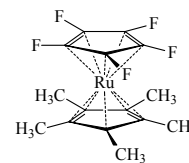


929 $\text{C}_{15}\text{H}_{15}\text{F}_5\text{Ru}$
ED, DFT
calculations

**1,2,3,4,5-Pentafluoro-1',2',3',4',5'-
pentamethylruthenocene**

C_5 assumed



r_a	\AA^a	θ_a	deg^a
$\text{Ru}-\text{C}^b$	2.178(2)	$\text{C}-\text{C}-\text{H}$	111.3(4) c
$\Delta(\text{Ru}-\text{C})^d$	0.053(8) c	φ_1^e	4.2(6)
$\text{C}-\text{C}^b$	1.429(3)	φ_2^f	2.1(11)
$\Delta(\text{C}-\text{C})^g$	0.012(6) c	twist(ring) h	-1.7(63)
$\text{C}(1')-\text{C}(\text{m})$	1.490(8)	twist(CH_3) i	-32(13)
$\text{C}-\text{H}$	1.096(4) c		
$\text{C}-\text{F}$	1.329(3)		

Local C_{3v} symmetry was assumed for the $\text{C}-\text{CH}_3$ groups.
The nozzle temperature was 454 K.

a) Estimated standard errors.

b) Mean value for two rings.

c) Restrained to the value from B3PW91/SDD calculations.

d) $[\text{Ru}-\text{C}(1')] - [\text{Ru}-\text{C}(1)]$.

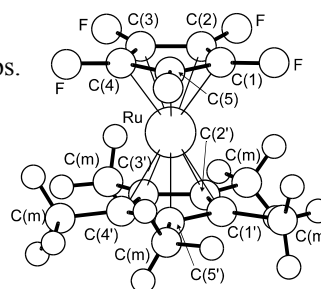
e) Angle between the ring plane and the $\text{C}-\text{F}$ bond, away from the Ru atom.

f) Angle between the ring plane and the $\text{C}(1')-\text{C}(\text{m})$ bond, away from the Ru atom.

g) $[\text{C}(1')-\text{C}(2')] - [\text{C}(1)-\text{C}(2)]$.

h) Clockwise twisting of the cyclopentadienyl rings, zero position when the rings are eclipsed.
The final result of the ED analysis is listed. The relative conformation of the two rings could not be determined by this ED analysis, but it appeared to support a more eclipsed conformation over a staggered one, and nearly free rotation was suggested.

i) Clockwise rotation of methyl group from the position when one of the $\text{C}-\text{H}$ bonds is *anti* with respect to the $\text{X}\dots\text{Ru}$ direction (X is the center of the ring).



Johnston, B.F., Rankin, D.W.H., Robertson, H.E., Hughes, R.P., Lompfrey, J.R.:
Organometallics **21** (2002) 4840.