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μ -(η -Diarseno- μ -As, μ -As')-bis(dicarbonyl- η ⁵-propylcyclopentadienylmolybdenum)-(Mo-Mo) and Bis- μ -(η -diarseno- μ -As, μ -As')-bis(carbonyl- η -cyclopentadienylmolybdenum)(Mo-Mo)

BY ANTHONY-J. DIMAIO, CYNTHIA J. BALDACCHINI AND ARNOLD L. RHEINGOLD*

Department of Chemistry, University of Delaware, Newark DE 18716, USA

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Abstract. $[Mo_2As_2(C_8H_{11})_2(CO)_4]$ (1), $M_r = 668.14$, monoclinic, I2/a, a = 17.297 (4), b = 7.302 (2), c =17.868 (5) Å, $\beta = 90.60$ (2)°, V = 2256.8 (10) Å³, Z =4, 0.5 molecules/asymmetric unit, $D_x = 1.97 \text{ g cm}^{-3}$, λ (Mo K α) = 0.71073 Å, μ = 41.8 cm⁻¹, F(000) = 1296, T = 296 K, $R_F = 2.66\%$ for 2284 reflections. The structure is the isopropyl substituted analogue of a previously reported cluster, $[Mo_2As_2(C_5H_5)_2(CO)_4]$ [Foley, Rheingold & Sullivan (1982). J. Am. Chem. Soc. 104, 4727-4729]. The heavy atoms of (1) form a distorted tetrahedral cluster with an *i*-PrCp group and two carbonyl units attached to each Mo atom with As - As = 2.302 (1), Mo - As = 2.576 (1) and 2.666 (1), and Mo-Mo = 3.064 (1) Å. $[Mo_2(As_2)_2 (C_5H_5)_2(CO)_2$ (2), $M_r = 677.78$, monoclinic, C2/c, a = 25.435 (6), b = 8.308 (2), c = 16.182 (4) Å, $\beta =$ 106.89 (2)°, V = 3272 (1) Å³, Z = 8, $D_x = 2.75$ g cm⁻¹, λ (Mo K α) = 0.71073 Å, $\mu = 99.7$ cm⁻¹ $D_r =$ $F(000) = 2510, T = 296 \text{ K}, R_F = 4.77\% \text{ for } 2113$ reflections. The structure is an analogue of the methylated bis(diarsenic) structure. $[(\eta^{5} -$ MeC₅H₄)Mo(CO)]₂, reported earlier [DiMaio & Rheingold (1987). J. Chem. Soc. Chem. Commun. pp. 404-405]. The structure contains two Mo₂As₂ tetrahedra sharing the Mo-Mo edge. Each tetrahedron resembles (1). The Mo-Mo bond forming the edge bridge is 2.959 (1) Å, and the As-As bond lengths are 2.272 (2) and 2.281 (2) Å. The four Mo-As bond lengths average 2.617(2) Å. In both (1) and (2), the As—As distances are very short, indicating considerable multiple bond character.

Experimental. For (1), red-orange crystals from methylene chloride/hexane $(0.18 \times 0.18 \times 0.30 \text{ mm})$; Nicolet R3m diffractometer with graphite monochromator; ω scans; lattice parameters from leastsquares fit of 25 reflections ($20 < 2\theta < 25^{\circ}$); empirical absorption correction (six reflections, ψ scan, 216 data), $T_{\text{max}}/T_{\text{min}} = 1.18$; $2\theta_{\text{max}} = 55^{\circ}$ ($h = \pm 23$, $k = \pm 10$, $l = \pm 24$); standard reflections 0.0.10, 040, $\overline{10}$, 0,4, < 1% intensity variation. 2895 reflections col-

lected, 2602 independent $(R_{\rm int} = 1.54\%), 2128$ observed with $F_o > 5\sigma(F_o)$, 474 unobserved reflections. Direct methods (SOLV) structure solution; least-squares refinement on 127 parameters; all

- Table 1. Atomic coordinates $(\times 10^4)$ and equivalent isotropic thermal parameters ($Å^2 \times 10^3$) for (1)
- U_{eq} is the equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ii} tensor.

