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DURENE-RHODIUM(I) COMPLEXES. CRYSTAL STRUCTURES OF THE COMPLEXES [Rh(durene)(diolefin)]ClO_4 (diolefin = tetrafluorobenzobarrelene or trimethyltetrafluorobenzobarrelene)

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Summary

The crystal structures of [Rh(durene)(diolefin)]ClO_4 (diolefin = tetrafluorobenzobarrelene (TFB) and trimethyltetrafluorobenzobarrelene (Me_3TFB)) have been solved by standard X-ray single crystal methods. The compounds crystallize in the space groups R_3c for the unmethylated TFB compound and $P2_1/n$ for the methylated one. The cell dimensions are 25.7586(5), 17.0059(4) Å and 12.6686(6), 11.5565(3), 16.7269(8) Å, β = 104.023(5)°, respectively. The refinement was taken to R values of 0.04 and 0.06, respectively. The arene in the TFB derivative has a distorted inverted boat conformation which becomes a skew one in the Me_3TFB compound. These puckering seems to be related to the tendency of rhodium(I) to achieve square-planar coordination.

Introduction

Several π-arene-rhodium(I) complexes have been structurally characterized recently [1—8]. In general, significant non-planarity is generated upon complexation to the metal. In order to obtain more information about the reasons for the different conformations and relative ring positions, we have solved by X-ray methods the crystal structures of the arene complexes, [Rh(durene)(diolefin)]ClO_4 (diolefin = TFB, Me_3TFB [9]). In these compounds two different positions of the durene relative to the diolefin moiety are observed.

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TABLE 1. CRYSTAL ANALYSIS PARAMETERS AT ROOM TEMPERATURE

Crystal data	Formulae	$[\mathrm{Rh(durene)(TFB)}]\mathrm{ClO_4}$	$[\mathrm{Rh(durene)(Me_3TFB)}]\mathrm{ClO_4}$
	Crystal habit	Yellow. Transparent. Sphere.	Yellow. Transparent. Prismatic.
	size (mm)	0,57 diameter	0,26 × 0,07 × 0,39
	Symmetry	$\bar{3}/m$ Rhombohedral $R\bar{3}c$. Acentric statistical test: N(Z), E's	$2/m$. Monoclinic $P2_1/n$
	Unit cell determination least-squares fit	46 reflexions $\theta(\mathrm{Cu}) \leqslant 45^\circ$	57 reflexions
	Unit cell dimensions (Å)	25,7586(5), 17,0059(4)	12,6686(6), 11,5565(3), 16,7269(8) $\beta = 104{,}023(5)^\circ$
	Packing: V (Å^3), Z	9771,7(3), 18	2375,9(1), 4
	D (g cm^{-3}), M, ($F000$)	1,72, 562,75, 5076	1,69, 604,83, 1224
Experimental data	Radiation, technique	Cu-$K_{\bar{\alpha}}$	Mo-$K_{\bar{\alpha}}$
		4-Circle PW1100 Philips-Diffractometer. Bisecting geometry.	
	Monochromator	Graphite oriented	
	Orientation	$0k0$: $\chi \sim -45^\circ$, $\phi \sim 359^\circ$ hhh: $\chi \sim -15^\circ$, $\phi \sim 315^\circ$	$0k0$: $\chi \sim 1^\circ$, $\phi \sim 96^\circ$ hhh: $\chi \sim 36^\circ$, $\phi \sim 61^\circ$
	Collection mode	$\theta \leqslant 25$	$\theta \leqslant 65$
	($\omega/2\theta$, 1°×1° det. apertures)	1,30, 1 min/reflex.	1,50, 1 min/reflex.
	Total, independent data	1963	4170
	Obs. data: $2\sigma_c(I)$	1791	2764
	Stability	Two reflexions every 90 min. No variation.	
	Absorption: faces	—	±010, ±102, ±$\bar{1}$02
	μ-Min., Mx. transmission	82,24, —	8,80, 0,943–0,792
Solution and refinement		[10]. X-Ray 70-System. Univac 1108.	
	Solution mode	Patterson	
	Refinement mode	Least-square on F's. Observed reflexions only. 4 blocks for the final L.S.	
	Final shift error	0,24	0,15
	Parameters: no. of variables,	368	420
	degrees of freedom,	1423	2344
	ratio of freedom	4,9	6,6
	w-scheme	Empirical as to give no trends in $\langle w\Delta^2\rangle$ vs. $\langle F_o\rangle$ or $\langle \sin\theta/\lambda\rangle$	
	ΔF	0,63	0,57
	Max. thermal values (Å^2)	$U_{33}(\mathrm{O2}) = 0{,}72(9)$	$U_{33}(\mathrm{O1}) = 0{,}32(2)$
	R, R_w	0,040, 0,045	0,060, 0,062
	Atomic factors	[11], International Tables for X-ray Crystallography; Neutral atoms; Real part of anomalous dispersion applied for Rh and Cl.	

