O(24)	0.2628 (3)	0.7619 (3)	0.3338 (7)	0.056 (2)
Fe(1A)	0.5081 (1)	1.3256 (1)	0.4330 (1)	0.038 (1)
Cl(1A)	0.5424 (1)	1.3890 (1)	0.1887 (3)	0.058 (1)
O(1A)	0.5592 (3)	1.1998 (3)	0.4243 (6)	0.049 (2)
C(2A)	0.5341 (4)	1.1072 (4)	0.3409 (8)	0.039 (3)
C(3A)	0.5954 (4)	1.0347 (4)	0.3349 (9)	0.046 (3)
C(4A)	0.5722 (5)	0.9361 (5)	0.240 (1)	0.056 (3)
C(5A)	0.4899 (5)	0.9092 (5)	0.154 (1)	0.058 (3)
C(6A)	0.4264 (5)	0.9801 (5)	0.1657 (9)	0.056 (3)
C(7A)	0.4472 (4)	1.0815 (4)	0.2571 (8)	0.041 (3)
C(8A)	0.3769 (4)	1.1500 (5)	0.2677 (9)	0.046 (3)
N(9A)	0.3868 (3)	1.2453 (3)	0.3372 (7)	0.038 (2)
C(10A)	0.3126 (4)	1.3058 (4)	0.3442 (9)	0.046 (3)
C(11A)	0.2304 (4)	1.2791 (5)	0.246 (1)	0.064 (4)
C(12A)	0.1642 (4)	1.3457 (6)	0.271 (1)	0.071 (4)
C(13A)	0.1761 (4)	1.4374 (6)	0.390 (1)	0.068 (4)
C(14A)	0.2578 (4)	1.4668 (5)	0.483 (1)	0.054 (3)
C(15A)	0.3277 (3)	1.4019 (4)	0.4634 (9)	0.041 (3)
N(16A)	0.4144 (3)	1.4238 (4)	0.5470 (7)	0.041 (2)
C(17A)	0.4337 (4)	1.5040 (5)	0.6702 (9)	0.045 (3)
C(18A)	0.5208 (4)	1.5367 (4)	0.7668 (9)	0.044 (3)
C(19A)	0.5319 (5)	1.6329 (5)	0.889 (1)	0.056 (3)
C(20A)	0.6096 (5)	1.6664 (5)	0.981 (1)	0.064 (4)
C(21A)	0.6828 (5)	1.6085 (5)	0.956 (1)	0.058 (3)
C(22A)	0.6753 (4)	1.5156 (5)	0.843 (1)	0.055 (3)
C(23A)	0.5952 (4)	1.4781 (4)	0.7417 (9)	0.044 (3)
O(24A)	0.5908 (3)	1.3880 (3)	0.6347 (6)	0.051 (2)
Fe(1B)	0.9557 (1)	0.1661 (1)	0.5114 (1)	0.044 (1)
Cl(1B)	1.0439 (1)	0.2854 (2)	0.6992 (3)	0.062 (1)
O(1B)	1.0285 (3)	0.0611 (4)	0.4199 (6)	0.061 (2)
C(2B)	1.0659 (4)	0.0325 (5)	0.2651 (9)	0.047 (3)
C(3B)	1.1235 (4)	−0.0458 (5)	0.249 (1)	0.054 (3)
C(4B)	1.1636 (4)	−0.0769 (5)	0.088 (1)	0.054 (3)
C(5B)	1.1503 (5)	−0.0313 (6)	−0.0610 (1)	0.062 (4)
C(6B)	1.0931 (4)	0.0433 (5)	−0.052 (1)	0.053 (3)
C(7B)	1.0503 (4)	0.0781 (5)	0.1090 (9)	0.043 (3)
C(8B)	0.9942 (4)	0.1600 (5)	0.1104 (9)	0.044 (3)
N(9B)	0.9541 (3)	0.2051 (4)	0.2516 (7)	0.042 (2)
C(10B)	0.9020 (4)	0.2892 (5)	0.2391 (9)	0.041 (2)
C(11B)	0.9142 (4)	0.3517 (5)	0.1120 (9)	0.052 (3)
C(12B)	0.8591 (4)	0.4300 (6)	0.115 (1)	0.065 (4)
C(13B)	0.7937 (5)	0.4469 (6)	0.238 (1)	0.072 (4)
C(14B)	0.7857 (4)	0.3904 (5)	0.365 (1)	0.059 (3)
C(15B)	0.8398 (4)	0.3094 (5)	0.3687 (9)	0.045 (3)
N(16B)	0.8378 (3)	0.2437 (4)	0.4954 (7)	0.042 (2)
C(17B)	0.7732 (4)	0.2422 (5)	0.6037 (9)	0.044 (3)
C(18B)	0.7688 (4)	0.1823 (5)	0.7383 (9)	0.046 (3)
C(19B)	0.7001 (5)	0.2013 (6)	0.860 (1)	0.057 (4)
C(20B)	0.6934 (5)	0.1498 (6)	1.002 (1)	0.069 (4)
C(21B)	0.7502 (5)	0.0742 (6)	1.018 (1)	0.061 (4)
C(22B)	0.8169 (4)	0.0513 (6)	0.895 (1)	0.056 (4)
C(23B)	0.8285 (4)	0.1080 (5)	0.7597 (9)	0.045 (3)
O(24B)	0.8946 (3)	0.0877 (3)	0.6524 (7)	0.060 (2)

