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Key indicators

Single-crystal X-ray study
T = 296 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.024
wR factor = 0.064
Data-to-parameter ratio = 14.2

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

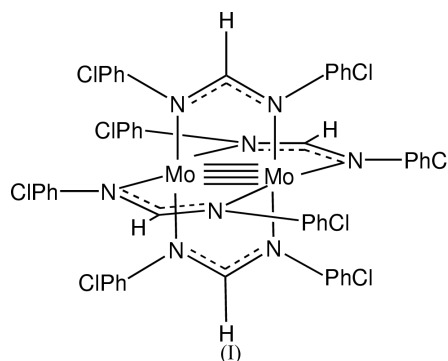
Tetrakis[μ -*N,N'*-bis(4-chlorophenyl)formamidinato-*N:N'*]dimolybdenum(II)

The title compound, $[\text{Mo}_2(\text{C}_{13}\text{H}_9\text{Cl}_2\text{N}_2)_4]$, is a tetra-chelate 'paddle wheel' complex of quadruply bonded dimolybdenum(II). Coordination of the four chloro-substituted formamidinate ligands occurs through the ligand N atoms. The centroid of the Mo—Mo bond is located on an inversion center. The Mo—Mo bond length is 2.0899 (12) Å.

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Comment

Metal–metal interactions are central to the behavior of a wide variety of molecules, clusters, interfaces, and materials. Our interest in the bonding of metal atoms to each other has led us to examine the electronic structures of numerous such systems *via* gas-phase photoelectron spectroscopy (Lichtenberger *et al.*, 1999, 2000). Part of this effort has been focused on understanding the effect of substitution of functional groups at the phenyl rings of the diphenylformamidinate ligand on the electronic structure of metal–metal bonded systems as a whole. As we intend to report shortly, the use of various substituents on the formamidinate ligand set affects the relative ease of the gas-phase oxidation of the various components of the Mo—Mo quadruple bond of $\text{Mo}_2(\text{form})_4$ [form = *N,N'*-bis(4-*X*-phenyl)formamidinate] and makes for an interesting comparison with the solution-phase oxidation potentials reported by Ren and coworkers (Lin *et al.*, 1995, 1996). The crystal structure of the 3-Cl-Ph derivative related closely to the title 4-Cl-Ph complex, (I), was determined by Lin *et al.* (1996).



Experimental

The substituted formamidines and the $\text{Mo}_2(\text{form})_4$ systems were prepared according to published syntheses (Cotton *et al.*, 1989). Crystals were grown by the diffusion of hexanes into dichloromethane solution.

Crystal data

[Mo₂(C₁₃H₉Cl₂N₂)₄]
M_r = 1248.37
 Triclinic, *P* $\bar{1}$
a = 10.347 (2) Å
b = 11.496 (2) Å
c = 12.569 (3) Å
 α = 106.61 (3)°
 β = 92.04 (3)°
 γ = 114.55 (3)°
V = 1282.7 (4) Å³

Z = 1
D_x = 1.616 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 25 reflections
 θ = 20–23°
 μ = 0.95 mm⁻¹
T = 296 (1) K
 Block, yellow
 0.33 × 0.33 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 ω -2 θ scans
 Absorption correction: ψ scan (North *et al.*, 1968)
*T*_{min} = 0.744, *T*_{max} = 0.833
 4498 measured reflections
 4498 independent reflections

4196 reflections with *I* > 2σ(*I*)
 θ_{max} = 25.0°
h = 0 → 12
k = -13 → 12
l = -14 → 14
 3 standard reflections
 frequency: 60 min
 intensity decay: 0.1%

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.024
wR (*F*²) = 0.064
S = 1.08
 4498 reflections
 316 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0330P)^2 + 0.5743P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Mo1—Mo1 ¹	2.0899 (12)	Mo1—N2 ¹	2.1602 (18)
Mo1—N3	2.1342 (19)	Mo1—N4 ¹	2.1751 (18)
Mo1—N1	2.1585 (18)		
Mo1 ¹ —Mo1—N3	93.63 (5)	Mo1 ¹ —Mo1—N2 ¹	91.62 (6)
Mo1 ¹ —Mo1—N1	93.78 (6)	Mo1 ¹ —Mo1—N4 ¹	91.91 (5)

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

H atoms were added at idealized positions, constrained to ride on the atom to which they are bonded and given displacement parameters equal to 1.2 or 1.5*U*_{iso} of that bonded atom.

Data collection: *CAD-4 Operations Manual* (Enraf–Nonius, 1977); cell refinement: *CAD-4 Operations Manual*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

This title structure was determined in the Molecular Structure Laboratory of the Department of Chemistry, University of Arizona, Tucson, USA.

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