Experimental

The complex [Rh(durene)(Me_3TFB)]ClO_4 was prepared as previously described [1]. The novel derivative [Rh(durene)(TFB)]ClO_4 was prepared analogously by treating $[RhCl(TFB)]_2$ [9] with $AgClO_4$ and durene. The yellow complexes were characterized by conventional methods [1,2]. All the relevant crystal structure data and procedures are listed in Table 1.

Results

Crystal structure parameters are given in Table 1. The final observed and calculated spectra were tested by δ-R_w plots [12], giving the values shown in Table 2. Figure 1 displays the atomic numbering. The most relevant bond distances, angles and selected torsion angles are shown in Tables 3 and 4, whilst final atomic coordinates are listed in Tables 5 and 6. The geometry of both molecules is compared by half normal probability plots of the interatomic dis-

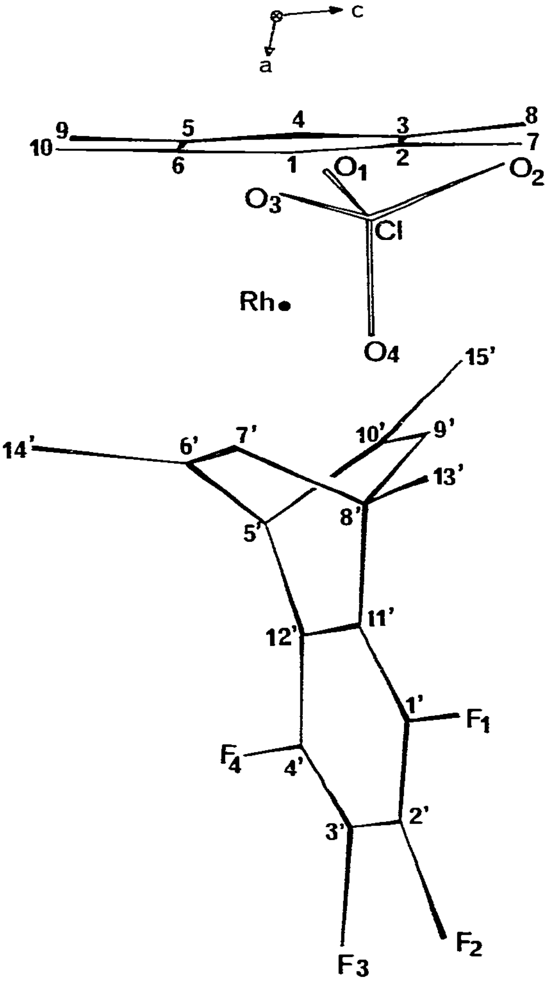

Fig. 1. A view of [Rh(durene)(Me_3TFB)]ClO_4 showing the atom numbering.

