.0)
11	PMe_2Menth	5.70	138	2055.4(1.6)	1986.7(10.0)	1973.4(9.6)	1980.05	1667.4(2.5)
12	PEt_3	6.30	132	2054.0(0.6)	1985.6(10.0)	1974.2(10.0)	1979.90	1664.0(2.1)
13	$P(CH_2–^{t}Bu)_3$	6.90	159	2053.8(1.3)	1985.6(10.0)	1970.4(9.4)	1977.75	1667.9(2.9)
14	$PPh(^{i}Pr)_2$	7.50	155	2055.6(1.9) 2060.8(sh)	1987.9(10.0)	1974.0(9.7)	1980.95	1665.8(3.4)
15	$PEt_2Benzyl$	7.65	134	2055.2(1.0)	1987.3(10.0)	1974.4(9.7)	1980.85	1665.3(3.1)
16	PPh_2SiMe_3	8.05	157	2054.5(0.8)	1997.4(10.0)	1986.1(9.5)	1991.70	1670.5(2.5)
17	$PPhEt_2$	9.30	136	2055.7(1.3)	1989.5(10.0)	1977.7(9.6)	1983.60	1665.9(3.3)

20	$PPhMe_2$	10.60	126	2060.1(0.8)	1991.3(10.0)	1980.4(9.7)	1985.85	1667.8(2.6)
21	$P(o\text{-Tol})_3$	10.65	194	2058.6(2.5)	1994.9(10.0)	1979.0(8.9)	1986.95	1668.7(2.5)
22	$PPh_2(^iPr)$	10.85	149	2058.2(1.9)	1991.3(10.0)	1977.5(9.6)	1984.40	1667.1(3.4)
23	$PPh_2(CH_2-^tBu)$	11.20	147	2058.6(1.6)	1992.0(10.0)	1978.2(9.4)	1985.10	1667.4(3.5)
24	$PPh(o\text{-Tol})_2$	11.90	178	2060.4(2.2)	1994.2(10.0)	1980.5(9.4)	1987.35	1668.3(3.2)
25	PPh_2Me	12.10	136	2059.3(1.4)	1991.4(10.0)	1979.5(9.7)	1985.45	1667.3(3.3)
26	$PPh_2(o\text{-Tol})$	12.75	161	2061.2(2.0)	1995.9(10.0)	1982.2(9.7)	1989.05	1667.7(3.6)
27	$P(O-^tBu)_3$	12.95	162	2062.6(0.9)	1994.8(10.0)	1981.9(9.5)	1988.35	1664.3(4.3)
28	$PPh_2(O-^tBu)$	13.85	160	2061.4(1.8) 2065.0(sh)	1995.9(10.0)	1978.3(9.5)	1987.10	1667.5(3.5)
29	$P(^tBu)(Menth)Cl$	16.00	162	2063.5(2.0)	2001.3(10.0)	1976.6(7.9)	1988.95	1669.5(2.3)
30	$PPh(O-^cPent)_2$	16.25	138	2063.3(1.1) 2069.2(sh)	1997.1(10.0)	1985.1(9.5)	1991.10	1667.3(4.3)
31	$PPh(OEt)_2$	18.10	116	2065.8(1.0) 2071.7(sh)	2000.4(10.0)	1987.5(9.6)	1993.95	1667.7(3.5)
32	$P(O-^cPent)_3$	18.50	135	2065.0(1.0)	2002.2(10.0)	1984.6(9.8)	1993.40	1666.9(3.1)
33	$P(O-^nBu)_3$	20.85	112	2069.6(0.9)	2004.7(10.0)	1986.4(9.8)	1995.55	1668.5(3.1)
34	$P(OEt)_3$	21.60	109	2069.1(0.9)	2004.6(10.0)	1985.4(9.8)	1995.00	1667.9(3.8)
35	$P(OMe)_3$	24.10	107	2072.6(0.9) 2075.5(sh)	2007.8(10.0)	1986.1(9.2)	1997.95	1670.8(3.3)
36	$P(O-o\text{-Tol})_3$	29.05	141	2077.2(1.3)	2011.7(10.0)	1997.9(9.4)	2004.80	1673.3(3.4)
37	$P(OPh)_3$	30.20	128	2079.7(1.4)	2011.4(10.0)	1998.6(8.6)	2005.00	1673.9(2.6)

[a] Assignments according to idealized C_{3v} symmetry [15], av = average.