Table 2. *Geometric parameters* (Å, °)

Fe(1)—Cl(1)	2.230 (2)	Fe(1A)—N(16A)	2.091 (5)
Fe(1)—O(1)	1.868 (4)	Fe(1A)—O(24A)	1.904 (4)
Fe(1)—N(9)	2.099 (4)	Fe(1B)—Cl(1B)	2.228 (2)
Fe(1)—N(16)	2.108 (5)	Fe(1B)—O(1B)	1.885 (5)
Fe(1)—O(24)	1.881 (4)	Fe(1B)—N(9B)	2.088 (5)
Fe(1A)—Cl(1A)	2.232 (2)	Fe(1B)—N(16B)	2.116 (5)
Fe(1A)—O(1A)	1.895 (4)	Fe(1B)—O(24B)	1.889 (5)
Fe(1A)—N(9A)	2.090 (4)		
O(1)—Fe(1)—Cl(1)	108.5 (2)	N(16A)—Fe(1A)—N(9A)	76.8 (2)
N(9)—Fe(1)—Cl(1)	103.1 (2)	O(24A)—Fe(1A)—Cl(1A)	106.7 (2)
N(9)—Fe(1)—O(1)	87.8 (2)	O(24A)—Fe(1A)—O(1A)	91.2 (2)
N(16)—Fe(1)—Cl(1)	101.0 (2)	O(24A)—Fe(1A)—N(9A)	149.4 (2)
N(16)—Fe(1)—O(1)	149.1 (2)	O(24A)—Fe(1A)—N(16A)	88.0 (2)
N(16)—Fe(1)—N(9)	76.6 (2)	O(1B)—Fe(1B)—Cl(1B)	106.7 (1)
O(24)—Fe(1)—Cl(1)	107.9 (2)	N(9B)—Fe(1B)—Cl(1B)	105.0 (1)
O(24)—Fe(1)—O(1)	92.0 (2)	N(9B)—Fe(1B)—O(1B)	87.6 (2)
O(24)—Fe(1)—N(9)	147.4 (2)	N(16B)—Fe(1B)—Cl(1B)	100.2 (2)
O(24)—Fe(1)—N(16)	87.5 (2)	N(16B)—Fe(1B)—O(1B)	151.6 (2)
O(1A)—Fe(1A)—Cl(1A)	110.0 (2)	N(16B)—Fe(1B)—N(9B)	76.5 (2)
N(9A)—Fe(1A)—Cl(1A)	102.4 (2)	O(24B)—Fe(1B)—Cl(1B)	109.9 (2)
N(9A)—Fe(1A)—O(1A)	87.6 (2)	O(24B)—Fe(1B)—O(1B)	92.9 (2)
N(16A)—Fe(1A)—Cl(1A)	101.9 (2)	O(24B)—Fe(1B)—N(9B)	143.4 (2)
N(16A)—Fe(1A)—O(1A)	146.8 (2)	O(24B)—Fe(1B)—N(16B)	86.5 (2)

The *x*, *y* and *z* coordinates of Fe(1) were fixed to define the origin of the structure. All H atoms were located geometrically (C—H 0.98 Å). Refinement was by the full-matrix least-squares method. The polarity was checked by inversion of all parameters; the refinement converged to identical *R* values in both cases. The polarity presented here was chosen arbitrarily.