TABLE 2

NORMAL PROBABILITY RESULTS

Type	$\|F_o\|$ vs. $\|F_c\|$ full normal	$d(Me_3TFB)$ vs. $d(TFB)$ half normal
Total points	1834	108
Excluded	3	5
Total *R*	0.041	0.015
Slope	0.859(1)	1.765(13)
Intercept	0.040(1)	−0.026(12)
Correlation	0.999	0.997
Dp. Max.	±3.0	3.5

tances (see Table 2). A list of structure factors and thermal parameters can be obtained from the authors.

Discussion

The Rh—C(arene) distances (Table 3), together with the values of the torsion angles within the ring (Table 4) and the deviations from the least squares plane of the ring atoms (Fig. 2 and 3) show that in the TFB derivative the durene ligand has a distorted inverted boat conformation [2], whilst in the Me_3TFB analogue the ring adopts a skew conformation. This is analogous to the conformations present in the 1,4-$C_6H_4Me_2$ derivatives [1,2]. In Table 7 we show an analysis of the conformations of the arene ring in rhodium complexes of the type [Rh(arene)(diolefin)]ClO_4, according to the puckering parameters (Cremer and Pople [13]).

In the complexes described in this paper, and in other related compounds [1,2], the two carbon atoms of the ring opposite to the olefinic bonds are

(Continued on p. 392)

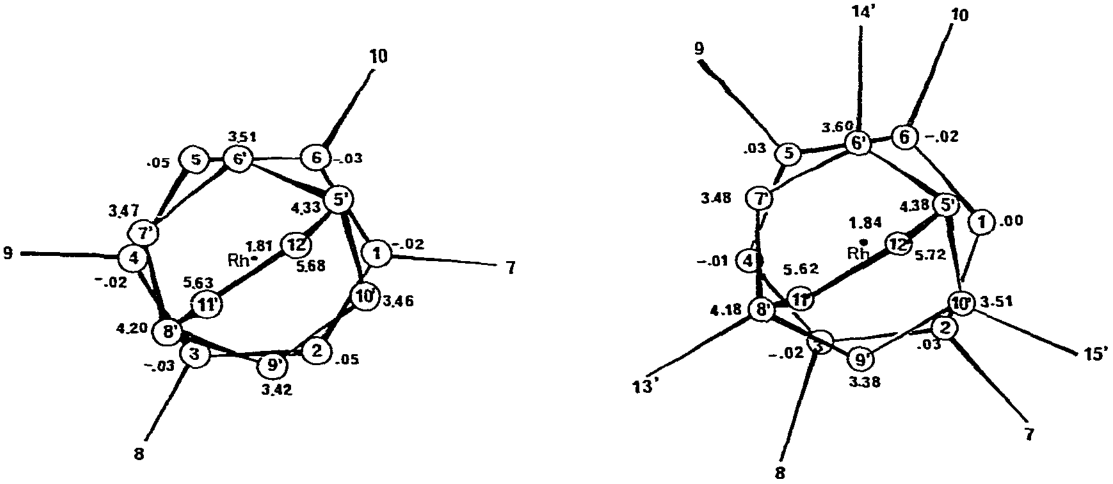

Fig. 2. Rhodium coordination as seen perpendicular to the arene ring, including deviations (Å) from the mean six-membered plane of the arene ring. Olefinic carbons of the coordinated TFB and Me_3TFB ligands are also included.

TABLE 3

BOND DISTANCES (Å) AND ANGLES (°)

