2.24. [Rh(7-PPh_2-8-Me-7,8-$C_2B_9H_{10}$)(C_8H_{12})], [Rh(nMePPh)(cod)].

Se disuelven 60.7 mg (0.12 mmol) de [$Rh_2(\mu$-Cl)$_2$(cod)$_2$] en 10 ml de cloruro de metileno desoxigenado y se le añaden 100 mg (0.246 mmol) de [NMe_4][nMePPh]. La mezcla se agita durante 10 minutos precipitando un sólido amarillo que se filtra y se lava con etanol en frio (10 ml). El resto de la disolución se concentra y se le añaden 10 ml de etanol, precipitando más sólido, que se filtra y lava igualmente (61 mg, 44% de rendimiento).

Análisis elemental

		%C	%H	%N
Calculado para	$C_{23}H_{35}B_9PRh$	50.91	6.46	
Experimental		49.84	6.25	

Espectro IR (KBr, bandas observadas en cm^{-1}).

2973,2931,2875 (Im), υ(C-H); 2586,2544,2502 (mI), υ(B-H); 2101 (pI), υ(B-H→Rh); 1435,1096(I), 969,821 (pI), 744,688,519 (Im), asignables a las fosfinas.

Espectro ^{1}H-RMN ($CDCl_3$).

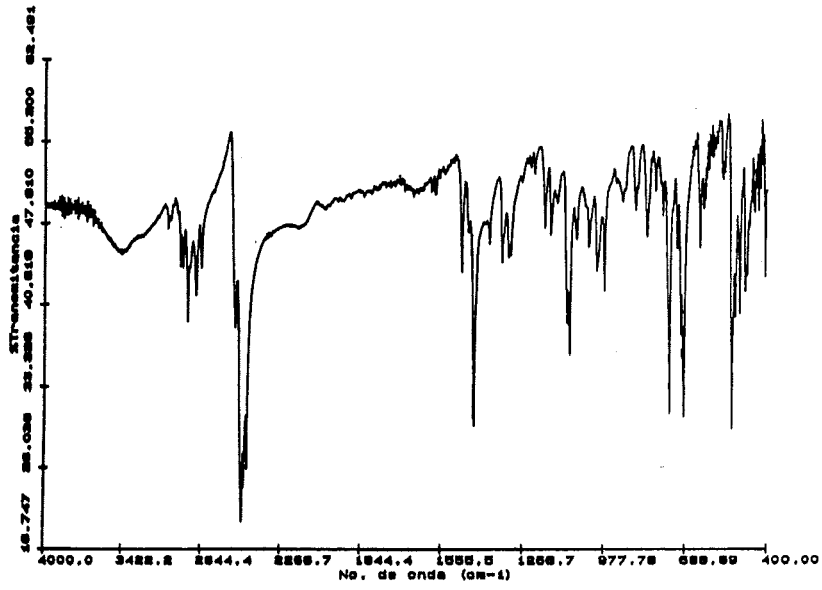
δ(ppm)	M	J(Hz)	Area relativa	Asignación
-2.45	a		1H	B-H-B
1.29	s		3H	BC-CH_3
2.37	m		8H	CH_2
3.57	a		2H	CH=CH
5.30	a		2H	CH=CH
7.20-7.75	m		10H	BC-P(C_6H_5)

Espectro $^{31}P\{^1H\}$-RMN ($CDCl_3$).

δ(ppm)	M	J(P,Rh)Hz)	Area relativa	Asignación
30.90	d	114		BC-P(C_6H_5)

Espectro ^{11}B-RMN ($CDCl_3$).

δ(ppm)	^{1}J(B,H)(Hz)	Area relativa	Asignación
-34.06	144.5	1B	
-31.45	108.8	1B	
-26.78		1B	
-22.67	138.6	1B	
-18.33	134.9	1B	
-12.67		1B	
-10.78		1B	
-8.27		1B	
-0.51	125.4	1B	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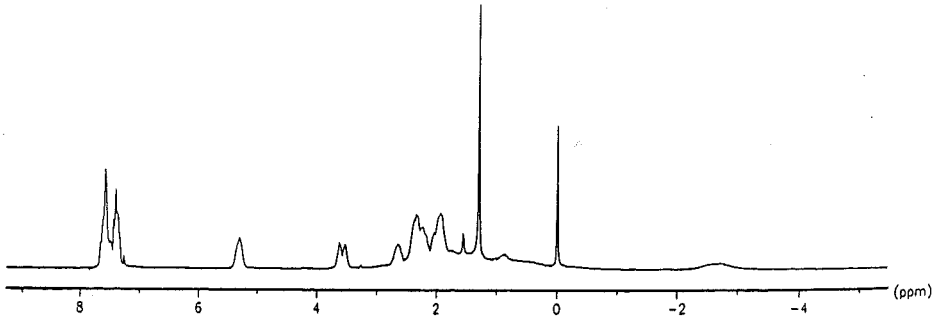
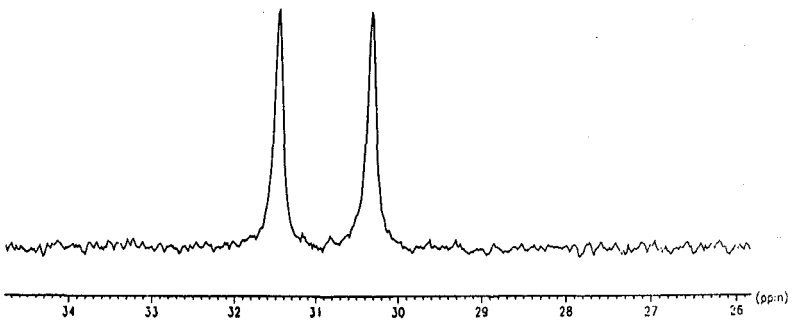
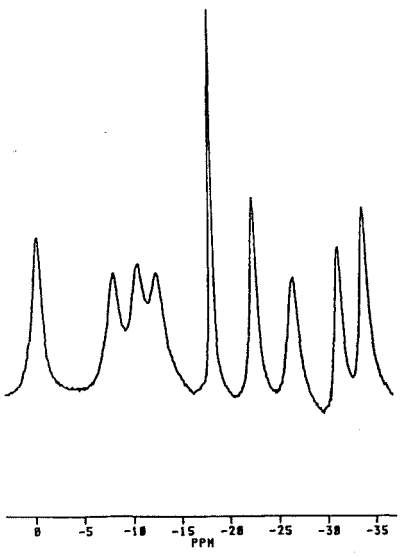
2266.7
1844.4
1555.5
1256.7
977.78
688.89
400.00
No. de onda (cm-1)


8
6
4
2
0
-2
-4
(ppm)


34
33
32
31
30
29
28
27
26
(pp:n)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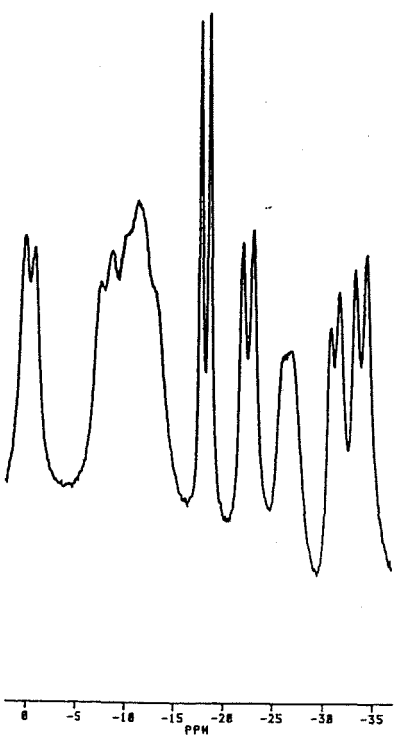
-5
-10
-15
-20
-25
-30
-35
PPM


0
-5
-10
-15
-20
-25
-30
-35
PPM

2.25. [Rh(7-PPh$_2$-7,8-C$_2$B$_9$H$_{10}$)(C$_8$H$_{12}$)], [Rh(nHPPh)(cod)].

Se disuelven 31 mg (0.062 mmol) de [Rh$_2$(μ-Cl)$_2$(cod)$_2$] en 8 ml de cloruro de metileno desoxigenado y se le añaden 50 mg (0.125 mmol) de [NMe$_4$][nHPPh]. La mezcla se agita durante 24 horas a temperatura ambiente precipitando un sólido amarillo que se filtra y se lava con agua (15 ml). El resto de la disolución se concentra obteniendo más sólido, que se filtra y lava igualmente (34 mg, 56% de rendimiento).

Análisis elemental

		%C	%H	%N
Calculado para	$C_{22}H_{33}B_9PRh$	49.99	6.25	
Experimental		50.12	6.15	

Espectro IR (KBr, bandas observadas en cm^{-1}).

3465 (pl), υ(arC-H); 2938 (pl), υ(C-H); 2546 (ml), υ(B-H); 2101 (pl), υ(B-H→Rh); 1436,1102 (l),999,744,695,522 (lm), asignables a las fosfinas.

Espectro $^1H\{^{11}B\}$-RMN (CDCl$_3$).

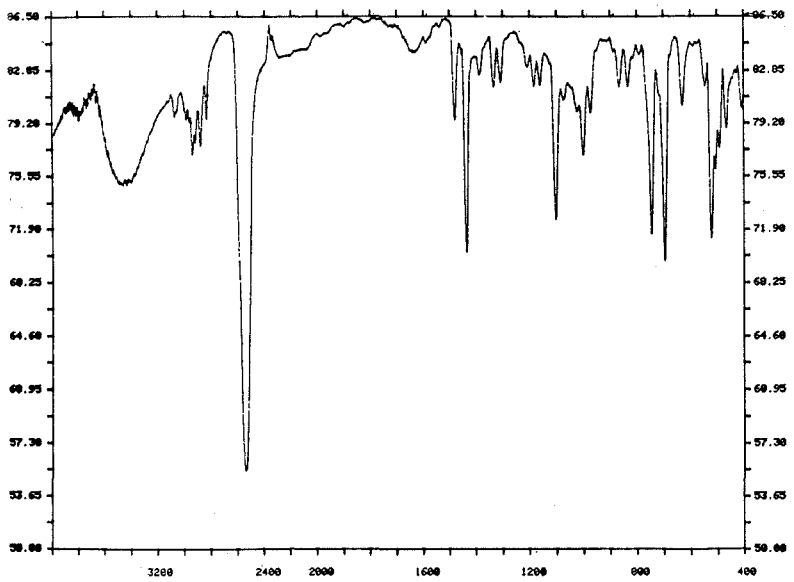
δ(ppm)	M	J(Hz)	Area relativa	Asignación
-2.84	a		1H	B-H-B
2.31	m		8H	CH_2
3.79	a		1H	CH=CH
4.02	a		1H	CH=CH
5.45	s		2H	CH=CH
7.38-7.59	m		10H	BC-P(C_6H_5)

Espectro $^{31}P\{^1H\}$-RMN (CDCl$_3$).

δ(ppm)	M	J(P,Rh)Hz)	Area relativa	Asignación
23.67	d	121		BC-P(C_6H_5)

Espectro ^{11}B-RMN (CDCl$_3$).

δ(ppm)	^{1}J(B,H)(Hz)	Area relativa	Asignación
-34.9	153.6	1B	
-32.0	124.8	1B	
-26.3		1B	
-24.2	153.6	1B	
-18.4	115.2	1B	
-16.9		1B	
-12.9	153.6	2B	
0.3	144.0	1B	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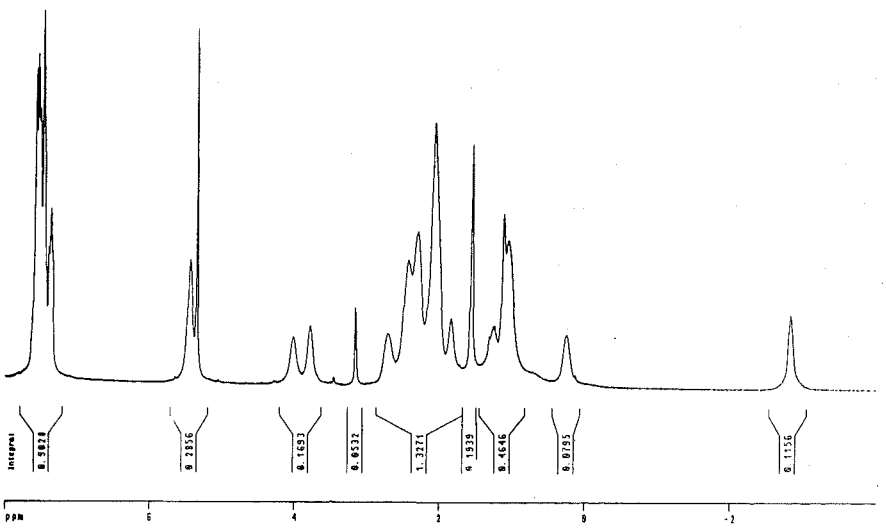
82.85
79.20
75.55
71.90
68.25
64.60
60.95
57.30
53.65
50.00
3200
2400
2000
1600
1200
800
400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1.3217
0.1939
0.4646
0.0795
0.1156
ppm
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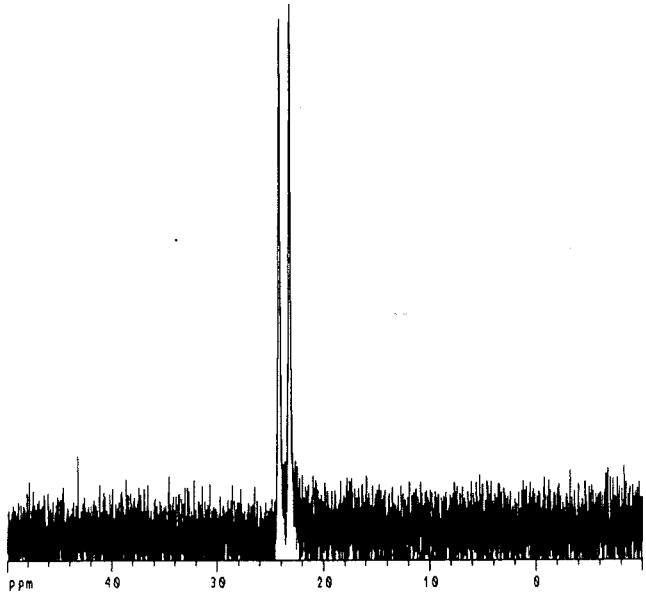
4
2
0
-2


ppm
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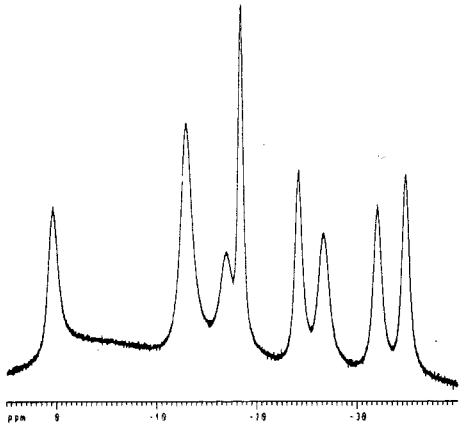
30
20
10
0


ppm
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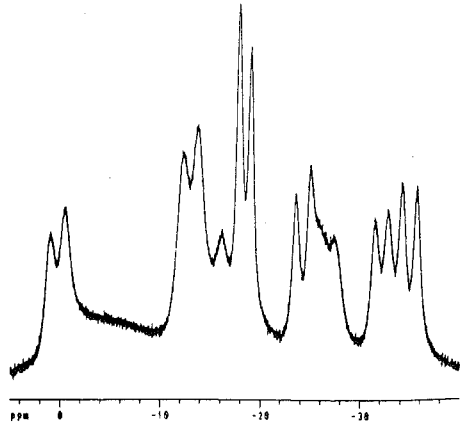
-10
-20
-30


ppm
0
-10
-20
-30

2.26. Reacción de [Rh(nMePPh)(COD)] con $Ph_2P(CH_2)_2PPh_2$.

a) Se disuelven 30 mg (0.055 mmol) de [Rh(nMePPh)(COD)] en 10 ml de CH_2Cl_2 desoxigenado y a esta disolución se le añaden 22 mg (0.055 mmol) de dppe. La mezcla se refluye durante 5 horas y se agita 18 horas más a temperatura ambiente. La disolución se concentra precipitando un sólido amarillo que se filtra y lava con 5 ml de etanol (10 mg).

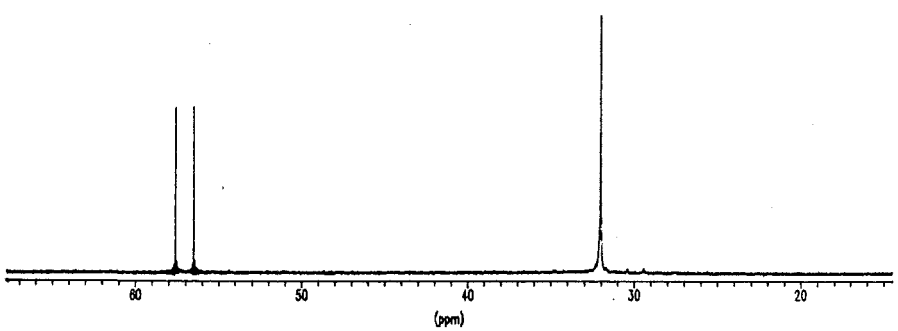
b) Se disuelven 30 mg (0.055 mmol) de [Rh(nMePPh)(COD)] en 6 ml de etanol desgasificado y se le añaden 22 mg (=.055 mmol) de dppe. La mezcla se refluye durante 1 hora, precipitando un sólido amarillo que se filtra y lava con 5 ml de etanol.

Espectro IR (KBr, bandas observadas en cm^{-1}).

3050 (pI), υ(arC-H); 2966,2931 (pI), υ(C-H); 2537 (mI), υ(B-H); 1434,1096,744,695,533 (mI), asignables a las fosfinas.

Espectro $^{31}P\{^1H\}$-RMN ($CDCl_3$).

δ(ppm)	M	J(P,Rh)(Hz)	Area relativa	Asignación
31.95	s			$BC\text{-}P(O)(C_6H_5)_2$
56.98	d	133		$\text{-}(CH_2)P(C_6H_5)$



2.27. Reacción de [Rh(nMePPh)(COD)] con piridina.

Se disuelven 25 mg (0.046 mmol) de [Rh(nMePPh)(COD)] en 6 ml de etanol desoxigenado y se le añaden 7.5 mg (0.095 mmol) de piridina. La mezcla se refluye durante 3 horas. Transcurrido este tiempo no se ha observado ningún cambio. La disolución se concentra precipitando un sólido amarillo que se filtra y lava con 5 ml de etanol.

3. Catálisis

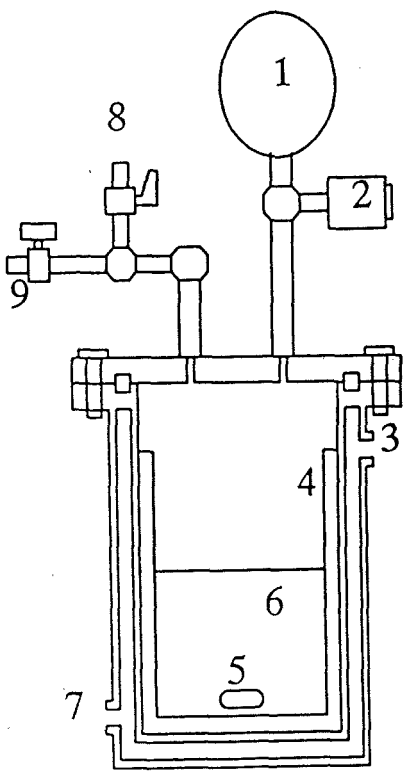
Se han llevado a cabo experimentos catalíticos en los que se utilizan como sistemas catalíticos algunos de los complejos de Rh(I), Ru(II) y Pd(II), descritos anteriormente. Las reacciones realizadas han sido:

-Hidrogenación de 1-hexeno.

-Hidrogenación de metaciclina.

-Hidroformilación de 1-hexeno y estireno.

Para ello, se diseñó, como parte del trabajo de esta tesis doctoral, un reactor que nos permitiera trabajar en atmósfera inerte, a presiones altas y temperaturas controladas y en contante agitación. En la figura VIII.1 se represnta el esquema del autoclave utilizado:



1. Manómetro
2. Disco de ruptura
3. Salida de agua termostatizada
4. Cámara de teflón interna
5. Núcleo magnético
6. Solución de reacción
7. entrada de agua termostatizada
8. Entrada de muestra y prurga
9. Entrada de gases

Figura VIII.1. *Esquema del reactor utilizado en las reacciones catalíticas.*

1. Hidrogenación de 1-hexeno.

En las reacciones de hidrogenación homogénea de 1-hexeno se han utilizado los siguientes precursores catalíticos de Rh(I): **a**,[Rh(nMePPh)$(PPh_3)_2$]; **b**,[Rh(nHPPh)$(PPh_3)_2$]; **c**,[Rh(nPhPPh)$(PPh_3)_2$]; **d**,[Rh(nMePEt)$(PPh_3)_2$]; **e**,[Rh(nMeP^{i}Pr)$(PPh_3)_2$]; **f**,[Rh(nMePPh)(cod)]. Los resultados obtenidos han sido comparados con el catalizador de Wilkinson, [RhCl$(PPh_3)_3$], en las mismas condiciones.

Se han realizado pruebas catalíticas en las mismas condiciones con los siguientes complejos de Ru(II): **a**,[RuCl(nMePPh)$(PPh_3)_2$]; **b**,[RuCl(nHPPh)$(PPh_3)_2$]; **c**[RuH(nMePPh)$(PPh_3)_2$]; **d**,[RuH(nHPPh)$(PPh_3)_2$]; **e**,[RuH(nPhPPh)$(PPh_3)_2$]; **f**,[Ru(nMePPh)$_2$], comparándose, a su vez, con los resultados obtenidos con **g**,[RuH(OAc)$(PPh_3)_3$] y **h**,[$RuCl_2(PPh_3)_3$].

Finalmente se probó el complejo [PdCl{n(PPh_2)MePPh}(PPh_3)].

Todas las hidrogenaciones se llevaron a cabo siguiendo este procedimiento:

En un balón Schlenk que contiene $5.21\cdot10^{-6}$ moles de complejo, bajo atmósfera de N_2, se añaden 10 ml de disolución de tolueno:1-hexeno ó THF:1-hexeno (1:1) (v/v), previamente preparada y desoxigenada. La suspensión resultante se agita magnéticamente hasta conseguir una total disolución del sólido*. Posteriormente, la disolución es transferida al autoclave, previamente purgado con N_2. Una vez traspasada, el reactor se conecta a un baño termostatizado donde se mantiene la temperatura deseada (66 °C o 25 °C), esperando en cada experimento 10 minutos para que se alcance la misma en el interior. Finalmente, se fija la presión de H_2 a 45 atm. Transcurrida una hora, se deja enfriar a temperatura ambiente, se despresuriza y se analiza la composición de la mezcla mediante cromatografía de gases. La reproducibilidad de los experimentos se comprobó repitiendo cada uno tres veces . En la tabla VIII. 1 se recogen los resultados obtenidos utilizando tolueno y T = 66 °C.

Isomerización de 1-hexeno.

En un balón tipo Schlenk se prepara una disolución de [Rh(nHPPh)$(PPh_3)_2$] ($5.21\cdot10^{-6}$ mol) en 10 ml de tolueno/1-hexeno (1:1), (v/v), previamente desgasificada. La disolución se transfiere al autoclave conectado a un baño termostatizado. La disolución se calienta a T = 66°C durante 10 minutos. Transcurrido este tiempo se enfría a temperatura ambiente y la muestra se analiza mediante cromatografía de gases.

Resultado: conversión del 0.5% (0.3% en 3-hexeno y 0.2% en trans-2-hexeno). No se observa cis-2-hexeno.

*En la mayoría de los ensayos fueron precisos 10 ó 20 minutos para disolver los complejos, dada la baja solubilidad de éstos, en otros no se consiguió una total disolución.

Complejo	% conv.	% n-hexano	% 2-c-hexeno	% 2-t-hexeno	% 3-hexeno
a	57.2	81.0	8.0	10.7	0.3
b	99.1	88.2	2.6	8.7	0.5
c	72.5	77.4	11.2	11.0	0.4
d	23.5	70.0	12.0	17.6	0.2
e	16.7	75.2	9.8	14.8	0.2
f	49.7	59.5	11.2	29.0	0.3
Wilkinson	99.4	98.6	0.0	0.3	1.1

Tabla VIII.1. *Hidrogenación e isomerización de 1-hexeno con complejos de rodio.*

Complejo	% conv.	% n-hexano	% c-hexeno	% t-hexeno	% 3-hexeno
a	35.5	89.6	5.6	4.7	0.1
b	89.1	83.7	8.7	7.6	0.0
c	92.4	91.8	2.4	5.2	0.6
d	75.0	95.7	1.5	2.2	0.6
e	37.0	83.0	6.3	10.7	0.0
e	49.7	64.4	14.2	21.1	0.3
f	99.7	99.1	0.1	0.8	0.0
h	99.4	94.8	2.8	2.3	01

Tabla VIII.2. *Hidrogenación e isomerización de 1-hexeno con complejos de rutenio.*

En la tabla VIII.3 y 4 se recogen los resultados obtenidos utilizando como disolvente THF, a la temperaturas de 66 °C y 25 °C, respectivamente..