	x	у	Z	\boldsymbol{U}
Mo(1)	3292 (1)	258 (1)	4624 (1)	39 (1)
As(1)	2758 (1)	2707 (1)	5597 (1)	46 (l)
O(1)	4580 (2)	3265 (4)	4581 (2)	72 (1)
O(2)	3975 (2)	- 846 (4)	6189 (2)	74 (l)
C(1)	4088 (2)	2210 (4)	4611 (2)	51 (1)
C(2)	3702 (2)	- 395 (5)	5628 (2)	54 (l)
C(3)	4130 (2)	- 1526 (5)	3950 (2)	55 (1)
C(4)	3589 (2)	- 2720 (4)	4278 (2)	66 (l)
C(5)	2860 (2)	- 2334 (4)	3955 (2)	61 (1)
C(6)	2940 (2)	-906 (5)	3430 (2)	52 (l)
C(7)	3734 (2)	- 385 (4)	3419 (2)	50 (l)
C(8)	4119 (2)	893 (6)	2878 (2)	57 (1)
C(9)	4307 (5)	-151 (11)	2160 (4)	97 (3)
C(0)	3658 (3)	2626 (7)	2703 (3)	75 (2)

Table 2. Atomic coordinates $(\times 10^4)$ and equivalent isotropic thermal parameters ($Å^2 \times 10^3$) for (2)

 U_{ex} is the equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ii} tensor.

	x	у	Z	U
Mo(1)	1216 (1)	3479 (1)	1280 (1)	32 (1)
Mo(2)	1231 (1)	1317 (1)	- 166 (1)	36 (I)
As(1)	940 (1)	406 (2)	1222 (1)	52 (Ú
As(2)	362 (1)	2077 (2)	264 (1)	48 (l)
As(3)	1103 (1)	4404 (2)	- 282 (1)	56 (l)
As(4)	1973 (1)	3599 (2)	439 (1)	67 (I)
C(1)	883 (6)	6022 (15)	1396 (8)	60 (6)
C(2)	537 (5)	4942 (15)	1650 (9)	58 (5)
C(3)	853 (6)	4193 (16)	2383 (8)	64 (6)
C(4)	1382 (6)	4811 (19)	2568 (9)	86 (6)
C(5)	1399 (6)	5948 (17)	1945 (9)	68 (6)
C(6)	587 (5)	309 (16)	- 1396 (7)	59 (5)
C(7)	900 (6)	1451 (16)	- 1679 (7)	60 (5)
C(8)	1436 (5)	928 (16)	- 1460 (7)	53 (5)
C(9)	1460 (7)	- 556 (19)	- 1052 (8)	75 (7)
C(10)	926 (7)	-923 (16)	- 1010 (8)	68 (6)
C(11)	1871 (6)	2338 (18)	1993 (8)	65 (5)
D(1)	2250 (4)	1724 (15)	2482 (6)	100 (5)
C(12)	1874 (6)	225 (19)	634 (8)	71 (6)
D(2)	2240 (4)	- 565 (16)	1024 (7)	108 (6)

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^{*} To whom correspondence should be addressed.

Table 3. Bond lengths (Å) and angles (°) for (1)

Table 4 (cont.)