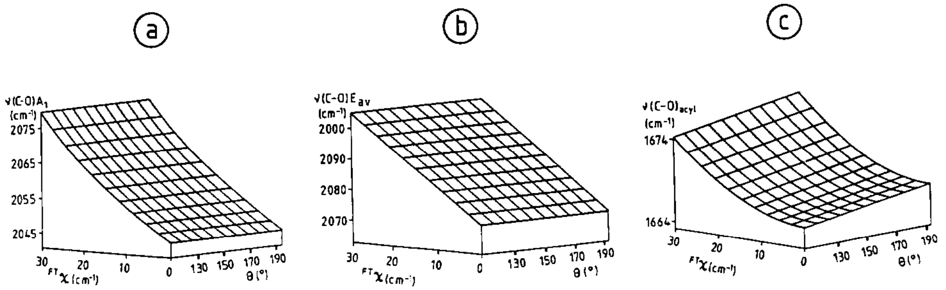


Fig. 1. Multidimensional regression analysis for the relationship between infrared ν(C–O) data for compounds IIa1–IIa37 and the steric (θ) and electronic ($^{FT}\chi$) parameters of the tertiary phosphines. (Standard deviations: *a*(5%), *b*(7%), *c*(6%)).

Table 2

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement factors (pm$^2 \times 10^7$)

	x	y	z	U_{eq}
Co	1700(1)	3837(1)	1739(1)	15(1) [a]
P	935(1)	2464(1)	3072(1)	15(1) [a]
O(1)	−682(2)	6634(1)	2136(1)	32(1) [a]
O(2)	1026(2)	2614(2)	283(1)	33(1) [a]
O(3)	4781(2)	2485(2)	2479(1)	32(1) [a]
O(4)	2881(2)	5919(1)	878(1)	30(1) [a]
O(5)	2633(2)	4907(2)	−277(1)	33(1) [a]
C(1)	250(2)	5541(2)	1981(1)	21(1) [a]
C(2)	1270(2)	3084(2)	849(1)	21(1) [a]
C(3)	3572(2)	3020(2)	2188(1)	21(1) [a]
C(4)	2480(2)	4994(2)	587(1)	20(1) [a]
C(5)	3347(2)	6945(2)	79(2)	30(1) [a]
C(6)	2004(2)	8435(2)	−158(2)	31(1) [a]
C(7)	2394(2)	9573(2)	−978(2)	36(1) [a]
C(8)	3683(3)	9852(2)	−729(2)	42(1) [a]
C(9)	1777	2168	4250	18(1) [a,b]
C(10)	1689(1)	3400(1)	4523(1)	26(1) [a,b]
C(11)	2330	3223	5408	31(1) [a,b]
C(12)	3059	1813	6020	31(1) [a,b]
C(13)	3147	581	5747	31(1) [a,b]
C(14)	2506	758	4862	24(1) [a,b]
C(15)	1447	605	2921	18(1) [a,b]
C(16)	2960(1)	−220(1)	2619(1)	25(1) [a,b]
C(17)	3386	−1629	2476	28(1) [a,b]
C(18)	2299	−2214	2635	27(1) [a,b]
C(19)	785	−1390	2937	27(1) [a,b]
C(20)	359	20	3080	22(1) [a,b]
C(21)	−1125	3174	3389	17(1) [a,b]
C(22)	−2127(1)	3960(1)	2604(1)	21(1) [a,b]
C(23)	−3709	4433	2810	24(1) [a,b]
C(24)	−4289	4119	3801	26(1) [a,b]
C(25)	−3287	3333	4586	26(1) [a,b]
C(26)	−1705	2860	4380	21(1) [a,b]

[a] Equivalent isotropic U defined as one-third of the trace of the orthogonalized U_{ih} tensor. [b] Atoms in rigid groups have standard deviations only for the pivot atom.