	TFB	Me_3TFB		TFB	Me_3TFB
Rh—C(1)	2,331(8)	2,311(9)	C(1')—C(2')	1,396(35)	1,374(11)
Rh—C(2)	2,224(9)	2,282(10)	C(1')—F(1)	1,328(31)	1,351(10)
Rh—C(3)	2,320(7)	2,331(11)	C(1')—C(11')	1,406(17)	1,378(9)
Rh—C(4)	2,326(10)	2,309(9)	C(2')—C(3')	1,321(50)	1,382(13)
Rh—C(5)	2,249(10)	2,295(9)	C(2')—F(2)	1,340(20)	1,341(9)
Rh—C(6)	2,346(9)	2,359(8)	C(3')—C(4')	1,420(22)	1,365(11)
Rh—C(6')	2,137(9)	2,162(7)	C(3')—F(3)	1,358(28)	1,343(10)
Rh—C(7')	2,151(8)	2,124(8)	C(4')—C(12')	1,399(21)	1,350(11)
Rh—C(9')	2,139(10)	2,101(6)	C(4')—F(4)	1,299(25)	1,353(10)
Rh—C(10')	2,138(12)	2,166(7)	C(5')—C(6')	1,546(19)	1,517(10)
C(1)—C(2)	1,421(13)	1,406(15)	C(5')—C(10')	1,539(16)	1,524(12)
C(2)—C(3)	1,428(15)	1,426(13)	C(5')—C(12')	1,526(13)	1,529(10)
C(3)—C(4)	1,410(17)	1,392(15)	C(6')—C(7')	1,390(16)	1,378(12)
C(4)—C(5)	1,433(16)	1,412(15)	C(7')—C(8')	1,542(18)	1,532(10)
C(5)—C(6)	1,424(18)	1,406(14)	C(8')—C(9')	1,522(16)	1,530(11)
C(6)—C(1)	1,404(19)	1,382(15)	C(8')—C(11')	1,531(16)	1,524(11)
C(3)—C(8)	1,497(15)	1,489(19)	C(9')—C(10')	1,409(16)	1,408(11)
C(6)—C(10)	1,497(20)	1,496(17)	C(11')—C(12')	1,361(23)	1,412(11)
C(1)—C(7)/C(2)—C(7)	1,509(21)	1,526(16)	C(8')—C(13')	—	1,524(13)
C(4)—C(9)/C(5)—C(9)	1,485(27)	1,508(19)	C(6')—C(14')	—	1,506(11)
Cl—O(1)	1,376(17)	1,362(12)	C(10')—C(15')	—	1,497(13)
Cl—O(2)	1,275(35)	1,368(15)			
Cl—O(3)	1,332(31)	1,361(14)			
Cl—O(4)	1,320(58)	1,400(7)			

TABLE 3 (cont.)