Mo(1)As(1)	2.666 (1)	Mo(1) - C(1)	1.982 (3)	C(3)—Mo(1)—C(11)	97.5 (5)	C(3)—Mo(1)—C(5)	58.8 (5)
Mo(1) - C(2)	1.981 (4)	Mo(1)-C(3)	2.300(3)	C(5) - Mo(1) - C(11)	97.7 (5)	Mo(2) - Mo(1) - C(11)	88·1 (4)
Mo(1)-Mo(1a)	3.064 (1)	Mo(1)-C(5)	2.356 (4)	Mo(1)— $Mo(2)$ — $As(2)$	55-2 (1)	As(2) - Mo(1) - C(11)	124.4 (4)
As(1) - Mo(1a)	2.576 (1)	Mo(1)-C(7)	2.339 (3)	Mo(1)— $Mo(2)$ — $As(3)$	54·9 (1)	As(4)—Mo(1)—C(11)	72.7 (4)
O(1)-C(1)	1.149 (4)	Mo(1)—As(1a)	2.576 (1)	As(2)—Mo(2)—As(3)	71.1 (1)	C(2)—Mo(1)—C(11)	131.6 (5)
C(3)—C(4)	1.412 (5)	As(1) - As(1a)	2.302 (1)	C(4) - Mo(1) - C(11)	78·4 (5)	C(6)—O(2)—C(8)	57.8 (5)
C(4)-C(5)	1.409 (6)	O(2)-C(2)	1.151 (4)	Mo(1)— $Mo(2)$ — $As(1)$	55.7 (1)	C(6)—Mo(2)—C(7)	34.7 (5)
C(6)-C(7)	1.425 (5)	C(3)-C(7)	1.431 (5)	As(1)—Mo(2)—As(2)	51.3 (1)	C(7)—Mo(2)—C(8)	34-3 (5)
C(8)-C(9)	1.531 (6)	C(5)—C(6)	1.410 (5)	As(1)—Mo(2)—As(3)	106.4 (1)	C(7)—Mo(2)—C(9)	57·5 (5)
Mo-CNT	2.002	C(7)-C(8)	1.505 (5)	Mo(1)—Mo(2)—As(4)	56-3 (1)	C(7)—Mo(2)—C(10)	57.6 (5)
		C(8)-C(0)	1.526 (6)	As(2)—Mo(2)—As(4)	107.3 (1)	C(9)—Mo(2)—C(10)	35.7 (6)
				C(6)—Mo(2)—C(9)	57.9 (5)	C(6)—Mo(2)—C(10)	34.2 (5)
As(1) - Mo(1) - C(1)	76.7 (1)	$A_{s(1)}-M_{o(1)}-C_{o(2)}$	72·2 (1)	C(8)—Mo(2)—C(9)	35.0 (5)	C(8)—Mo(2)—C(10)	58.6 (5)
C(1) - Mo(1) - C(2)	86·6 (1)	As(1) - Mo(1) - C(3)	161.2 (1)	Mo(1) - Mo(2) - C(12)	87.7 (4)	As(1) - Mo(2) - C(12)	72.6 (5)
C(1) - Mo(1) - C(3)	87·7 (1)	C(2) - Mo(1) - C(3)	96.7 (1)	As(2) - Mo(2) - C(12)	123.0 (5)	As(3)—Mo(2)—C(12)	124.3 (4)
As(1) - Mo(1) - C(4)	151.9 (1)	C(1) - Mo(1) - C(4)	121.0 (1)	As(4)-Mo(2)-C(12)	73.9 (4)	C(6)—Mo(2)—C(12)	129.3 (5)
C(2) - Mo(1) - C(4)	86·4 (1)	C(3) - Mo(1) - C(4)	35.6 (1)	C(7) - Mo(2) - C(12)	132.8 (6)	C(8) - Mo(2) - C(12)	99.5 (5)
As(1) - Mo(1) - C(5)	139.4 (1)	C(1) - Mo(1) - C(5)	142 0 (1)	C(9) - Mo(2) - C(12)	77.8 (5)	C(10) - Mo(2) - C(12)	95-1 (5)
C(2) - Mo(1) - C(5)	112.0 (1)	C(3) - Mo(1) - C(5)	58·5 (1)	Mo(1) - As(1) - Mo(2)	67.7 (1)	Mo(1)— $As(1)$ — $As(2)$	63·0 (1)
C(4) - Mo(1) - C(5)	35.1 (1)	As(1) - Mo(1) - C(6)	137.7 (1)	$M_0(2) - A_s(1) - A_s(2)$	62.3(1)	Mo(1) - As(2) - Mo(2)	69·8 (1)
C(1) - Mo(1) - C(6)	114.8 (1)	C(2) - Mo(1) - C(6)	144.6 (1)	Mo(1) - As(2) - As(1)	65·5 (1)	Mo(2) - As(2) - As(1)	66.4 (1)
C(3) - Mo(1) - C(6)	58.9 (1)	C(4) - Mo(1) - C(6)	58·6 (1)	Mo(1) - As(3) - Mo(2)	69·9 (1)	Mo(1)—As(3)—As(4)	66.1 (1)
C(5) - Mo(1) - C(6)	34.7 (1)	As(1) - Mo(1) - C(7)	148.6 (1)	Mo(2)—As(3)—As(4)	65.7 (1)	Mo(1) - As(4) - Mo(2)	67.7 (1)
