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#### Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.016$  Å  
Disorder in main residue  
 $R$  factor = 0.064  
 $wR$  factor = 0.110  
Data-to-parameter ratio = 14.7

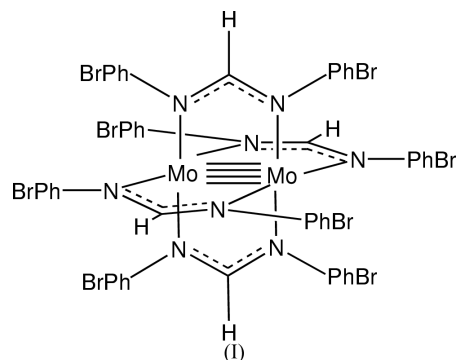
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Tetrakis[ $\mu$ - $N,N'$ -bis(4-bromophenyl)formamidinato- $N:N'$ ]dimolybdenum(II)

The title compound,  $[\text{Mo}_2(\text{C}_{13}\text{H}_9\text{Br}_2\text{N}_2)_4]$ , is a tetra-chelate 'paddle wheel' complex of quadruply bonded dimolybdenum(II). The centroid of the Mo—Mo bond is located on an inversion center and the bond length is 2.0869 (19) Å.

#### Comment

The present structural report is the complement of the accompanying communication of tetrakis[ $\mu$ - $N,N'$ -bis(4-chlorophenyl)formamidinato- $N:N'$ ]dimolybdenum(II) (Lynn *et al.*, 2001). Both reports describe the structural determination of Mo—Mo bound compounds studied by Lichtenberger and colleagues *via* gas-phase photoelectron spectroscopy (Lichtenberger *et al.*, 1999, 2000). Compounds of the general form  $\text{Mo}_2(\text{form})_4$  [form =  $N,N'$ -bis(4- $X$ -phenyl)formamidinate] feature a quadruple metal–metal bond with unique electronic characteristics. Thorough investigation of such systems will elucidate some of the subtle nature of metal–metal interactions, which are of fundamental interest to a wide range of research efforts (Lin *et al.*, 1995, 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 a dichloro-methane solution.

#### Crystal data

$[\text{Mo}_2(\text{C}_{13}\text{H}_9\text{Br}_2\text{N}_2)_4]$   
 $M_r = 1604.05$   
Triclinic,  $P\bar{1}$   
 $a = 10.437$  (2) Å  
 $b = 11.610$  (2) Å  
 $c = 12.801$  (3) Å  
 $\alpha = 107.00$  (3)°  
 $\beta = 92.56$  (3)°  
 $\gamma = 113.31$  (3)°  
 $V = 1339.4$  (5) Å<sup>3</sup>

$Z = 1$   
 $D_x = 1.989$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 25 reflections  
 $\theta = 10$ – $15^\circ$   
 $\mu = 6.48$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
Plate, yellow  
 $0.18 \times 0.12 \times 0.03$  mm

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## Data collection

Enraf–Nonius CAD-4 diffractometer	2283 reflections with $I > 2\sigma(I)$
$\omega$ -2 $\theta$ scans	$\theta_{\max} = 25.0^\circ$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$h = 0 \rightarrow 12$
$T_{\min} = 0.601$ , $T_{\max} = 0.825$	$k = -13 \rightarrow 12$
4717 measured reflections	$l = -15 \rightarrow 15$
4717 independent reflections	3 standard reflections
	frequency: 60 min
	intensity decay: 1.2%

## Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2]$
$wR(F^2) = 0.110$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\max} = 0.003$
4717 reflections	$\Delta\rho_{\max} = 0.58 \text{ e } \text{\AA}^{-3}$
320 parameters	$\Delta\rho_{\min} = -0.75 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Mo1—Mo1 <sup>1</sup>	2.0869 (19)	Mo1—N4	2.171 (7)
Mo1—N1	2.117 (7)	Mo1—N3 <sup>1</sup>	2.178 (7)
Mo1—N2 <sup>1</sup>	2.144 (7)		
Mo1 <sup>1</sup> —Mo1—N1	93.60 (19)	Mo1 <sup>1</sup> —Mo1—N4	91.3 (2)
Mo1 <sup>1</sup> —Mo1—N2 <sup>1</sup>	93.7 (2)	Mo1 <sup>1</sup> —Mo1—N3 <sup>1</sup>	91.98 (19)

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

One of the bromine substituents (Br1) of a formamidinate ligand was found to be disordered. This disorder was likely due to librational motion of the entire PhBr group perpendicular to the PhBr plane. To address the disorder, Br1 was split into two sites (Br1 and Br1'), which were forced to have identical displacement parameters. Subsequent refinement of the bromine site-occupancy factors resulted in occupancies of 0.828 and 0.172 (4) for Br1 and Br1', respectively. The least occupied site (Br1') is out of the PhBr plane, while the Br1 site is in the plane. The sites of the phenyl ring C atoms

were not split as an approximation. 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 times  $U_{\text{iso}}$  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 structure was determined in the Molecular Structure Laboratory of the Department of Chemistry, University of Arizona, Tucson, USA.

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