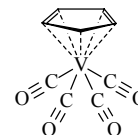


867
ED $\text{C}_9\text{H}_5\text{O}_4\text{V}$ **Cyclopentadienyltetracarbonylvanadium**

(see comment)

Tetracarbonyl(η^5 -2,4-cyclopentadien-1-yl)vanadium

r_g	\AA^a	θ^b	deg a
V–C(6)	1.963(7)	V–C(6)≡O(6) c	177(11)
C(6)≡O(6)	1.135(4)	X...V–C(6) d	120.1(22)
C–C (ring)	1.405(6)	X...C–H d e	171(19)
C–H	1.123 f	C(6)–V–C(7) g	75.4(20)
V–C(1)	2.282(13) g	τ^d h	9 i



Local C_{4v} symmetry for the $\text{V}(\text{CO})_4$ moiety and local C_{5v} symmetry for the VC_5H_5 group were assumed. The relative positions of these two groups could not be determined unequivocally. The models with an eclipsed or staggered configuration fitted the experimental data equally as well as a model which allows for free rotation of the C_5H_5 ring with respect to the $\text{V}(\text{CO})_4$ group. The parameters are given here for the staggered model.

The sample temperature was 95 °C.

a) Twice the estimated standard errors.

b) Unidentified, possibly θ_a .

c) C≡O bent towards the ring.

d) X is the center of the cyclopentadienyl ring.

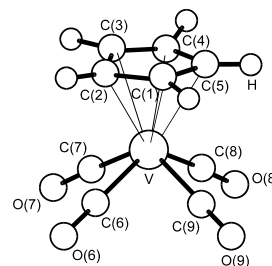
e) C–H bent away from the vanadium atom.

f) Kept constant in the final refinement.

g) Dependent parameter.

h) Torsional angle, C(6)–V...X...C(1); $\tau = 0^\circ$ for the *syn* position.

i) Assumed.



Almond, M.J., Page, E.M., Rice, D.A., Hagen, K.: J. Organomet. Chem. **511** (1996) 303.