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Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71052 (114 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SH1030]

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Redetermination of the Structure of μ_6-Acetonato-1:2:3κ^3C^1;4:5:6κ^3C^3-bis[nonacarbonyl-1κ^3C,2κ^3C,3κ^3C-*triangulo*-tricobalt(3 *Co–Co*)] at 128 K

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Abstract

The structure of the carbonyl-bridged dicluster compound $OC[CCo_3(CO)_9]_2$ has been redetermined from diffractometer data recorded at 128 K. The broad

features of the structure agree with those reported previously [Allegra & Valle (1969). *Acta Cryst.* **B25**, 107–119] but the lengths of the C—C bonds linking the apical carbyne C atoms of the Co_3C cluster units to the bridging keto group do not differ significantly from one another as found in the original determination. This observation is in keeping with the known electrochemical behaviour of the molecule.

Comment

The structure of $OC[CCo_3(CO)_9]_2$ was originally reported (Allegra & Valle, 1969) from multiple film data ($R = 0.12$). Our interest in the detailed structure stems from the fact that this molecule displays electrochemical responses indicating an interaction between the two reducible Co_3C cluster centres (Worth, Robinson & Simpson, 1992*a*). A common feature of dicluster systems with interacting redox centres is the observation that the apical carbyne atoms of the Co_3C units are linked through short C—C bonds. Such behaviour could be predicted for molecules in which there was significant delocalization over the linking carbon–carbon bonds as evidenced by short C—C distances (Worth, Robinson & Simpson, 1990, 1992*b*). Surprisingly, the previously determined C_{apical}—C(O)—C_{apical} bond distances in this molecule showed apparently significant differences (1.60 and 1.42 Å, respectively).

The title compound was prepared in good yield from the thermolysis of $BrCCo_3(CO)_9$ with Ph_3As in an atmosphere of CO (Worth, Robinson & Simpson, 1992*a*) and recrystallized from dichloromethane. The overall structural form of the molecule is similar to that reported earlier, with the central C—C(O)—C group strictly planar and the two cluster carbonyl units oriented to minimize steric repulsions between the carbonyl ligands and the apical carbonyl substituent [shortest intramolecular contacts O(2)···C(21) 2.919 (6), O(2)···C(42) 2.864 (6) and O(2)···C(51) 2.877 (6) Å]. However, the present study reveals that the C—C distances, linking the C_{apical} atoms to the central carbonyl C atom, are C(1)—C(2) 1.477 (5) and C(2)—C(3) 1.485 (6) Å, commensurate with some electron delocalization between the cluster redox centres. Furthermore, the Co—C_{apical} distances are essentially equivalent in both cluster moieties [mean 1.902 (8) Å] and while the Co—C≡O angles show significant variation, the mean value, 177.3 (11)°, deviates far less from the anticipated 180° than previously determined.

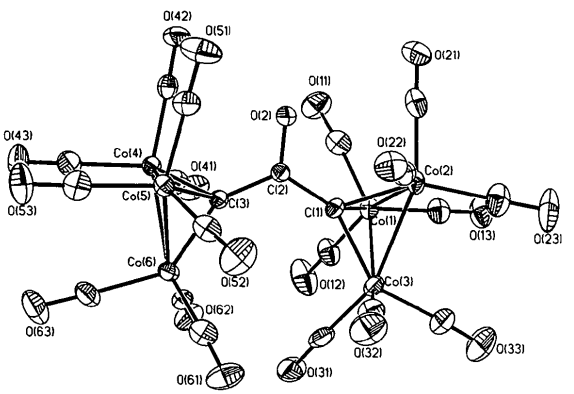

Fig. 1. View of the title compound showing the atom-numbering scheme.

