CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.
CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.
EVANS, H. T., APPLEMAN, D. E. & HANDWERKER, D. S. (1963). *LSUCRE*. Least-squares unit-cell refinement. Annu. Meet. Program 42, Am. Crystallogr. Assoc., Cambridge, MA.
KETTERER, J. (1985). Thesis, Univ. of Freiburg.
KETTERER, J., KELLER, E. & KRÄMER, V. (1985). *Z. Kristallogr.* **172**, 63–70.
SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.
SILLÉN, L. G. (1941). *Sven. Kem. Tidskr.* **53**, 39–43.
WELLS, A. F. (1984). *Structural Inorganic Chemistry*, 5th ed. Oxford Univ. Press.

Acta Cryst. (1986). C**42**, 1099–1100

Space group of octadecacarbonyl-1,2,3:4,5,6-bis-μ_3-[(η-toluene)cuprio]-*octahedro*-hexaruthenium.

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Abstract

The structure of $(C_6H_5CH_3)_2Cu_2Ru_6(CO)_{18}$ should be described in $P\bar{1}$ and not in $P1$ as originally reported by Ansell, Modrick & Bradley [*Acta Cryst.* (1984), C**40**, 365–368].

During the preparation of a brief review (Jones, 1986) of noncentrosymmetric structures published in *Acta Crystallographica*, Section C, 1984, it was noticed that some structures were probably centrosymmetric. One such case is presented here.

The structure of the title compound was described by Ansell, Modrick & Bradley (AMB; 1984) in space group $P1$ with $Z = 2$; $a = 10{\cdot}236$, $b = 10{\cdot}395$, $c = 19{\cdot}267$ Å, $\alpha = 82{\cdot}64$, $\beta = 75{\cdot}27$, $\gamma = 82{\cdot}44°$. Inspection of AMB's atomic coordinates suggested strongly that both independent molecules in fact lay on centres of symmetry in $P\bar{1}$. Refinement of a centrosymmetric model, using the deposited structure factors and applying a coordinate shift of −0·985, 0·057, −0·003 from AMB's coordinates, confirmed this hypothesis. Details of refinement: 4357 observed reflections, unit weights, $R = 0{\cdot}039$, 272 parameters (*cf.* AMB's refinement; $R = 0{\cdot}038$, 495 parameters), max. Δ/σ 0·011, program system *SHELXTL* (Sheldrick, 1983). The increased stability of refinement in $P\bar{1}$ allowed the resolution of a twofold disorder of the toluene group of the second molecule; atoms C(1′)–C(7′), s.o.f. 0·64 (2), form the major component, and

Table 1. *Atom coordinates* (×10⁴) *and isotropic temperature factors* (Å² × 10³)

