chelation is found in $Mo_2[(C_6H_5)_2PC(S)N(CH_3)]_4$ and both *S,N*- and *P,N*-coordination modes exist in an isomer of that compound (Ambrosius, Cotton, Falvello, Hintzen, Melton, Schwotzer, Tomas & Van Der Linden, 1984). A tridentate bridging mode, as well as a bidentate (*P,S*-) mode, has been reported in the dimer: $\{Mo(CO)_2[(C_6H_5)_2PC(S)N(CH_3)]_2\}_2$ (Bosman, Noordik, Ambrosius & Cras, 1980; Ambrosius, Willemse, Cras, Bosman & Noordik, 1984).

We are grateful for a Commonwealth Postgraduate Research Award to PAJ.

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Acta Cryst. (1987). C**43**, 2441–2442

Structure of the Aluminium Alkoxide Complex [Al(O-iPr)(3,5-heptanedione)$_2$]$_2$

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(*Received* 25 *November* 1986; *accepted* 1 *July* 1987)

Abstract. 1,1,2,2-Tetrakis(3,5-heptanedionato)-di-μ-isopropoxy-dialuminium(III), $[Al(C_7H_{11}O_2)_2(C_3H_7O)]_2$, $M_r = 734{\cdot}8$, triclinic, $P\bar{1}$, $a = 9{\cdot}150\ (4)$, $b = 10{\cdot}08\ (1)$, $c = 12{\cdot}574\ (7)$ Å, $\alpha = 96{\cdot}64\ (7)$, $\beta = 111{\cdot}15\ (4)$, $\gamma = 112{\cdot}62\ (7)°$, $V = 954{\cdot}0$ Å^3, $Z = 2$, $D_x = 2{\cdot}56$ g cm^{-3}, $\lambda(\text{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $\mu = 3{\cdot}4$ cm^{-1}, $F(000) = 788$, $T = 173$ K, $R = 0{\cdot}0837$, $wR = 0{\cdot}0672$ for 1534 unique observed reflections. Centrosymmetric dimer, with half of the molecule being the asymmetric unit. Aluminium sites contain octahedral coordination with bridging isopropoxide ligands occupying a diastereotopic position. This is the final compound in a series of aluminium alkoxides.

Experimental. Compound obtained by reaction of 3,5-heptanedione with $[Al(O\text{-}iPr)_3]_4$ in dry methylene chloride (Wengrovius, Garbauskas, Williams, Going, Donohue & Smith, 1986), recrystallized from methy lene chloride/pentane at 243 K. Crystal size 0·3 × 0·3 × 0·1 mm plate. Poorly diffracting (hence high *R* value). Crystal sealed in capillary under dry nitrogen due to moisture sensitivity. Nicolet *P3F* automated diffractometer. ω/θ scan with variable scan speeds. Cell parameters determined from 14 reflections $5 < 2\theta < 22°$. No absorption correction applied. Data collection: $4 < 2\theta < 45°$. $0 \le h \le 10$, $-11 \le k \le 11$, $-14 \le l \le 14$. Standard reflections: 100 and $\bar{1}\bar{1}\bar{1}$ varied less than 1% during data collection. 2689 reflections collected, 2500 unique reflections, 1534 unique reflections observed with $F > 3\sigma(F)$. Structure solved by direct methods, refined on *F*. H atoms located by

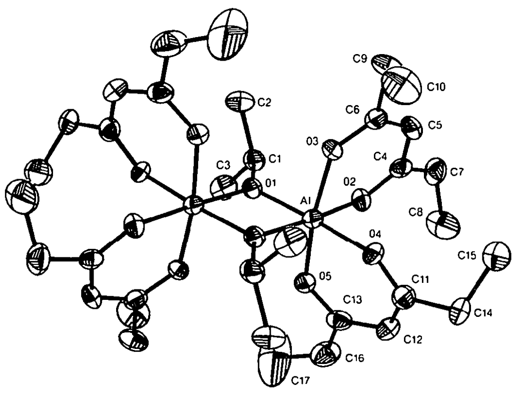

Fig. 1. Thermal-ellipsoid (50% probability) plot.

