SHORT-FORMAT PAPERS

Contributions intended for publication under this heading should follow the format given in the Chechlist for Authors [*Acta Cryst.* (1985). C**41**, 1–4].

Acta Cryst. (1985). C**41**, 995–996

An Organomolybdenum Complex

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(*Received* 10 *October* 1984; *accepted* 25 *February* 1985)

Abstract. (η-Allyl)bromodicarbonyl(*N,N'*-dicyclohexylethanediimine)molybdenum(II), [$MoBr(C_3H_5)(CO)_2(C_{14}H_{24}N_2)$], $M_r = 493{\cdot}30$, orthorhombic, *Pnam*, $a = 12{\cdot}541$ (1), $b = 8{\cdot}318$ (1), $c = 19{\cdot}503$ (1) Å, $V = 2034{\cdot}5$ Å^3, $Z = 4$, $D_x = 1{\cdot}611$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 7{\cdot}322$ mm^{-1}, $F(000) = 1000$, $T = 293$ K, final $R = 0{\cdot}088$ for 1267 unique observed reflections. The Mo atom shows octagonal coordination with a mirror plane passing through it, the Br atom and the central C atom of the η-allyl group. Bonds to Mo are Mo—Br = 2·649 (2), Mo—N = 2·221 (8), Mo—C(allyl) = 2·179 (17), and Mo—C(carbonyl) = 1·965 (14) Å.

Experimental. Tabular crystal, 0·13 × 0·10 × 0·05 mm, non-standard setting of space group *Pnma* (No. 62) used, Enraf–Nonius CAD-4 diffractometer, Ni-filtered radiation, moving-crystal/moving-counter technique, $2\theta < 140°$, lattice parameters from θ measurements on 45 reflections, no absorption corrections, $h = -15$ to 15, $k = -10$ to 10, $l = 0$ to 23, reflection 402 as intensity standard, average count 5484·5 with σ (calculated from distribution of measurements) = 103·9. 4215 reflections measured and merged using *SHELX*76 (Sheldrick, 1976), 1651 unique reflections, merging $R_{int} = 0{\cdot}072$, 384 excluded during refinement [$F_o < 3\sigma(F_o)$]. Mo and Br positions from Patterson function, other non-H atoms from Fourier syntheses, based on phases defined by Mo and Br; least-squares refinement, F magnitudes; isotropic and then anisotropic temperature factors gave $R = 0{\cdot}088$, $wR = 0{\cdot}0676$ including H atoms at calculated positions. Weights given by $w = 1/[\sigma^2(F) +$

Table 1. *Atom coordinates* (×10^4) *and equivalent isotropic temperature factors* (Å^2 ×10^4)

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Mo	1126 (1)	5274 (2)	2500	306
Br	3189 (1)	4591 (3)	2500	522
C(1)	1463 (9)	7021 (14)	1857 (7)	386
C(2)	−610 (14)	5195 (25)	2500	560
C(3)	−406 (10)	5976 (16)	3097 (7)	530
C(10)	940 (9)	1797 (13)	2124 (6)	419
C(11)	1129 (10)	3129 (12)	1061 (6)	379
C(12)	179 (8)	2351 (16)	702 (7)	443
C(13)	308 (10)	2458 (16)	−68 (6)	453
C(14)	1350 (9)	1652 (15)	−295 (7)	446
C(15)	2289 (9)	2335 (17)	78 (7)	491
C(16)	2161 (9)	2307 (17)	854 (7)	465
O(1)	1676 (9)	8076 (11)	1491 (5)	720
N(1)	1017 (7)	3131 (10)	1824 (5)	302

Table 2. *Bond lengths* (Å) *and angles* (°)