Complejo	% conversión	% n-hexano	% Isomeros
a	81.1	74.8	25.2
b	99.1	90.6	9.4
d	92.2	88.5	11.5
e	96.3	85.9	14.1

Tabla VIII.3. *Conversión de 1-hexeno con complejos de rodio a 66 °C en THF.*

Complejo	% conversión	% n-hexano	% Isomeros
a	6.0	95.7	4.3
b	12.6	94.7	5.3
d	0.5	84.6	15.4
e	2.5	94.8	5.2

Tabla VIII.4. *Conversión de 1-hexeno con complejos de rodio a 25 °C en THF.*

Reacciones con PPh_3.

En el primer experimento se prepara una disolución de $[Rh(nHPPh)(PPh_3)_2]$ ($5.21 \cdot 10^{-6}$ mmol) y PPh_3 ($5.21 \cdot 10^{-6}$ mmol) en 10 ml de THF:hexeno (1:1). La disolución se transfiere al reactor y se calienta durante 10 minutos a 40.8°C, hasta alcanzar dicha temperatura en el interior. Se conecta a la linea de alta presión de H_2, ajustando ésta a 45 atm y dejandola 1 hora. En el segundo experimento se procede del mismo modo pero aumentando a 4 equivalentes de PPh_3, es decir, $20.84 \cdot 10^{-6}$ mmol de PPh_3.

Los resultados de conversión de n-hexeno son los siguientes:

	Sin PPh_3	+1 PPh_3	+4 PPh_3
$[Rh(nHPPh)(PPh_3)_2]$	40%	22%	20%

2. Hidrogenación de la metaciclina.

Los experimentos de hidrogenación de la metaciclina se han llevado a cabo utilizando los siguientes precursores catalíticos: $[Rh(nMePPh)(PPh_3)_2]$, $[Rh(nHPPh)(PPh_3)_2]$, $[RuCl(nMePPh)(PPh_3)_2]$, $[RuCl(nHPPh)(PPh_3)_2]$, $[RuH(nMePPh)(PPh_3)_2]$, $[RuH(nHPPh)(PPh_3)_2]$.

En todos los casos el procedimiento experimental fue el siguiente:

En un balón Schlenck que contiene $5.21 \cdot 10^{-6}$ moles de complejo y 62.5 mg de metaciclina, bajo nitrógeno, se añaden 6 ml de una disolución de MeOH:tolueno (2:1), previamente desoxigenada. Se agita, calentando si es necesario, hasta conseguir una total disolución. Se transfiere al reactor, purgado con N_2 y se conecta al baño termostatizado donde se ha fijado una temperatura de 75 °C. Se deja 10 minutos para que se alcance la temperatura y se conecta a la linea de alta presión de H_2, ajustando una presión de 45 atm. Transcurridas 7 horas, el autoclave se enfria a temperatura ambiente , se descompresiona y la muestra se analiza por cromatografía líquida (HPLC).

Como fase móvil de la separación por HPLC, se preparó una mezcla de 500 ml de una disolución tampón de fosfato monosódico (0.1 M) y EDTA (0.01 M), 500 ml de metanol y 6 ml de N,N-dimetiloctilamina, ajustada a pH = 8 con una solución acuosa de NaOH al 20%.

En la tabla VIII.5 se recogen los resultados obtenidos en la hidrogenación de metaciclina.

Catalizador	% Metaciclina	% Doxiciclina
$[Rh(nMePPh)(PPh_3)_2]$	15.0	85.0
$[Rh(nHPPh)(PPh_3)_2]$	0.3	99.7
$[RuCl(nMePPh)(PPh_3)_2]$	98.2	1.8
$[RuCl(nHPPh)(PPh_3)_2]$	98.3	1.7
$[RuH(nMePPh))(PPh_3)_2]$	98.7	0.3
$[RuH(nHPPh)(PPh_3)_2]$	98.0	2.0

Tabla VIII.5. *Hidrogenación de metaciclina a doxiciclina.*

3. Hidroformilación de Alquenos.

Las reacciones de hidroformilación se llevaron a cabo en la misma relación sustrato/catalizador que las de hidrogenación (S/C = 7677).

En un Schlenk que contiene $5.3 \cdot 10^{-6}$ mmol de [Rh(nMePPh)(PPh_3)] se añaden 25 ml de una disolución de tolueno:1-hexeno (20:5) previamente desgasificada.. La disolución se transfiere al reactor purgado con N_2 y se somete a 45 atm de presión de gas CO/H_2 (1:1), variando la temperatura y el tiempo de reacción.

Sustrato	T	Tiempo(h)	%Conversión	%2-metil-hexanal	%n-heptanal
1-hexeno	50	3	4	2	2
1-hexeno	50	25	39	15	24
1-hexeno	85	3	20	8	12
1-hexeno	85	25	94	35	59
estireno	50	1	-	-	-

Tabla VIII.2. *Hidroformilación de olefinas con el complejo [Rh(nMePPh)(PPh_3)$_2$].*

4. Estructuras cristalinas.

4.1 Estructura cristalina de cMePPh.

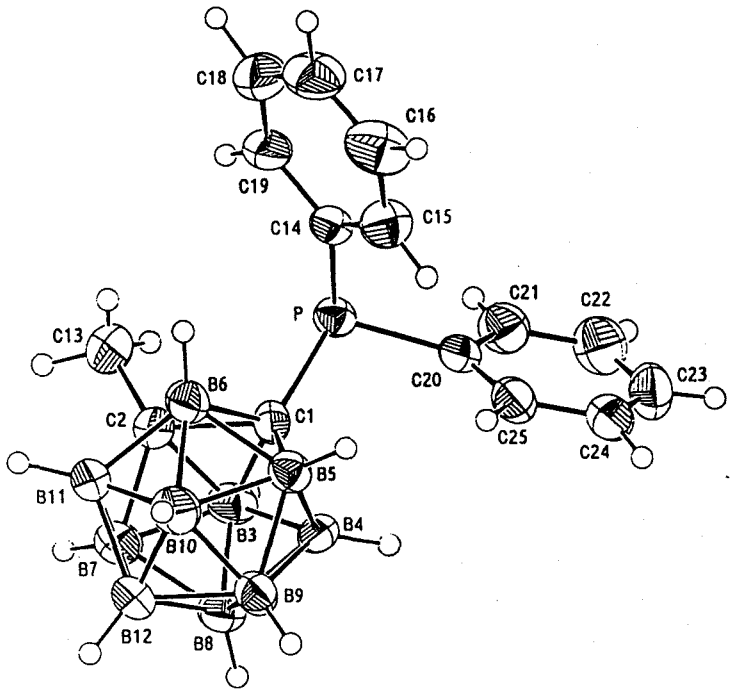


Tabla 1. *Datos cristalográficos para [1-(C_6H_5)$_2$-2-CH_3-1,2-$C_2B_{10}H_{10}$].*

Fórmula química	$C_{15}H_{23}B_{10}P$
peso molecular	342.4 g/mol
a =	11.057 (3) Å
b =	12.937 (2) Å
c =	13.639 (4) Å
V =	1951.0 (8) Å^3
Z =	4
Grupo espacial:	ortorrómbico $Pna2_1$ (No. 33)
T =	23 °C
λ =	0.71069 Å
ρ =	1.106 g cm^{-3}
μ =	1.3 cm^{-1}
coefic. de transmisión =	0.948 - 1.000
$R(F_o)$	0.048
$R_w(F_o)$ =	0.047

Tabla 2. *Coordenadas fraccionarias y desviación estándar (entre paréntesis) para [1-P(C_6H_5)$_2$-2-CH_3-1,2-$C_2B_{10}H_{10}$].*

	x/a	y/b	z/c	U
P	0.16126(9)	0.38418(7)	0.30000	* 0.0352(3)
C(1)	0.0879(3)	0.5048(3)	0.3498(3)	* 0.034(1)
C(2)	-0.0656(4)	0.5028(3)	0.3414(4)	* 0.042(1)
B(3)	0.0147(5)	0.5752(4)	0.2582(4)	* 0.043(2)
B(4)	0.1387(4)	0.6267(4)	0.3249(4)	* 0.038(2)
B(5)	0.1306(4)	0.5792(4)	0.4465(4)	* 0.037(1)
B(6)	0.0023(5)	0.4968(4)	0.4542(5)	* 0.045(2)
B(7)	-0.1204(5)	0.6221(4)	0.3104(6)	* 0.053(2)
B(8)	0.0079(4)	0.7030(4)	0.3022(6)	* 0.046(2)
B(9)	0.0781(5)	0.7065(4)	0.4183(5)	* 0.043(2)
B(10)	-0.0059(5)	0.6251(4)	0.4994(5)	* 0.051(2)
B(11)	-0.1276(5)	0.5742(4)	0.4328(5)	* 0.050(2)
B(12)	-0.0807(5)	0.7028(4)	0.4112(5)	* 0.049(2)
C(13)	-0.1281(5)	0.4066(4)	0.3040(8)	* 0.062(2)
C(14)	0.1831(4)	0.3052(3)	0.4098(3)	* 0.039(1)
C(15)	0.2693(5)	0.3198(4)	0.4812(4)	* 0.051(2)
C(16)	0.2779(6)	0.2515(5)	0.5607(5)	* 0.068(2)
C(17)	0.1994(6)	0.1695(4)	0.5673(4)	* 0.066(2)
C(18)	0.1142(5)	0.1537(4)	0.4961(4)	* 0.060(2)
C(19)	0.1048(4)	0.2209(3)	0.4184(4)	* 0.049(2)
C(20)	0.3141(4)	0.4238(3)	0.2643(3)	* 0.039(1)
C(21)	0.3531(5)	0.3820(4)	0.1765(4)	* 0.052(2)
C(22)	0.4691(5)	0.3999(5)	0.1418(5)	* 0.065(2)
C(23)	0.5452(5)	0.4621(5)	0.1930(5)	* 0.062(2)
C(24)	0.5100(5)	0.5057(4)	0.2803(5)	* 0.058(2)
C(25)	0.3942(4)	0.4873(3)	0.3153(4)	* 0.046(2)

Tabla 3. *Distancias de enlace (Å) para [1-P(C_6H_5)$_2$-2-CH_3-1,2-$C_2B_{10}H_{10}$].*

P-C(1)	1.885(4)
P-C(14)	1.829(4)
P-C(20)	1.832(4)
C(1)-C(2)	1.702(6)
C(1)-B(3)	1.745(7)
C(1)-B(4)	1.709(6)
C(1)-B(5)	1.700(7)
C(1)-B(6)	1.714(8)
C(2)-B(3)	1.718(7)
C(2)-B(6)	1.715(8)
C(2)-B(7)	1.711(7)
C(2)-B(11)	1.696(8)
C(2)-C(13)	1.513(7)

Tabla 4. *Angulos de enlace (°) para [1-P(C_6H_5)$_2$-2-CH_3-1,2-$C_2B_{10}H_{10}$].*

C(1)-P-C(14)	102.9(2)
C(1)-P-C(20)	105.1(2)
C(14)-P-C(20)	104.6(2)
P-C(1)-C(2)	113.1(3)
P-C(1)-B(3)	112.0(3)
P-C(1)-B(4)	123.4(3)
P-C(1)-B(5)	129.0(3)
P-C(1)-B(6)	119.2(3)
C(1)-C(2)-C(13)	119.4(4)
P-C(14)-C(15)	126.5(3)
P-C(14)-C(19)	115.0(4)
P-C(20)-C(21)	114.1(3)
P-C(20)-C(25)	128.2(3)

4.2. Estructura cristalina de 2(cMe)PPh.

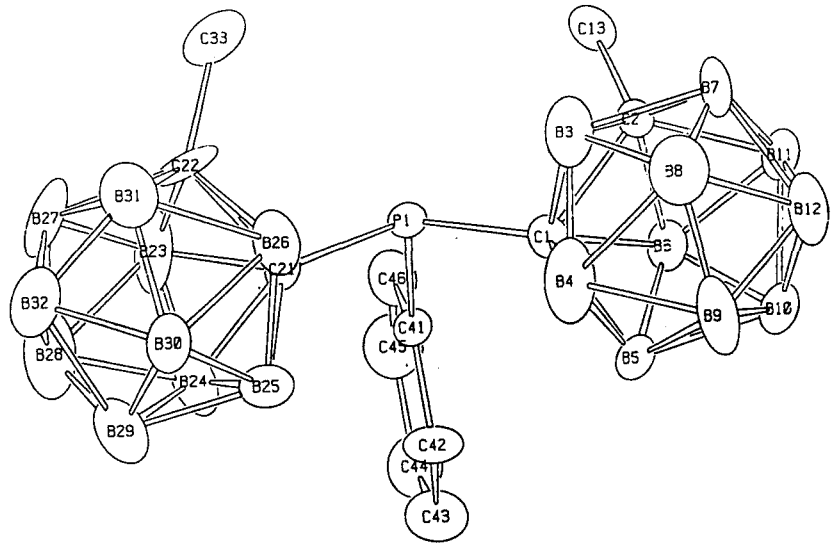


Table 5. *Datos cristalográficos para [1-CH_3-1,2-$C_2B_{10}H_{10}$]$_2$P(C_6H_5).*

Fórmula química	$C_{12}H_{31}B_{20}P$
peso molecular	422.55 g/mol
a =	11.716 (7) Å
b =	14.306 (7) Å
c =	15.183 (4) Å
β =	94.10 (3)°
V =	2538 (2) Å^3
Z =	4
Grupo espacial:	monoclínico, $P2_1/c$ (No. 14)
T =	23 °C
λ =	0.71069 Å
ρ =	1.106 g cm^{-3}
μ =	1.07 cm^{-1}
coefic. de transmisión	0.71 - 1.26
$R(F_o)$	0.101
$R_w(F_o)$ =	0.113

Tabla 6. *Coordenadas fraccionarias y desviación estándar (entre paréntesis) para* $[1\text{-}CH_3\text{-}1,2\text{-}C_2B_{10}H_{10}]_2P(C_6H_5)$.

	x/a	y/b	z/c	U
P(1)	0.2422(3)	0.3704(2)	0.2131(2)	* 0.050(1)
C(1)	0.3899(9)	0.3366(8)	0.2580(7)	* 0.054(5)
C(2)	0.4262(9)	0.402(1)	0.3525(7)	* 0.078(6)
B(3)	0.394(1)	0.291(1)	0.360(1)	* 0.12(1)
B(4)	0.450(1)	0.229(1)	0.270(2)	* 0.14(1)
B(5)	0.510(1)	0.324(1)	0.201(1)	* 0.108(9)
B(6)	0.484(1)	0.433(1)	0.256(1)	* 0.084(8)
B(7)	0.510(1)	0.345(2)	0.422(1)	* 0.109(9)
B(8)	0.525(2)	0.236(2)	0.386(1)	* 0.14(1)
B(9)	0.599(1)	0.249(2)	0.286(2)	* 0.14(1)
B(10)	0.625(1)	0.373(2)	0.267(1)	* 0.106(9)
B(11)	0.570(1)	0.431(1)	0.362(1)	* 0.075(7)
B(12)	0.639(1)	0.323(1)	0.369(1)	* 0.114(9)
C(13)	0.341(1)	0.478(1)	0.381(1)	* 0.146(9)
C(21)	0.1640(9)	0.2611(8)	0.1752(7)	* 0.054(5)
C(22)	0.048(1)	0.241(1)	0.228(1)	* 0.150(9)
B(23)	0.026(2)	0.295(2)	0.135(2)	* 0.15(1)
B(24)	0.112(2)	0.251(1)	0.067(1)	* 0.13(1)
B(25)	0.204(1)	0.167(1)	0.116(1)	* 0.077(7)
B(26)	0.176(1)	0.158(1)	0.229(1)	* 0.095(8)
B(27)	-0.063(1)	0.201(1)	0.159(2)	* 0.16(1)
B(28)	-0.023(2)	0.202(2)	0.058(2)	* 0.18(1)
B(29)	0.085(2)	0.129(1)	0.050(1)	* 0.12(1)
B(30)	0.122(1)	0.074(1)	0.149(1)	* 0.082(7)
B(31)	0.033(2)	0.112(2)	0.233(1)	* 0.17(1)
B(32)	-0.023(1)	0.092(1)	0.130(2)	* 0.12(1)
C(33)	0.025(2)	0.301(2)	0.313(1)	* 0.26(2)
C(41)	0.2600(8)	0.4356(8)	0.1121(7)	* 0.053(5)
C(42)	0.319(1)	0.407(1)	0.0416(8)	* 0.083(6)
C(43)	0.325(1)	0.468(1)	-0.0310(9)	* 0.103(7)
C(44)	0.270(1)	0.555(1)	-0.032(1)	* 0.109(7)
C(45)	0.210(1)	0.581(1)	0.041(1)	* 0.106(7)
C(46)	0.206(1)	0.5221(8)	0.1120(8)	* 0.073(6)

Tabla 7. *Distancias de enlace (Å) para [1-CH_3-1,2-$C_2B_{10}H_{10}$]$_2$P(C_6H_5).*

P(1)-C(1)	1.88(1)	P(1)-C(21)	1.88(1)
P(1)-C(41)	1.82(1)	C(1)-C(2)	1.74(2)
C(1)-B(3)	1.69(2)	C(1)-B(4)	1.70(2)
C(1)-B(5)	1.72(2)	C(1)-B(6)	1.77(2)
C(2)-B(3)	1.64(3)	C(2)-B(6)	1.71(2)
C(2)-B(7)	1.61(2)	C(2)-B(11)	1.73(2)
C(2)-C(13)	1.56(2)	C(21)-C(22)	1.66(2)
C(21)-B(23)	1.75(2)	C(21)-B(24)	1.72(2)
C(21)-B(25)	1.70(2)	C(21)-B(26)	1.69(2)
C(22)-B(23)	1.61(3)	C(22)-B(26)	1.92(2)
C(22)-B(27)	1.71(3)	C(22)-B(31)	1.86(3)
C(22)-C(33)	1.58(3)	C(41)-C(42)	1.38(2)
C(41)-C(46)	1.39(2)	C(42)-C(43)	1.41(2)
C(43)-C(44)	1.41(2)	C(44)-C(45)	1.40(2)
C(45)-C(46)	1.38(2)		

Tabla 8. *Ángulos de enlace (°) para [1-CH_3-1,2-$C_2B_{10}H_{10}$]$_2$P(C_6H_5).*

C(1)-P(1)-C(2)1	108.2(5)	C(1)-P(1)-C(41)	106.2(5)
C(21)-P(1)-C(41)	104.5(5)	P(1)-C(1)-C(2)	109.0(7)
P(1)-C(1)-B(3)	113.4(8)		
P(1)-C(1)-B(4)	129.7(9)		
P(1)-C(1)-B(5)	128.0(8)		
P(1)-C(1)-B(6)	110.8(8)		
C(1)-C(2)-C(13)	118.5(9)		
P(1)-C(21)-C(22)	113.1(8)		
P(1)-C(21)-B(23)	107.1(9)		
P(1)-C(21)-B(24)	119.8(9)		
P(1)-C(21)-B(25)	132.3(8)		
P(1)-C(21)-B(26)	123.7(8)		
C(21)-C(22)-C(33)	120(1)		
C(1)-C(41)-C(42)	126.5(9)		
P(1)-C(41)-C(46)	112.2(8)		
C(42)-C(41)-C(46)	121(1)		
C(41)-C(42)-C(43)	119(1)		
C(42)-C(43)-C(44)	120(1)		
C(43)-C(44)-C(45)	119(1)		
C(44)-C(45)-C(46)	120(1)		
C(41)-C(46)-C(45)	120(1)		

4.3. Estructura cristalina de cHPPh.

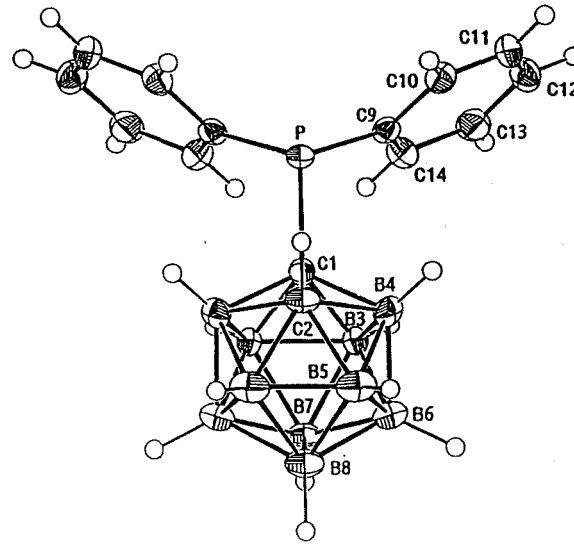


Tabla 9. *Datos cristalográficos para [1-P(C_6H_5)$_2$-1,2-$C_2B_{10}H_{11}$].*

Fórmula química	$C_{14}H_{21}B_{10}P$
peso molecular	328.39 g/mol
sistema cristalino	ortorrómbico
grupo espacial	Cmc21 (No. 36)
a, Å	16.037(3)
b, Å	8.769(4)
c, Å	12.804(3)
V, Å3	1801(1)
Z	4
p(calcd), gcm-3	1.211
myy, mm-1	0.14
T, C	-120
lambda, Å	0.71073
R(F)	0.062
wR(F)	0.045

Tabla 10. *Coordenadas fraccionarias y desviación estándar (entre paréntesis) para [1-P(C_6H_5)$_2$-1,2-$C_2B_{10}H_{11}$].*

	x/a	y/b	z/c	U
P	1/2	0.5177(2)	0.30000	* 0.0208(4)
C(1)	1/2	0.7261(7)	0.3314(5)	* 0.021(2)
C(2)	1/2	0.7464(7)	0.4608(5)	* 0.025(2)
B(3)	0.4443(3)	0.8737(5)	0.2746(4)	* 0.023(2)
B(4)	0.4103(3)	0.7869(6)	0.3936(4)	* 0.025(2)
B(5)	0.4443(4)	0.9014(6)	0.5005(5)	* 0.032(2)
B(6)	0.4097(3)	0.9873(6)	0.3817(4)	* 0.027(2)
B(7)	1/2	1.0415(7)	0.3107(7)	* 0.022(2)
B(8)	1/2	1.0593(9)	0.4470(6)	* 0.030(3)
C(9)	0.4092(3)	0.4908(5)	0.2157(3)	* 0.022(1)
C(10)	0.3533(3)	0.3806(5)	0.2525(4)	* 0.028(1)
C(11)	0.2822(3)	0.3428(6)	0.1975(4)	* 0.035(2)
C(12)	0.2659(3)	0.4129(6)	0.1033(4)	* 0.034(2)
C(13)	0.3206(3)	0.5208(6)	0.0640(4)	* 0.036(2)
C(14)	0.3932(3)	0.5586(5)	0.1198(4)	* 0.026(1)

Tabla 11. *Distancias de enlace (Å) para [1-P(C_6H_5)$_2$-1,2-$C_2B_{10}H_{11}$].*

P-C(1)	1.871(6)
P-C(9)	1.828(4)
P-C(9)	1.828(4)
C(1)-C(2)	1.666(9)
C(1)-B(3)	1.732(7)
C(1)-B(4)	1.729(6)
C(2)-B(4)	1.714(6)
C(2)-B(5)	1.705(8)
C(9)-C(10)	1.400(6)
C(9)-C(14)	1.388(6)
C(10)-C(11)	1.379(7)
C(11)-C(12)	1.379(7)
C(12)-C(13)	1.385(7)
C(13)-C(14)	1.407(7)

Tabla 12. *Ángulos de enlace (°) para (1-P(C_6H_5)$_2$-1,2-$C_2B_{10}H_{10}$).*

C(1)-P-C(9)	104.7(2)
C(9)-P-C(9)	105.6(2)
P-C(1)-C(2)	108.5(4)
P-C(1)-B(3)	129.8(3)
P-C(1)-B(4)	113.6(3)
P-C(9)-C(10)	113.6(3)
P-C(9)-C(14)	127.9(3)
C(10)-C(9)-C(14)	118.3(4)
C(9)-C(10)-C(11)	121.6(5)
C(10)-C(11)-C(12)	119.7(5)
C(11)-C(12)-C(13)	120.1(5)
C(12)-C(13)-C(14)	120.1(5)
C(9)-C(14)-C(13)	120.1(4)

(*) Symmetry code: 1-x, y, z

4.4. Estructura cristalina de cMeP^{i}Pr.

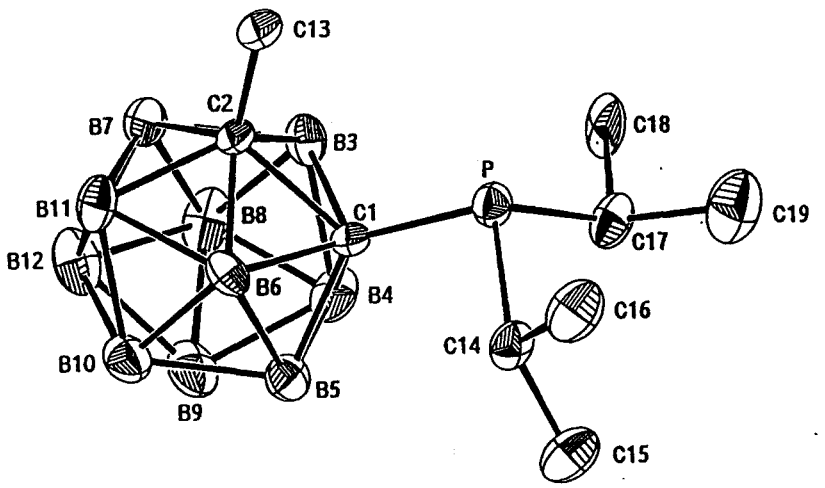


Tabla 13. *Datos cristalográficos para [1-P{CH(CH$_3$)$_2$}$_2$-2-CH$_3$-1,2-C$_2$B$_{10}$H$_{10}$].*