Experimental

Crystal data

$[Co_6(C_3O)(CO)_{18}]$
$M_r = 909.82$
Orthorhombic
$P2_12_12_1$
$a = 9.775$ (2) Å
$b = 30.857$ (10) Å
$c = 9.698$ (2) Å
$V = 2925$ (1) Å^3
$Z = 4$
$D_x = 2.04$ Mg m^{-3}
Mo radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 4.9$–$33.2°$
$\mu = 3.54$ mm^{-1}
$T = 128$ (5) K
Block
0.4 × 0.2 × 0.2 mm
Brown-black

Data collection

Nicolet *R3m* diffractometer
ω scans
Absorption correction: empirical
$T_{min} = 0.618$, $T_{max} = 0.788$
3945 measured reflections
3792 independent reflections
3630 observed reflections [$I > 2\sigma(I)$]
$R_{int} = 0.0273$
$\theta_{max} = 55°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 41$
$l = 0 \rightarrow 13$
3 standard reflections monitored every 100 reflections
intensity variation: <1%

Refinement

Refinement on F
Final $R = 0.0316$
$wR = 0.0470$
3630 reflections
415 parameters
$w = (\sigma^2F + 0.002949F^2)^{-1}$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.66$ e Å^{-3}
Atomic scattering factors from *SHELX*76 for C and O and *International Tables for X-ray Crystallography* (1974, Vol. IV) for Co

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

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

	x	y	z	U_{eq}
C(1)	0.9533 (4)	0.3883 (1)	−0.0307 (5)	0.019
C(2)	0.8972 (5)	0.3457 (1)	−0.0710 (1)	0.018
O(2)	0.9446 (4)	0.3132 (1)	−0.0129 (4)	0.029

C(3)	0.7870 (5)	0.3394 (1)	−0.1745 (4)	0.018
Co(1)	0.9101 (1)	0.4169	0.1383 (1)	0.021
Co(2)	1.1333 (1)	0.3958	0.0418 (1)	0.021
Co(3)	0.9864 (1)	0.4463	−0.0855 (1)	0.024
Co(4)	0.6350 (1)	0.3027	−0.1469 (1)	0.019
Co(5)	0.8118 (1)	0.3016	−0.3281 (1)	0.019
Co(6)	0.6628 (1)	0.3651	−0.3013 (1)	0.021
C(11)	0.8540 (6)	0.3695 (2)	0.2314 (5)	0.031
O(11)	0.8091 (6)	0.3404 (1)	0.2861 (4)	0.046
C(12)	0.7426 (6)	0.4409 (2)	0.1297 (6)	0.034
O(12)	0.6380 (4)	0.4552 (2)	0.1223 (6)	0.055
C(13)	0.9960 (6)	0.4508 (2)	0.2664 (6)	0.031
O(13)	1.0521 (5)	0.4716 (1)	0.3447 (5)	0.042
C(21)	1.1518 (5)	0.3525 (2)	0.1641 (5)	0.031
O(21)	1.1664 (5)	0.3248 (1)	0.2395 (4)	0.040
C(22)	1.2157 (5)	0.3696 (2)	−0.1008 (5)	0.028
O(22)	1.2601 (4)	0.3519 (1)	−0.1916 (4)	0.037
C(23)	1.2604 (6)	0.4341 (2)	0.1089 (7)	0.039
O(23)	1.3365 (4)	0.4581 (2)	0.1559 (7)	0.058
C(31)	0.8265 (6)	0.4675 (1)	−0.1472 (6)	0.034
O(31)	0.7280 (4)	0.4818 (1)	−0.1843 (6)	0.047
C(32)	1.0749 (6)	0.4408 (2)	−0.2476 (6)	0.035
O(32)	1.1286 (5)	0.4364 (2)	−0.3498 (5)	0.049
C(33)	1.0590 (6)	0.4969 (2)	−0.0195 (7)	0.043
O(33)	1.0949 (7)	0.5287 (1)	0.0230 (7)	0.071
C(41)	0.5507 (5)	0.3316 (2)	−0.0103 (5)	0.028
O(41)	0.5032 (5)	0.3509 (1)	0.0766 (4)	0.044
C(42)	0.7066 (5)	0.2599 (2)	−0.0427 (5)	0.026
O(42)	0.7488 (4)	0.2326 (1)	0.0235 (4)	0.036
C(43)	0.4970 (6)	0.2722 (2)	−0.2339 (5)	0.031
O(43)	0.4183 (5)	0.2531 (2)	−0.2910 (5)	0.045
C(51)	0.9188 (6)	0.2600 (2)	−0.2548 (5)	0.028
O(51)	0.9883 (6)	0.2338 (1)	−0.2122 (4)	0.048
C(52)	0.9461 (5)	0.3287 (2)	−0.4231 (5)	0.027
O(52)	1.0310 (5)	0.3461 (2)	−0.4766 (5)	0.048
C(53)	0.7209 (6)	0.2696 (2)	−0.4581 (5)	0.032
O(53)	0.6623 (5)	0.2491 (2)	−0.5338 (4)	0.046
C(61)	0.7575 (6)	0.4033 (2)	−0.4007 (5)	0.031
O(61)	0.8126 (5)	0.4288 (1)	−0.4660 (5)	0.049
C(62)	0.5568 (5)	0.4019 (2)	−0.2059 (5)	0.028
O(62)	0.4855 (4)	0.4252 (1)	−0.1494 (5)	0.039
C(63)	0.5375 (7)	0.3484 (2)	−0.4301 (6)	0.038
O(63)	0.4605 (6)	0.3370 (2)	−0.5103 (6)	0.060