Mo—Br	2·649 (2)	C(11)—N(1)	1·494 (14)
C(1)—Mo	1·965 (14)	C(11)—C(12)	1·527 (15)
C(2)—Mo	2·179 (17)	C(12)—C(13)	1·513 (16)
N(1)—Mo	2·221 (8)	C(13)—C(14)	1·534 (17)
C(1)—O(1)	1·162 (13)	C(14)—C(15)	1·497 (16)
C(2)—C(3)	1·358 (16)	C(15)—C(16)	1·521 (16)
C(10)—N(1)	1·259 (12)	C(16)—C(11)	1·519 (16)
C(10)—C(10′)	1·465 (23)		
C(2)—Mo—Br	165·9 (6)	N(1)—C(11)—C(12)	112·6 (10)
C(2)—Mo—C(1)	103·7 (5)	N(1)—C(11)—C(16)	110·2 (10)
C(2)—Mo—N(1)	85·1 (5)	C(12)—C(11)—C(16)	110·6 (9)
Br—Mo—C(1)	87·1 (3)	C(11)—C(12)—C(13)	110·3 (11)
Br—Mo—N(1)	83·6 (2)	C(12)—C(13)—C(14)	110·6 (11)
C(1)—Mo—N(1)	103·2 (4)	C(13)—C(14)—C(15)	111·4 (11)
C(3)—C(2)—Mo	78·3 (10)	C(14)—C(15)—C(16)	113·3 (11)
C(10)—N(1)—Mo	115·9 (8)	C(15)—C(16)—C(11)	110·4 (11)
C(11)—N(1)—Mo	125·9 (7)	C(1)—Mo—C(1′)	79·3 (7)
O(1)—C(1)—Mo	178·1 (11)	N(1)—Mo—C(1′)	170·1 (4)
C(3)—C(2)—C(3′)	118·1 (11)	N(1)—Mo—N(1′)	72·8 (6)
C(11)—N(1)—C(10)	118·0 (9)		

A prime denotes the equivalent position $x, y, \frac{1}{2} - z$.

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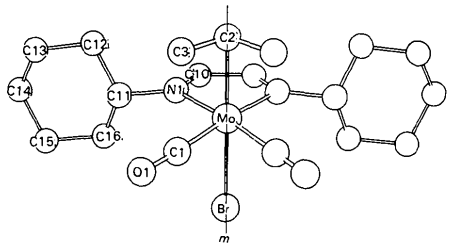

Fig. 1. Diagram of the molecule showing numbering scheme.

$0{\cdot}000407F^2$]. In final cycle max. LS shift/error 0·029, average 0·002. Final difference synthesis max. and min. peaks 1·53 and $-1{\cdot}33$ e Å^{-3} respectively. Scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1* gives the atom parameters and Table 2 bond lengths and angles. Fig. 1 shows the molecule and numbering scheme; Fig. 2 the packing in the unit cell.

Related literature. This compound is one of a series as prepared by Hsieh & West (1976). Previous structures of the series are listed in Graham, Akrigg & Sheldrick (1983).

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares-plane values have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42082 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

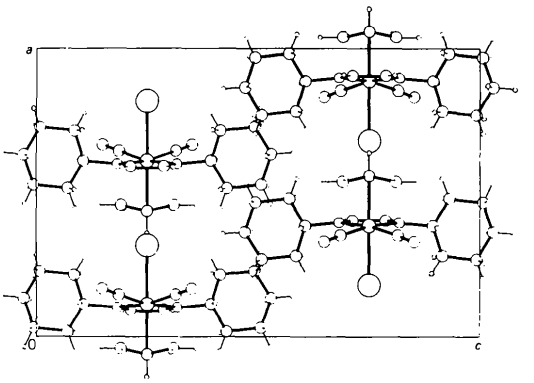

Fig. 2. *b*-axis-projection packing diagram (*PLUTO*78, Motherwell & Clegg, 1978).

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1985). C**41**, 996

Structure d'un polyphosphate mixte de lithium et de potassium, $LiK(PO_3)_2$: errata.

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(*Reçu le* 3 *septembre* 1984, *accepté le* 8 *février* 1985)

Abstract

Two errors and two omissions are corrected in the paper by El-Horr, Bagieu & Tordjman [*Acta Cryst.* (1983), C**39**, 1597–1599]. The correct absorption coefficient μ calculated for $\lambda = 0{\cdot}7107$ Å is 1·480 mm^{-1}.

Dans *Environnement du potassium* la phrase quatrième doit être 'Les polyèdres de coordination de K(1) et de K(2) partagent une face commune: O(*E*11)–O(*E*21)–O(*L*12)' et la sixième 'Les polyèdres de coordination autour de deux atomes K symétriques par rapport à l'axe 2_1 peuvent être reliés entre eux soit par un sommet, soit par une arête'. Dans *Enchaînement des polyèdres* LiO_4 *et* KO_9 la phrase troisième doit être 'L'enchaînement peut se faire par la mise en commun soit d'un sommet, soit d'une arête selon **c**'.

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