Fórmula química	$C_9H_{27}B_{10}P$
peso molecular	274.39 g/mol
sistema cristalino	ortorrómbico
grupo espacial	Pbca (No. 61)
a, Å	18.278(12)
b, Å	13.866(7)
c, Å	13.520(5)
V, Å3	3427(3)
Z	8
p(calcd), gcm-3	1.064
myy, mm-1	0.14
T, C	-80
lambda, Å	0.71073
R(F)	0.095
wR(F)	0.082

Tabla 14. *Coordenadas fraccionarias y desviación estándar (entre paréntesis) para [1-P{CH(CH$_3$)$_2$}$_2$-2-CH$_3$-1,2-C$_2$B$_{10}$H$_{10}$].*

	x/a	y/b	z/c	U
P	0.8564(1)	0.6286(2)	0.3454(1)	* 0.0243(5)
C(1)	0.7789(3)	0.6203(5)	0.4360(5)	* 0.020(2)
C(2)	0.6935(3)	0.6038(5)	0.3834(5)	* 0.020(2)
B(3)	0.7343(4)	0.5095(7)	0.4439(6)	* 0.026(3)
B(4)	0.7796(5)	0.5616(8)	0.5480(6)	* 0.034(3)
B(5)	0.7680(5)	0.6876(7)	0.5395(6)	* 0.027(3)
B(6)	0.7150(4)	0.7126(6)	0.4321(6)	* 0.023(3)
B(7)	0.6398(5)	0.5348(7)	0.4572(6)	* 0.034(3)
B(8)	0.6934(5)	0.5068(8)	0.5633(7)	* 0.034(3)
B(9)	0.7127(5)	0.6195(8)	0.6207(6)	* 0.038(3)
B(10)	0.6738(5)	0.7148(7)	0.5495(6)	* 0.031(3)
B(11)	0.6281(4)	0.6606(7)	0.4487(7)	* 0.031(3)
B(12)	0.6272(5)	0.6019(7)	0.5651(7)	* 0.037(4)
C(13)	0.6873(4)	0.5965(6)	0.2721(5)	* 0.033(3)
C(14)	0.8932(3)	0.7514(6)	0.3758(5)	* 0.028(2)
C(15)	0.9472(4)	0.7605(6)	0.4609(6)	* 0.042(3)
C(16)	0.9239(4)	0.7963(6)	0.2814(6)	* 0.042(3)
C(17)	0.9287(4)	0.5460(6)	0.3930(5)	* 0.031(3)
C(18)	0.9070(4)	0.4387(6)	0.3899(6)	* 0.041(3)
C(19)	0.9955(4)	0.5605(6)	0.3258(7)	* 0.053(3)

Tabla 15. *Distancias de enlace (Å) para [1-P{CH(CH$_3$)$_2$}$_2$-2-CH$_3$-1,2-C$_2$B$_{10}$H$_{10}$].*

P-C(1)	1.876(6)
P-C(14)	1.876(8)
P-C(17)	1.863(7)
C(1)-C(2)	1.731(9)
C(1)-B(3)	1.74(1)
C(1)-B(4)	1.72(1)
C(1)-B(5)	1.69(1)
C(1)-B(6)	1.73(1)
C(2)-C(13)	1.512(9)
C(14)-C(15)	1.52(1)
C(14)-C(16)	1.53(1)
C(17)-C(18)	1.54(1)
C(17)-C(19)	1.53(1)

Tabla 16. *Ángulos de enlace (°) para [1-P{CH(CH$_3$)$_2$}$_2$-2-CH$_3$-1,2-C$_2$B$_{10}$H$_{10}$].*

C(1)-P-C(14)	100.6(3)
C(1)-P-C(17)	105.8(3)
C(14)-P-C(17)	103.2(3)
P-C(1)-C(2)	114.9(4)
P-C(1)-B(3)	116.6(5)
P-C(1)-B(4)	126.8(5)
P-C(1)-B(5)	126.5(5)
P-C(1)-B(6)	116.4(5)
C(1)-C(2)-C(13)	119.0(5)
B(3)-C(2)-C(13)	117.2(6)
B(6)-C(2)-C(13)	117.7(6)
B(7)-C(2)-C(13)	120.3(6)
B(11)-C(2)-C(13)	120.0(6)
P-C(14)-C(15)	118.3(6)
P-C(14)-C(16)	108.5(5)
C(15)-C(14)-C(16)	111.1(6)
P-C(17)-C(18)	113.8(5)
P-C(17)-C(19)	106.3(5)
C(18)-C(17)-C(19)	108.3(6)

4.5. Estructura cristalina de cPhP^{i}Pr.

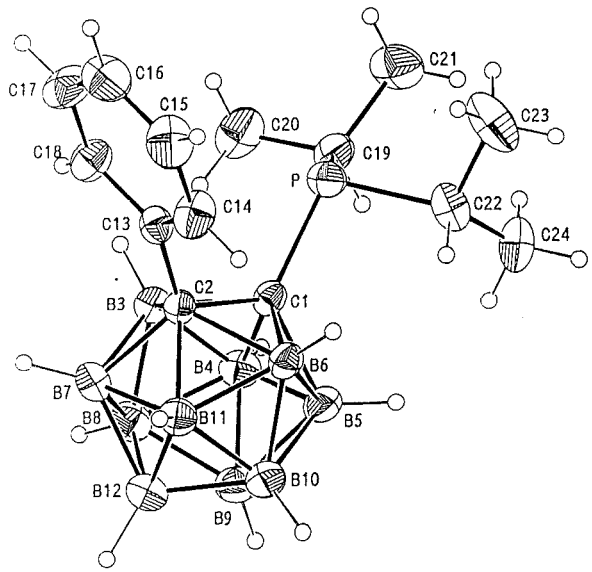


Tabla 17. *Datos cristalográficos para [1-P{CH(CH$_3$)$_2$}$_2$-2-C$_6$H$_5$-1,2-C$_2$B$_{10}$H$_{10}$].*

Fórmula química	$C_{14}H_{29}B_{10}P$
peso molecular	335.95 g/mol
sistema cristalino	monoclínico
grupo espacial	$P2_1/n$ (No 14)
a, Å	9.673 (1)
b, Å	20.021 (2)
c, Å	10.571 (2)
β	90.89 (1)
V, Å^3	2047.0 (5)
Z	4
p(calcd), gcm-3	1.092
myy, mm-1	0.14
T, K	295
lambda, Å	0.71069
R(F)	0.057
wR(F)	0.058

Tabla 18. *Coordenadas fraccionarias y desviación estándar (entre paréntesis) para [1-P{CH(CH$_3$)$_2$}$_2$-2-C$_6$H$_5$-1,2-C$_2$B$_{10}$H$_{10}$].*

	x	*y*	*z*	U_{eq}
P	0.1080(1)	0.07041(5)	0.20574(9)	0.0503(3)
C(1)	0.2075(3)	0.1416(2)	0.2787(3)	0.042(1)
C(2)	0.3296(3)	0.1775(2)	0.1759(3)	0.041(1)
B(3)	0.3833(4)	0.1295(2)	0.3017(4)	0.047(1)
B(4)	0.2716(5)	0.1468(2)	0.4300(4)	0.053(2)
B(5)	0.1455(5)	0.2039(2)	0.3737(4)	0.056(2)
B(6)	0.1798(4)	0.2197(2)	0.2125(4)	0.048(2)
B(7)	0.4699(5)	0.2043(2)	0.2613(4)	0.051(2)
B(8)	0.4347(5)	0.1857(2)	0.4214(4)	0.059(2)
B(9)	0.2873(5)	0.2328(2)	0.4648(5)	0.063(2)
B(10)	0.2298(5)	0.2779(2)	0.3309(5)	0.060(2)
B(11)	0.3424(5)	0.2609(2)	0.2058(4)	0.053(2)
B(12)	0.4092(5)	0.2680(2)	0.3620(4)	0.061(2)
C(13)	0.3453(3)	0.1515(2)	0.0437(3)	0.046(1)
C(14)	0.2772(4)	0.1812(2)	-0.0567(4)	0.069(2)
C(15)	0.2961(5)	0.1589(3)	-0.1780(4)	0.087(2)
C(16)	0.3820(6)	0.1069(3)	-0.2026(4)	0.085(2)
C(17)	0.4512(5)	0.0774(2)	-0.1044(4)	0.080(2)
C(18)	0.4339(4)	0.0996(2)	0.0187(4)	0.062(2)
C(19)	0.1088(4)	0.0046(2)	0.3308(3)	0.058(1)
C(20)	0.2495(5)	-0.0277(2)	0.3505(4)	0.085(2)
C(21)	0.0054(5)	-0.0494(2)	0.2870(4)	0.087(2)
C(22)	-0.0737(4)	0.1039(2)	0.2065(4)	0.065(2)
C(23)	-0.1547(5)	0.0741(3)	0.0929(4)	0.103(2)
C(24)	-0.1560(4)	0.0988(2)	0.3277(4)	0.090(2)

$U_{eq}=1/3\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*a_i\cdot a_j$.

Tabla 19. *Distancias de enlace (Å) para [1-P{CH(CH$_3$)$_2$}$_2$-2-C$_6$H$_5$-1,2-C$_2$B$_{10}$H$_{10}$].*

P-C(1)	1.879(3)	C(1)-B(6)	1.731(5)
P-C(19)	1.866(4)	C(2)-C(13)	1.501(5)
P-C(22)	1.881(4)	C(19)-C(20)	1.519(6)
C(1)-C(2)	1.769(4)	C(19)-C(21)	1.540(6)
C(1)-B(3)	1.730(5)	C(22)-C(23)	1.544(6)
C(1)-B(4)	1.710(5)	C(22)-C(24)	1.522(6)

Tabla 20. *Ángulos de enlace (°) para [1-P{CH(CH$_3$)$_2$}$_2$-2-C$_6$H$_5$-1,2-C$_2$B$_{10}$H$_{10}$].*

C(1)-P-C(19)	104.4(2)	B(6)-C(2)-C(13)	118.4(3)
C(1)-P-C(22)	101.5(2)	B(7)-C(2)-C(13)	120.7(3)
C(19)-P-C(22)	104.0(2)	B(11)-C(2)-C(13)	120.4(3)
P-C(1)-C(2)	113.5(2)	C(2)-C(13)-C(14)	120.9(3)
P-C(1)-B(3)	116.6(2)	C(2)-C(13)-C(18)	120.9(3)
P-C(1)-B(4)	127.3(2)	P-C(19)-C(20)	113.1(3)
P-C(1)-B(5)	127.6(2)	P-C(19)-C(21)	106.7(3)
P-C(1)-B(6)	116.3(2)	P-C(22)-C(23)	108.8(3)
C(1)-C(2)-C(13)	120.5(3)	P-C(22)-C(24)	118.7(3)
B(3)-C(2)-C(13)	119.5(3)		

Ángulos diedros

C(19)-P-C(1)-C(2)	134.9(2)	C(1)-C(2)-C(13)-C(14)	95.6(4)
C(22)-P-C(1)-C(2)	-117.2(2)	C(1)-C(2)-C(13)-C(18)	-88.0(4)
P-C(1)-C(2)-C(13)	0.7(4)		

4.6. Estructura cristalina de cPhP(O)Ph.

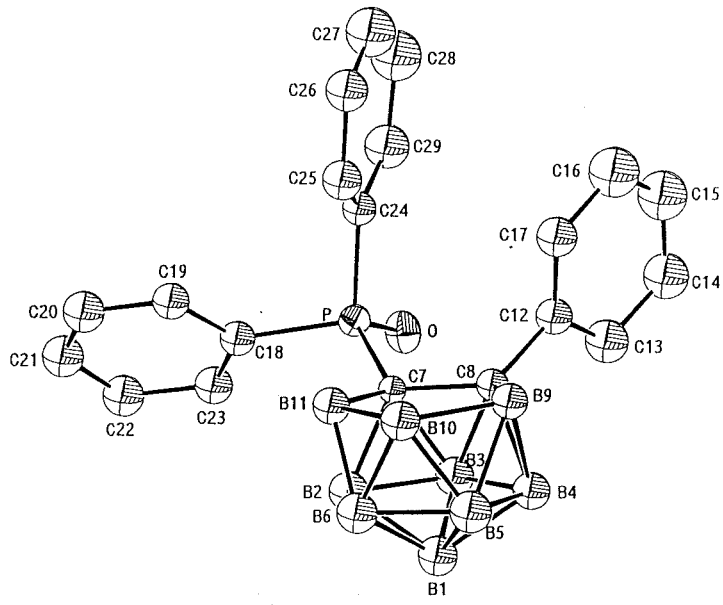


Table 21. *Datos cristalográficos para* $[N(CH_2CH_2CH_2CH_3)_4]$ $[7\text{-}P(O)(C_6H_5)_2\text{-}8\text{-}C_6H_5\text{-}7,8\text{-}C_2B_9H_{10}]$.

Fórmula química	$[C_{20}H_{25}B_9OP][C_{16}H_{36}N]$
peso molecular	652.15
a, Å	13.884 (7)
b, Å	21.485 (4)
c, Å	13.404 (7)
V, Å^3	3998 (3)
Z	4
sistema cristalino	ortorrómbico
grupo espacial	$P2_12_12_1$
T, °C	21
λ, Å	0.71069
ρ_{calcd}, g cm^{-3}	1.083
μ, cm^{-1}	0.9
$R(F_o)$	0.099
$R_w(F_o)$	0.090

Tabla 22. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para* - *$[N(CH_2CH_2CH_2CH_3)_4][7\text{-}P(O)(C_6H_5)_2\text{-}8\text{-}C_6H_5\text{-}7,8\text{-}C_2B_9H_{10}]$.*

	x/a	y/b	z/c	U	PP
P	0.4834(3)	0.5408(2)	0.5384(3)	* 0.040(1)	
O	0.5219(7)	0.5692(4)	0.4469(6)	* 0.056(4)	
N	0.6225(8)	0.6442(5)	0.2059(8)	* 0.061(5)	
B(1)	0.655(1)	0.6366(8)	0.761(1)	0.063(6)	
B(2)	0.617(1)	0.5645(8)	0.711(1)	0.065(6)	
B(3)	0.605(1)	0.6330(8)	0.642(1)	0.061(6)	
B(4)	0.576(1)	0.6947(8)	0.724(1)	0.057(5)	
B(5)	0.568(1)	0.6624(9)	0.841(1)	0.073(6)	
B(6)	0.595(1)	0.5813(8)	0.833(1)	0.068(6)	
C(7)	0.5122(9)	0.5822(5)	0.6544(8)	0.031(3)	
C(8)	0.4845(9)	0.6534(5)	0.6607(9)	0.042(4)	
B(9)	0.458(1)	0.6755(8)	0.772(1)	0.053(5)	
B(10)	0.473(1)	0.6055(8)	0.850(1)	0.063(6)	
B(11)	0.503(1)	0.5483(8)	0.761(1)	0.056(5)	
C(12)	0.425(1)	0.6850(6)	0.577(1)	0.053(4)	
C(13)	0.471(1)	0.7187(7)	0.503(1)	0.076(5)	
C(14)	0.4121(9)	0.7497(7)	0.431(1)	0.086(6)	
C(15)	0.317(1)	0.7409(8)	0.439(1)	0.101(7)	
C(16)	0.270(1)	0.7102(8)	0.512(1)	0.103(7)	
C(17)	0.328(1)	0.6810(7)	0.587(1)	0.065(5)	
C(18)	0.5236(9)	0.4600(6)	0.548(1)	0.049(4)	
C(19)	0.474(1)	0.4138(6)	0.5992(9)	0.054(4)	
C(20)	0.504(1)	0.3527(6)	0.597(1)	0.070(5)	
C(21)	0.582(1)	0.3375(6)	0.539(1)	0.070(5)	
C(22)	0.635(1)	0.3800(7)	0.489(1)	0.069(5)	
C(23)	0.604(1)	0.4431(6)	0.491(1)	0.057(5)	
C(24)	0.3544(9)	0.5341(6)	0.533(1)	0.047(4)	
C(25)	0.294(1)	0.5259(7)	0.614(1)	0.065(5)	
C(26)	0.193(1)	0.5209(7)	0.605(1)	0.073(5)	
C(27)	0.156(1)	0.5256(8)	0.511(1)	0.101(6)	
C(28)	0.209(1)	0.5394(8)	0.428(1)	0.104(7)	
C(29)	0.312(1)	0.5417(7)	0.441(1)	0.079(5)	
C(30)	0.680(1)	0.6412(7)	0.304(1)	0.068(5)	
C(31)	0.783(1)	0.6325(7)	0.292(1)	0.073(5)	
C(32)	0.835(1)	0.6244(7)	0.388(1)	0.084(6)	
C(33)	0.942(1)	0.6230(8)	0.385(1)	0.093(6)	
C(34)	0.632(1)	0.5841(7)	0.149(1)	0.067(5)	
C(35)	0.601(1)	0.5258(8)	0.201(1)	0.088(6)	
C(36)	0.604(1)	0.4689(8)	0.137(1)	0.103(6)	
C(37)	0.567(2)	0.413(1)	0.186(1)	0.142(9)	
C(38)	0.656(1)	0.6963(6)	0.140(1)	0.056(4)	
C(39)	0.645(1)	0.7613(7)	0.178(1)	0.085(6)	
C(40)	0.689(1)	0.8066(8)	0.105(1)	0.107(7)	

C(41)	0.670(2)	0.8732(9)	0.137(1)	0.132(8)	
C(42)	0.515(1)	0.6543(6)	0.233(1)	0.062(5)	
C(43)	0.443(1)	0.6532(8)	0.149(1)	0.111(7)	
C(44)	0.337(1)	0.6656(9)	0.191(1)	0.16(1)	
C(45A)	0.345(4)	0.726(2)	0.143(4)	0.11(2)	0.34(2)
C(45B)	0.258(4)	0.630(3)	0.230(6)	0.13(4)	0.25(2)
C(45C)	0.265(3)	0.671(2)	0.119(3)	0.12(2)	0.41(3)

Tabla 23. *Distancias de enlace (Å) para* $[N(CH_2CH_2CH_2CH_3)_4][7\text{-}P(O)(C_6H_5)_2\text{-}8\text{-}C_6H_5\text{-}7,8\text{-}C_2B_9H_{10}]$.

P-O	1.470(9)	P-C7	1.84(1)
P-C18	1.83(1)	P-C24	1.80(1)
B1-B2	1.77(3)	B1-B3	1.74(3)
B1-B4	1.74(3)	B1-B5	1.72(3)
B1-B6	1.74(3)	B1-H1	1.10
B2-B3	1.75(3)	B2-B6	1.70(3)
B2-C7	1.69(2)	B2-B11	1.76(3)
B2-H2	1.10	B3-B4	1.76(2)
B3-C7	1.69(2)	B3-C8	1.74(2)
B3-H3	1.10	B4-B5	1.72(3)
B4-C8	1.77(2)	B4-B9	1.80(2)
B4-H4	1.10	B5-B6	1.79(3)
B5-B9	1.80(3)	B5-B10	1.80(3)
B5-H5	1.10	B6-B10	1.78(3)
B6-B11	1.75(3)	B6-H6	1.10
C7-C8	1.58(2)	C7-B11	1.60(2)
C8-B9	1.61(2)	C8-C12	1.55(2)
B9-B10	1.84(2)	B9-H9	1.10
B10-B11	1.77(2)	B10-H10A	1.10
B11-H11	1.10	C12-C13	1.38(2)
C12-C17	1.35(2)	C13-C14	1.43(2)
C13-H13	.95	C14-C15	1.34(2)
C14-H14	.95	C15-C16	1.35(2)
C15-H15	.95	C16-C17	1.43(2)
C16-H16	.95	C17-H17	.95
C18-C19	1.39(2)	C18-C23	1.41(2)
C19-C20	1.38(2)	C19-H19	.95
C20-C21	1.36(2)	C20-H20	.95
C21-C22	1.35(2)	C21-H21	.95
C22-C23	1.42(2)	C22-H22	.95
C23-H23	.95	C24-C25	1.39(2)
C24-C29	1.37(2)	C25-C26	1.42(2)
C25-H25	.95	C26-C27	1.36(2)
C26-H26	.95	C27-C28	1.36(2)
C27-H27	.95	C28-C29	1.44(2)
C28-H28	.95	C29-H29	.95
N-C30	1.54(2)	N-C34	1.50(2)
N-C38	1.50(2)	N-C42	1.54(2)

C30-C31	1.46(2)	C30-H30A	.95
C30-H30B	.95	C31-C32	1.49(2)
C31-H31A	.95	C31-H31B	.95
C32-C33	1.48(2)	C32-H32A	.95
C32-H32B	.95	C33-H33A	.95
C33-H33B	.95	C33-H33C	.95
C34-C35	1.49(2)	C34-H34A	.95
C34-H34B	.95	C35-C36	1.49(2)
C35-H35A	.95	C35-H35B	.95
C36-C37	1.47(3)	C36-H36A	.95
C36-H36B	.95	C37-H37A	.95
C37-H37B	.95	C37-H37C	95
C38-C39	.50(2)	C38-H38A	.95
C38-H38B	.95	C39-C40	1.51(2)
C39-H39A	.95	C39-H39B	.95
C40-C41	1.52(3)	C40-H40A	.95
C40-H40B	.95	C41-H41A	.95
C41-H41B	.95	C41-H41C	95
C42-C43	1.51(2)	C42-H42A	95
C42-H42B	.95	C43-C44	1.59(3)
C43-H43A	.95	C43-H43B	.95
C44-C45A	1.45(4)	C44-C45B	1.44(7)
C44-C45C	1.40(4)	C44-H44A	.95
C44-H44B	.95	C44-H44C	.95
C45A-C45C	1.65(6)	C45B-C45C	1.74(8)
P-B2	3.01(2)	P-B3	2.95(2)
P-C7	1.84(1)	P-C8	2.92(1)
P-B11	3.00(2)	P-C12	3.24(1)
P-C13	3.85(1)	P-C17	3.76(2)
P-C18	1.83(1)	P-C19	2.85(1)
P-C23	2.76(1)	P-C24	1.80(1)
P-C25	2.84(2)	P-C29	2.71(2)
P-H2	3.287	P-H3	3.171
P-H11	3.187	P-H13	3.986
P-H17	3.859	P-H19	2.966
P-H23	2.825	P-H25	2.954
P-H29	2.761	P-H30B	3.835
P-H42A	3.905	O-P	1.470(9)
O-B3	3.17(2)	O-C7	2.80(1)
O-C8	3.43(1)	O-C12	3.32(2)
O-C13	3.37(2)	O-C18	2.71(1)
O-C23	3.00(2)	O-C24	2.70(2)
O-C29	2.98(2)	O-C30	3.30(2)
O-C42	3.40(2)	O-H3	3.351
O-H23	2.614	O-H29	2.547
O-H30A	3.449	O-H30B	2.472
O-H35A	3.238	O-H35B	3.110
O-H42A	2.552	N-C30	1.54(2)
N-C31	2.53(2)	N-C34	1.50(2)

Tabla 24. *Ángulos de enlace (°) para* $[N(CH_2CH_2CH_2CH_3)_4][7\text{-}P(O)(C_6H_5)_2\text{-}8\text{-}C_6H_5\text{-}7,8\text{-}C_2B_9H_{10}]$.