	TFB	Me$_3$TFB		TFB	Me$_3$TFB
C(6)—C(1)—C(2)	118,7(10)	122,1(9)	C(6′)—C(5′)—C(10′)	97,1(9)	100,5(6)
C(1)—C(2)—C(3)	123,1(10)	119,7(9)	C(5′)—C(6′)—C(7′)	113,6(10)	112,5(6)
C(2)—C(3)—C(4)	118,0(9)	118,1(9)	C(6′)—C(7′)—C(8′)	113,8(10)	114,9(7)
C(3)—C(4)—C(5)	118,3(9)	121,1(9)	C(7′)—C(8′)—C(11′)	107,6(10)	110,3(6)
C(4)—C(5)—C(6)	123,0(10)	120,7(9)	C(7′)—C(8′)—C(9′)	98,6(9)	96,6(6)
C(5)—C(6)—C(1)	118,2(10)	118,2(9)	C(9′)—C(8′)—C(11′)	108,1(10)	107,8(6)
C(2)—C(3)—C(8)	119,6(10)	122,4(10)	C(8′)—C(9′)—C(10′)	114,3(10)	114,8(6)
C(4)—C(3)—C(8)	122,4(10)	119,5(10)	C(5′)—C(10′)—C(9′)	112,8(10)	111,2(6)
C(1)—C(6)—C(10)	122,6(13)	120,2(10)	C(1′)—C(11′)—C(8′)	123,7(13)	130,0(7)
C(5)—C(6)—C(10)	119,2(13)	121,6(10)	C(8′)—C(11′)—C(12′)	113,3(12)	111,9(6)
C(2)—C(1)—C(7)/C(1)—C(2)—C(7)	117,0(10)	121,2(9)	C(1′)—C(11′)—C(12′)	123,0(14)	117,8(7)
C(6)—C(1)—C(7)/C(3)—C(2)—C(7)	124,3(11)	118,9(9)	C(5′)—C(12′)—C(11′)	115,8(12)	114,0(6)
C(3)—C(4)—C(9)/C(4)—C(5)—C(9)	123,8(12)	117,4(10)	C(4′)—C(12′)—C(11′)	120,9(13)	120,1(7)
C(5)—C(4)—C(9)/C(6)—C(5)—C(9)	117,9(12)	121,8(10)	C(4′)—C(12′)—C(5′)	123,3(13)	125,7(7)
C(11′)—C(1′)—F(1)	122,5(16)	121,8(7)	C(11′)—C(8′)—C(13′)	—	117,2(7)
C(2′)—C(1′)—F(1)	122,6(18)	117,1(7)	C(7′)—C(8′)—C(13′)	—	112,0(7)
C(2′)—C(1′)—C(11′)	114,9(18)	121,1(7)	C(9′)—C(8′)—C(13′)	—	111,0(7)
C(1′)—C(2′)—F(2)	116,5(20)	119,6(8)	C(5′)—C(6′)—C(14′)	—	118,6(7)
C(1′)—C(2′)—C(3′)	123,1(23)	120,1(8)	C(7′)—C(6′)—C(14′)	—	125,1(7)
C(3′)—C(2′)—F(2)	120,4(22)	120,3(8)	C(9′)—C(10′)—C(15′)	—	126,3(7)
C(2′)—C(3′)—F(3)	121,7(22)	118,1(8)	C(5′)—C(10′)—C(15′)	—	119,5(7)
C(2′)—C(3′)—C(4′)	122,4(22)	119,0(8)	O(1)—Cl—O(2)	109,9(18)	112,0(8)
C(4′)—C(3′)—F(3)	115,8(20)	122,9(8)	O(1)—Cl—O(3)	114,0(18)	106,6(9)
C(3′)—C(4′)—F(4)	119,8(17)	117,9(8)	O(1)—Cl—O(4)	115,6(21)	110,0(8)
C(3′)—C(4′)—C(12′)	115,7(17)	121,8(8)	O(2)—Cl—O(3)	117,3(26)	106,9(8)
C(12′)—C(4′)—F(4)	124,5(15)	120,3(8)	O(2)—Cl—O(4)	92,7(29)	111,5(7)
C(10′)—C(5′)—C(12′)	107,9(10)	106,4(6)	O(3)—Cl—O(4)	105,7(33)	109,7(8)
C(6′)—C(5′)—C(12′)	107,9(10)	110,6(6)			

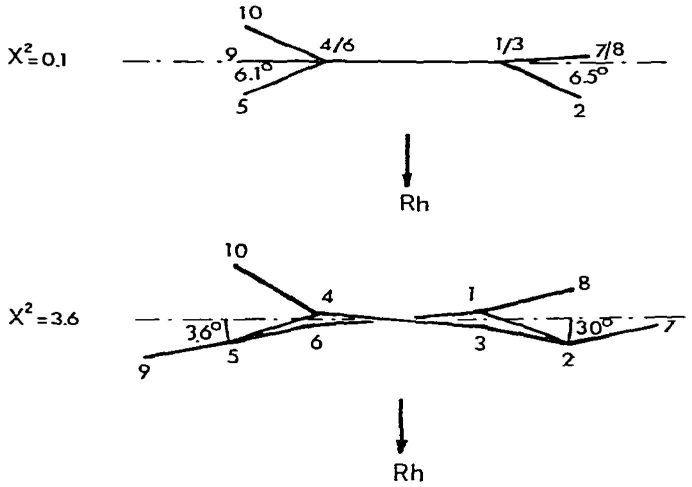

Fig. 3. The puckering of the arene rings in the TFB (above) and Me$_3$TFB (below) compounds, to show the different conformations and the angular deviations of the atoms of the cation.