0108-2701/87/122441-02$01.50

Table 1. *Atom coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2 \times 10^3$)

	x	y	z	U_{eq}*
Al	3752 (3)	4402 (2)	3739 (2)	25 (1)
O(1)	6083 (5)	4914 (4)	4756 (3)	25 (2)
O(2)	1293 (5)	3873 (4)	2860 (4)	29 (2)
O(3)	4338 (6)	6327 (4)	3473 (4)	28 (3)
O(4)	3825 (5)	3747 (4)	2295 (3)	29 (2)
O(5)	2865 (5)	2365 (4)	3779 (3)	30 (2)
C(1)	7486 (8)	4808 (7)	4524 (6)	31 (4)
C(2)	7034 (9)	3165 (7)	4024 (6)	46 (5)
C(3)	7952 (9)	5791 (7)	3760 (6)	45 (4)
C(4)	599 (9)	4446 (7)	2089 (5)	29 (4)
C(5)	1561 (9)	5826 (7)	1965 (6)	34 (4)
C(6)	3376 (10)	6705 (7)	2684 (6)	34 (4)
C(7)	−1372 (9)	3590 (7)	1337 (6)	43 (4)
C(8)	−2055 (10)	1914 (7)	974 (7)	67 (5)
C(9)	4328 (10)	8259 (7)	2557 (7)	44 (5)
C(10)	5723 (10)	8333 (8)	2164 (7)	64 (6)
C(11)	2961 (9)	2401 (7)	1546 (6)	35 (4)
C(12)	2075 (9)	1125 (7)	1797 (6)	38 (4)
C(13)	2089 (8)	1155 (7)	2915 (6)	34 (4)
C(14)	3073 (10)	2315 (7)	377 (5)	45 (4)
C(15)	2640 (11)	3446 (8)	−182 (6)	59 (5)
C(16)	1150 (11)	−271 (7)	3172 (7)	55 (5)
C(17)	1763 (15)	−269 (9)	4347 (8)	170 (9)

* Equivalent isotropic U defined as one-third of the trace of the orthogonalized U_{ij} tensor.

difference map and constrained to have C—H = 0·96 Å and isotropic thermal parameters, $U = 0{\cdot}06$ Å^2. 208 parameters refined. All non-H atoms treated as anisotropic. $R_{int} = 0{\cdot}0302$; $R = 0{\cdot}0837$; $wR = 0{\cdot}0672$; $w^{-1} = \sigma^2(F) + 0{\cdot}0003F^2$. $(\Delta/\sigma)_{max} = 0{\cdot}094$, $(\Delta\rho)_{max} = 0{\cdot}37$, $(\Delta\rho)_{min} = -0{\cdot}40$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Programs: *SHELXTL* (Sheldrick, 1981). Atomic coordinates are contained in Table 1.* Bond lengths and angles, structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited. Fig. 1 illustrates the molecule with the numbering scheme employed. Note that the large thermal motion for C(17) leads to an incorrect bond distance for C(16)—C(17). Efforts to refine this disorder were unsuccessful.

Related literature. For additional information on structures and chemistry of aluminium alkoxide and siloxide complexes, see Garbauskas, Wengrovius, Going & Kasper (1984) and Wengrovius *et al.* (1986).

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* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44206 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1987). C**43**, 2442–2443

The Silver Salt of Cyanourea

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(*Received* 16 *June* 1987; *accepted* 11 *August* 1987)

Abstract. $Ag^+.C_2H_2N_3O^-$, $M_r = 191{\cdot}93$, orthorhombic, *Pbca*, $a = 6{\cdot}530$ (6), $b = 9{\cdot}882$ (4), $c = 12{\cdot}973$ (3) Å, $Z = 8$, $V/Z = 104{\cdot}6$ (2) Å^3; $D_x = 3{\cdot}045$ (5), $D_m > 2{\cdot}96$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71073$ Å, $\mu = 46{\cdot}2$ cm^{-1}, $F(000) = 720$, $T = 297$ (2) K, $R = 0{\cdot}040$ for 909 reflections. The anion is formed from the neutral cyanourea molecule by loss of the H ion attached to the central N atom. The bond distances indicate considerable electron delocalization in the anion. The NH_2 group is bent out of the plane of the N_2CO fragment by 23 (6)° and the nitrile group is bent out of the same plane by 4·5 (3)°. The NH_2 H atoms are both involved in hydrogen bonds to O atoms in adjacent anions. The Ag ion has two close contacts [2·143 (4) Å to a nitrile N atom and 2·180 (4) Å to a central N atom] 144·7 (2)° apart as well as two longer contacts [2·576 (3) Å to an O atom and 2·733 (5) Å to another nitrile N atom].

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