O-P-C7	115.2(5)	O-P-C18	110.2(6)
O-P-C24	111.2(6)	C7-P-C18	109.4(6)
C7-P-C24	106.8(6)	C18-P-C24	103.4(6)
B2-B1-B3	60(1)	B2-B1-B4	109(1)
B2-B1-B5	108(1)	B2-B1-B6	58(1)
B2-B1-H1	121	B3-B1-B4	61(1)
B3-B1-B5	108(1)	B3-B1-B6	106(1)
B3-B1-H1	123	B4-B1-B5	60(1)
B4-B1-B6	110(1)	B4-B1-H1	121
B5-B1-B6	62(1)	B5-B1-H1	121
B6-B1-H1	121	B1-B2-B3	59(1)
B1-B2-B6	60(1)	B1-B2-C7	103(1)
B1-B2-B11	107(1)	B1-B2-H2	122
B3-B2-B6	108(1)	B3-B2-C7	59.1(9)
B3-B2-B11	106(1)	B3-B2-H2	122
B6-B2-C7	103(1)	B6-B2-B11	61(1)
B6-B2-H2	121	C7-B2-B11	55.4(9)
C7-B2-H2	127	B11-B2-H2	122
B1-B3-B2	61(1)	B1-B3-B4	59(1)
B1-B3-C7	104(1)	B1-B3-C8	104(1)
B1-B3-H3	124	B2-B3-B4	109(1)
B2-B3-C7	58.8(9)	B2-B3-C8	104(1)
B2-B3-H3	124	B4-B3-C7	105(1)
B4-B3-C8	60.5(9)	B4-B3-H3	119
C7-B3-C8	54.7(8)	C7-B3-H3	126
C8-B3-H3	124	B1-B4-B3	60(1)
B1-B4-B5	59(1)	B1-B4-C8	103(1)
B1-B4-B9	108(1)	B1-B4-H4	124
B3-B4-B5	106(1)	B3-B4-C8	59.2(9)
B3-B4-B9	105(1)	B3-B4-H4	119
B5-B4-C8	101(1)	B5-B4-B9	61(1)
B5-B4-H4	128	C8-B4-B9	53.4(8)
C8-B4-H4	124	B9-B4-H4	124
B1-B5-B4	61(1)	B1-B5-B6	60(1)
B1-B5-B9	109(1)	B1-B5-B10	110(1)
B1-B5-H5	121	B4-B5-B6	109(1)
B4-B5-B9	62(1)	B4-B5-B10	112(1)
B4-B5-H5	118	B6-B5-B9	107(1)
B6-B5-B10	60(1)	B6-B5-H5	124
B9-B5-B10	62(1)	B9-B5-H5	121
B10-B5-H5	121	B1-B6-B2	62(1)
B1-B6-B5	58(1)	B1-B6-B10	109(1)
B1-B6-B11	109(1)	B1-B6-H6	123
B2-B6-B5	108(1)	B2-B6-B10	111(1)
B2-B6-B11	61(1)	B2-B6-H6	122
B5-B6-B10	61(1)	B5-B6-B11	106(1)

B5-B6-H6	122	B10-B6-B11	60(1)
B10-B6-H6	118	B11-B6-H6	122
P-C7-B2	117.3(9)	P-C7-B3	113.3(9)
P-C7-C8	117.5(8)	P-C7-B11	121.0(9)
B2-C7-B3	62(1)	B2-C7-C8	114(1)
B2-C7-B11	64(1)	B3-C7-C8	64.2(9)
B3-C7-B11	116(1)	C8-C7-B11	112(1)
B3-C8-B4	60.4(9)	B3-C8-C7	61.1(9)
B3-C8-B9	115(1)	B3-C8-C12	121(1)
B4-C8-C7	110(1)	B4-C8-B9	64.5(9)
B4-C8-C12	121(1)	C7-C8-B9	113(1)
C7-C8-C12	121(1)	B9-C8-C12	115(1)
B4-B9-B5	57(1)	B4-B9-C8	62.1(9)
B4-B9-B10	107(1)	B4-B9-H9	122
B5-B9-C8	104(1)	B5-B9-B10	59(1)
B5-B9-H9	127	C8-B9-B10	105(1)
C8-B9-H9	123	B10-B9-H9	123
B5-B10-B6	60(1)	B5-B10-B9	59(1)
B5-B10-B11	105(1)	B5-B10-H10A	124
B6-B10-B9	106(1)	B6-B10-B11	59(1)
B6-B10-H10A	124	B9-B10-B11	102(1)
B9-B10-H10A	124	B11-B10-H10A	124
B2-B11-B6	58(1)	B2-B11-C7	60(1)
B2-B11-B10	109(1)	B2-B11-H11	121
B6-B11-C7	104(1)	B6-B11-B10	61(1)
B6-B11-H11	126	C7-B11-B10	108(1)
C7-B11-H11	121	B10-B11-H11	121
C8-C12-C13	120(1)	C8-C12-C17	115(1)
C13-C12-C17	124(1)	C12-C13-C14	117(1)
C12-C13-H13	121	C14-C13-H13	121
C13-C14-C15	117(1)	C13-C14-H14	122
C15-C14-H14	122	C14-C15-C16	126(2)
C14-C15-H15	117	C16-C15-H15	117
C15-C16-C17	117(1)	C15-C16-H16	121
C17-C16-H16	121	C12-C17-C16	118(1)
C12-C17-H17	121	C16-C17-H17	121
P-C18-C19	124(1)	P-C18-C23	116.7(9)
C19-C18-C23	119(1)	C18-C19-C20	121(1)
C18-C19-H19	119	C20-C19-H19	119
C19-C20-C21	119(1)	C19-C20-H20	121
C21-C20-H20	121	C20-C21-C22	123(1)
C20-C21-H21	118	C22-C21-H21	118
C21-C22-C23	118(1)	C21-C22-H22	121
C23-C22-H22	121	C18-C23-C22	120(1)
C18-C23-H23	120	C22-C23-H23	120
P-C24-C25	125(1)	P-C24-C29	117(1)
C25-C24-C29	117(1)	C24-C25-C26	123(1)

C24-C25-H25	119	C26-C25-H25	119
C25-C26-C27	117(1)	C25-C26-H26	122
C27-C26-H26	122	C26-C27-C28	124(2)
C26-C27-H27	118	C28-C27-H27	118
C27-C28-C29	117(1)	C27-C28-H28	122
C29-C28-H28	122	C24-C29-C28	122(1)
C24-C29-H29	119	C28-C29-H29	119
C30-N-C34	110(1)	C30-N-C38	112(1)
C30-N-C42	108(1)	C34-N-C38	108(1)
C34-N-C42	109(1)	C38-N-C42	110(1)
N-C30-C31	115(1)	N-C30-H30A	108
N-C30-H30B	108	C31-C30-H30A	108
C31-C30-H30B	108	H30A-C30-H30B	109
C30-C31-C32	113(1)	C30-C31-H31A	108
C30-C31-H31B	108	C32-C31-H31A	108
C32-C31-H31B	108	H31A-C31-H31B	109
C31-C32-C33	108	C31-C32-H32B	108
C33-C32-H32A	108	C33-C32-H32B	108
H32A-C32-H32B	108	C32-C33-H33B	108
C32-C33-H33C	117	H33A-C33-H33B	109
H33A-C33-H33C	108	H33B-C33-H33C	108
N-C34-C35	117(1)	N-C34-H34A	107
N-C34-H34B	107	C35-C34-H34A	107
C35-C34-H34B	107	H34A-C34-H34B	109
C34-C35-C36	114(1)	C34-C35-H35A	108
C34-C35-H35B	108	C36-C35-H35A	108
C36-C35-H35B	108	H35A-C35-H35B	109
C35-C36-C37	114(2)	C35-C36-H36A	108
C37-C36-H36A	108	C37-C36-H36B	108
H36A-C36-H36B	109	C36-C37-H37A	108
H44A-C44-H44C	109	C36-C37-H37B	108
H44B-C44-H44C	109	C36-C37-H37C	114
H37A-C37-H37B	109	H37A-C37-H37C	108
H37B-C37-H37C	108	N-C38-C39	117(1)
N-C38-H38A	107	N-C38-H38B	107
C39-C38-H38A	107	C39-C38-H38B	107
H38A-C38-H38B	109	C38-C39-C40	110(1)
C38-C39-H39A	109	C38-C39-H39B	109
C40-C39-H39A	109	C40-C39-H39B	109
H39A-C39-H39B	109	C39-C40-C41	110(1)
C39-C40-H40A	109	C39-C40-H40B	109
C41-C40-H40A	109	C41-C40-H40B	109
H40A-C40-H40B	109	C40-C41-H41A	109
C40-C41-H41B	109	C40-C41-H41C	110
H41A-C41-H41B	109	H41A-C41-H41C	109
H41B-C41-H41C	109	N-C42-C43	118(1)
N-C42-H42A	107	N-C42-H42B	107
C43-C42-H42A	107	C43-C42-H42B	107
H42A-C42-H42B	109	C42-C43-C44	110(1)

4.7 Estructura cristalina de nMeP(H)^{i}Pr.

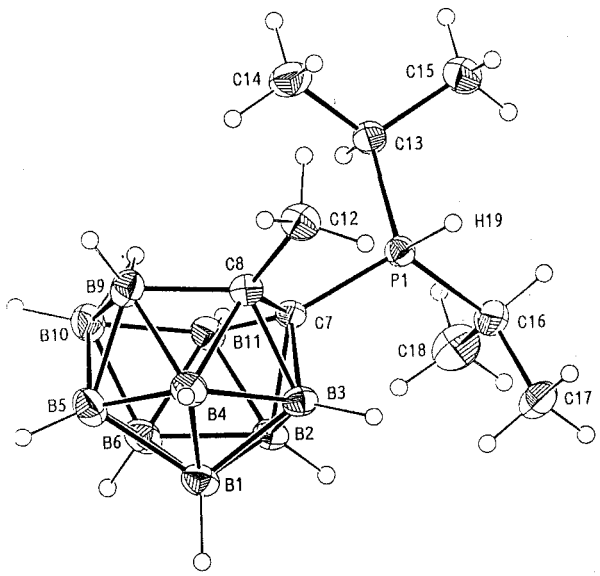


Tabla 25. *Datos cristalográficos para* $[7\text{-}PH\{CH(CH_3)_2\}_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{10}]$.

Fórmula química:	$C_9H_{28}B_9P$
peso molecular	264.57
a =	11.1860 (9) Å
b =	9.363 (1) Å
c =	16.167 (1) Å
β =	93.090 (7)°
V =	1690.8 (2) Å^3
Z =	4
grupo espacial:	$P2_1/c$ (No. 14)
T =	21 °C
λ =	0.71069 Å
ρ =	1.039 g cm^{-3}
μ =	1.4 cm^{-1}
transm coeff	0.756 - 1.000
$R(F_o)$ =	0.046
$R_w(F_o)$ =	0.055

Tabla 26. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para [7-PH{CH(CH$_3$)$_2$}$_2$-8-CH$_3$-7,8-C$_2$B$_9$H$_{10}$].*

P(1)	0.78285(5)	0.68598(6)	0.20166(4)	* 0.0309(2)
B(1)	0.8304(3)	0.2675(3)	0.3197(2)	* 0.041(1)
B(2)	0.7539(2)	0.3675(3)	0.2424(2)	* 0.0360(9)
B(3)	0.8969(2)	0.4249(3)	0.2836(2)	* 0.0346(9)
B(4)	0.9047(3)	0.3844(3)	0.3894(2)	* 0.0404(9)
B(5)	0.7686(3)	0.3120(3)	0.4174(2)	* 0.045(1)
B(6)	0.6736(3)	0.3011(3)	0.3235(2)	* 0.043(1)
C(7)	0.7778(2)	0.5435(2)	0.2748(1)	* 0.0292(7)
C(8)	0.8648(2)	0.5526(2)	0.3562(1)	* 0.0326(7)
B(9)	0.7964(3)	0.4950(3)	0.4356(2)	* 0.041(1)
B(10)	0.6470(3)	0.4308(4)	0.3998(2)	* 0.047(1)
B(11)	0.6461(2)	0.4771(3)	0.2905(2)	* 0.0382(9)
C(12)	0.9580(2)	0.6705(3)	0.3675(1)	* 0.0433(8)
C(13)	0.6772(2)	0.8254(2)	0.2251(1)	* 0.0368(7)
C(14)	0.6840(3)	0.8635(3)	0.3168(2)	* 0.057(1)
C(15)	0.6956(2)	0.9570(3)	0.1713(2)	* 0.052(1)
C(16)	0.7654(2)	0.6420(3)	0.0923(1)	* 0.0439(9)
C(17)	0.8681(3)	0.5500(3)	0.0634(2)	* 0.057(1)
C(18)	0.6414(3)	0.5851(4)	0.0643(2)	* 0.065(1)
H(1)	0.870(2)	0.158(2)	0.307(1)	0.046(7)
H(2)	0.748(2)	0.341(2)	0.178(1)	0.048(7)
H(3)	0.975(2)	0.440(2)	0.244(1)	0.036(6)
H(4)	0.993(2)	0.371(2)	0.424(1)	0.050(7)
H(5)	0.765(2)	0.236(2)	0.465(1)	0.061(8)
H(6)	0.607(2)	0.215(3)	0.312(1)	0.051(7)
H(9)	0.821(2)	0.541(2)	0.494(1)	0.050(7)
H(10A)	0.566(2)	0.418(2)	0.437(1)	0.051(7)
H(10B)	0.685(2)	0.547(3)	0.396(2)	0.082(9)
H(11)	0.567(2)	0.511(2)	0.252(1)	0.041(6)
H(12A)	1.0129	0.6736	0.3248	0.052
H(12B)	0.9219	0.7616	0.3729	0.052
H(12C)	1.0039	0.6537	0.4176	0.052
H(13)	0.5991	0.7899	0.2116	0.070
H(14A)	0.6667	0.7807	0.3479	0.070
H(14B)	0.7627	0.8956	0.3321	0.070
H(14C)	0.6287	0.9365	0.3291	0.070
H(15A)	0.7749	0.9917	0.1817	0.070
H(15B)	0.6841	0.9312	0.1147	0.070
H(15C)	0.6404	1.0300	0.1836	0.070
H(16)	0.7727	0.7304	0.0641	0.070
H(17A)	0.9410	0.6006	0.0732	0.070
H(17B)	0.8708	0.4638	0.0945	0.070
H(17C)	0.8590	0.5270	0.0062	0.070
H(18A)	0.6266	0.5013	0.0953	0.070
H(18B)	0.5838	0.6559	0.0760	0.070
H(18C)	0.6323	0.5621	0.0071	0.070
H(19)	0.896(2)	0.749(3)	0.209(1)	0.050(7)

Tabla 27. *Distancias de enlace (Å) para* $[7\text{-}PH\{CH(CH_3)_2\}_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{10}]$.

P1-C7	1.786(2)	P1-C13	1.814(2)
P1-C16	1.816(2)	P1-H19	1.39(2)
B1-B2	1.748(4)	B1-B3	1.764(4)
B1-B4	1.748(4)	B1-B5	1.806(4)
B1-B6	1.786(4)	B1-H1	1.14(2)
B2-B3	1.781(4)	B2-B6	1.743(4)
B2-C7	1.745(3)	B2-B11	1.792(4)
B2-H2	1.08(2)	B3-B4	1.749(4)
B3-C7	1.734(3)	B3-C8	1.727(4)
B3-H3	1.12(2)	B4-B5	1.748(4)
B4-C8	1.715(4)	B4-B9	1.788(4)
B4-H4	1.11(2)	B5-B6	1.808(4)
B5-B9	1.763(4)	B5-B10	1.768(4)
B5-H5	1.04(2)	B6-B10	1.767(5)
B6-B11	1.754(4)	B6-H6	1.10(2)
C7-C8	1.597(3)	C7-B11	1.632(4)
C8-B9	1.621(4)	C8-C12	1.523(3)
B9-B10	1.840(4)	B9-H9	1.07(2)
B9-H10B	1.46(2)	B10-B11	1.819(4)
B10-H10A	1.12(2)	B10-H10B	1.17(3)
B11-H11	1.10(2)	C12-H12A	.950(2)
C12-H12B	.949(2)	C12-H12C	.948(2)
C13-C14	1.523(4)	C13-C15	1.528(3)
C13-H13	.950(2)	C14-H14A	.950(3)
C14-H14B	.950(3)	C14-H14C	.950(3)
C15-H15A	.950(3)	C15-H15B	.950(3)
C15-H15C	.950(3)	C16-C17	1.528(4)
C16-C18	1.531(4)	C16-H16	.950(3)
C17-H17A	.950(3)	C17-H17B	.950(3)
C17-H17C	.950(3)	C18-H18A	.950(3)
C18-H18B	.950(3)	C18-H18C	.950(3)
P1-B2	3.074(3)	P1-B3	3.029(3)
P1-C7	1.786(2)	P1-C8	2.898(2)
P1-B11	2.910(3)	P1-C12	3.238(2)
P1-C13	1.814(2)	P1-C14	2.770(3)
P1-C15	2.753(3)	P1-C16	1.816(2)
P1-C17	2.785(3)	P1-C18	2.819(3)
P1-H2	3.27(2)	P1-H3	3.20(2)
P1-H10B	3.62(3)	P1-H11	3.06(2)
P1-H12A	3.1695(6)	P1-H12B	3.1806(6)
P1-H13	2.2881(6)	P1-H14A	2.8979(6)
P1-H14B	2.8978(6)	P1-H14C	3.6200(6)
P1-H15A	2.8813(7)	P1-H15B	2.8813(6)
P1-H15C	3.5986(7)	P1-H16	2.2587(6)
P1-H17A	2.9122(6)	P1-H17B	2.9122(6)
P1-H17C	3.6356(6)	P1-H18A	2.9459(6)

P1-H18B	2.9459(6)	P1-H18C	3.6745(6)
P1-H19	1.39(2)	P1-H1	3.90(2)
P1-H3	3.67(2)	P1-H4	3.74(2)
H10B-B9	1.46(2)	H10B-B10	1.17(3)
H10B-B11	1.85(3)	H10B-H10A	1.95(3)
H19-P1	1.39(2)	H19-C7	2.59(2)
H19-C12	2.73(2)	H19-C13	2.57(2)
H19-C16	2.52(2)	H19-C17	3.00(2)
H19-H12A	2.34(2)	H19-H12B	2.66(2)
H19-H14B	2.90(2)	H19-H15A	2.67(2)
H19-H16	2.65(2)	H19-H17A	2.66(2)
H19-B3	2.84(2)	H19-H1	2.78(3)
H19-H3	2.40(3)	H19-H4	2.78(3)

Tabla 28. *Ángulos de enlace (°) para [7-PH{CH(CH$_3$)$_2$}$_2$-8-CH$_3$-7,8-C$_2$B$_9$H$_{10}$].*

C7-P1-C13	110.8(1)	C7-P1-C16	118.0(1)
C7-P1-H19	108.9(9)	C13-P1-C16	109.3(1)
C13-P1-H19	106(1)	C16-P1-H19	102.9(9)
B2-B1-B3	60.9(2)	B2-B1-B4	108.8(2)
B2-B1-B5	107.8(2)	B2-B1-B6	59.1(2)
B2-B1-H1	122(1)	B3-B1-B4	59.7(2)
B3-B1-B5	106.6(2)	B3-B1-B6	107.2(2)
B3-B1-H1	121(1)	B4-B1-B5	58.9(2)
B4-B1-B6	107.5(2)	B4-B1-H1	120(1)
B5-B1-B6	60.4(2)	B5-B1-H1	122(1)
B6-B1-H1	124(1)	B1-B2-B3	60.0(2)
B1-B2-B6	61.5(2)	B1-B2-C7	103.3(2)
B1-B2-B11	108.1(2)	B1-B2-H2	125(1)
B3-B2-B6	108.3(2)	B3-B2-C7	58.9(1)
B3-B2-B11	106.1(2)	B3-B2-H2	116(1)
B6-B2-C7	100.8(2)	B6-B2-B11	59.5(2)
B6-B2-H2	130(1)	C7-B2-B11	54.9(1)
C7-B2-H2	121(1)	B11-B2-H2	123(1)
B1-B3-B2	59.1(2)	B1-B3-B4	59.1(2)
B1-B3-C8	104.3(2)	B1-B3-H3	131(1)
B2-B3-B4	107.3(2)	B2-B3-C7	59.5(1)
B2-B3-C8	104.3(2)	B2-B3-H3	122(1)
B4-B3-C7	102.5(2)	B4-B3-C8	59.1(1)
B4-B3-H3	126(1)	C7-B3-C8	54.9(1)
C7-B3-H3	119(1)	C8-B3-H3	120(1)
B1-B4-B3	60.6(2)	B1-B4-B5	62.2(2)
B1-B4-C8	105.5(2)	B1-B4-B9	108.8(2)
B1-B4-H4	129(1)	B3-B4-B5	109.8(2)
B3-B4-C8	59.8(1)	B3-B4-B9	106.5(2)
B3-B4-H4	121(1)	B5-B4-C8	102.8(2)
B5-B4-B9	59.8(2)	B5-B4-H4	126(1)

C8-B4-B9	55.1(2)	C8-B4-H4	118(1)
B9-B4-H4	117(1)	B1-B5-B4	58.9(2)
B1-B5-B6	59.2(2)	B1-B5-B9	107.3(2)
B1-B5-B10	109.4(2)	B1-B5-H5	121(1)
B4-B5-B6	106.6(2)	B4-B5-B9	61.2(2)
B4-B5-B10	112.8(2)	B4-B5-H5	121(1)
B6-B5-B9	106.6(2)	B6-B5-B10	59.2(2)
B6-B5-H5	122(1)	B9-B5-B10	62.8(2)
B9-B5-H5	124(1)	B10-B5-H5	119(1)
B1-B6-B2	59.4(2)	B1-B6-B5	60.3(2)
B1-B6-B10	110.3(2)	B1-B6-B11	108.2(2)
B1-B6-H6	121(1)	B2-B6-B5	107.9(2)
B2-B6-B10	113.1(2)	B2-B6-B11	61.7(2)
B2-B6-H6	120(1)	B5-B6-B10	59.3(2)
B5-B6-B11	106.7(2)	B5-B6-H6	123(1)
B10-B6-B11	62.2(2)	B10-B6-H6	119(1)
B11-B6-H6	122(1)	P1-C7-B2	121.1(2)
P1-C7-B3	118.8(2)	P1-C7-C8	117.8(1)
P1-C7-B11	116.7(2)	B2-C7-B3	61.6(1)
B2-C7-C8	112.0(2)	B2-C7-B11	64.0(2)
B3-C7-C8	62.3(1)	B3-C7-B11	116.0(2)
C8-C7-B11	114.1(2)	B3-C8-B4	61.1(2)
B3-C8-C7	62.8(1)	B3-C8-B9	115.6(2)
B3-C8-C12	114.7(2)	B4-C8-C7	110.2(2)
B4-C8-B9	64.8(2)	B4-C8-C12	117.6(2)
C7-C8-B9	110.0(2)	C7-C8-C12	121.4(2)
B9-C8-C12	119.7(2)	B4-B9-B5	59.0(2)
B4-B9-C8	60.1(2)	B4-B9-B10	107.7(2)
B4-B9-H9	117(1)	B4-B9-H10B	126(1)
B5-B9-C8	106.1(2)	B5-B9-B10	58.7(2)
B5-B9-H9	125(1)	B5-B9-H10B	96(1)
C8-B9-B10	108.6(2)	C8-B9-H9	117(1)
C8-B9-H10B	88(1)	B10-B9-H9	127(1)
B10-B9-H10B	39(1)	H9-B9-H10B	16(2)
B5-B10-B6	61.5(2)	B5-B10-B9	58.5(2)
B5-B10-B11	105.7(2)	B5-B10-H10A	119(1)
B5-B10-H10B	109(1)	B6-B10-B9	105.0(2)
B6-B10-B11	58.5(2)	B6-B10-H10A	118(1)
B6-B10-H10B	122(1)	B9-B10-B11	100.7(2)
B9-B10-H10A	128(1)	B9-B10-H10B	52(1)
B11-B10-H10A	126(1)	B11-B10-H10B	73(1)
H10A-B10-H10B	116(2)	B2-B11-B6	58.9(2)
B2-B11-C7	61.1(2)	B2-B11-B10	108.4(2)
B2-B11-H11	117(1)	B6-B11-C7	105.1(2)
B6-B11-B10	59.3(2)	B6-B11-H11	124(1)
C7-B11-B10	106.5(2)	C7-B11-H11	120(1)
B10-B11-H11	126(1)	C8-C12-H12A	113.6(2)
C8-C12-H12B	111.8(2)	C8-C12-H12C	108.5(2)
H12A-C12-H12B	109.5(2)	H12A-C12-H12C	106.5(2)

H12B-C12-H12C	106.6(2)	P1-C13-C14	111.9(2)
P1-C13-C15	110.6(2)	P1-C13-H13	107.6(2)
C14-C13-C15	111.3(2)	C14-C13-H13	107.6(2)
C15-C13-H13	107.6(2)	C13-C14-H14A	108.9(2)
C13-C14-H14B	108.9(3)	C13-C14-H14C	111.9(2)
H14A-C14-H14B	109.5(3)	H14A-C14-H14C	108.9(3)
H14B-C14-H14C	108.9(3)	C13-C15-H15A	109.2(2)
C13-C15-H15B	109.2(2)	C13-C15-H15C	110.6(2)
H15A-C15-H15B	109.5(3)	H15A-C15-H15C	109.2(3)
H15B-C15-H15C	109.2(3)	P1-C16-C17	112.5(2)
P1-C16-C18	114.4(2)	P1-C16-H16	105.1(2)
C17-C16-C18	113.4(2)	C17-C16-H16	105.1(2)
C18-C16-H16	105.1(2)	C16-C17-H17A	108.7(2)
C16-C17-H17B	108.7(3)	C16-C17-H17C	112.5(3)
H17A-C17-H17B	109.5(3)	H17A-C17-H17C	108.7(3)
H17B-C17-H17C	108.7(3)	C16-C18-H18A	108.2(2)
C16-C18-H18B	108.2(3)	C16-C18-H18C	114.4(3)
H18A-C18-H18B	109.5(3)	H18A-C18-H18C	108.2(3)
H18B-C18-H18C	108.2(3)	B9-H10B-B10	88(2)

Ángulos diedros

C12-C7-C8-P1	6.0(3)
C8-C7-P1-C13	-89.9(2)
C8-C7-P1-C16	143.1(2)

4.8. Estructura cristalina de trans-[Ru(nMePPh)$_2$].

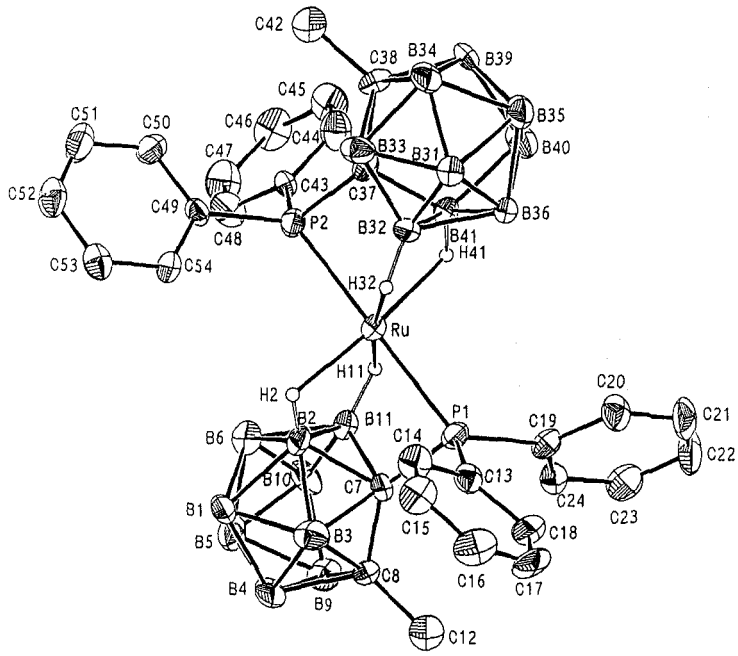


Tabla 29. *Datos cristalográficos para [Ru(7-P(C$_6$H$_5$)$_2$-8-CH$_3$-7,8-C$_2$B$_9$H$_{10}$)$_2$]·2(CH$_3$)$_2$CO*