Table 2. *Geometric parameters* (Å, °)

C(1)—C(2)	1.477 (5)	Co(2)—C(23)	1.833 (6)
C(2)—O(2)	1.241 (5)	C(23)—O(23)	1.145 (7)
C(2)—C(3)	1.485 (6)	Co(3)—C(31)	1.798 (6)
Co(1)—Co(2)	2.462 (1)	C(31)—O(31)	1.118 (7)
Co(1)—Co(3)	2.467 (1)	Co(3)—C(32)	1.802 (6)
Co(2)—Co(3)	2.452 (1)	C(32)—O(32)	1.130 (8)
Co(4)—Co(5)	2.466 (1)	Co(3)—C(33)	1.831 (6)
Co(4)—Co(6)	2.456 (1)	C(33)—O(33)	1.122 (7)
Co(5)—Co(6)	2.457 (1)	Co(4)—C(41)	1.797 (5)
C(1)—Co(1)	1.909 (4)	C(41)—O(41)	1.132 (7)
C(1)—Co(2)	1.910 (4)	C(42)—O(42)	1.134 (6)
C(3)—Co(4)	1.887 (4)	Co(4)—C(43)	1.849 (5)
C(3)—Co(5)	1.909 (4)	C(43)—O(43)	1.115 (7)
C(3)—Co(6)	1.902 (4)	Co(5)—C(51)	1.801 (5)
Co(1)—C(11)	1.804 (5)	C(51)—O(51)	1.133 (7)
C(11)—O(11)	1.133 (7)	Co(5)—C(52)	1.809 (5)
Co(1)—C(12)	1.799 (5)	C(52)—O(52)	1.117 (7)
C(12)—O(12)	1.117 (7)	Co(5)—C(53)	1.831 (6)
Co(1)—C(13)	1.829 (5)	C(53)—O(53)	1.126 (7)
C(13)—O(13)	1.135 (7)	Co(6)—C(61)	1.781 (5)
Co(2)—C(21)	1.796 (6)	C(61)—O(61)	1.144 (7)
C(21)—O(21)	1.133 (7)	Co(6)—C(62)	1.794 (5)
Co(2)—C(22)	1.793 (5)	C(62)—O(62)	1.141 (6)
C(22)—O(22)	1.124 (6)	Co(6)—C(63)	1.824 (6)
		C(63)—O(63)	1.138 (7)