Table 3

Bond lengths and angles in IIa1 (with standard deviations)

Bond lengths (pm)			
Co–P	222.9(1)	Co–C(1)	178.5(2)
Co–C(2)	181.6(2)	Co–C(3)	177.0(2)
Co–C(4)	196.7(2)	P–C(9)	183.2(1)
P–C(15)	183.2(1)	P–C(21)	182.2(1)
O(1)–C(1)	114.6(2)	O(2)–C(2)	113.4(3)
O(3)–C(3)	114.4(2)	O(4)–C(4)	135.5(3)
O(4)–C(5)	146.7(3)	O(5)–C(4)	120.1(2)
O(5)–C(6)	150.8(2)	C(6)–C(7)	152.2(3)
C(7)–C(8)	151.4(4)		
Bond angles (deg)			
P–Co–C(1)	93.6(1)	P–Co–C(2)	92.9(1)
C(1)–Co–C(2)	116.7(1)	P–Co–C(3)	91.0(1)
C(1)–Co–C(3)	122.9(1)	C(2)–Co–C(3)	119.8(1)
P–Co–C(4)	177.1(1)	C(1)–Co–C(4)	88.2(1)
C(2)–Co–C(4)	88.3(1)	C(3)–Co–C(4)	86.2(1)
Co–P–C(9)	113.8(1)	Co–P–C(15)	112.8(1)
C(9)–P–C(15)	104.9(1)	Co–P–C(21)	116.1(1)
C(9)–P–C(21)	104.0(1)	C(15)–P–C(21)	104.0(1)
C(4)–O(4)–C(5)	117.3(2)	Co–C(1)–O(1)	180.0(1)
Co–C(2)–O(2)	178.7(2)	Co–C(3)–O(3)	179.7(2)
Co–C(4)–O(4)	111.8(1)	Co–C(4)–O(5)	126.2(2)
O(4)–C(4)–O(5)	122.0(2)	O(4)–C(5)–C(6)	109.9(2)
C(5)–C(6)–C(7)	113.3(2)	C(6)–C(7)–C(8)	113.9(2)

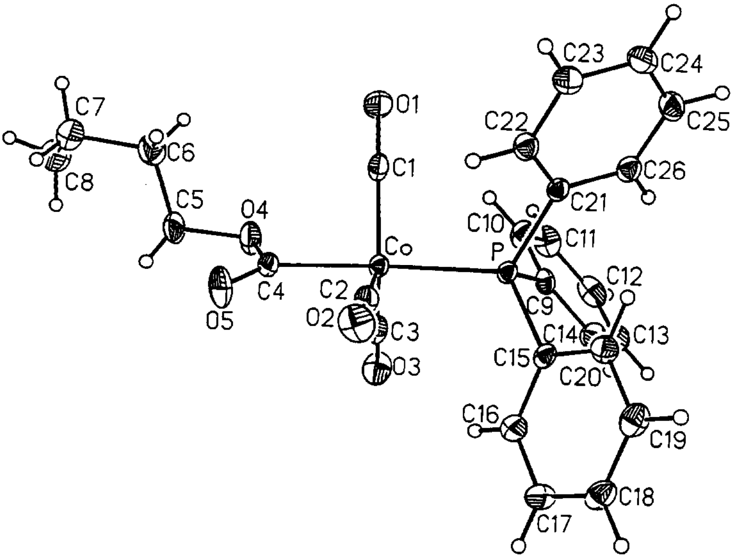
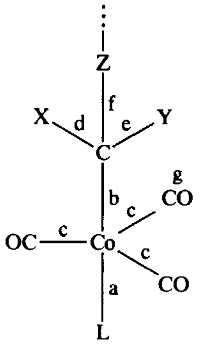


Fig. 2. ORTEP diagram of the structure of ^{n}BuOC(O)Co(CO)$_3$PPh$_3$ (IIa1).

Table 4

Comparison of some structural parameters of organocobalt carbonyls $RCo(CO)_3L$



Ligands		Distance (pm)							Angles (deg)		Ref.
R	L	*a*	*b*	c_{av}	*d*	*e*	*f*	g_{av}	bc_{av}	df	
^{n}BuOC(O)–	PPh_3	229.9 (1)	196.7 (2)	179.0	120.1	–	135.5 (3)	113.8	87.6	122.0	This work
MeOC(O)–	PPh_3	223.2	197.6	178.6	119.6	–	134.2	113.8	ng	(bd) 112.9	[3a]
η^6-Cr(CO)$_3$–C_6H_5–CH_2–	CO	180.6 (8)	212.6 (7)	180.9	nd	nd	149.8 (9)	112.1 [a]	86.4	112.3	[6b]
$ClCH_2$–	PPh_3	222.3 (1)	202.2 (3)	178.3	nd	nd	179.4 (3)	113.8	92.5	(bf) 114.9 (1)	[11]
PhOC(O)CH_2–	PPh_3	221.1 (2)	210.9 (8)	177.4	ng	ng	154.0 [b]	114.3	ng	ng	[17]
$ClCH_2C(O)$–	PPh_3	225.4 (1)	199.9 (5)	178.7	118.0 (7)	–	149.9 [c] (8)	113.4	88.2	117.2 (5)	[11]
2,6-Cl_2–C_6H_3–$CH_2C(O)$–	PPh_3	225.9 (1)	199.6 (4)	178.4	119.3 (5)	–	153.7 (7)	113.8	88.0	119.9 (4)	[6b]
HCF_2CF_2–	PPh_3	227.0 (1)	195.0 (3)	181.0	143.0 (3)	139.0 (3)	159.0 (4)	111.0	87.0	104.5	[18]