Fórmula química:	$C_{30}H_{46}B_{18}P_2Ru \cdot 2(CH_3)_2CO$
peso molecular	880.45
a =	11.664 (9) Å
b =	9.773 (7) Å
c =	41.59 (3) Å
β =	91.61 (6)°
V =	4739 (6) Å^3
Z =	4
grupo espacial:	monoclínico, $P2_1/n$ (No. 14)
T =	23 °C
λ =	0.71069 Å
ρ =	1.234 g cm^{-3}
μ =	4.2 cm^{-1}
transm coeff =	0.903 - 1.000
$R(F_o)$	0.067
$R_w(F_o)$ =	0.060

Tabla 30. *Coordenadas fraccionarias y desviación estandard (entre paréntesis para* $[Ru(7\text{-}P(C_6H_5)_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{10})_2]\cdot 2(CH_3)_2CO$.

	x/a	y/b	z/c	U_{eq} [a]
Ru	0.96172(9)	0.3078(1)	0.63494(2)	0.0376(3)
P(1)	1.0811(3)	0.2092(4)	0.59588(7)	0.042(1)
B(1)	0.734(1)	0.241(1)	0.5600(3)	0.049(6)
B(2)	0.848(1)	0.259(1)	0.5890(3)	0.047(6)
B(3)	0.867(1)	0.151(2)	0.5559(3)	0.057(7)
B(4)	0.802(1)	0.237(2)	0.5229(3)	0.064(7)
B(5)	0.746(1)	0.394(2)	0.5361(3)	0.061(7)
B(6)	0.770(1)	0.402(2)	0.5778(3)	0.053(6)
C(7)	0.9709(9)	0.271(1)	0.5675(2)	0.040(5)
C(8)	0.9459(9)	0.254(1)	0.5306(2)	0.048(5)
B(9)	0.882(1)	0.394(2)	0.5176(3)	0.056(6)
B(10)	0.856(1)	0.504(2)	0.5519(3)	0.058(6)
B(11)	0.917(1)	0.406(1)	0.5836(3)	0.036(5)
C(12)	1.034(3)	0.180(3)	0.5103(7)	0.065(4)
C(13)	1.1011(9)	0.028(1)	0.5928(2)	0.045(5)
C(14)	1.023(1)	-0.060(1)	0.6072(3)	0.057(5)
C(15)	1.028(1)	-0.200(1)	0.6045(3)	0.069(6)
C(16)	1.112(1)	-0.256(1)	0.5864(3)	0.076(6)
C(17)	1.194(1)	-0.177(1)	0.5725(3)	0.067(5)
C(18)	1.190(1)	-0.032(1)	0.5751(3)	0.062(6)
C(19)	1.2152(9)	0.287(1)	0.5860(2)	0.041(4)
C(20)	1.318(1)	0.254(1)	0.6031(3)	0.061(6)
C(21)	1.418(1)	0.315(2)	0.5956(3)	0.081(6)
C(22)	1.425(1)	0.415(1)	0.5720(3)	0.074(6)
C(23)	1.328(1)	0.450(1)	0.5554(3)	0.066(6)
C(24)	1.2240(9)	0.387(1)	0.5623(3)	0.051(5)
P(2)	0.8438(3)	0.4146(3)	0.67264(7)	0.040(1)
B(31)	1.082(1)	0.136(1)	0.7195(3)	0.038(5)
B(32)	1.014(1)	0.218(2)	0.6863(3)	0.042(6)
B(33)	0.944(1)	0.211(2)	0.7225(3)	0.056(6)
B(34)	1.048(1)	0.235(2)	0.7528(3)	0.052(6)
B(35)	1.185(1)	0.262(1)	0.7354(3)	0.053(6)
B(36)	1.162(1)	0.243(2)	0.6931(3)	0.049(6)
C(37)	0.9540(9)	0.366(1)	0.7017(2)	0.037(4)
C(38)	0.971(1)	0.375(1)	0.7386(2)	0.047(5)
B(39)	1.107(1)	0.409(2)	0.7472(3)	0.057(7)
B(40)	1.185(1)	0.411(2)	0.7099(3)	0.057(6)
B(41)	1.072(1)	0.376(1)	0.6813(3)	0.035(5)

C(42)	0.873(2)	0.431(4)	0.7588(8)	0.063(4)
C(43)	-0.8317(9)	0.601(1)	0.6739(2)	0.038(5)
C(44)	0.908(1)	0.678(1)	0.6912(3)	0.065(5)
C(45)	0.898(1)	0.821(1)	0.6907(3)	0.072(6)
C(46)	0.812(1)	0.884(1)	0.6738(3)	0.066(6)
C(47)	0.738(1)	0.806(1)	0.6571(3)	0.073(6)
C(48)	0.746(1)	0.665(1)	0.6568(3)	0.062(5)
C(49)	0.7027(9)	0.353(1)	0.6822(2)	0.037(4)
C(50)	0.636(1)	0.418(1)	0.7046(3)	0.059(5)
C(51)	0.529(1)	0.363(1)	0.7120(3)	0.069(6)
C(52)	0.489(1)	0.244(1)	0.6973(3)	0.065(6)
C(53)	0.555(1)	0.179(1)	0.6746(3)	0.060(5)
C(54)	0.6597(9)	0.236(1)	0.6676(3)	0.049(5)
O(55)	1.426(1)	0.873(1)	0.6467(3)	0.193(6)
C(56)	1.354(1)	0.797(2)	0.6531(4)	0.132(6)
C(57)	1.248(1)	0.823(2)	0.6692(4)	0.119(6)
C(58)	1.391(1)	0.647(2)	0.6425(3)	0.111(6)
O(59)	0.602(2)	-0.178(2)	0.5638(4)	0.340(8)
C(60)	0.548(2)	-0.173(3)	0.5371(4)	0.340(8)
C(61)	0.613(3)	-0.178(5)	0.5064(4)	0.340(8)
C(62)	0.420(2)	-0.160(5)	0.5360(7)	0.340(8)

[a] $U_{eq} = 1/3\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* a_i \cdot a_j$

Tabla 31. *Distancias de enlace (Å) para* $[Ru(7\text{-}P(C_6H_5)_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{10})_2]\cdot 2(CH_3)_2CO$.

Ru-P(1)	2.373(3)	Ru-P(2)	2.358(3)
Ru-B(2)	2.34(1)	Ru-B(11)	2.39(1)
Ru-B(32)	2.38(1)	Ru-B(41)	2.38(1)
Ru-H(2)	1.88	Ru-H(11)	1.95
Ru-H(32)	1.94	Ru-H(41)	1.93
P(1)-C(7)	1.82(1)	P(1)-C(13)	1.79(1)
P(1)-C(19)	1.80(1)	P(2)-C(37)	1.80(1)
P(2)-C(43)	1.82(1)	P(2)-C(49)	1.81(1)
B(3)-C(7)	1.74(2)	B(3)-C(8)	1.74(2)
C(7)-C(8)	1.56(1)	C(7)-B(11)	1.62(2)
C(8)-B(9)	1.64(2)	C(8)-C(12)	1.53(3)
B(9)-B(10)	1.81(2)	B(10)-B(11)	1.76(2)
B(33)-C(37)	1.75(2)	B(33)-C(38)	1.76(2)
C(37)-C(38)	1.55(1)	C(37)-B(41)	1.64(2)
C(38)-B(39)	1.65(2)	C(38)-C(42)	1.53(3)
B(39)-B(40)	1.82(2)	B(40)-B(41)	1.79(2)

Tabla 32. *Ángulos de enlace (°) para* $[Ru\{7\text{-}P(C_6H_5)_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{10})\}_2]\cdot 2(CH_3)_2CO$.

P(1)-Ru-P(2)	177.6(1)	H(2)-Ru-H(41)	172
H(11)-Ru-H(32)	173	Ru-P(1)-C(7)	83.8(4)
Ru-P(1)-C(13)	122.0(4)	Ru-P(1)-C(19)	121.0(4)
C(7)-P(1)-C(13)	111.7(5)	C(7)-P(1)-C(19)	108.4(5)
C(13)-P(1)-C(19)	106.7(5)	Ru-P(2)-C(37)	84.9(4)
Ru-P(2)-C(43)	120.5(4)	Ru-P(2)-C(49)	123.3(4)
C(37)-P(2)-C(43)	107.3(5)	C(37)-P(2)-C(49)	113.6(5)
C(43)-P(2)-C(49)	104.8(5)	C(7)-B(3)-C(8)	53.3(6)
P(1)-C(7)-B(2)	103.0(7)	P(1)-C(7)-B(3)	115.6(8)
P(1)-C(7)-C(8)	135.4(8)	P(1)-C(7)-B(11)	106.1(7)
C(8)-C(7)-B(11)	115.1(9)	C(7)-C(8)-B(9)	108.0(9)
C(7)-C(8)-C(12)	119(1)	B(9)-C(8)-C(12)	121(1)
C(8)-B(9)-B(10)	108.4(9)	B(9)-B(10)-B(11)	102(1)
C(7)-B(11)-B(10)	106.5(9)	C(37)-B(33)-C(38)	52.2(7)
P(2)-C(37)-B(32)	105.2(7)	P(2)-C(37)-B(33)	120.3(7)
P(2)-C(37)-C(38)	135.9(8)	P(2)-C(37)-B(41)	103.1(7)
C(38)-C(37)-B(41)	115.3(9)	C(37)-C(38)-B(39)	108.6(9)
C(37)-C(38)-C(42)	119(1)	B(39)-C(38)-C(42)	122(1)
C(38)-B(39)-B(40)	108.9(9)		
B(39)-B(40)-B(41)	100.6(9)		
C(37)-B(41)-B(40)	106.3(9)		

4.9. Estructura cristalina de cis-[Ru(nMePPh)$_2$].

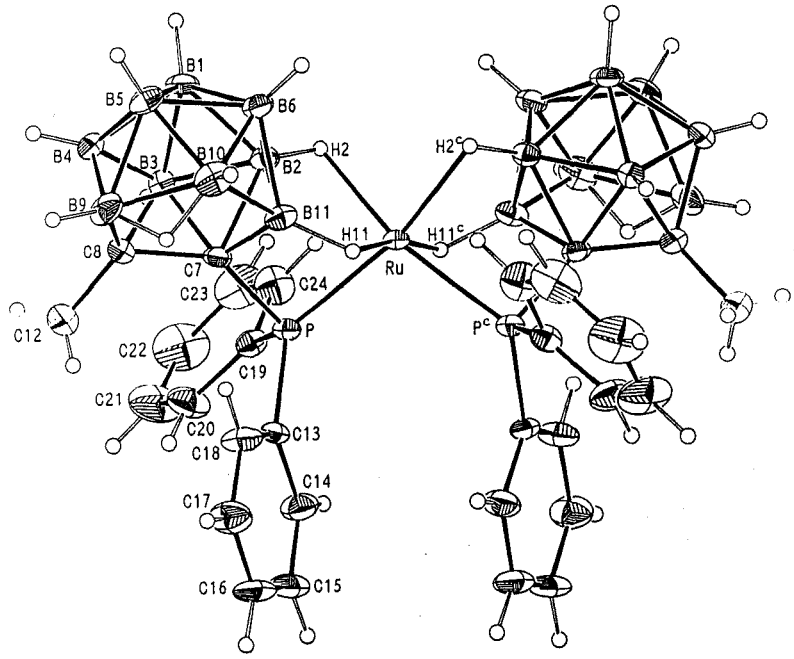


Tabla 33. *Datos cristalográficos para [Ru(7-P(C$_6$H$_5$)$_2$-8-CH$_3$-7,8-C$_2$B$_9$H$_{10}$)$_2$]·1.486CHCl$_3$*

Fórmula química:	$C_{30}H_{46}B_{18}P_2Ru \cdot 1.486CHCl_3$
peso molecular	941.4
a =	20.674 (3) Å
b =	11.539 (2) Å
c =	20.976 (3) Å
β =	110.92 (1)°
V =	4674 (2) Å^3
Z =	4
grupo espacial:	monoclínico, C2/c
T =	23 °C
λ =	0.71069 Å
ρ =	1.338 g cm^{-3}
μ =	6.8 cm^{-1}
transm coeff =	0.91 - 1.000
$R(F_o)$	0.066
$R_w(F_o)$ =	0.068

Tabla 34. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para* $[Ru(7\text{-}P(C_6H_5)_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{10})_2]\cdot 1.486CHCl_3$.

	x/a	y/b	z/c	U_{eq}[a]
Ru	1/2	0.83192(7)	1/4	0.0258(3)
P	0.5072(1)	0.7112(2)	0.3394(1)	0.0298(7)
B(1)	0.5756(5)	1.0473(7)	0.4201(5)	0.042(4)
B(2)	0.5399(4)	0.9449(7)	0.3550(4)	0.032(3)
B(3)	0.5397(4)	0.9152(7)	0.4372(4)	0.034(3)
B(4)	0.6185(5)	0.9670(8)	0.4936(5)	0.041(4)
B(5)	0.6686(5)	1.0260(8)	0.4488(5)	0.045(4)
B(6)	0.6162(5)	1.0166(7)	0.3597(5)	0.037(4)
C(7)	0.5693(3)	0.8126(6)	0.3933(3)	0.031(3)
C(8)	0.6099(4)	0.8237(6)	0.4704(3)	0.039(3)
B(9)	0.6862(5)	0.8813(8)	0.4817(5)	0.047(4)
B(10)	0.6882(5)	0.9192(9)	0.3954(5)	0.049(4)
B(11)	0.6043(4)	0.8653(7)	0.3427(5)	0.036(4)
C(12)	0.6026(5)	0.7304(8)	0.5180(4)	0.066(4)
C(13)	0.5495(4)	0.5707(6)	0.3498(4)	0.035(3)
C(14)	0.5110(4)	0.4700(7)	0.3307(4)	0.053(4)
C(15)	0.5445(5)	0.3634(7)	0.3395(5)	0.065(4)
C(16)	0.6148(5)	0.3572(6)	0.3676(5)	0.067(5)
C(17)	0.6536(4)	0.4572(7)	0.3858(5)	0.062(4)
C(18)	0.6207(4)	0.5630(6)	0.3766(5)	0.052(4)
C(19)	0.4348(4)	0.6941(6)	0.3675(4)	0.039(3)
C(20)	0.4358(5)	0.6135(8)	0.4183(5)	0.064(4)
C(21)	0.3847(6)	0.6127(9)	0.4447(6)	0.095(7)
C(22)	0.3324(6)	0.690(1)	0.4240(6)	0.097(6)
C(23)	0.3304(5)	0.7713(9)	0.3766(6)	0.077(5)
C(24)	0.3820(4)	0.7723(8)	0.3481(5)	0.060(4)
Cl(1)[b]	0.6874(3)	0.6691(5)	0.7171(3)	0.153(3)
Cl(2)[b]	0.6125(3)	0.8793(5)	0.6808(2)	0.144(3)
Cl(3)[b]	0.7553(3)	0.8674(6)	0.7012(3)	0.172(4)
C(25)[b]	0.6931(8)	0.827(2)	0.7287(7)	0.118(9)

[a] $U_{eq} = 1/3\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* a_i \cdot a_j$

[b] Site occupation parameter 0.743(4)

Tabla 35. *Distancias de enlace (Å) para [Ru(7-P(C_6H_5)$_2$-8-CH_3-7,8-$C_2B_9H_{10}$)$_2$]·1.486$CHCl_3$.*

Ru-P	2.298(2)	Ru-B(2)	2.436(8)
Ru-B(11)	2.363(8)	Ru-H(2)	2.01(7)
Ru-H(11)	1.69(4)	P-C(7)	1.806(6)
P-C(13)	1.818(7)	P-C(19)	1.805(9)
B(2)-H(2)	1.23(6)	B(3)-C(7)	1.74(1)
B(3)-C(8)	1.73(1)	C(7)-C(8)	1.538(9)
C(7)-B(11)	1.60(1)	C(8)-B(9)	1.65(1)
C(8)-C(12)	1.51(1)	B(9)-B(10)	1.88(2)
B(10)-B(11)	1.80(1)	B(11)-H(11)	1.27(4)

Tabla 36. *Ángulos de enlace (°) para [Ru(7-P(C_6H_5)$_2$-8-CH_3-7,8-$C_2B_9H_{10}$)$_2$]·1.486$CHCl_3$*

P-Ru-H(2)	84(2)
P-Ru-H(11)	81(2)
P-Ru-P[c]	105.33(8)
P-Ru-H(2)[c]	165(2)
P-Ru-H(11)[c]	92(2)
H(2)-Ru-H(11)	102(2)
H(2)-Ru-H(2)[c]	89(3)
H(2)-Ru-H(11)[c]	87(2)
H(11)-Ru-H(11)[c]	169(2)
Ru-P-C(7)	86.7(2)
Ru-P-C(13)	121.8(3)
Ru-P-C(19)	120.9(2)
C(7)-P-C(13)	107.4(3)
C(7)-P-C(19)	110.7(4)
C(13)-P-C(19)	106.5(4)
C(7)-B(3)-C(8)	52.6(4)
P-C(7)-B(2)	103.1(4)
P-C(7)-B(3)	117.8(5)
P-C(7)-C(8)	135.4(6)
P-C(7)-B(11)	102.6(5)
C(8)-C(7)-B(11)	117.3(6)
C(7)-C(8)-B(9)	108.7(7)
C(7)-C(8)-C(12)	119.3(6)
B(9)-C(8)-C(12)	120.6(6)
C(8)-B(9)-B(10)	107.7(6)
B(9)-B(10)-B(11)	99.4(7)
C(7)-B(11)-B(10	106.7(6)

[c]Symmetry code 1-x, y, 1/2-z

4.10. Estructura cristalina para [RuCl(nMePPh)(PPh_3)$_2$].

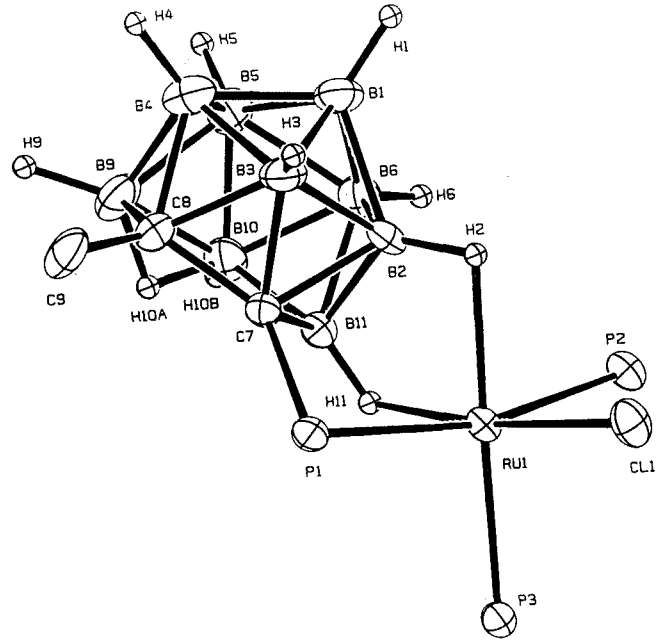


Tabla 37. *Datos cristalográficos para [RuCl(7-PPh_2-8-Me-7,8-$C_2B_9H_{10}$)(PPh_3)$_2$].*

Fórmula química:	$C_{51}H_{53}B_9ClP_3Ru$
peso molecular	992.71
a =	10.626(2) Å
b =	19.270(3) Å
c =	24.105(2) Å
α =	
β =	97.74(1)°
γ =	
V =	4891(1) Å^3
Z =	4
grupo espacial:	monoclínico
	$P2_1/n$ (No. 14)
T =	23 °C
λ =	0.71069Å
ρ =	1.348 g cm^{-3}
μ =	5.00 cm^{-1}
transm coeff =	0.91 - 1.00
$R(F_o)$ =	0.041
$R_w(F_o)$ =	0.056

Tabla 38. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para* $[RuCl(7\text{-}PPh_2\text{-}8\text{-}Me\text{-}7,8\text{-}C_2B_9H_{10})(PPh_3)_2]$.

átomo	x	y	z	B_{eq}
Ru(1)	0.94689(4)	0.21524(3)	0.68816(2)	2.15(2)
Cl(1)	0.7438(1)	0.1877(1)	0.71673(7)	3.47(7)
P(1)	0.8780(1)	0.25476(9)	0.59160(7)	2.31(7)
P(2)	1.0404(1)	0.2067(1)	0.78401(7)	2.65(7)
P(3)	0.9852(2)	0.10217(9)	0.66411(7)	2.42(7)
C(7)	0.9693(6)	0.3321(3)	0.6131(2)	2.5(3)
C(8)	0.9911(6)	0.4014(3)	0.5822(3)	3.3(3)
C(9)	0.9234(8)	0.4139(4)	0.5236(3)	4.7(4)
C(11)	0.9476(6)	0.2268(3)	0.5297(2)	2.5(3)
C(12)	1.0652(6)	0.2519(4)	0.5194(3)	3.4(3)
C(13)	1.1196(7)	0.2287(4)	0.4733(3)	4.2(4)
C(14)	1.0581(8)	0.1819(4)	0.4371(3)	4.4(4)
C(15)	0.9409(7)	0.1561(4)	0.4463(3)	3.9(3)
C(16)	0.8868(6)	0.1788(3)	0.4922(3)	3.2(3)
C(21)	0.7148(6)	0.2776(3)	0.5640(3)	2.7(3)
C(22)	0.6746(6)	0.2919(4)	0.5077(3)	4.3(4)
C(23)	0.5520(8)	0.3130(5)	0.4898(3)	6.6(5)
C(24)	0.4693(8)	0.3224(5)	0.5279(4)	6.8(5)
C(25)	0.5067(8)	0.3087(5)	0.5820(4)	6.7(5)
C(26)	0.6289(6)	0.2864(4)	0.6016(3)	4.4(3)
C(31)	1.2147(6)	0.1988(3)	0.8002(3)	2.9(3)
C(32)	1.2932(6)	0.2136(4)	0.7596(3)	3.7(3)
C(33)	1.4240(6)	0.2099(4)	0.7722(3)	4.4(4)
C(34)	1.4792(7)	0.1900(4)	0.8248(4)	5.0(4)
C(35)	1.4033(7)	0.1757(4)	0.8650(3)	5.0(4)
C(36)	1.2735(7)	0.1796(4)	0.8533(3)	3.9(3)
C(41)	1.0063(6)	0.2842(4)	0.8247(2)	3.1(3)
C(42)	0.8849(7)	0.3109(4)	0.8198(3)	3.9(3)
C(43)	0.8579(8)	0.3684(5)	0.8505(3)	5.0(4)
C(44)	0.954(1)	0.4009(5)	0.8854(4)	6.9(5)
C(45)	1.0753(9)	0.3759(5)	0.8889(4)	6.6(5)
C(46)	1.1032(7)	0.3174(4)	0.8599(3)	4.7(4)
C(51)	0.9864(6)	0.1362(4)	0.8280(3)	3.3(3)
C(52)	0.8739(6)	0.1430(4)	0.8515(3)	3.9(3)
C(53)	0.8346(8)	0.0901(5)	0.8847(3)	5.4(4)
C(54)	0.909(1)	0.0326(5)	0.8966(4)	6.0(5)
C(55)	1.0178(8)	0.0248(4)	0.8731(4)	5.3(4)
C(56)	1.0568(7)	0.0761(4)	0.8390(3)	4.1(4)
C(61)	0.9609(6)	0.0246(3)	0.7065(3)	3.1(3)
C(62)	1.0329(7)	-0.0359(4)	0.7010(3)	4.3(4)
C(63)	1.0046(9)	-0.0968(4)	0.7272(4)	5.6(4)
C(64)	0.905(1)	-0.0994(5)	0.7578(4)	6.0(5)
C(65)	0.8328(8)	-0.0411(5)	0.7623(3)	5.4(4)
C(66)	0.8594(7)	0.0210(4)	0.7366(3)	3.9(3)
C(71)	1.1494(6)	0.0935(3)	0.6498(3)	2.6(3)

C(72)	1.2442(7)	0.0722(4)	0.6913(3)	3.9(3)
C(73)	1.3712(7)	0.0751(4)	0.6836(3)	5.1(4)
C(74)	1.4035(7)	0.1010(5)	0.6342(4)	5.4(4)
C(75)	1.3107(7)	0.1227(4)	0.5930(3)	4.6(4)
C(76)	1.1840(6)	0.1187(3)	0.6000(3)	3.4(3)
C(81)	0.8806(6)	0.0720(3)	0.6018(2)	2.5(3)
C(82)	0.7551(6)	0.0941(3)	0.5924(3)	2.9(3)
C(83)	0.6714(6)	0.0671(4)	0.5489(3)	3.6(3)
C(84)	0.7105(7)	0.0172(4)	0.5145(3)	3.6(3)
C(85)	0.8335(8)	-0.0063(4)	0.5237(3)	4.0(4)
C(86)	0.9184(7)	0.0206(3)	0.5670(3)	3.5(3)
B(1)	0.9990(9)	0.4312(4)	0.6950(4)	3.9(4)
B(2)	0.9626(7)	0.3431(4)	0.6838(3)	2.9(3)
B(3)	0.8945(8)	0.4055(4)	0.6342(3)	3.4(4)
B(4)	1.013(1)	0.4675(5)	0.6296(4)	4.5(4)
B(5)	1.1532(9)	0.4436(5)	0.6729(4)	4.4(4)
B(6)	1.1175(8)	0.3670(4)	0.7097(3)	3.3(4)
B(9)	1.1400(9)	0.4253(5)	0.6006(4)	4.1(4)
B(10)	1.2132(8)	0.3608(5)	0.6543(4)	3.7(4)
B(11)	1.0847(7)	0.3033(4)	0.6574(3)	2.7(3)
H(1)	0.965(6)	0.461(3)	0.723(3)	4.7
H(2)	0.889(5)	0.311(3)	0.704(2)	3.4
H(3)	0.789(6)	0.417(3)	0.617(2)	4.4
H(4)	0.987(6)	0.519(4)	0.610(3)	5.5
H(5)	1.218(6)	0.479(4)	0.686(3)	5.3
H(6)	1.165(6)	0.356(3)	0.746(3)	3.9
H(9)	1.196(6)	0.459(3)	0.566(3)	5.1
H(10A)	1.176(6)	0.373(4)	0.599(3)	5.1
H(10B)	1.304(6)	0.354(3)	0.662(3)	4.4
H(11)	1.081(5)	0.255(3)	0.665(2)	2.6