C(1)—C(2)—C(3)	124.4 (4)	Co(5)—Co(4)—Co(6)	59.9 (1)
C(1)—C(2)—O(2)	117.4 (4)	C(3)—Co(4)—Co(5)	49.9 (1)
O(2)—C(2)—C(3)	118.2 (4)	C(3)—Co(4)—Co(6)	49.9 (1)
C(2)—C(1)—Co(1)	123.8 (3)	C(3)—Co(4)—C(41)	99.6 (2)
C(2)—C(1)—Co(2)	123.2 (3)	C(3)—Co(4)—C(42)	102.3 (2)
C(2)—C(1)—Co(3)	146.1 (3)	C(3)—Co(4)—C(43)	144.6 (2)
Co(1)—Co(2)—Co(3)	60.3 (1)	C(3)—Co(5)—Co(4)	49.1 (1)
Co(1)—Co(3)—Co(2)	60.1 (1)	C(3)—Co(5)—Co(6)	49.7 (1)
Co(2)—Co(1)—Co(3)	59.7 (1)	C(3)—Co(5)—C(51)	101.6 (2)
Co(1)—C(1)—Co(2)	80.3 (2)	C(3)—Co(5)—C(52)	102.0 (2)
Co(1)—C(1)—Co(3)	80.9 (2)	C(3)—Co(5)—C(53)	143.6 (2)
Co(2)—C(1)—Co(3)	80.3 (2)	C(3)—Co(6)—Co(4)	49.3 (1)
C(2)—C(3)—Co(4)	123.7 (3)	C(3)—Co(6)—Co(5)	50.0 (1)
C(2)—C(3)—Co(5)	121.0 (3)	C(3)—Co(6)—C(61)	107.1 (2)
C(2)—C(3)—Co(6)	147.7 (3)	C(3)—Co(6)—C(62)	107.4 (2)
Co(4)—C(3)—Co(5)	81.0 (2)	C(3)—Co(6)—C(63)	138.9 (2)
Co(4)—C(3)—Co(6)	80.8 (2)	Co(1)—C(11)—O(11)	174.7 (5)
Co(5)—C(3)—Co(6)	80.3 (2)	Co(1)—C(12)—O(12)	178.5 (6)
C(1)—Co(1)—Co(2)	49.9 (1)	Co(1)—C(13)—O(13)	178.5 (5)
C(1)—Co(1)—Co(3)	49.3 (1)	Co(2)—C(21)—O(21)	178.2 (5)
C(1)—Co(1)—C(11)	97.0 (2)	Co(2)—C(22)—O(22)	175.8 (5)
C(1)—Co(1)—C(12)	110.6 (2)	Co(2)—C(23)—O(23)	177.1 (6)
C(1)—Co(1)—C(13)	138.3 (2)	Co(3)—C(31)—O(31)	178.2 (5)
C(1)—Co(2)—Co(1)	49.8 (1)	Co(3)—C(32)—O(32)	178.3 (5)
C(1)—Co(2)—Co(3)	49.6 (1)	Co(3)—C(33)—O(33)	175.3 (7)
C(1)—Co(2)—C(21)	104.2 (2)	Co(4)—C(41)—O(41)	176.7 (5)
C(1)—Co(2)—C(22)	94.3 (2)	Co(4)—C(42)—O(42)	178.5 (4)
C(1)—Co(2)—C(23)	146.5 (2)	Co(4)—C(43)—O(43)	176.7 (5)
C(1)—Co(3)—Co(1)	49.8 (1)	Co(5)—C(51)—O(51)	177.9 (5)
C(1)—Co(3)—Co(2)	50.2 (1)	Co(5)—C(52)—O(52)	177.0 (5)
C(1)—Co(3)—C(31)	106.9 (2)	Co(5)—C(53)—O(53)	177.2 (5)
C(1)—Co(3)—C(32)	103.8 (2)	Co(6)—C(61)—O(61)	176.8 (5)
C(1)—Co(3)—C(33)	140.7 (2)	Co(6)—C(62)—O(62)	177.2 (5)
Co(4)—Co(5)—Co(6)	59.8 (1)	Co(6)—C(63)—O(63)	178.4 (5)
Co(4)—Co(6)—Co(5)	60.2 (1)		

The structure was solved by Patterson methods using *SHELXS*-86 (Sheldrick, 1986). Refinement was performed with a version of *SHELX*76 (Sheldrick, 1976) amended for the refinement of large structures (Rabinovich & Reich, 1979). Programs used: *PARST* (Nardelli, 1983), *SHELX*400 (Rabinovich & Reich, 1979), *SHELX*76, *SHELXTL* (Sheldrick, 1980) and *SHELXS*86.

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Lists of structure factors, anisotropic thermal parameters, complete geometry and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71003 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HL1020]

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