$C(1) - M_0(1) - C(7)$	84.3 (1)	C(2) - Mo(1) - C(7)	131.9 (1)	Mo(1) - As(4) - As(3)	62·3 (1)	Mo(2)-As(4)-As(3)	62.7 (1)
C(3) - Mo(1) - C(7)	35.9 (1)	C(4) - Mo(1) - C(7)	59·4 (1)	$M_0(1) - C(1) - C(2)$	73.4 (8)	Mo(1) - C(1) - C(5)	72.7 (8)
C(5) - Mo(1) - C(7)	58.4 (1)	$C(6) - M_0(1) - C(7)$	35.2 (1)	C(2) - C(1) - C(5)	110.5 (12)	Mo(1) - C(2) - C(1)	71.5 (8)
As(1) - Mo(1) - Mo(1a)	52.9(1)	O(1)-Mo(1)-Mo(1a)	129·0 (1)	$M_0(1) - C(2) - C(3)$	72.1 (9)	C(1) - C(2) - C(3)	106.4 (11)
C(2) - Mo(1) - Mo(1a)	85·2 (1)	C(1) - Mo(1) - As(1a)	89.3 (1)	$M_0(1) - C(3) - C(2)$	73.4 (9)	Mo(1) - C(3) - C(4)	71.5 (9)
Mo(1) - C(4) - C(5)	73.9 (2)	Mo(1)— $As(1)$ — $Mo(1a)$	71·5 (1)	C(2) - C(3) - C(4)	107.8 (13)	Mo(1) - C(4) - C(3)	73.4 (8)
Mo(1) - C(5) - C(4)	71.0 (2)	Mo(a)—As(1)—As(1a)	66·0 (1)	$M_0(1) - C(4) - C(5)$	72.8 (8)	C(3) - C(4) - C(5)	109.1 (11)
Mo(1a) - Mo(1) - As(1a)	55.6 (1)	$M_0(1) - C(2) - O(2)$	175.5 (3)	$M_0(1) - C(5) - C(1)$	73·0 (8)	$M_0(1) - C(5) - C(4)$	71.9 (8)
$Mo(1) \rightarrow As(1) \rightarrow As(1a)$	62.0(1)	$M_0(1) - C(3) - C(7)$	73.5 (2)	C(1) - C(5) - C(4)	106.1 (13)	Mo(2) - C(6) - C(7)	73.2 (6)
$M_0(1) - C(1) - O(1)$	175.7 (3)	$M_0(1) - C(4) - C(3)$	71.4 (2)	$M_0(2) - C(6) - C(10)$	71.7 (7)	C(7) - C(6) - C(10)	108.4 (13)
$M_0(1) - C(3) - C(4)$	73.0 (2)	C(3)-C(4)-C(5)	107.5 (3)	$M_0(2) - C(7) - C(6)$	72.1 (6)	Mo(2) - C(7) - C(8)	71.8 (6)
C(4) - C(3) - C(7)	108.6 (3)	$M_0(1) - C(5) - C(6)$	73.2 (2)	C(6)C(7)-C(8)	108 5 (12)	Mo(2) - C(8) - C(7)	73.9 (7)
As(1) - Mo(1) - As(1a)	$52 \cdot 1 (1)$	Mo(1)C(6)C(5)	72.1 (2)	$M_0(2) - C(8) - C(9)$	71.6 (8)	C(7) - C(8) - C(9)	107.7 (13)
C(2)—Mo(1)—As(1a)	123.4(1)	C(5)C(6)C(7)	107.9 (3)	$M_0(2) - C(9) - C(8)$	73.4 (8)	$M_0(2) - C(9) - C(10)$	72.3 (9)
C(4) - C(5) - C(6)	109·1 (3)	$M_{0}(1) - C(7) - C(6)$	73.6 (2)	C(8) - C(9) - C(10)	107.7 (13)	Mo(2) - C(10) - C(6)	74.1 (7)
$M_0(1) - C(6) - C(7)$	71.2(2)	$M_0(1) - C(7) - C(8)$	128.2 (2)	$M_0(2) - C(10) - C(9)$	72.0 (8)	C(6)-C(10)-C(9)	107.7 (13)
$M_0(1) - C(7) - C(3)$	70·5 (2)	C(6)-C(7)-C(8)	127.4 (3)	$M_0(1) - C(11) - O(1)$	173.7 (13)	$M_0(2) - C(12) - O(2)$	171.4 (12)
C(3) - C(7) - C(5)	106.9 (3)	C(7) - C(8) - C(0)	114.3 (3)				
C(3) - C(7) - C(8)	125-0 (3)	CNT-Mo(1a)-Mo(1)	116.7	CNT—Mo(2)—As(1)	128.1	CNT-Mo(2)-As(2)	113-1
C(7) - C(8) - C(9)	109.2 (4)	CNT-Mo(1a)-As(1)	167-2	CNT-Mo(2)-As(3)	112.9	CNT-Mo(1)-As(3)	112.4
C(9) - C(8) - C(0)	110.8 (4)			CNT-Mo(2)-As(4)	126.9	CNT-Mo(1)-As(4)	128-2
CNT-Mo-As(1a)	117.00			CNT-Mo(1)-As(2)	112.0	CNT-Mo(1)-Mo(2)	162.9
· · ·				CNT - Mo(1) - As(1)	126.7		