[a] ax(C–O) 113.2(10) pm; [b] Average for disordered species. [c] C–Cl 171.4(7). nd = not determined; ng = not given.

Preparation of $^{n}BuOC(O)Co(CO)_4$ (Ia)

See ref. 1a.

Preparation of $^{n}BuOC(O)Co(CO)_3ER_3$ complexes IIa1–IIa37

A solution of Ia (2.5 10^{-2} *M*) in n-heptane was treated with a stoichiometric amount of ER_3 at 20–25 °C. The mixture was stirred for 1 h. In the case of compound IIa1, $ER_3 = PPh_3$, the solution was concentrated and filtered, and the product isolated analytically pure in 87% yield by recrystallization at approx. −20 °C from Et_2O/n-hexane (1 : 1), and identified by IR (Table 1, [1a]) and ^1H NMR [1a] spectroscopy and elemental analyses. Anal. Found: Co, 11.6; P, 6.1. $C_{26}CoH_{24}O_5P$ calc.: Co, 11.64; P, 6.12%. The other compounds (IIa2–IIa37) were prepared in solution by essentially the same method and identified from their IR spectra (Table 1). The solutions were generally pure, the amount of cobalt carbonyls other than IIa (starting compound and/or traces of $Co_2(CO)_8$) was < 5% of that of the main product, except in 4 cases in which the starting compound was still present to the extent of 10–20%; the good separation of the bands allowed precise determination of the absorption maxima of the products even in these cases.

Preparation of $^{n}BuOC(O)Co(CO)_2L_2$ ($L = PEt_3$, IIIa1; $P(OMe)_3$, IIIa2)

A solution of IIa12 (90.5 mg, 0.25 mmol) in 10 ml of n-heptane was treated with an excess (up to 5-fold) of the ligand (L) at 40 °C and the mixture was stirred for 1 h at this temperature. Compound IIIa2 was prepared similarly from IIa35. The compounds IIIa1 and IIIa2 were identified from their IR spectra (Table 5).

X-ray structure determination of IIa1

Approximate crystal size: $0.09 \times 0.25 \times 0.26$ mm^3, Nicolet R3 m/V diffractometer, Mo-K_α radiation (graphite monochromator), $T = 125$ K, cell dimensions: $a = 971.6(1)$, $b = 1037.3(1)$, $c = 1381.1(2)$ pm, $\alpha = 73.67(1)$, $\beta = 80.23(1)$, $\gamma = 63.72(1)°$, $V = 1.1962(3) \times 10^9$ pm^3, $Z = 2$, $d_{calc.} = 1.409$ g/cm^3, $\mu = 0.81$ cm^{-1}, triclinic, space group $P\bar{1}$; data collection (2θ max = 50 °) of 4249 independent intensities, 3983 of which were treated as observed ($F_o \geqslant 4\sigma(F)$), empirical absorption correction (min/max transmission 0.787/0.987), structure solution by Patterson methods and full matrix least squares refinement using SHELXTL-PLUS. Phenyl rings and hydrogen atoms were treated as rigid groups and all non-hydrogen atoms given anisotropic displacement parameters; 269 parameters were refined, $R = 0.029$, $R_w = 0.035$, $w^{-1} = (\sigma^2(F) + 5 \times 10^{-4} F^2)$ maximum residual electron density 0.41 e/(pm$^3 \times 10^6$).

Table 5

Infrared ν(C–O) spectra of IIIa1 and IIIa2 in n-heptane

Compound	IR ν(C–O)	Absorption maxima (cm^{-1})	Intensity $\nu(C–O)_{acyl}$
IIIa1	1961.2(4.0)	1903.4(10.0)	1610.0(2.0)
IIIa2	2019.7(4.5)	1964.3(10.0)	1647.6(3.1)

Lists of hydrogen atom coordinates, thermal parameters, and structure factors are available from the authors.

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