[a] $B_{eq} = 4/3\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j$

Tabla 39. *Distancias (Å) y ángulos de enlace (°) para [RuCl(7-PPh$_2$-8-Me-7,8-C$_2$B$_9$H$_{10}$)(PPh$_3$)$_2$].*

Ru(1) - Cl(1)	2.411(2)	Ru(1) - P(1)	2.465(2)
Ru(1) - P(2)	2.395(2)	Ru(1) - P(3)	2.305(2)
Ru(1) - B(2)	2.473(8)	Ru(1) - B(11)	2.422(8)
Ru(1) - H(2)	2.00(6)	Ru(1) - H(11)	1.78(5)
P(1) - C(7)	1.815(6)	P(1) - C(11)	1.834(6)
P(1) - C(21)	1.826(6)	P(2) - C(31)	1.847(6)
P(2) - C(41)	1.850(7)	P(2) - C(51)	1.861(7)
P(3) - C(61)	1.848(7)	P(3) - C(71)	1.831(6)
P(3) - C(81)	1.838(6)	C(7) - C(8)	1.561(8)
C(7) - B(2)	1.730(9)	C(7) - B(11)	1.613(9)
C(8) - B(9)	1.65(1)	B(9) - B(10)	1.89(1)
B(10) - B(11)	1.77(1)		

Cl(1) - Ru(1) - P(1)	100.05(6)	P(1)-C(7)-B(11)	103.6(4)
Cl(1) - Ru(1) - P(2)	88.88(6)	C(8)-C(7)-B(2)	113.2(5)
Cl(1) - Ru(1) - P(3)	93.37(6)	C(8)-C(7)-B(11)	117.5(5)
Cl(1) - Ru(1) - H(2)	80(2)		
Cl(1) - Ru(1) - H(11)	167(2)		
P(1) - Ru(1) - P(2)	164.63(6)		
P(1) - Ru(1) - P(3)	95.43(6)		
P(1) - Ru(1) - H(2)	81(2)		
P(1) - Ru(1) - H(11)	73(2)		
P(2) - Ru(1) - P(3)	96.52(6)		
P(2) - Ru(1) - H(2)	89(2)		
P(2) - Ru(1) - H(11)	95(2)		
P(3) - Ru(1) - H(2)	172(2)		
P(3) - Ru(1) - H(11)	99(2)		
H(2) - Ru(1) - H(11)	87(2)		
Ru(1) - P(1) - C(7)	84.6(2)		
Ru(1) - P(1) - C(11)	125.2(2)		
Ru(1) - P(1) - C(21)	124.4(2)		
P(1) - C(7) - C(8)	132.4(4)		
P(1) - C(7) - B(2)	106.9(4)		

4.11. Estructura cristalina para [RuCl(nMePPh)(EtOH)(PPh_3)].

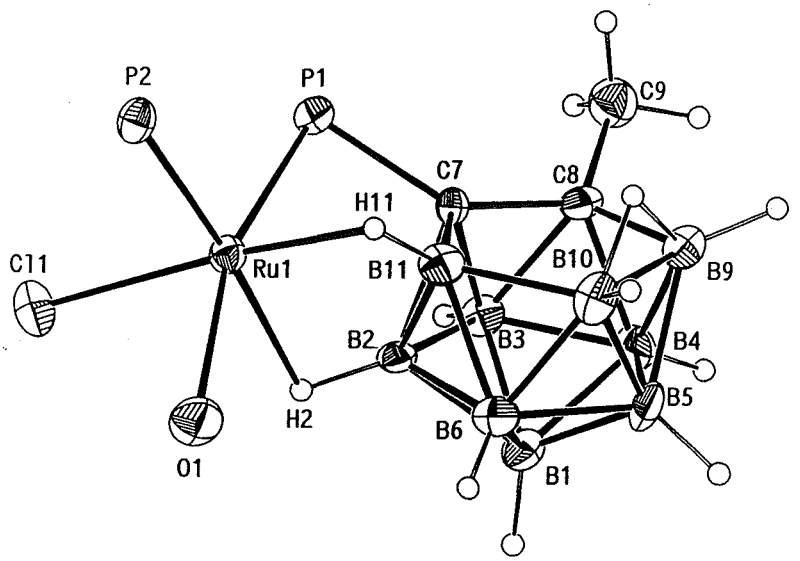


Tabla 40. *Datos cristalográficos para [RuCl(nMePPh)(EtOH)(PPh_3)]·0.64$(Me)_2CO$.*

Fórmula química:	$C_{35}H_{44}B_9OClP_2Ru{\cdot}0.64(Me)_2CO$
peso molecular	813.66
a =	16.878 (4) Å
b =	19.377 (5) Å
c =	13.811 (3) Å
α =	103.15 (2)°
β =	97.14 (2)°
γ =	79.31 (2)°
V =	4306 (4) $Å^3$
Z =	4
grupo espacial:	triclínico
	$P\bar{1}$ (No. 2)
T =	23 °C
λ =	0.71069 Å
ρ =	1.255 g cm^{-3}
μ =	5.2 cm^{-1}
transm coeff =	0.936 - 1.000
$R(F_o)$ =	0.071
$R_w(F_o)$ =	0.077

Table 41. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para [RuCl(nMePPh)(EtOH)(PPh_3)]·0.64(Me_2CO) (2).*

Molécula I

	x/a	y/b	z/c	U_{eq}[a], Å^2
Ru(1)	0.07497(5)	0.27063(5)	0.53138(7)	0.0300(3)
Cl(1)	0.1954(2)	0.2072(2)	0.4537(2)	0.050(1)
P(1)	0.0454(2)	0.1945(1)	0.6201(2)	0.030(1)
P(2)	-0.0071(2)	0.2399(2)	0.3908(2)	0.034(1)
O(1)	0.1032(5)	0.3671(4)	0.4894(6)	0.056(4)
C(1A)[b]	0.051(2)	0.433(2)	0.480(2)	0.081(9)
C(1B)[b]	0.181(1)	0.387(2)	0.485(5)	0.28(3)
C(2A)[b]	0.117(3)	0.486(2)	0.479(3)	0.15(2)
C(2B)[b]	0.267(1)	0.352(2)	0.524(3)	0.20(2)
C(7)	0.0381(6)	0.2692(5)	0.7262(7)	0.029(4)
C(8)	0.0222(6)	0.2821(5)	0.8368(8)	0.034(4)
C(9)	0.010(1)	0.2190(9)	0.880(1)	0.049(3)
C(31)	0.1146(6)	0.1183(4)	0.6545(5)	0.048(1)
C(32)	0.0877(3)	0.0745(6)	0.7066(5)	0.048(1)
C(33)	0.1427(6)	0.0215(4)	0.7438(5)	0.048(1)
C(34)	0.2246(5)	0.0125(4)	0.7290(5)	0.048(1)
C(35)	0.2515(3)	0.0564(6)	0.6770(5)	0.048(1)
C(36)	0.1964(7)	0.1093(4)	0.6397(5)	0.048(1)
C(37)	-0.0521(6)	0.165(1)	0.5989(7)	0.048(1)
C(38)	-0.119(1)	0.2087(4)	0.6417(5)	0.048(1)
C(39)	-0.1947(7)	0.1860(7)	0.6231(7)	0.048(1)
C(40)	-0.2027(6)	0.1193(9)	0.5619(7)	0.048(1)
C(41)	-0.135(1)	0.0751(3)	0.5191(5)	0.048(1)
C(42)	-0.0601(7)	0.0978(8)	0.5376(7)	0.048(1)
C(43)	-0.1160(3)	0.254(1)	0.4072(9)	0.054(1)
C(44)	-0.152(1)	0.321(1)	0.4599(6)	0.054(1)
B(1)	0.1271(8)	0.3737(7)	0.828(1)	0.040(6)
B(2)	0.1083(8)	0.3194(7)	0.7074(9)	0.033(5)
B(3)	0.1210(8)	0.2805(7)	0.8143(9)	0.033(5)
B(4)	0.0736(8)	0.3454(8)	0.9069(9)	0.041(6)
B(5)	0.0320(9)	0.4237(7)	0.860(1)	0.044(6)
B(6)	0.0568(8)	0.4070(7)	0.736(1)	0.045(6)
B(9)	-0.0326(8)	0.3618(7)	0.869(1)	0.040(5)
B(10)	-0.0436(9)	0.4067(7)	0.759(1)	0.046(6)
B(11)	0.0092(7)	0.3361(7)	0.671(1)	0.037(5)
C(45)	-0.235(1)	0.3347(4)	0.4690(6)	0.054(1)
C(46)	-0.2823(3)	0.282(1)	0.4254(8)	0.054(1)
C(47)	-0.247(1)	0.2157(8)	0.3727(6)	0.054(1)
C(48)	-0.164(1)	0.2017(6)	0.3635(7)	0.054(1)
C(49)	0.0155(5)	0.1505(3)	0.3124(5)	0.046(1)
C(50)	-0.0168(4)	0.1382(4)	0.2132(6)	0.046(1)
C(51)	0.0017(4)	0.0707(4)	0.1513(4)	0.046(1)
C(52)	0.0525(5)	0.0154(3)	0.1886(5)	0.046(1)
C(53)	0.0847(4)	0.0277(4)	0.2879(5)	0.046(1)

C(54)	0.0663(5)	0.0953(4)	0.3497(4)	0.046(1)
C(55)	-0.0034(7)	0.2945(4)	0.3004(6)	0.057(1)
C(56)	-0.0697(4)	0.3408(6)	0.2678(5)	0.057(1)
C(57)	-0.0603(5)	0.3828(4)	0.2016(5)	0.057(1)
C(58)	0.0154(6)	0.3786(4)	0.1681(5)	0.057(1)
C(59)	0.0817(4)	0.3324(5)	0.2007(5)	0.057(1)
C(60)	0.0724(5)	0.2904(4)	0.2669(5)	0.057(1)

Molécula II

	x/a	y/b	z/c	U_{eq}*, Å^2
Ru(2)	0.53244(5)	0.23543(5)	0.10241(7)	0.0323(4)
Cl(2)	0.5044(2)	0.3039(2)	0.2660(2)	0.053(1)
P(3)	0.5936(2)	0.3068(1)	0.0353(2)	0.031(1)
P(4)	0.4041(2)	0.2672(2)	0.0379(2)	0.036(1)
O(2)	0.5082(5)	0.1479(4)	0.1647(6)	0.058(4)
C(3)	0.486(1)	0.084(1)	0.119(1)	0.118(6)
C(4)	0.518(2)	0.024(1)	0.178(2)	0.165(8)
C(27)	0.6720(6)	0.2298(5)	0.0021(7)	0.027(4)
C(28)	0.7505(6)	0.2152(6)	-0.0504(8)	0.037(5)
C(29)	0.779(1)	0.2738(8)	-0.084(1)	0.047(3)
C(61)	0.6409(4)	0.3820(4)	0.1073(5)	0.048(1)
C(62)	0.6733(5)	0.4260(4)	0.0609(4)	0.048(1)
C(63)	0.7166(4)	0.4781(4)	0.1180(5)	0.048(1)
C(64)	0.7275(4)	0.4863(3)	0.2215(5)	0.048(1)
C(65)	0.6950(4)	0.4424(4)	0.2680(4)	0.048(1)
C(66)	0.6517(4)	0.3902(4)	0.2109(5)	0.048(1)
C(67)	0.5543(5)	0.3349(4)	-0.0808(5)	0.049(1)
C(68)	0.5722(4)	0.2892(3)	-0.1719(6)	0.049(1)
C(69)	0.5442(4)	0.3114(3)	-0.2610(4)	0.049(1)
C(70)	0.4982(4)	0.3793(4)	-0.2591(4)	0.049(1)
C(71)	0.4802(4)	0.4250(3)	-0.1681(6)	0.049(1)
C(72)	0.5083(5)	0.4028(4)	-0.0789(4)	0.049(1)
C(73)	0.3913(5)	0.2502(5)	-0.0992(4)	0.055(1)
C(74)	0.4196(4)	0.1819(4)	-0.1535(6)	0.055(1)
C(75)	0.4079(5)	0.1671(3)	-0.2575(6)	0.055(1)
C(76)	0.3679(5)	0.2205(4)	-0.3071(4)	0.055(1)
C(77)	0.3395(4)	0.2888(4)	-0.2527(6)	0.055(1)
C(78)	0.3512(5)	0.3036(3)	-0.1488(6)	0.055(1)
C(79)	0.352(2)	0.3592(7)	0.0789(9)	0.047(1)
C(80)	0.268(2)	0.373(1)	0.0628(5)	0.047(1)
C(81)	0.2259(3)	0.442(2)	0.0958(9)	0.047(1)
C(82)	0.268(2)	0.4970(6)	0.1449(8)	0.047(1)
C(83)	0.352(2)	0.483(1)	0.1611(6)	0.047(1)
C(84)	0.3942(3)	0.414(2)	0.128(1)	0.047(1)
C(85)	0.3335(4)	0.2150(4)	0.0687(6)	0.058(2)
C(86)	0.3250(5)	0.2225(4)	0.1699(6)	0.058(2)
C(87)	0.2738(5)	0.1840(4)	0.2000(4)	0.058(2)
C(88)	0.2311(4)	0.1380(4)	0.1288(6)	0.058(2)
C(89)	0.2395(5)	0.1305(4)	0.0275(5)	0.058(2)
C(90)	0.2907(5)	0.1690(4)	-0.0025(5)	0.058(2)

B(21)	0.7740(8)	0.1295(7)	0.088(1)	0.042(6)
B(22)	-0.6786(8)	0.1833(7)	0.0965(9)	0.033(5)
B(23)	0.7619(7)	0.2198(7)	0.076(1)	0.034(5)
B(24)	0.8185(7)	0.1518(7)	-0.003(1)	0.037(5)
B(25)	0.7717(8)	0.0747(7)	-0.036(1)	0.048(6)
B(26)	0.6834(8)	0.0945(7)	0.033(1)	0.040(6)
B(29)	0.7592(8)	0.1345(8)	-0.120(1)	0.047(6)
B(30)	0.6719(8)	0.0914(7)	-0.098(1)	0.045(6)
B(31)	0.6218(7)	0.1648(6)	-0.016(1)	0.032(5)

[a] $U_{eq} = 1/3\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* a_i \cdot a_j$
[b] Site occupation parameter 0.50
[c] Site occupation parameter 0.28

Tabla 42. *Distancias (Å) y ángulos de enlace (°) para [RuCl(nMePPh)(EtOH)(PPh_3)]·0.64(Me_2CO).*

Molécula I

Ru(1)-Cl(1)	2.410(3)	Ru(1)-P(1)	2.276(4)
Ru(1)-P(2)	2.270(3)	Ru(1)-O(1)	2.224(9)
Ru(1)-B(2)	2.44(1)	Ru(1)-B(11)	2.34(1)
Ru(1)-H(2)	2.06	Ru(1)-H(11)	1.83
P(1)-C(7)	1.808(9)	P(1)-C(31)	1.820(9)
P(1)-C(37)	1.81(1)	P(2)-C(43)	1.842(7)
P(2)-C(49)	1.824(6)	P(2)-C(55)	1.82(1)
C(7)-C(8)	1.54(1)	C(7)-B(11)	1.62(2)
C(8)-C(9)	1.53(2)	C(8)-B(9)	1.64(2)
B(9)-B(10)	1.89(2)	B(10)-B(11)	1.79(2)
Cl(1)-Ru(1)-P(1)	104.3(1)	Cl(1)-Ru(1)-P(2)	93.1(1)
Cl(1)-Ru(1)-H(11)	174	P(1)-Ru(1)-P(2)	98.6(1)
P(1)-Ru(1)-O(1)	162.8(2)	P(2)-Ru(1)-H(2)	175
H(2)-Ru(1)-H(11)	92	Ru(1)-P(1)-C(7)	87.5(4)
Ru(1)-P(1)-C(31)	125.7(4)	Ru(1)-P(1)-C(37)	120.9(5)
P(1)-C(7)-C(8)	137.1(8)	P(1)-C(7)-B(2)	103.2(6)
P(1)-C(7)-B(3	120.2(6)	P(1)-C(7)-B(11)	101.0(7)
C(8)-C(7)-B(11)	117.1(8)	C(7)-C(8)-B(9)	109.0(9)
C(8)-B(9)-B(10)	107.2(9)	B(9)-B(10)-B(11)	100.1(9)
C(7)-B(11)-B(10)	106(1)		

Molécula II

Ru(2)-Cl(2)	2.400(3)	Ru(2)-P(3)	2.277(4)
Ru(2)-P(4)	2.267(3)	Ru(2)-O(2)	2.189(9)
Ru(2)-B(22)	2.49(1)	Ru(2)-B(31)	2.38(1)
Ru(2)-H(22)	2.11	Ru(2)-H(31)	1.85
P(3)-C(27)	1.814(9)	P(3)-C(61)	1.824(7)
P(3)-C(67)	1.819(8)	P(4)-C(73)	1.838(6)
P(4)-C(79)	1.83(2)	P(4)-C(85)	1.84(1)
C(27)-C(28)	1.54(2)	C(27)-B(31)	1.60(2)
C(28)-C(29)	1.49(2)	C(28)-B(29)	1.63(2)
B(29)-B(30)	1.91(2)	B(30)-B(31)	1.75(2)
Cl(2)-Ru(2)-P(3)	104.7(1)	Cl(2)-Ru(2)-P(4)	92.6(1)
Cl(2)-Ru(2)-H(31)	175	P(3)-Ru(2)-P(4)	98.1(1)
P(3)-Ru(2)-O(2)	163.5(2)	P(4)-Ru(2)-H(22)	177
H(22)-Ru(2)-H(31)	91	Ru(2)-P(3)-C(27)	87.6(4)
Ru(2)-P(3)-C(61)	124.6(3)	Ru(2)-P(3)-C(67)	122.7(3)
P(3)-C(27)-C(28)	135.6(8)	P(3)-C(27)-B(22)	104.4(7)
P(3)-C(27)-B(23)	120.8(6)	P(3)-C(27)-B(31)	101.4(6)
C(28)-C(27)-B(31)	116.6(8)	C(27)-C(28)-B(29)	108.6(9)
C(28)-B(29)-B(30)	107.5(9)	B(29)-B(30)-B(31)	98.6(9)
C(27)-B(31)-B(30)	108.5(9)		

4.12. Estructura cristalina para [PdCl{n(PPh$_2$)MePPh}(PPh$_3$)].

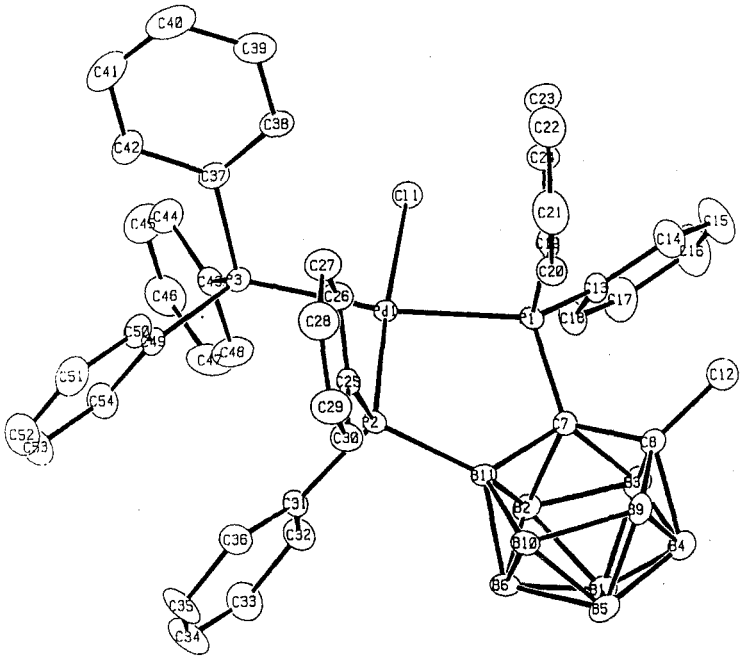


Tabla 43. *Datos cristalográficos para [PdCl{7-PPh$_2$-8-Me-11-PPh$_2$-7,8-C$_2$B$_9$H$_{10}$}(PPh$_3$)].*

Fórmula química	$[C_{45}H_{47}B_9ClP_3Pd]\cdot C_7H_8$
peso molecular	1012.01
a =	19.007 (6) Å
b =	10.863 (5) Å
c =	25.454 (7) Å
β =	96.15 (2)°
V =	5225 (3) Å^3
Z	4
grupo espacial	$P2_1/n$ (No. 14)
T =	-80 °C
λ =	0.71069 Å
ρ =	1.286 g cm^{-3}
μ =	5.3 cm^{-1}
coef. transm.	0.885 - 1.000
$R(F_o)$ =	0.070
$R_w(F_o)$ =	0.068

Table 44. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para [PdCl{n(PPh$_2$)MePPh}(PPh$_3$)].*

	x/a	y/b	z/c	U
Pd	0.49327(2)	0.35401(4)	0.72975(2)	* 0.0230(1)
Cl	0.42167(8)	0.5311(1)	0.72294(6)	* 0.0370(5)
P(1)	0.47400(8)	0.3357(1)	0.81781(6)	* 0.0258(5)
P(2)	0.55912(8)	0.1796(1)	0.74238(6)	* 0.0244(5)
P(3)	0.49175(8)	0.3737(2)	0.63791(6)	* 0.0288(5)
B(1)	0.6759(4)	0.2344(9)	0.9070(3)	* 0.046(3)
B(2)	0.6277(4)	0.2885(8)	0.8479(3)	* 0.035(2)
B(3)	0.5930(4)	0.3062(8)	0.9095(3)	* 0.043(3)
B(4)	0.6159(4)	0.1751(8)	0.9471(3)	* 0.045(3)
B(5)	0.6629(4)	0.0713(8)	0.9111(3)	* 0.045(3)
B(6)	0.6714(3)	0.1450(8)	0.8485(3)	* 0.038(3)
C(7)	0.5423(3)	0.2428(5)	0.8556(2)	* 0.027(2)
C(8)	0.5345(3)	0.1859(6)	0.9116(2)	* 0.038(2)
B(9)	0.5694(4)	0.0482(9)	0.9151(3)	* 0.044(3)
B(10)	0.6111(4)	0.0218(7)	0.8529(3)	* 0.036(3)
B(11)	0.5851(3)	0.1593(7)	0.8169(3)	* 0.027(2)
C(12)	0.4708(9)	0.213(2)	0.9410(8)	0.043(2)
C(13)	0.4635(3)	0.4809(6)	0.8511(2)	* 0.034(2)
C(14)	0.4135(4)	0.5002(7)	0.8863(3)	* 0.049(3)
C(15)	0.4103(5)	0.6138(8)	0.9114(3)	* 0.071(4)
C(16)	0.4560(5)	0.7053(8)	0.9024(3)	* 0.075(4)
C(17)	0.5061(4)	0.6863(7)	0.8682(3)	* 0.059(3)
C(18)	0.5097(3)	0.5760(6)	0.8424(3)	* 0.042(2)
C(19)	0.3918(3)	0.2496(6)	0.8141(2)	* 0.035(2)
C(20)	0.3927(3)	0.1224(6)	0.8208(3)	* 0.039(2)
C(21)	0.3306(4)	0.0544(8)	0.8098(3)	* 0.063(3)
C(22)	0.2689(4)	0.1130(9)	0.7927(3)	* 0.074(4)
C(23)	0.2673(4)	0.2390(9)	0.7854(3)	* 0.070(4)
C(24)	0.3289(3)	0.3072(7)	0.7960(3)	* 0.048(3)
C(25)	0.5059(3)	0.0463(5)	0.7200(2)	* 0.027(2)
C(26)	0.4367(3)	0.0608(6)	0.6982(3)	* 0.035(2)
C(27)	0.3943(4)	-0.0399(7)	0.6840(3)	* 0.047(3)
C(28)	0.4225(4)	-0.1575(7)	0.6910(3)	* 0.053(3)
C(29)	0.4910(4)	-0.1746(6)	0.7135(3)	* 0.053(3)
C(30)	0.5325(3)	-0.0733(6)	0.7281(3)	* 0.038(2)
C(31)	0.6407(3)	0.1785(6)	0.7105(2)	* 0.031(2)
C(32)	0.6839(3)	0.2811(7)	0.7186(3)	* 0.046(3)
C(33)	0.7490(4)	0.2845(8)	0.6975(3)	* 0.064(3)
C(34)	0.7693(4)	0.1848(9)	0.6699(4)	* 0.077(4)
C(35)	0.7270(4)	0.0846(9)	0.6604(3)	* 0.071(4)
C(36)	0.6619(3)	0.0794(7)	0.6812(3)	* 0.046(3)
C(37)	0.4030(3)	0.3547(6)	0.6049(2)	* 0.039(2)
C(38)	0.3461(3)	0.3316(6)	0.6332(3)	* 0.042(2)

C(39)	0.2798(4)	0.3062(8)	0.6072(3)	* 0.063(3)
C(40)	-0.2703(4)	0.304(1)	0.5531(4)	* 0.085(4)
C(41)	0.3256(5)	0.3304(9)	0.5247(3)	* 0.077(4)
C(42)	0.3917(4)	0.3528(7)	0.5498(3)	* 0.051(3)
C(43)	0.5243(3)	0.5259(6)	0.6220(2)	* 0.036(2)
C(44)	0.4888(4)	0.6032(7)	0.5852(3)	* 0.052(3)
C(45)	0.5182(5)	0.7151(8)	0.5737(3)	* 0.066(3)
C(46)	0.5830(4)	0.7488(7)	0.5989(3)	* 0.065(3)
C(47)	0.6184(4)	0.6764(7)	0.6362(4)	* 0.061(3)
C(48)	0.5884(4)	0.5636(7)	0.6479(3)	* 0.052(3)
C(49)	0.5396(3)	0.2686(6)	0.5986(2)	* 0.034(2)
C(50)	0.5126(4)	0.1529(7)	0.5871(2)	* 0.045(2)
C(51)	0.5460(4)	0.0707(7)	0.5572(3)	* 0.056(3)
C(52)	0.6085(5)	0.1032(8)	0.5380(3)	* 0.074(4)
C(53)	0.6365(4)	0.2163(9)	0.5486(3)	* 0.068(3)
C(54)	0.6033(4)	0.3007(7)	0.5798(3)	* 0.048(3)
C(55)	0.2796(5)	0.2330(9)	0.9624(4)	* 0.095(4)
C(56)	0.3214(5)	0.2688(9)	1.0066(4)	* 0.080(4)
C(57)	0.3284(5)	0.3849(9)	1.0226(4)	* 0.095(5)
C(58)	0.2898(6)	0.472(1)	0.9953(4)	* 0.096(5)
C(59)	0.2451(5)	0.443(1)	0.9506(4)	* 0.094(5)
C(60)	0.2362(5)	0.328(1)	0.9319(4)	* 0.095(5)
C(61)	0.2661(7)	0.118(1)	0.9433(5)	0.144(5)

Tabla 45. *Distancias de enlace (Å) para* $[PdCl\{n(PPh_2)MePPh\}(PPh_3)]$.