TABLE 4

SELECTED TORSION ANGLES (°)

	TFB	Me$_3$TFB
6—1—2—3	7.3(15)	−2.6(15)
1—2—3—4	−7.4(15)	4.3(14)
2—3—4—5	0.4(14)	−1.3(14)
3—4—5—6	6.8(16)	−3.3(15)
4—5—6—1	−7.1(16)	4.9(14)
5—6—1—2	0.0(15)	−2.0(15)
11′—8′—5′—12′	0.2(9)	−0.8(5)
11′—8′—5′—10′	125.1(10)	−121.4(5)
11′—8′—5′—6′	−125.1(9)	126.2(5)
7′—8′—5′—12′	124.0(9)	−127.6(6)
7′—8′—5′—10′	−111.0(7)	111.8(6)
7′—8′—5′—6′	−1.2(5)	−0.6(5)
9′—8′—5′—12′	−124.3(10)	122.3(5)
9′—8′—5′—10′	0.7(7)	1.7(4)
9′—8′—5′—6′	110.5(6)	−110.7(5)
5′—6′—7′—8′	−2.3(14)	−1.2(9)
6′—7′—8′—9′	−58.1(11)	60.3(8)
7′—8′—9′—10′	58.7(12)	−61.1(8)
8′—9′—10′—5′	1.2(14)	3.1(9)
9′—10′—5′—6′	−60.9(11)	58.3(7)
10′—5′—6′—7′	61.8(11)	−59.9(8)
5′—6′—7′—8′	−2.3(14)	−1.2(9)
6′—7′—8′—11′	54.1(13)	−51.4(9)
7′—8′—11′—12′	−53.1(14)	51.7(8)
8′—11′—12′—5′	0.3(17)	−1.5(9)
11′—12′—5′—6′	51.6(15)	−51.1(9)
12′—5′—6′—7′	−49.6(13)	52.1(9)
5′—10′—9′—8′	1.2(14)	3.1(9)
10′—9′—8′—11′	−53.1(13)	52.6(8)
9′—8′—11′—12′	52.5(14)	−52.6(8)
8′—11′—12′—5′	0.3(17)	−1.5(9)
11′—12′—5′—10′	−52.3(15)	57.2(8)
12′—5′—10′—9′	50.5(13)	−57.1(8)

TABLE 5

FINAL ATOMIC COORDINATES FOR [Rh(durene)(TFB)]ClO$_4$

Atom	x	y	z
Rh	0.45812(1)	−0.03212(1)	0.25000(0)
C(1)	0.36126(4C)	−0.10719(42)	0.28181(50)
C(2)	0.36581(43)	−0.08769(43)	0.20268(57)
C(3)	0.40354(37)	−0.09324(35)	0.14580(44)
C(4)	0.44300(42)	−0.11266(35)	0.17190(57)
C(5)	0.44274(44)	−0.12605(37)	0.25375(69)
C(6)	0.40032(52)	−0.12675(43)	0.30803(52)
C(7)	0.31626(59)	−0.10232(72)	0.33347(100)
C(8)	0.40252(78)	−0.07528(65)	0.06236(65)
C(9)	0.48711(80)	−0.11707(78)	0.12027(157)
C(10)	0.39939(135)	−0.14745(91)	0.39056(93)
C(1′)	0.62748(59)	0.19229(57)	0.22049(151)
F(1)	0.64143(46)	0.20020(42)	0.14459(105)
C(2′)	0.65778(71)	0.23725(65)	0.27635(231)
F(2)	0.70168(43)	0.28995(32)	0.24945(113)
C(3′)	0.64405(80)	0.23002(74)	0.35191(194)
F(3)	0.67516(47)	0.27424(43)	0.40503(113)
C(4′)	0.59872(57)	0.17470(57)	0.38333(125)
F(4)	0.58710(52)	0.17009(50)	0.45818(80)
C(5′)	0.51943(43)	0.06550(46)	0.35174(72)
C(6′)	0.53706(40)	0.02068(41)	0.31821(65)
C(7′)	0.55271(38)	0.02974(40)	0.23909(71)
C(8′)	0.54663(45)	0.08082(44)	0.20118(76)
C(9′)	0.48043(43)	0.05693(38)	0.21768(63)
C(10′)	0.46503(43)	0.04780(43)	0.29802(69)
C(11′)	0.58288(43)	0.13715(43)	0.25114(101)
C(12′)	0.56820(46)	0.12855(46)	0.32877(89)
Cl	0.29653(10)	0.03257(10)	0.18895(14)
O(1)	0.31270(105)	0.09220(61)	0.19016(123)
O(2)	0.24662(118)	0.00228(101)	0.15335(344)
O(3)	0.30274(206)	0.01175(149)	0.25792(122)
O(4)	0.32525(242)	0.01775(200)	0.13744(200)