Table 4. Bond lengths (Å) and angles (°) for (2)

Mo(1) - Mo(2) $Mo(1) - As(2)$ $Mo(1) - As(4)$ $Mo(1) - C(11)$ $Mo(2) - As(2)$ $Mo(2) - As(4)$ $Mo(2) - As(4)$	2·959 (1) 2·588 (1) 2·661 (2) 1·972 (13) 2·580 (2) 2·653 (2) 1·986 (13)	Mo(1)-As(1)Mo(1)-As(3)Mo(2)-As(1)Mo(2)-As(3)As(1)-As(2)C(1)-C(2)C(2)-C(3)	2·642 (2) 2·577 (2) 2·670 (2) 2·586 (2) 2·272 (2) 1·400 (21) 1·374 (17)
As(3) - As(4) C(1)-C(5)	2·281 (2) 1·355 (18)	C(4) - C(5) C(6) - C(10) C(6) - C(10)	1.392(21) 1.367(18) 1.202(20)
C(3) - C(4) C(6) - C(7) C(7) - C(8) C(9) - C(10)	1·387 (21) 1·398 (20) 1·378 (18) 1·412 (24)	C(8) - C(9) C(11) - O(1) CNT - Mo(2) CNT - Mo(1)	1·392 (20) 1·171 (16) 2·001 1·985
C(12) - O(2) Mo(2) - Mo(1) - As(1)	1.163(17) 56.6(1)	As(1)—Mo(2)—As(4)	103.5 (1)
As(1) - Mo(1) - As(2) As(1) - Mo(1) - As(3) Mo(2) - Mo(1) - As(4)	51.5(1) 107.5(1) 56.0(1)	As(3) - Mo(2) - As(4) Mo(2) - Mo(1) - As(2) Mo(2) - Mo(1) - As(3)	51.6 (1) 55.0 (1) 55.2 (1)
As(2) - Mo(1) - As(4) C(1) - Mo(1) - C(2) C(1) - Mo(1) - C(3)	$ \begin{array}{c} 106.9 (1) \\ 35.2 (5) \\ 57.5 (5) \end{array} $	As(2) - Mo(1) - As(3) As(1) - Mo(1) - As(4) As(3) - Mo(1) - As(4)	71·2 (1) 104·0 (1) 51·6 (1)
$\begin{array}{c} C(1) & MO(1) & C(3) \\ C(2) - MO(1) - C(4) \\ C(2) - MO(1) - C(5) \\ C(4) - MO(1) - C(5) \\ C(1) - MO(1) - C(11) \end{array}$	57.8 (5) 58.6 (5) 35.3 (5) 131.4 (5)	$\begin{array}{c} C(2) - Mo(1) - C(3) \\ C(1) - Mo(1) - C(4) \\ C(3) - Mo(1) - C(4) \\ C(1) - Mo(1) - C(5) \end{array}$	$34 \cdot 4 (5) 57 \cdot 1 (5) 35 \cdot 1 (5) 34 \cdot 2 (4)$

non-H atoms anisotropic, H atoms idealized and updated (C--H = 0.96 Å, U = 1.2U of attached C); $R_F = 2.66\%, \ wR_F = 2.72\%, \ S = 1.237, \ w^{-1} = \sigma^2(F_o)$ $+gF_o^2$, g = 0.0002; $(\Delta/\sigma)_{max} = 0.026$; $\Delta\rho_{max} = 0.361$, $\Delta\rho_{min} = -0.317 \text{ e } \text{Å}^{-3}$; atomic scattering factors from International Tables for X-ray Crystallography (1974); SHELXTL computer program (Sheldrick, 1985).