Pd-Cl	2.352(2)	Pd-P1	2.318(2)
Pd-P2	2.274(2)	Pd-P3	2.345(2)
P1-C7	1.833(6)	P1-C13	1.812(7)
P1-C19	1.815(6)	P2-B11	1.920(7)
P2-C25	1.822(6)	P2-C31	1.826(6)
P3-C37	1.814(6)	P3-C43	1.826(7)
P3-C49	1.823(7)	B1-B2	1.78(1)
B1-B3	1.77(1)	B1-B4	1.73(1)
B1-B5	1.79(1)	B1-B6	1.77(1)
B1-H1	1.07(6)	B2-B3	1.77(1)
B2-B6	1.77(1)	B2-C7	1.729(9)
B2-B11	1.76(1)	B2-H2	1.13(6)
B3-B4	1.74(1)	B3-C7	1.732(9)
B3-C8	1.72(1)	B3-H3	1.04(6)
B4-B5	1.75(1)	B4-C8	1.71(1)
B4-B9	1.79(1)	B4-H4	1.04(6)
B5-B6	1.81(1)	B5-B9	1.81(1)
B5-B10	1.77(1)	B5-H5	1.07(6)
B6-B10	1.77(1)	B6-B11	1.755(9)
B6-H6	1.11(4)	C7-C8	1.574(9)
C7-B11	1.622(9)	C8-B9	1.64(1)
C8-C12	1.52(2)	B9-B10	1.87(1)
B9-H9	1.13(6)	B9-H10b	1.35(5)
B10-B11	1.79(1)	B10-H10a	1.07(6)
B10-H10b	1.22(5)	C12-H12a	.95(3)
C12-H12b	.95(5)	C12-H12c	.95(4)
C13-C14	1.39(1)	C13-C18	1.389(9)
C14-C15	1.39(1)	C14-H14	.950(7)
C15-C16	1.36(1)	C15-H15	.950(9)
C16-C17	1.37(1)	C16-H16	.950(9)
C17-C18	1.37(1)	C17-H17	.950(8)
C18-H18	.950(7)	C19-C20	1.392(9)
C19-C24	1.383(9)	C20-C21	1.39(1)
C20-H20	.950(6)	C21-C22	1.36(1)
C21-H21	.950(8)	C22-C23	1.38(1)
C22-H22	.950(8)	C23-C24	1.39(1)
C23-H23	.950(8)	C24-H24	.950(8)
C25-C26	1.381(8)	C25-C30	1.401(9)
C26-C27	1.384(9)	C26-H26	.950(6)
C27-C28	1.39(1)	C27-H27	.950(7)
C28-C29	1.38(1)	C28-H28	.950(7)
C29-C30	1.381(9)	C29-H29	.950(7)
C30-H30	.950(6)	C31-C32	1.387(9)
C31-C36	1.39(1)	C32-C33	1.40(1)
C32-H32	.950(7)	C33-C34	1.37(1)
C33-H33	.950(8)	C34-C35	1.36(1)
C34-H34	.950(8)	C35-C36	1.40(1)
C35-H35	.950(9)	C36-H36	.950(7)

C37-C38	1.385(9)	C37-C42	1.396(9)
C38-C39	1.387(9)	C38-H38	.950(7)
C39-C40	1.37(1)	C39-H39	.950(8)
C40-C41	1.37(1)	C40-H40	.950(8)
C41-C42	1.37(1)	C41-H41	.950(8)
C42-H42	.950(7)	C43-C44	1.380(9)
C43-C48	1.383(9)	C44-C45	1.38(1)
C44-H44	.950(7)	C45-C46	1.38(1)
C45-H45	.950(8)	C46-C47	1.35(1)
C46-H46	.950(8)	C47-C48	1.40(1)
C47-H47	.950(7)	C48-H48	.950(7)
C49-C50	1.38(1)	C49-C54	1.39(1)
C50-C51	1.37(1)	C50-H50	.950(7)
C51-C52	1.38(1)	C51-H51	.950(8)
C52-C53	1.36(1)	C52-H52	.950(9)
C53-C54	1.41(1)	C53-H53	.950(8)
C54-H54	.950(7)	C55-C56	1.36(1)
C55-C60	1.49(1)	C55-C61	1.35(2)
C56-C57	1.33(1)	C56-H56	.950(9)
C57-C58	1.35(1)	C57-H57	.95(1)
C58-C59	1.38(1)	C58-H58	.95(1)
C59-C60	1.35(2)	C59-H59	.95(1)
C60-H60	.950(9)	C61-H61a	.95(1)
C61-H61b	.95(1)	C61-H61c	.95(1)

Tabla 46. *Ángulos de enlace (°) para [PdCl{n(PPh$_2$)MePPh}(PPh$_3$)].*

Cl-Pd-P1	89.49(6)	Cl-Pd-P2	175.55(6)
Cl-Pd-P3	84.65(6)	P1-Pd-P2	86.19(6)
P1-Pd-P3	170.26(6	P2-Pd-P3	99.48(6)
Pd-P1-C7	112.2(2)	Pd-P1-C13	114.5(2)
Pd-P1-C19	102.6(2)	C7-P1-C13	109.9(3)
C7-P1-C19	107.5(3)	C13-P1-C19	109.6(3)
Pd-P2-B11	108.4(2)	Pd-P2-C25	109.8(2)
Pd-P2-C31	115.0(2)	B11-P2-C25	107.0(3)
B11-P2-C31	107.3(3)	C25-P2-C31	108.9(3)
Pd-P3-C37	111.3(2)	Pd-P3-C43	109.6(2)
Pd-P3-C49	122.4(2)	C37-P3-C43	108.7(3)
C37-P3-C49	99.7(3)	C43-P3-C49	104.2(3)
B2-B1-B3	60.2(4)	B2-B1-B4	108.0(5)
B2-B1-B5	108.3(6)	B2-B1-B6	59.7(4)
B2-B1-H1	120(3)	B3-B1-B4	59.8(5)
B3-B1-B5	107.8(6)	B3-B1-B6	108.0(5)
B3-B1-H1	117(3)	B4-B1-B5	59.6(5)
B4-B1-B6	108.3(6)	B4-B1-H1	121(3)
B5-B1-B6	60.9(5)	B5-B1-H1	125(3)
B6-B1-H1	125(3)	B1-B2-B3	59.6(4)
B1-B2-B6	60.1(4)	B1-B2-C7	102.4(5)

B1-B2-B11	106.7(6)	B1-B2-H2	128(3)
B3-B2-B6	107.9(6)	B3-B2-C7	59.2(4)
B3-B2-B11	106.6(5)	B3-B2-H2	117(3)
B6-B2-C7	101.1(5)	B6-B2-B11	59.6(4)
B6-B2-H2	130(3)	C7-B2-B11	55.3(4)
C7-B2-H2	120(3)	B11-B2-H2	122(3)
B1-B3-B2	60.2(4)	B1-B3-B4	59.1(5)
B1-B3-C7	102.7(5)	B1-B3-C8	104.3(6)
B1-B3-H3	129(3)	B2-B3-B4	107.5(6)
B2-B3-C7	59.1(4)	B2-B3-C8	104.3(5)
B2-B3-H3	122(3)	B4-B3-C7	101.2(6)
B4-B3-C8	59.2(4)	B4-B3-H3	126(3)
C7-B3-C8	54.3(4)	C7-B3-H3	122(3)
C8-B3-H3	121(3)	B1-B4-B3	61.0(5)
B1-B4-B5	61.9(5)	B1-B4-C8	106.2(5)
B1-B4-B9	110.1(6)	B1-B4-H4	123(3)
B3-B4-B5	110.5(6)	B3-B4-C8	59.7(4)
B3-B4-B9	107.3(5)	B3-B4-H4	114(3)
B5-B4-C8	104.5(5)	B5-B4-B9	61.4(5)
B5-B4-H4	130(3)	C8-B4-B9	55.7(4)
C8-B4-H4	118(3)	B9-B4-H4	123(3)
B1-B5-B4	58.5(5)	B1-B5-B6	59.0(5)
B1-B5-B9	106.5(6)	B1-B5-B10	108.6(6)
B1-B5-H5	120(3)	B4-B5-B6	105.9(6)
B4-B5-B9	60.2(5)	B4-B5-B10	111.3(5)
B4-B5-H5	119(3)	B6-B5-B9	107.0(5)
B6-B5-B10	59.3(4)	B6-B5-H5	124(3)
B9-B5-B10	62.9(4)	B9-B5-H5	123(3)
B10-B5-H5	122(3)	B1-B6-B2	60.3(5)
B1-B6-B5	60.1(5)	B1-B6-B10	109.6(5)
B1-B6-B11	107.2(5)	B1-B6-H6	124(2)
B2-B6-B5	108.2(5)	B2-B6-B10	111.1(5)
B2-B6-B11	60.1(4)	B2-B6-H6	120(3)
B5-B6-B10	59.4(4)	B5-B6-B11	106.1(5)
B5-B6-H6	125(3)	B10-B6-B11	61.1(4)
B10-B6-H6	119(3)	B11-B6-H6	120(2)
P1-C7-B2	113.8(4)	P1-C7-B3	120.0(4)
P1-C7-C8	124.2(4)	P1-C7-B11	111.2(4)
B2-C7-B3	61.7(4)	B2-C7-C8	113.3(4)
B2-C7-B11	63.4(4)	B3-C7-C8	62.5(4)
B3-C7-B11	115.5(5)	C8-C7-B11	115.6(5)
B3-C8-B4	61.1(4)	B3-C8-C7	63.2(4)
B3-C8-B9	115.9(5)	B3-C8-C12	115(1)
B4-C8-C7	109.7(5)	B4-C8-B9	64.5(5)
B4-C8-C12	118.4(8)	C7-C8-B9	109.4(5)
C7-C8-C12	121.9(9)	B9-C8-C12	119(1)
B4-B9-B5	58.4(5)	B4-B9-C8	59.8(5)
B4-B9-B10	105.7(6)	B4-B9-H9	120(3)
B4-B9-H10b	134(2)	B5-B9-C8	105.4(6)
B5-B9-B10	57.7(4)	B5-B9-H9	117(3)

B5-B9-H10b	98(2)	C8-B9-B10	107.5(5)
C8-B9-H9	128(3)	C8-B9-H10b	96(2)
B10-B9-H9	120(3)	B10-B9-H10b	41(2)
H9-B9-H10b	105(4)	B5-B10-B6	61.3(4)
B5-B10-B9	59.4(4)	B5-B10-B11	105.8(5)
B5-B10-H10a	117(3)	B5-B10-H10b	106(3)
B6-B10-B9	105.8(5)	B6-B10-B11	59.0(4)
B6-B10-H10a	118(3)	B6-B10-H10b	132(3)
B9-B10-B11	100.7(5)	B9-B10-H10a	126(3)
B9-B10-H10b	46(2)	B11-B10-H10a	127(3)
B11-B10-H10b	86(3)	H10a-B10-H10b	108(4)
P2-B11-B2	114.1(4)	P2-B11-B6	126.3(5)
P2-B11-C7	116.3(4)	P2-B11-B10	128.9(5)
B2-B11-B6	60.2(4)	B2-B11-C7	61.2(4)
B2-B11-B10	110.2(5)	B6-B11-C7	106.0(5)
B6-B11-B10	59.9(4)	C7-B11-B10	106.5(5)
C8-C12-H12a	115(4)	C8-C12-H12b	113(3)
C8-C12-H12c	106(3)	H12a-C12-H12b	109(6)
H12a-C12-H12c	106(5)	H12b-C12-H12c	106(5)
P1-C13-C14	123.4(5)	P1-C13-C18	118.0(5)
C14-C13-C18	118.6(6)	C13-C14-C15	119.7(7)
C13-C14-H14	120.2(7)	C15-C14-H14	120.2(8)
C14-C15-C16	120.7(8)	C14-C15-H15	119.6(8)
C16-C15-H15	119.6(8)	C15-C16-C17	119.9(8)
C15-C16-H16	120(1)	C17-C16-H16	120.1(9)
C16-C17-C18	120.6(7)	C16-C17-H17	119.7(8)
C18-C17-H17	119.7(8)	C13-C18-C17	120.6(7)
C13-C18-H18	119.7(7)	C17-C18-H18	119.7(7)
P1-C19-C20	120.4(5)	P1-C19-C24	119.5(5)
C20-C19-C24	119.2(6)	C19-C20-C21	120.2(6)
C19-C20-H20	119.9(6)	C21-C20-H20	119.9(7)
C20-C21-C22	119.8(8)	C20-C21-H21	120.1(7)
C22-C21-H21	120.1(8)	C21-C22-C23	120.7(7)
C21-C22-H22	119.6(9)	C23-C22-H22	119.6(8)
C22-C23-C24	119.8(7)	C22-C23-H23	118.7(8)
C24-C23-H23	114.2(9)	C19-C24-C23	120.3(7)
C19-C24-H24	119.9(6)	C23-C24-H24	119.9(7)
P2-C25-C26	120.5(5)	P2-C25-C30	120.8(4)
C26-C25-C30	118.5(5)	C25-C26-C27	121.2(6)
C25-C26-H26	119.4(6)	C27-C26-H26	119.4(6)
C26-C27-C28	119.2(6)	C26-C27-H27	120.4(7)
C28-C27-H27	120.4(7)	C27-C28-C29	120.8(7)
C27-C28-H28	119.6(7)	C29-C28-H28	119.6(7)
C28-C29-C30	119.4(6)	C28-C29-H29	120.3(7)
C30-C29-H29	120.3(7)	C25-C30-C29	120.9(6)
C25-C30-H30	119.5(6)	C29-C30-H30	119.5(6)
P2-C31-C32	116.5(5)	P2-C31-C36	123.4(5)
C32-C31-C36	120.0(6)	C31-C32-C33	119.9(7)
C31-C32-H32	120.0(7)	C33-C32-H32	120.0(7)

C32-C33-C34	118.9(8)	C32-C33-H33	120.5(8)
C34-C33-H33	120.5(8)	C33-C34-C35	122.1(8)
C33-C34-H34	118.9(9)	C35-C34-H34	118.9(9)
C34-C35-C36	119.7(8)	C34-C35-H35	120.1(8)
C36-C35-H35	120.2(8)	C31-C36-C35	119.3(7)
C31-C36-H36	120.4(7)	C35-C36-H36	120.4(8)
P3-C37-C38	121.2(5)	P3-C37-C42	120.2(5)
C38-C37-C42	118.4(6)	C37-C38-C39	120.5(6)
C37-C38-H38	119.8(6)	C39-C38-H38	119.7(7)
C38-C39-C40	120.0(7)	C38-C39-H39	120.0(8)
C40-C39-H39	120.0(7)	C39-C40-C41	120.0(7)
C39-C40-H40	120.0(9)	C41-C40-H40	120.0(9)
C40-C41-C42	120.7(8)	C40-C41-H41	119.7(8)
C42-C41-H41	119.7(8)	C37-C42-C41	120.4(7)
C37-C42-H42	119.8(6)	C41-C42-H42	119.8(7)
P3-C43-C44	123.3(5)	P3-C43-C48	117.7(5)
C44-C43-C48	118.9(6)	C43-C44-C45	120.0(7)
C43-C44-H44	120.0(7)	C45-C44-H44	120.0(7)
C44-C45-C46	119.8(7)	C44-C45-H45	120.1(8)
C46-C45-H45	120.1(8)	C45-C46-C47	121.7(8)
C45-C46-H46	119.1(8)	C47-C46-H46	119.1(8)
C46-C47-C48	118.3(7)	C46-C47-H47	120.9(8)
C48-C47-H47	120.9(8)	C43-C48-C47	121.2(7)
C43-C48-H48	119.4(7)	C47-C48-H48	119.4(7)
P3-C49-C50	119.5(5)	P3-C49-C54	122.3(5)
C50-C49-C54	118.2(6)	C49-C50-C51	121.8(7)
C49-C50-H50	119.1(7)	C51-C50-H50	119.1(7)
C50-C51-C52	119.9(7)	C50-C51-H51	120.0(8)
C52-C51-H51	120.0(8)	C51-C52-C53	119.7(8)
C51-C52-H52	120.2(9)	C53-C52-H52	120.2(9)
C52-C53-C54	120.9(8)	C52-C53-H53	119.5(9)
C54-C53-H53	119.5(9)	C49-C54-C53	119.3(7)
C49-C54-H54	120.3(7)	C53-C54-H54	120.3(7)
C56-C55-C60	118.4(9)	C56-C55-C61	129(1)
C60-C55-C61	112.2(9)	C55-C56-C57	123.7(9)
C55-C56-H56	118.1(9)	C57-C56-H56	118.1(9)
C56-C57-C58	118.7(9)	C56-C57-H57	121(1)
C58-C57-H57	121(1)	C57-C58-C59	121(1)
C57-C58-H58	119(1)	C59-C58-H58	119(1)
C58-C59-C60	123(1)	C58-C59-H59	118(1)
C60-C59-H59	118.4(9)	C55-C60-C59	114.8(8)
C55-C60-H60	123(1)	C59-C60-H60	123(1)
B9-H10b-B10	93(3)	C55-C61-H61a	104(1)
C55-C61-H61b	104(1)	C55-C61-H61c	129(1)
H61a-C61-H61b	109(1)	H61a-C61-H61c	104(1)
H61b-C61-H61c	104(1)		

4.13. Estructura cristalina para [Rh(nHPPh)(PPh_3)$_2$].

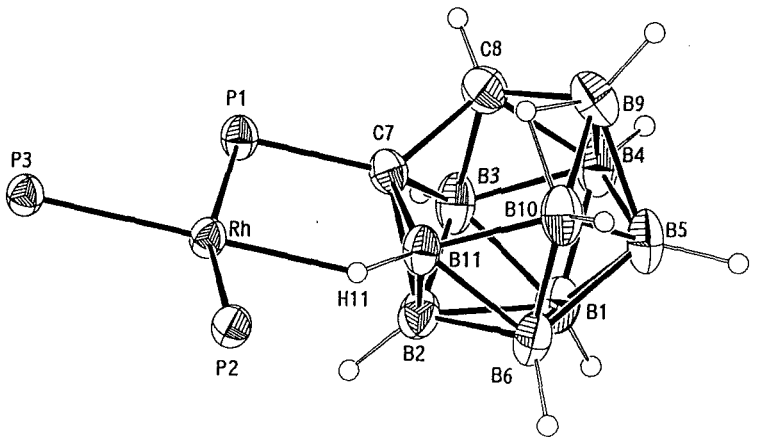


Tabla 47. *Datos cristalográficos para [Rh(7-PPh_2-7,8-$C_2B_9H_{11}$)(PPh_3)$_2$]·3CH_2Cl_2.*

Fórmula química:	$C_{50}H_{51}B_9P_3Rh{\cdot}3CH_2Cl_2$
peso molecular	1199.80
a =	15.987(5) Å
b =	18.496(4) Å
c =	19.320(4) Å
β =	91.22(2)°
V =	5712(2) Å^3
Z =	4
grupo espacial:	monoclínico, $P2_1/n$ (No. 14)
T =	23 °C
λ =	0.71069 Å
ρ =	1.395 g cm^{-3}
μ =	7.0 cm^{-1}
coef. transm. =	0.956-1.000
$R(F_o)$ =	0.064
$R_w(F_o)$ =	0.068

Table 48. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para* $[Rh(7\text{-}PPh_2\text{-}7,8\text{-}C_2B_9H_{11})(PPh_3)_2]\cdot 3CH_2Cl_2$.

	x/a	*y/b*	*z/c*	U_{eq} [a]
Rh	0.43590(3)	0.23466(3)	0.15148(3)	0.0361(2)
Cl(1)	0.4186(2)	0.2184(2)	0.6078(2)	0.149(2)
Cl(2)	0.4282(2)	0.1238(2)	0.4927(2)	0.156(2)
Cl(3)	0.6701(3)	0.5381(4)	0.3116(3)	0.285(4)
Cl(4)	0.5325(4)	0.5954(5)	0.3355(4)	0.412(7)
Cl(5)	0.4130(3)	0.3457(3)	0.3802(2)	0.227(3)
Cl(6)	0.5266(4)	0.3633(6)	0.4809(3)	0.420(7)
P(1)	0.5692(1)	0.1960(1)	0.17235(9)	0.0391(6)
P(2)	0.2924(1)	0.2381(1)	0.12528(9)	0.0417(6)
P(3)	0.4655(1)	0.3410(1)	0.10410(9)	0.0389(6)
B(1)	0.5111(6)	0.0249(5)	0.3190(4)	0.056(3)
B(2)	0.4946(6)	0.1121(5)	0.2879(4)	0.052(3)
B(3)	0.5924(6)	0.0702(5)	0.2787(5)	0.057(3)
B(4)	0.5734(6)	-0.0215(5)	0.2641(5)	0.064(4)
B(5)	0.4655(6)	-0.0362(5)	0.2577(5)	0.062(4)
B(6)	0.4142(6)	0.0487(5)	0.2739(5)	0.055(3)
C(7)	0.5421(4)	0.1093(3)	0.2088(3)	0.041(2)
C(8)	0.5886(4)	0.0367(4)	0.1979(4)	0.053(3)
B(9)	0.5217(6)	-0.0269(5)	0.1806(5)	0.065(4)
B(10)	0.4163(5)	0.0136(5)	0.1897(5)	0.056(3)
B(11)	0.4431(5)	0.1039(4)	0.2064(4)	0.041(3)
C(12)	0.6196(4)	0.1756(4)	0.0920(3)	0.045(2)
C(13)	0.5814(5)	0.1223(4)	0.0507(4)	0.065(3)
C(14)	0.6091(6)	0.1081(5)	-0.0140(4)	0.085(4)
C(15)	0.6738(7)	0.1456(5)	-0.0386(4)	0.097(5)
C(16)	0.7115(6)	0.1987(5)	-0.0000(4)	0.088(4)
C(17)	0.6847(5)	0.2143(4)	0.0654(4)	0.061(3)
C(18)	0.6453(4)	0.2399(4)	0.2297(3)	0.050(2)
C(19)	0.7313(5)	0.2340(4)	0.2249(4)	0.065(3)
C(20)	0.7846(5)	0.2735(5)	0.2692(5)	0.089(4)
C(21)	0.7515(7)	0.3153(5)	0.3192(5)	0.104(5)
C(22)	0.6670(6)	0.3177(5)	0.3272(4)	0.092(4)
C(23)	0.6135(5)	0.2818(4)	0.2826(4)	0.069(3)
C(24)	0.2292(4)	0.2375(4)	0.2027(3)	0.045(2)
C(25)	0.2680(4)	0.2256(4)	0.2660(4)	0.055(3)
C(26)	0.2230(5)	0.2246(5)	0.3248(4)	0.070(3)
C(27)	0.1386(5)	0.2371(5)	0.3218(4)	0.077(3)

C(28)	0.0986(5)	0.2486(5)	0.2603(5)	0.080(4)
C(29)	-0.1437(4)	0.2491(4)	0.2000(4)	0.063(3)
C(30)	0.2374(4)	0.3040(4)	0.0709(3)	0.044(2)
C(31)	0.2148(4)	0.3704(4)	0.0970(4)	0.055(3)
C(32)	0.1746(5)	0.4218(4)	0.0567(4)	0.071(3)
C(33)	0.1574(5)	0.4069(4)	-0.0115(5)	0.074(3)
C(34)	0.1781(5)	0.3411(5)	-0.0387(4)	0.071(3)
C(35)	0.2189(5)	0.2899(4)	0.0016(4)	0.055(3)
C(36)	0.2684(4)	0.1521(4)	0.0818(4)	0.048(3)
C(37)	0.1981(5)	0.1108(5)	0.0956(5)	0.083(4)
C(38)	0.1849(6)	0.0478(5)	0.0593(6)	0.109(5)
C(39)	0.2342(7)	0.0269(5)	0.0081(6)	0.105(5)
C(40)	0.3036(6)	0.0662(5)	-0.0047(5)	0.086(4)
C(41)	0.3212(5)	0.1286(4)	0.0313(4)	0.066(3)
C(42)	0.5734(4)	0.3732(4)	0.0964(4)	0.047(3)
C(43)	0.6138(5)	0.3792(4)	0.0344(4)	0.062(3)
C(44)	0.6952(5)	0.4038(5)	0.0319(5)	0.078(4)
C(45)	0.7361(5)	0.4228(5)	0.0919(5)	0.086(4)
C(46)	0.6977(5)	0.4193(4)	0.1541(5)	0.074(4)
C(47)	0.6159(5)	0.3953(4)	0.1559(4)	0.059(3)
C(48)	0.4203(4)	0.4183(3)	0.1474(4)	0.047(3)
C(49)	0.3739(5)	0.4072(4)	0.2057(4)	0.058(3)
C(50)	0.3382(5)	0.4657(5)	0.2386(4)	0.074(4)
C(51)	0.3498(6)	0.5348(5)	0.2153(5)	0.081(4)
C(52)	0.3986(6)	0.5459(4)	0.1597(4)	0.074(4)
C(53)	0.4354(5)	0.4889(4)	0.1267(4)	0.057(3)
C(54)	0.4308(4)	0.3440(4)	0.0138(3)	0.043(2)
C(55)	0.3898(5)	0.4023(4)	-0.0172(4)	0.055(3)
C(56)	0.3720(5)	0.4004(5)	-0.0872(4)	0.074(4)
C(57)	0.3942(6)	0.3421(5)	-0.1259(4)	0.075(4)
C(58)	0.4326(5)	0.2839(4)	-0.0952(4)	0.062(3)
C(59)	0.4501(4)	0.2847(4)	-0.0263(4)	0.049(3)
C(60)	0.4692(7)	0.1507(7)	0.5719(6)	0.126(6)
C(61)	0.561(1)	0.5158(8)	0.313(1)	0.29(1)
C(62)	0.453(1)	0.314(1)	0.4500(9)	0.36(2)

[a] $U_{eq} = 1/3\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$

Tabla 49. *Distancias de enlace (Å) para* $[Rh(7\text{-}PPh_2\text{-}7,8\text{-}C_2B_9H_{11})(PPh_3)_2]\cdot 3CH_2Cl_2$.