closer to the rhodium atom. It is noteworthy that with the sole exception of [Rh(durene)(Me$_3$TFB)]ClO$_4$, in all the complexes of the type [Rh(C$_6$H$_{6-x}$Me$_x$)-(diolefin)]ClO$_4$ the diolefin is not situated opposite to the substituted carbon atoms, which have a relatively lower π-electron density. In other words, the slight tendency of the coordinated arene to depart from planarity seems to be related to the π-electron density of the arene ring and to the tendency of rhodium(I) to achieve square-planar coordination.

The reason for the different disposition of the [Rh(durene)(Me$_3$TFB)]ClO$_4$ is not clear, but steric interaction cannot be excluded. There is no isomorphism with the related [Rh(1,4-C$_6$H$_4$Me$_2$)(Me$_3$TFB)]ClO$_4$ derivatives [1] although pseudoisomorphism is observed for the [Rh(durene)(TFB)]ClO$_4$ complex and all the [Rh(arene)(TFB)]ClO$_4$ complexes previously reported [2].

The rhodium distances to the best least squares plane through the durene ring is shorter for the TFB complex than for the Me$_3$TFB analogue (Fig. 2), as previously observed in [Rh(1,4-C$_6$H$_4$Me$_2$)(diolefin)]ClO$_4$ (diolefin = TFB or Me$_3$TFB) complexes, in spite of the higher lability in solution of the rhodium—

TABLE 6

FINAL ATOMIC COORDINATES FOR [Rh(durene)(Me$_3$TFB)]ClO$_4$

Atom	x	y	z
Rh	0.27228(3)	0.24690(7)	0.04720(2)
C(1)	0.12399(74)	0.36975(82)	0.01658(67)
C(2)	0.13172(69)	0.32051(78)	0.09464(61)
C(3)	0.12628(74)	0.19794(84)	0.10268(63)
C(4)	0.12071(71)	0.13048(76)	0.03287(63)
C(5)	0.11816(78)	0.18182(84)	−0.04420(63)
C(6)	0.11550(71)	0.30279(87)	−0.05317(61)
C(7)	0.13721(84)	0.39600(101)	0.17037(71)
C(8)	0.12928(122)	0.14071(143)	0.18292(89)
C(9)	0.11176(106)	0.10198(144)	−0.11655(87)
C(10)	0.10339(113)	0.35894(126)	−0.13548(76)
C(1′)	0.67639(50)	0.11574(71)	0.16790(45)
C(2′)	0.77499(65)	0.17036(87)	0.17755(54)
C(3′)	0.78019(63)	0.27912(71)	0.14431(56)
C(4′)	0.68637(67)	0.33050(71)	0.10175(54)
C(5′)	0.47839(59)	0.33288(65)	0.05173(45)
C(6′)	0.40917(45)	0.24905(87)	−0.00879(34)
C(7′)	0.40056(61)	0.14231(69)	0.02583(45)
C(8′)	0.46352(59)	0.13014(65)	0.11598(45)
C(9′)	0.40407(50)	0.22646(63)	0.15011(42)
C(10′)	0.41420(59)	0.33727(67)	0.11783(45)
C(11′)	0.58122(59)	0.16808(65)	0.12624(44)
C(12′)	0.58853(59)	0.27878(63)	0.09228(45)
C(13′)	0.44428(89)	0.01305(84)	0.15187(76)
C(14′)	0.39246(84)	0.27192(93)	−0.09965(52)
C(15′)	0.40083(82)	0.45037(84)	0.15787(63)
F(1)	0.67686(39)	0.01023(43)	0.20269(28)
F(2)	0.86578(38)	0.11817(47)	0.22025(32)
F(3)	0.87816(38)	0.32978(54)	0.15579(40)
F(4)	0.69367(41)	0.43685(45)	0.06972(37)
Cl	0.80130(16)	0.23602(25)	−0.08195(63)
O(1)	0.85317(91)	0.33600(95)	−0.05224(100)
O(2)	0.83776(82)	0.19246(122)	−0.14644(56)
O(3)	0.82702(118)	0.15699(109)	−0.01992(71)
O(4)	0.68861(56)	0.25384(99)	−0.10371(54)