	x	*y*	*z*	U_{iso}
Ru(1)	3168 (1)	4928 (1)	4774·2 (4)	25 (1)*
Ru(2)	4551 (1)	6956 (1)	5125·9 (5)	25 (1)*
Ru(3)	5907 (1)	5394 (1)	3924·2 (4)	25 (1)*
Cu(1)	3741 (1)	7098 (1)	3911 (1)	40 (1)*
O(1*a*)	2210 (9)	4391 (9)	3483 (5)	56 (2)
O(1*b*)	1779 (9)	2596 (9)	5564 (5)	55 (2)
O(1*c*)	452 (10)	6524 (9)	5154 (5)	57 (2)
O(2*a*)	1914 (10)	8677 (10)	5506 (5)	65 (3)
O(2*b*)	5138 (9)	7757 (9)	6457 (5)	56 (2)
O(2*c*)	5720 (9)	9368 (9)	4288 (5)	57 (2)
O(3*a*)	5049 (9)	4944 (9)	2590 (5)	55 (2)
O(3*b*)	8610 (9)	3829 (9)	3411 (5)	55 (2)
O(3*c*)	7130 (10)	7758 (10)	3025 (5)	65 (3)
C(1*a*)	2663 (12)	4638 (11)	3953 (6)	36 (3)
C(1*b*)	2390 (11)	3465 (11)	5289 (6)	35 (3)
C(1*c*)	1528 (11)	5988 (11)	5006 (6)	35 (3)
C(2*a*)	2902 (12)	7957 (12)	5340 (7)	42 (3)
C(2*b*)	4947 (12)	7359 (11)	5965 (6)	40 (3)
C(2*c*)	5292 (12)	8419 (11)	4569 (6)	39 (3)
C(3*a*)	5317 (11)	5114 (11)	3125 (6)	36 (3)
C(3*b*)	7574 (12)	4390 (11)	3656 (6)	38 (3)
C(3*c*)	6617 (12)	6886 (11)	3400 (6)	39 (3)
C(1)	3517 (14)	8197 (13)	2907 (7)	52 (3)
C(2)	3302 (14)	9266 (13)	3315 (8)	54 (3)
C(3)	1978 (13)	9688 (12)	3695 (7)	46 (3)
C(4)	890 (13)	9000 (12)	3668 (7)	48 (3)
C(5)	1129 (16)	7934 (15)	3270 (8)	64 (4)
C(6)	2431 (16)	7548 (15)	2894 (8)	64 (4)
C(7)	1702 (16)	10847 (15)	4132 (8)	65 (4)

Table 1 (*cont.*)

	x	*y*	*z*	U_{iso}
Ru(1′)	859 (1)	4948 (1)	8917·7 (4)	30 (1)*
Ru(2′)	−1916 (1)	5146 (1)	9828·0 (5)	31 (1)*
Ru(3′)	−39 (1)	6991 (1)	9904·7 (5)	31 (1)*
Cu(1′)	−1016 (2)	6908 (1)	8756 (1)	42 (1)*
O(1*a*′)	−194 (10)	4183 (10)	7706 (6)	63 (3)
O(1*b*′)	2373 (10)	6930 (9)	7834 (5)	59 (2)
O(1*c*′)	3247 (10)	2928 (10)	8506 (5)	62 (3)
O(2*a*′)	−4264 (11)	7277 (10)	10036 (6)	71 (3)
O(2*b*′)	−3802 (11)	3452 (10)	10885 (6)	72 (3)
O(2*c*′)	−3100 (11)	4376 (10)	8671 (6)	69 (3)
O(3*a*′)	1488 (11)	8993 (11)	8843 (6)	77 (3)
O(3*b*′)	958 (11)	8024 (11)	11045 (6)	74 (3)
O(3*c*′)	−2286 (12)	9187 (11)	10130 (6)	76 (3)
C(1*a*′)	146 (13)	4493 (12)	8201 (7)	46 (3)
C(1*b*′)	1757 (12)	6215 (11)	8265 (6)	39 (3)
C(1*c*′)	2347 (13)	3672 (12)	8716 (7)	44 (3)
C(2*a*′)	−3299 (14)	6520 (13)	9938 (7)	48 (3)
C(2*b*′)	−3005 (13)	4078 (12)	10506 (7)	47 (3)
C(2*c*′)	−2569 (13)	4709 (12)	9083 (7)	48 (3)
C(3*a*′)	897 (13)	8161 (13)	9223 (7)	49 (3)
C(3*b*′)	593 (13)	7521 (13)	10632 (7)	47 (3)
C(3*c*′)	−1484 (13)	8292 (13)	10025 (7)	48 (3)
C(1′)	−1035 (9)	8481 (17)	7885 (9)	37 (5)
C(2′)	−1825 (9)	9472 (17)	8273 (9)	47 (5)
C(3′)	−3235 (9)	9480 (17)	8478 (9)	43 (5)
C(4′)	−3854 (9)	8497 (17)	8296 (9)	65 (7)
C(5′)	−3064 (9)	7506 (17)	7907 (9)	60 (7)
C(6′)	−1654 (9)	7498 (17)	7702 (9)	48 (6)
C(7′)	−4049 (30)	10591 (29)	8976 (16)	86 (9)
C(1″)	−2571 (42)	9745 (22)	8423 (16)	54 (6)
C(2″)	−3660 (42)	9054 (22)	8442 (16)	54 (6)
C(3″)	−3432 (42)	7888 (22)	8122 (16)	54 (6)
C(4″)	−2115 (42)	7414 (22)	7784 (16)	54 (6)
C(5″)	−1026 (42)	8105 (22)	7765 (16)	54 (6)
C(6″)	−1253 (42)	9271 (22)	8085 (16)	54 (6)
C(7″)	−5049 (39)	9684 (37)	8757 (21)	54 (6)