Rh-P(1)	2.276(2)
Rh-P(2)	2.340(2)
Rh-P(3)	2.224(2)
Rh-B(2)	3.586(8)
Rh-B(11)	2.643(8)
Rh-H(11)	1.81(5)
P(1)-C(7)	1.804(7)
P(1)-C(12)	1.804(7)
P(1)-C(18)	1.819(7)
B(3)-C(7)	1.72(1)
B(3)-C(8)	1.68(1)
C(7)-C(8)	1.551(9)
C(7)-B(11)	1.59(1)
C(8)-B(9)	1.62(1)
B(9)-B(10)	1.86(1)
B(10)-B(11)	1.75(1)
B(11)-H(11)	1.12(5)

Tabla 50. *Ángulos de enlace (°) para* $[Rh(7\text{-}PPh_2\text{-}7,8\text{-}C_2B_9H_{11})(PPh_3)_2]\cdot 3CH_2Cl_2$.

P(1)-Rh-P(2)	163.14(7)	C(7)-B(11)-B(10)	107.8(6)
P(1)-Rh-P(3)	98.29(7)	C(7)-B(11)-H(11)	122(3)
P(1)-Rh-H(11)	86(2)	B(10)-B(11)-H(11)	119(3)
P(2)-Rh-P(3)	95.93(7)		
P(2)-Rh-H(11)	79(2)		
P(3)-Rh-H(11)	174(2)		
Rh-P(1)-C(7)	96.7(2)		
Rh-P(1)-C(12)	110.3(2)		
Rh-P(1)-C(18)	125.4(2)		
Rh-P(2)-C(24)	112.3(2)		
Rh-P(2)-C(30)	127.0(2)		
Rh-P(2)-C(36)	105.7(2)		
Rh-P(3)-C(42)	122.0(2)		
Rh-P(3)-C(48)	114.6(2)		
Rh-P(3)-C(54)	111.0(2)		
P(1)-C(7)-B(2)	115.6(5)		
P(1)-C(7)-B(3)	124.6(5)		
P(1)-C(7)-C(8)	126.6(5)		
P(1)-C(7)-B(11)	107.0(4)		
C(8)-C(7)-B(11)	115.0(5)		
C(7)-C(8)-B(9)	109.9(6)		
C(8)-B(9)-B(10)	106.5(6)		
B(9)-B(10)-B(11)	100.6(6)		

4.14.. Estructura cristalina para [Rh(nMePPh)(COD)].

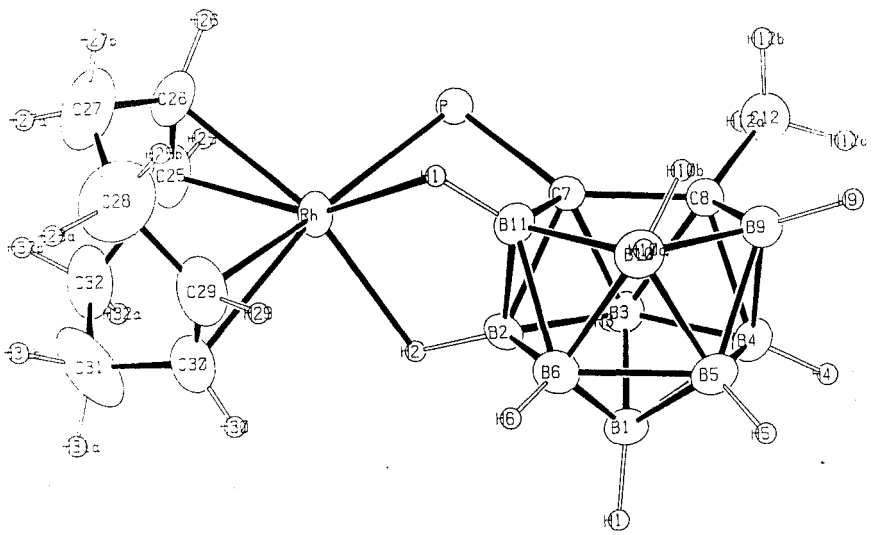


Tabla 51. *Datos cristalográficos para [Rh(7-P(C_6H_5)$_2$-8-CH_3-7,8-$C_2B_9H_{11}$)(C_8H_{12})].*

Fórmula química:	$C_{23}H_{35}B_9PRh$
peso molecular	542.68
a =	12.925 (2) Å
b =	10.568 (2) Å
c =	19.352 (1) Å
β =	90.438 (6)°
V =	2643.2 (7) Å^3
Z =	4
grupo espacial:	$P2_1/n$ (No. 14)
T =	20 °C
λ =	0.71069 Å
ρ =	1.364 g cm^{-3}
μ =	7.2 cm^{-1}
$R(F_o)$ =	0.037
$R_w(F_o)$ =	0.040

Table 52. *Coordenadas fraccionarias y desviación estandard (entre paréntesis) para* $[Rh(7\text{-}P(C_6H_5)_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{11})(C_8H_{12})]$.

	x/a	y/b	z/c	U
Rh	0.38234(2)	0.70017(3)	0.86897(2)	* 0.0378(1)
P	0.51981(7)	0.83201(9)	0.84882(5)	* 0.0304(3)
B(1)	0.4043(3)	0.7275(6)	0.6494(2)	* 0.052(2)
B(2)	0.4022(3)	0.7283(5)	0.7404(2)	* 0.038(1)
B(3)	0.4694(3)	0.8483(5)	0.6958(2)	* 0.043(2)
B(4)	0.5278(4)	0.7778(6)	0.6248(2)	* 0.052(2)
B(5)	0.5015(4)	0.6136(6)	0.6242(3)	* 0.056(2)
B(6)	0.4194(4)	0.5854(5)	0.6968(3)	* 0.049(2)
C(7)	0.5288(3)	0.7660(3)	0.7629(2)	* 0.031(1)
C(8)	0.5979(3)	0.8000(4)	0.6990(2)	* 0.038(1)
B(9)	0.6232(3)	0.6686(5)	0.6581(3)	* 0.049(2)
B(10)	0.5514(4)	0.5371(5)	0.6997(3)	* 0.052(2)
B(11)	0.4945(3)	0.6199(4)	0.7711(2)	* 0.040(1)
C(12)	0.6749(3)	0.9071(4)	0.7044(3)	0.055(1)
H(12a)	0.650(2)	0.989(1)	0.717(1)	0.055(1)
H(12b)	0.731(2)	0.884(3)	0.734(1)	0.055(1)
H(12c)	0.702(2)	0.914(3)	0.6591(6)	0.055(1)
C(13)	0.5014(3)	1.0026(3)	0.8456(2)	* 0.036(1)
C(14)	0.5835(3)	1.0858(4)	0.8454(2)	* 0.052(2)
C(15)	0.5673(3)	1.2137(4)	0.8341(3)	* 0.070(2)
C(16)	0.4701(4)	1.2582(4)	0.8238(3)	* 0.070(2)
C(17)	0.3874(3)	1.1769(4)	0.8251(3)	* 0.063(2)
C(18)	0.4027(3)	1.0499(4)	0.8365(2)	* 0.046(1)
C(19)	0.6447(3)	0.8099(3)	0.8913(2)	* 0.034(1)
C(20)	0.6640(3)	0.8677(4)	0.9539(2)	* 0.055(2)
C(21)	0.7595(4)	0.8571(5)	0.9852(2)	* 0.064(2)
C(22)	0.8352(3)	0.7868(5)	0.9557(2)	* 0.062(2)
C(23)	0.8170(3)	0.7254(5)	0.8952(2)	* 0.060(2)
C(24)	0.7208(3)	0.7364(4)	0.8622(2)	* 0.048(1)
C(25)	0.3189(4)	0.7984(4)	0.9527(2)	* 0.061(2)
C(26)	0.3844(4)	0.7020(5)	0.9771(2)	* 0.066(2)
C(27)	0.3438(6)	0.5786(6)	1.0085(3)	* 0.107(3)
C(28)	0.3061(6)	0.4830(6)	0.9580(4)	* 0.131(4)
C(29)	0.2860(4)	0.5263(5)	0.8873(3)	* 0.077(2)
C(30)	0.2209(4)	0.6173(5)	0.8684(3)	* 0.074(2)
C(31)	0.1538(4)	0.6905(7)	0.9171(4)	* 0.121(3)
C(32)	0.2009(5)	0.7971(6)	0.9514(3)	* 0.093(2)

Tabla 53. *Distancias de enlace (Å) para* $[Rh(7\text{-}P(C_6H_5)_2\text{-}8\text{-}CH_3\text{-}7,8\text{-}C_2B_9H_{11})(C_8H_{12})]$.

Rh-P	2.294(1)	Rh-B2	2.520(4)

Rh-B11	2.540(4)	Rh-C25	2.096(4)
Rh-C26	2.093(4)	Rh-C29	2.249(5)
Rh-C30	2.263(5)	Rh-H2	2.01(3)
Rh-H11	2.07(4)	P-C7	1.808(3)
P-C13	1.820(4)	P-C19	1.821(4)
B1-B2	1.763(6)	B1-B3	1.771(7)
B1-B4	1.752(7)	B1-B5	1.809(8)
B1-B6	1.770(8)	B1-H1	1.09(4)
B2-B3	1.766(7)	B2-B6	1.745(7)
B2-C7	1.735(5)	B2-B11	1.753(6)
B2-H2	1.14(3)	B3-B4	1.740(7)
B3-C7	1.736(6)	B3-C8	1.738(6)
B3-H3	1.04(4	B4-B5	1.767(8)
B4-C8	1.708(6)	B4-B9	1.804(7)
B4-H4	1.06(3)	B5-B6	1.791(7)
B5-B9	1.797(7)	B5-B10	1.785(7)
B5-H5	1.07(4)	B6-B10	1.780(7)
B6-B11	1.766(6)	B6-H6	1.00(4)
C7-C8	1.572(5)	C7-B11	1.614(6)
C8-B9	1.633(7)	C8-C12	1.510(6)
B9-B10	1.858(7)	B9-H9	1.11(3)
B9-H10b	1.32(4)	B10-B11	1.798(7)
B10-H10a	1.07(4)	B10-H10b	1.16(3)
B11-H11	1.09(4)	C12-H12a	.95(2)
C12-H12b	.95(2)	C12-H12c	.95(2)
C13-C14	1.378(5)	C13-C18	1.380(5)
C14-C15	1.385(6)	C14-H14	.83(4)
C15-C16	1.354(7)	C15-H15	.87(5)
C16-C17	1.372(6)	C16-H16	.91(5)
C17-C18	1.375(6)	C17-H17	.84(4)
C18-H18	.84(3)	C19-C20	1.379(6)
C19-C24	1.377(5)	C20-C21	1.374(6)
C20-H20	.84(4)	C21-C22	1.358(7)
C21-H21	.85(4)	C22-C23	1.358(7)
C22-H22	.86(4)	C23-C24	1.397(6)
C23-H23	.86(4)	C24-H24	.97(3)
C25-C26	1.404(7)	C25-C32	1.525(8)
C25-H25	.97(4)	C26-C27	1.533(8)
C26-H26	.96(4)	C27-C28	1.48(1)
C27-H27a	.80(6)	C27-H27b	.94(5)
C28-C29	1.463(9)	C28-H28a	.92(6)
C28-H28b	1.01(6)	C29-C30	1.327(7)
C29-H29	.89(6)	C30-C31	1.501(9)
C30-H30	.86(4)	C31-C32	1.440(9)
C31-H31a	.93(7)	C31-H31b	1.04(7)
C32-H32a	.98(6)	C32-H32b	.91(5)

Tabla 54. *Ángulos de enlace (°) para [Rh(7-P(C_6H_5)$_2$-8-CH_3-7,8-$C_2B_9H_{11}$)(C_8H_{12})].*

P-Rh-B2	71.1(1)	P-Rh-B11	68.2(1)
P-Rh-C25	98.0(1)	P-Rh-C26	99.2(1)
P-Rh-C29	162.5(1)	P-Rh-C30	161.8(1)
P-Rh-H2	82.9(8)	P-Rh-H11	77(1)
B2-Rh-B11	40.5(1)	B2-Rh-C25	138.4(2)
B2-Rh-C26	170.1(2)	B2-Rh-C29	108.2(2)
B2-Rh-C30	98.1(2)	B2-Rh-H2	26.3(8)
B2-Rh-H11	65(1)	B11-Rh-C25	166.1(2)
B11-Rh-C26	138.3(2)	B11-Rh-C29	99.5(2)
B11-Rh-C30	113.5(2)	B11-Rh-H2	66.4(8)
B11-Rh-H11	25(1)	C25-Rh-C26	39.2(2)
C25-Rh-C29	93.6(2)	C25-Rh-C30	80.2(2)
C25-Rh-H2	115.1(9)	C25-Rh-H11	154(1)
C26-Rh-C29	81.5(2)	C26-Rh-C30	90.8(2)
C26-Rh-H2	154.3(9)	C26-Rh-H11	116(1)
C29-Rh-C30	34.2(2)	C29-Rh-H2	104.1(9)
C29-Rh-H11	86(1)	C30-Rh-H2	81.6(8)
C30-Rh-H11	112(1)	H2-Rh-H11	90(1)
Rh-P-C7	88.7(1)	Rh-P-C13	120.4(1)
Rh-P-C19	122.0(1)	C7-P-C13	111.1(2)
C7-P-C19	107.6(2)	C13-P-C19	104.9(2)
B2-B1-B3	60.0(3)	B2-B1-B4	106.9(3)
B2-B1-B5	106.7(3)	B2-B1-B6	59.2(3)
B2-B1-H1	121(2)	B3-B1-B4	59.2(3)
B3-B1-B5	106.7(3)	B3-B1-B6	107.3(3)
B3-B1-H1	122(2)	B4-B1-B5	59.5(3)
B4-B1-B6	107.5(3)	B4-B1-H1	124(2)
B5-B1-B6	60.1(3)	B5-B1-H1	124(2)
B6-B1-H1	121(2)	Rh-B2-B1	171.3(3)
Rh-B2-B3	128.4(3)	Rh-B2-B6	112.9(3)
Rh-B2-C7	83.3(2)	Rh-B2-B11	70.3(2)
Rh-B2-H2	51(1)	B1-B2-B3	60.2(3)
B1-B2-B6	60.6(3)	B1-B2-C7	103.3(3)
B1-B2-B11	108.6(3)	B1-B2-H2	127(1)
B3-B2-B6	108.7(3)	B3-B2-C7	59.4(2)
B3-B2-B11	107.4(3)	B3-B2-H2	116(2)
B6-B2-C7	101.3(3)	B6-B2-B11	60.6(3)
B6-B2-H2	130(2)	C7-B2-B11	55.1(2)
C7-B2-H2	119(2)	B11-B2-H2	120(2)
B1-B3-B2	59.8(3)	B1-B3-B4	59.9(3)
B1-B3-C7	102.9(3)	B1-B3-C8	104.9(3)
B1-B3-H3	128(2)	B2-B3-B4	107.2(4)
B2-B3-C7	59.4(2)	B2-B3-C8	104.2(3)
B2-B3-H3	118(2)	B4-B3-C7	100.6(3)
B4-B3-C8	58.8(2)	B4-B3-H3	130(2)
C7-B3-C8	53.8(2)	C7-B3-H3	120(2)
C8-B3-H3	124(2)	B1-B4-B3	60.9(3)
B1-B4-B5	61.9(3)	B1-B4-C8	107.0(3)

B1-B4-B9	109.4(4)	B1-B4-H4	122(2)
B3-B4-B5	109.9(3)	B3-B4-C8	60.5(2)
B3-B4-B9	107.0(3)	B3-B4-H4	119(2)
B5-B4-C8	104.0(3)	B5-B4-B9	60.4(3)
B5-B4-H4	124(2)	C8-B4-B9	55.3(3)
C8-B4-H4	122(2)	B9-B4-H4	123(2)
B1-B5-B4	58.7(3)	B1-B5-B6	58.9(3)
B1-B5-B9	107.2(4)	B1-B5-B10	109.2(3)
B1-B5-H5	122(2)	B4-B5-B6	105.9(4)
B4-B5-B9	60.8(3)	B4-B5-B10	111.8(4)
B4-B5-H5	122(2)	B6-B5-B9	106.9(3)
B6-B5-B10	59.7(3)	B6-B5-H5	122(2)
B9-B5-B10	62.5(3)	B9-B5-H5	123(2)
B10-B5-H5	119(2)	B1-B6-B2	60.2(3)
B1-B6-B5	61.1(3)	B1-B6-B10	111.2(3)
B1-B6-B11	107.7(3)	B1-B6-H6	127(2)
B2-B6-B5	108.3(4)	B2-B6-B10	111.0(3)
B2-B6-B11	59.9(3)	B2-B6-H6	125(2)
B5-B6-B10	60.0(3)	B5-B6-B11	106.2(3)
B5-B6-H6	122(2)	B10-B6-B11	60.9(3)
B10-B6-H6	112(2)	B11-B6-H6	119(2)
P-C7-B2	104.6(2)	P-C7-B3	117.6(2)
P-C7-C8	132.5(3)	P-C7-B11	105.0(2)
B2-C7-B3	61.2(2)	B2-C7-C8	113.3(3)
B2-C7-B11	63.0(3)	B3-C7-C8	63.2(2)
B3-C7-B11	115.6(3)	C8-C7-B11	117.0(3)
B3-C8-B4	60.7(3)	B3-C8-C7	63.0(2)
B3-C8-B9	115.3(3)	B3-C8-C12	114.3(3)
B4-C8-C7	109.1(3)	B4-C8-B9	65.3(3)
B4-C8-C12	120.4(3)	C7-C8-B9	107.7(3)
C7-C8-C12	119.7(3)	B9-C8-C12	122.5(3)
B4-B9-B5	58.8(3)	B4-B9-C8	59.3(3)
B4-B9-B10	106.9(3)	B4-B9-H9	114(2)
B4-B9-H10b	133(2)	B5-B9-C8	105.9(3)
B5-B9-B10	58.4(3)	B5-B9-H9	119(2)
B5-B9-H10b	96(2)	C8-B9-B10	108.9(3)
C8-B9-H9	121(2)	C8-B9-H10b	98(2)
B10-B9-H9	127(2)	B10-B9-H10b	38(1)
H9-B9-H10b	112(2)	B5-B10-B6	60.3(3)
B5-B10-B9	59.1(3)	B5-B10-B11	105.1(3)
B5-B10-H10a	117(2)	B5-B10-H10b	104(2)
B6-B10-B9	104.7(3)	B6-B10-B11	59.1(3)
B6-B10-H10a	118(2)	B6-B10-H10b	131(2)
B9-B10-B11	100.2(3)	B9-B10-H10a	127(2)
B9-B10-H10b	45(2)	B11-B10-H10a	128(2)
B11-B10-H10b	86(2)	H10a-B10-H10b	110(3)
Rh-B11-B2	69.1(2)	Rh-B11-B6	111.3(3)
Rh-B11-C7	85.0(2)	Rh-B11-B10	167.2(3)
Rh-B11-H11	53(2)	B2-B11-B6	59.5(3)

B2-B11-C7	61.9(2)	B2-B11-B10	109.8(3)
B2-B11-H11	120(2)	B6-B11-C7	105.5(3)
B6-B11-B10	59.9(3)	B6-B11-H11	129(2)
C7-B11-B10	106.0(3)	C7-B11-H11	119(2)
B10-B11-H11	124(2)	C8-C12-H12a	118(2)
C8-C12-H12b	110(2)	C8-C12-H12c	104(2)
H12a-C12-H12b	109(2)	H12a-C12-H12c	107(2)
H12b-C12-H12c	107(2)	P-C13-C14	122.1(3)
P-C13-C18	118.9(3)	C14-C13-C18	118.7(4)
C13-C14-C15	120.5(4)	C13-C14-H14	122(3)
C15-C14-H14	117(3)	C14-C15-C16	120.1(4)
C14-C15-H15	112(3)	C16-C15-H15	127(3)
C15-C16-C17	120.1(4)	C15-C16-H16	118(3)
C17-C16-H16	122(3)	C16-C17-C18	120.2(4)
C16-C17-H17	116(3)	C18-C17-H17	124(3)
C13-C18-C17	120.4(4)	C13-C18-H18	119(2)
C17-C18-H18	121(2)	P-C19-C20	119.6(3)
P-C19-C24	121.4(3)	C20-C19-C24	119.0(3)
C19-C20-C21	120.5(4)	C19-C20-H20	117(3)
C21-C20-H20	123(3)	C20-C21-C22	120.4(4)
C20-C21-H21	121(2)	C22-C21-H21	119(2)
C21-C22-C23	120.2(4)	C21-C22-H22	123(3)
C23-C22-H22	116(3)	C22-C23-C24	120.1(4)
C22-C23-H23	127(3)	C24-C23-H23	113(3)
C19-C24-C23	119.7(4)	C19-C24-H24	119(2)
C23-C24-H24	122(2)	Rh-C25-C26	70.3(3)
Rh-C25-C32	112.3(3)	Rh-C25-H25	107(2)
C26-C25-C32	126.8(4)	C26-C25-H25	111(2)
C32-C25-H25	118(2)	Rh-C26-C25	70.5(2)
Rh-C26-C27	112.7(3)	Rh-C26-H26	107(2)
C25-C26-C27	122.9(5)	C25-C26-H26	122(2)
C27-C26-H26	111(2)	C26-C27-C28	115.5(5)
C26-C27-H27a	108(5)	C26-C27-H27b	108(3)
C28-C27-H27a	109(4)	C28-C27-H27b	102(3)
H27a-C27-H27b	114(5)	C27-C28-C29	117.2(5)
C27-C28-H28a	115(4)	C27-C28-H28b	101(4)
C29-C28-H28a	110(4)	C29-C28-H28b	104(4)
H28a-C28-H28b	108(5)	Rh-C29-C28	108.0(4)
Rh-C29-C30	73.4(3)	Rh-C29-H29	99(4)
C28-C29-C30	126.3(5)	C28-C29-H29	120(4)
C30-C29-H29	113(4)	Rh-C30-C29	72.3(3)
Rh-C30-C31	109.5(4)	Rh-C30-H30	105(3)
C29-C30-C31	124.6(5)	C29-C30-H30	122(3)
C31-C30-H30	111(3)	C30-C31-C32	116.7(5)
C30-C31-H31a	107(5)	C30-C31-H31b	103(4)
C32-C31-H31a	117(5)	C32-C31-H31b	111(4)
H31a-C31-H31b	100(6)	C25-C32-C31	115.7(5)
C25-C32-H32a	101(3)	C25-C32-H32b	102(3)
C31-C32-H32a	114(3)	C31-C32-H32b	120(3)
H32a-C32-H32b	101(4)	Rh-H2-B2	103(2)

B9-H10b-B10	97(2)	Rh-H11-B11	102(3)