TABLE 7

PUCKERING COMPARISON OF THE ARENE DISTRIBUTIONS (q_2, q_3 and Q values in Å, ϕ and θ in (°))

Compound	Cremer and Pople found parameters (n being any integer)				
	q_3	q_2	ϕ_2	θ	Q
Theoretical Boat	0	q_2	0+60.n	90	q_2
Theoretical Skew	0	q_2	30+60.n	90	q_2
[Rh(durene)(TFB)]ClO$_4$	−0.002	0.086	241.5	91.0	0.086
[Rh(C$_6$H$_4$Me$_2$)(TFB)]ClO$_4$	0.016	0.077	242.9	79.0	0.078
[Rh(C$_6$H$_3$Me$_3$)(TFB)]ClO$_4$	−0.022	0.072	229.0	106.9	0.075
[Rh(C$_6$Me$_6$)(TFB)]ClO$_4$	0.000	0.073	331.4	90.3	0.073
[Rh(durene)(Me$_3$TFB)]ClO$_4$	−0.003	0.050	81.3	93.0	0.050
[Rh(C$_6$H$_4$Me$_2$)(Me$_3$TFB)]ClO$_4$	−0.003	0.087	81.8	92.2	0.087

TABLE 8

OLEFINIC C—C DISTANCES FOR [Rh(arene)(diolefin)]ClO_4 COMPLEXES

Compound	Olefinic C—C distances (Å) with σ's	Reference
Free TFB ligand	1.302(4), 1.306(5)	[14]
[Rh(durene)(TFB)]ClO_4	1.390(16), 1.409(16)	This work
[Rh($C_6H_4Me_2$)(TFB)]ClO_4	1.409(18), 1.423(14)	[2]
[Rh($C_6H_3Me_3$)(TFB)]ClO_4	1.332(26), 1.399(19)	[2]
[Rh(C_6Me_6)(TFB)]ClO_4	1.381(21), 1.423(18)	[2]
[Rh(durene)(Me_3TFB)]ClO_4	1.378(12), 1.408(11)	This work
[Rh($C_6H_4Me_2$)(Me_3TFB)]ClO_4	1.388(11), 1.390(12)	[1]

arene bond in TFB derivatives [1]. These rhodium—arene distances seem to be related to the ancillary ligand and increase in the order: TFB (1.81—1.83 Å) [2] < Me_3TFB (1.83—1.84 Å) [1] < P-donor ligands (1.86—1.88 Å) [3,5,6,8].

A significant increase of the olefinic C—C distances compared with those in the free ligand is observed for [Rh(durene)(TFB)]ClO_4, as well as for other related derivatives [1,2]. Various lengths of the olefinic C—C bonds is observed in the complexes shown in Table 8.

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