

Charles B. Duke III,^a Tung T. To,^a
 Charles R. Ross II^b and
 Theodore J. Burkey^{a*}

^aDepartment of Chemistry, University of Memphis, 213 Smith Chemistry Building, Memphis, TN 38152-3550, USA, and ^bSt. Jude Children's Research Hospital, 332 North Lauderdale, Memphis, TN 38105-2794, USA

Correspondence e-mail: tburkey@memphis.edu

Key indicators

Single-crystal X-ray study
 T = 173 K
 Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
 R factor = 0.026
 wR factor = 0.070
 Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

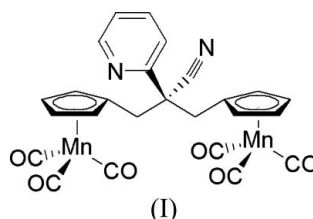
{ μ -1,1'-[2-Cyano-2-(2-pyridyl)propane-1,3-diyl]-di- η^5 -cyclopentadienyl}bis[tricarbonylmanganese(II)]

The dinuclear title compound, $[\text{Mn}_2(\text{C}_{19}\text{H}_{16}\text{N}_2)(\text{CO})_6]$, was isolated *en route* to other photochromic organometallic targets. The structure features two bridged half-sandwich cyclopentadienylmanganese centers.

Received 27 March 2007
 Accepted 18 April 2007

Comment

The synthesis of photochromic organometallic systems has led us to a variety of functionalized arene-metal-carbonyl complexes and several unexpected side-products. In the present work, a condensation of the anion of 2-pyridine-acetonitrile with cymantrene methyl chloride, $[\text{Mn}(\eta^5\text{-C}_5\text{H}_4\text{CH}_2\text{Cl})(\text{CO})_3]$, led to the title compound, (I), an unexpected dinuclear complex (To *et al.*, 2007).



In the structure of (I), atoms Mn1 and Mn2 are 1.770 (1) and 1.769 (1) Å from the respective least-squares planes of their arene rings. The average distances from the metal atoms to the ring C atoms are 2.143 (4) and 2.141 (4) Å for Mn1 and Mn2, respectively. Individual Mn–C distances are in the ranges 2.140 (2)–2.146 (2) Å for Mn1 and 2.138 (2)–2.144 (2) Å for Mn2, indicating no significant distortion of the Mn–arene bonds. The average Mn–CO distances are

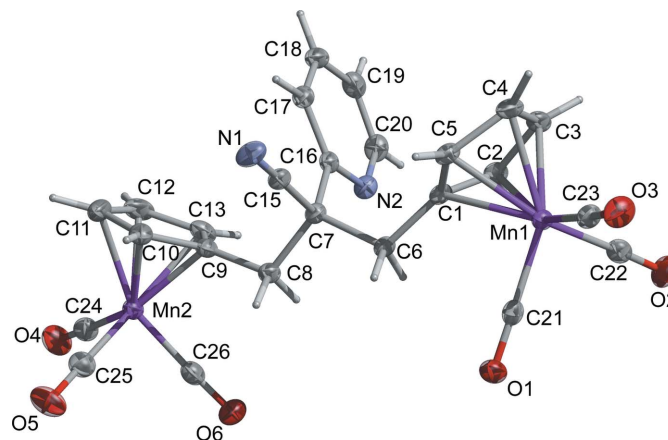


Figure 1
 The molecular structure of (I), showing 50% probability displacement ellipsoids and the labeling scheme used.

1.802 (3) and 1.798 (3) Å for Mn1 and Mn2, respectively. The nearly 90° angles between adjacent CO ligands show that the geometries about the metal centers are pseudooctahedral.

Experimental

Thorough experimental details for the synthesis of (I) and its ¹H and ¹³C NMR spectra will be submitted elsewhere (To *et al.*, 2007). Diffraction-quality crystals were obtained from evaporation of an ethyl acetate–hexanes (1:4) solution.

Crystal data

[Mn ₂ (C ₁₀ H ₁₆ N ₂)(CO) ₆]	$V = 2295.0 (1) \text{ \AA}^3$
$M_r = 550.28$	$Z = 4$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation
$a = 12.3281 (3) \text{ \AA}$	$\mu = 9.35 \text{ mm}^{-1}$
$b = 14.9809 (4) \text{ \AA}$	$T = 173 (2) \text{ K}$
$c = 12.7137 (3) \text{ \AA}$	$0.19 \times 0.12 \times 0.05 \text{ mm}$
$\beta = 102.202 (1)^\circ$	

Data collection

Bruker X8 PROTEUM CCD diffractometer	45918 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	4204 independent reflections
$T_{\min} = 0.259$, $T_{\max} = 0.626$	3998 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$	316 parameters
$wR(F^2) = 0.070$	H-atom parameters constrained
$S = 1.05$	$\Delta\rho_{\max} = 0.38 \text{ e \AA}^{-3}$
4204 reflections	$\Delta\rho_{\min} = -0.22 \text{ e \AA}^{-3}$

All H atoms were treated using an isotropic idealized riding model, with C–H distances in the range 0.95–0.99 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *PROTEUM2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SADABS* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997), Mercury (Version 1.4.2, Build 2; Macrae *et al.*, 2006) and *RASTER3D* (Merritt & Bacon, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *publCIF* (Westrip, 2007).

The authors acknowledge support provided by the National Institute of Standards and Technology (grant No. 70NANB4H1093) and the National Science Foundation (grant No. CHE-0227475 to TJB, CBD, TTT). Support of this research by the Cancer Center Support CORE Grant (No. P30 CA-21765) and the American Lebanese Syrian Associated Charities (ALSAC) is gratefully acknowledged by CRR.

References

- Bruker (2000). *SADABS*. Version 2.03. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2005). *SAINT* (Version 7.12a) and *PROTEUM2* (Version 1.0). Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
- Merritt, E. A. & Bacon, D. J. (1997). *Methods in Enzymology*, Vol. 277, *Macromolecular Crystallography*, Part B, edited by C. W. Carter Jr & R. M. Sweet, pp. 505–524. New York: Academic Press.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- To, T. T., Duke, C. B. III, Junker, C. S., O'Brien, C. M., Ross, C. R. II, Barnes, C. E., Webster, C. E. & Burkey, T. J. (2007). *Organometallics*. In preparation.
- Westrip, S. P. (2007). *publCIF*. In preparation.