For (2), red-orange crystals from methylene chloride/hexane $(0.30 \times 0.32 \times 0.34 \text{ mm})$; Nicolet R3m diffractometer with graphite monochromator; ω scans; lattice parameters from least-squares fit of 25 reflections ($20 < 2\theta < 25^{\circ}$); empirical absorption correction (six reflections, ψ scan, 216 data); T_{max} / $T_{\min} = 2.28, \ 2\theta_{\max} = 52^{\circ}$ $(h = \pm 32, \ k = \pm 11, \ l =$ +20); standard reflections $\overline{7}$, 3, 10, $\overline{9}$ 53, $\overline{17}$, 1, 7, <1% intensity variation. 3575 reflections collected, 3215 independent ($R_{int} = 2.76\%$), 2113 observed with $F_o >$ $5\sigma(F_{o})$, 1102 unobserved reflections. Direct methods (SOLV) structure solution; least-squares refinement



Fig. 1. Molecular structure and labelling scheme for (1).



Fig. 2. Molecular structure and labelling scheme for (2).

on 181 parameters; all non-H atoms anisotropic, H atoms idealized and updated (C—H = 0.96 Å, U =1.2U of attached C). $R_F = 4.77\%$, $wR_F = 5.03\%$, S =1.276, $w^{-1} = \sigma^2(F_o) + gF_o^2$, g = 0.001; $(\Delta/\sigma)_{max} =$ 0.043; $\Delta\rho_{max} = 1.009$, $\Delta\rho_{min} = -1.208$ eÅ⁻³; atomic scattering factors from *International Tables for X-ray* *Crystallography* (1974); *SHELXTL* computer program (Sheldrick, 1985).

Atomic coordinates and equivalent isotropic thermal parameters for (1) and (2) are given in Tables 1 and 2 respectively. Bond lengths and angles for (1) are given in Table 3. Bond lengths and angles for (2) are given in Table 4. Figs. 1 and 2 show the labelled molecular structures for (1) and (2) respectively.*

Related literature. (1) is an analogue of a structure previously reported by Foley, Rheingold & Sullivan (1982). (2) is an analogue of a structure previously reported by DiMaio & Rheingold (1987). Three similar Mo—As clusters have been reported by Scherer, Sitzmann & Wolmershauser (1986).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters, and figures showing unit-cell packing have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52328 (35 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- DIMAIO, A.-J. & RHEINGOLD, A. L. (1987). J. Chem. Soc. Chem. Commun. pp. 404-405.
- FOLEY, M. J., RHEINGOLD, A. L. & SULLIVAN, P. J. (1982). J. Am. Chem. Soc. 104, 4727–4729.
- International Tables for X-ray Crystallography (1974). Vol. IV, pp. 99, 149. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- SCHERER, O. J., SITZMANN, H. & WOLMERSHAUSER, G. (1986). J. Organomet. Chem. 309, 77–86.
- SHELDRICK, G. M. (1985). SHELXTL Users Manual, version 5.1. Nicolet XRD Corp., Madison, WI, USA.

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Structure of $[(1,2,3-\eta)$ -Cyclotridecenyl]bis(triphenylphosphine)rhodium Benzene Solvate

BY A. W. CORDES, S. SIEGEL, S.-T. LIN, L. MARTIN AND M. C. NOBLE

Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR 72701, USA

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Abstract. [Rh(C₁₃H₂₃){P(C₆H₅)₃}₂].0·5C₆H₆, $M_r = 845.9$, triclinic, $P\overline{1}$, a = 12.260 (6), b = 13.05 (1), c = 15.91 (1) Å, $\alpha = 71.30$ (6), $\beta = 76.24$ (6), $\gamma = 67.71$ (5)°, V = 2211 (3) Å³, Z = 2, $D_x = 1.27$ g cm⁻³,

 λ (Mo K α) = 0.71073 Å, μ = 4.8 cm⁻¹, F(000) = 886, T = 293 K, R = 0.043 for 6030 reflections with $F_o^2 > 3\sigma(F_o^2)$. The Rh atom is η^3 -bonded to the allyl portion of the 13-carbon-ring ligand. The ring atoms © 1990 International Union of Crystallography

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