* Equivalent isotropic U calculated from anisotropic U.

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C(1'')–C(7''), s.o.f. 0·36 (2), the minor component. Both rings were refined as rigid hexagons with C–C 1·395 Å; all temperature factors of the minor component were constrained equal. (Problems in the refinement of these groups were noted by AMB.) Final atomic coordinates are presented in Table 1.* Molecule (1) is associated with the symmetry centre 0·5, 0·5, 0·5 and molecule (2) (primed atoms) with 0, 0·5, 1 (see also Figs. 1–3 of AMB).

The molecular geometry after the new refinement is more regular than that of AMB, as would be expected. Examples of some bond length and angle ranges follow (AMB's values in brackets): Cu–Ru 2·641–2·665 Å (2·631–2·722 Å); Ru–Ru in capped triangular faces 2·923–2·943 Å (2·901–2·958 Å); Ru–Ru between these faces 2·865–2·875 Å (2·846–2·895 Å); Ru–C–O 170·7–175·0° (150–170°).

The coordination of toluene to the Cu atoms is distorted η^2, both for Cu(1) and for both disorder components at Cu(1').

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* Lists of structure factors, bond lengths and angles, and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42904 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

ANSELL, G. B., MODRICK, M. A. & BRADLEY, J. S. (1984). *Acta Cryst.* C**40**, 365–368.

JONES, P. G. (1986). *Acta Cryst.* C**42**, 924–925.

SHELDRICK, G. M. (1983). *SHELXTL Users Manual*, revision 4. Nicolet XRD Corporation, Madison, Wisconsin.

International Union of Crystallography

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Commission on Journals Author Grievance Procedure

The Commission on Journals has recently instituted a formal appeals procedure in which an author who believes his paper has been unjustifiably rejected by the Co-editor of an IUCr journal may appeal initially to the Editor of that journal for a new review and, finally, to the Editor of the other journal if the author is still aggrieved by the decision.

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Commission on Journals Equivalent Value of the Anisotropic Temperature Factor Coefficients

Anisotropic temperature factor coefficients have been published in *Acta Cryst.* since 1979 only if the table of values is very short, or they are necessary for understanding the paper, or they possess unusual features. In all other cases, the table of values has been deposited and a brief discussion of the deposited values given instead, including the maximum and minimum values found and the presence of any nonpositive-definite coefficients determined. In addition, the equivalent values of the anisotropic temperature factors have been published, together with the list of atomic coordinates and a definition of the equivalent values in terms of the individual coefficients with source reference, see *Notes for Authors* [*Acta Cryst.* (1983), A**39**, 174–186].

Authors have been encouraged to use their definition of choice. Among the acceptable definitions are those given by W. C. Hamilton [*Acta Cryst.* (1959), **12**, 609–610] and by B. T. M. Willis & A. W. Pryor [*Thermal Vibrations in Crystallography* (1975), pp. 101–102. Cambridge Univ. Press]. Arithmetic or geometric mean values for non-orthogonal crystal axes are correct only if derived from the principal axes of the thermal ellipsoid. Values of U_{eq} are to be preferred over B_{eq}.

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Appointments in the IUCr Office

A notice concerning recent appointments in the IUCr office appeared in the July 1986 issue of *Acta Crystallographica*, section A, p. 288.