

**Data collection**

Nicolet P3 diffractometer	$h = 0 \rightarrow 8; 0 \rightarrow 8$
$\omega$ scans	$k = -12 \rightarrow 0; 0 \rightarrow 12$
2237 measured reflections	$l = -21 \rightarrow 0; 0 \rightarrow 21$
1099 independent reflections	4 standard reflections
1023 observed reflections	monitored every 96 reflections
$[F > 4.0\sigma(F)]$	intensity variation: 1.28%
$R_{\text{int}} = 0.0086$	
$\theta_{\text{max}} = 55.0^\circ$	

**Refinement**

Refinement on $F$	$\Delta\rho_{\text{max}} = 0.38 \text{ e } \text{\AA}^{-3}$
Final $R = 0.0349$	$\Delta\rho_{\text{min}} = -0.16 \text{ e } \text{\AA}^{-3}$
$wR = 0.0499$	Extinction correction:
$S = 1.9613$	$F^* = F[1 + 0.002\chi F^2$
1023 reflections	$/\sin(2\theta)]^{-1/4}$
129 parameters	Extinction coefficient:
All H-atom parameters refined	0.0012
Calculated weights $w =$	Atomic scattering factors
$1/[\sigma^2(F) + 0.0004F^2]$	from <i>International Tables</i>
$(\Delta/\sigma)_{\text{max}} = 0.065$	for <i>X-ray Crystallography</i>
	(1974, Vol. IV, Table 2.3.1)

Data collection: *SHELXTL-Plus* (Sheldrick, 1991). Cell refinement: *SHELXTL-Plus*. Data reduction: *SHELXTL-Plus*. Program(s) used to solve structure: *SHELXTL-Plus*. Program(s) used to refine structure: *SHELXTL-Plus*. Molecular graphics: *SHELXTL-Plus*. Software used to prepare material for publication: *PLATON* (Spek, 1990).

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters ( $\text{\AA}^2$ )

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	$x$	$y$	$z$	$U_{\text{eq}}$
S	0.3566 (1)	0.04553 (8)	0.04855 (4)	0.0411 (2)
N	0.3627 (4)	-0.1937 (3)	0.1787 (1)	0.0355 (6)
C2'	0.1411 (4)	-0.0868 (3)	0.0655 (1)	0.0279 (6)
C3'	-0.0322 (5)	-0.0699 (3)	0.0066 (2)	0.0361 (7)
C4'	0.0111 (5)	0.0481 (3)	-0.0518 (2)	0.0420 (8)
C5'	0.2145 (6)	0.1218 (3)	-0.0372 (2)	0.0423 (8)
C2	0.1616 (4)	-0.1991 (3)	0.1344 (1)	0.0286 (6)
C3	-0.0133 (5)	-0.3025 (4)	0.1520 (2)	0.0391 (8)
C4	0.0202 (6)	-0.4077 (4)	0.2165 (2)	0.0465 (9)
C5	0.2279 (5)	-0.4045 (4)	0.2618 (2)	0.0434 (8)
C6	0.3867 (5)	-0.2933 (4)	0.2388 (2)	0.0397 (8)

Table 2. Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

S—C5'	1.712 (3)	C2—C3	1.386 (4)
S—C2'	1.723 (3)	C2—N	1.353 (3)
C5'—C4'	1.360 (5)	N—C6	1.294 (4)
C4'—C3'	1.407 (4)	C3—C4	1.385 (4)
C3'—C2'	1.369 (4)	C4—C5	1.393 (4)
C2'—C2	1.469 (3)	C5—C6	1.387 (4)
C5'—S—C2'	92.3 (1)	C2'—C2—C3	121.9 (2)
S—C5'—C4'	111.0 (2)	N—C2—C3	123.0 (2)
C5'—C4'—C3'	113.3 (3)	C2—C3—C4	118.8 (3)
C4'—C3'—C2'	112.9 (2)	C3—C4—C5	118.6 (3)
C3'—C2'—C2	128.9 (2)	C4—C5—C6	116.7 (3)
C3'—C2'—S	110.5 (2)	C5—C6—N	126.5 (3)
S—C2'—C2	120.6 (2)	C6—N—C2	116.3 (2)
C2'—C2—N	115.1 (2)		

SHS acknowledges the support of the Robert A. Welch Foundation (grant F-0017).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55767 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST1039]

**References**

- Chao, M. & Schempp, E. (1977). *Acta Cryst.* **B33**, 1557–1564.  
 Destro, R., Pilati, T. & Simonetta, M. (1975). *Acta Cryst.* **B31**, 2883–2885.  
 Golić, L., Leban, I., Stanovnik, B. & Tišler, M. (1979). *Acta Cryst.* **B35**, 2256–2258.  
 Kvik, Å. & Noordik, J. (1977). *Acta Cryst.* **B33**, 2862–2866.  
 Nakai, H. (1990). *Acta Cryst.* **C46**, 1951–1953.  
 Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.  
 Shiro, M. (1990). *Acta Cryst.* **C46**, 1152–1153.  
 Spek, A. L. (1990). 40th Meet. Am. Crystallogr. Assoc., New Orleans, LA, USA. Abstract PM04.  
 Tenon, A. J., Ebby, N., Degny, E., Viani, R. & Bodot, H. (1988). *Acta Cryst.* **C44**, 95–97.

*Acta Cryst.* (1993). **C49**, 1032–1035

## Structures of Tetradecyltrimethylammonium Salicylate Monohydrate (1) and Hexadecyltrimethylammonium Salicylate Monohydrate (2)

L. L. KOH, Y. XU, L. M. GAN, C. H. CHEW AND K. C. LEE

*Chemistry Department, Faculty of Science, National University of Singapore, Singapore 0511*

(Received 10 August 1992; accepted 9 December 1992)

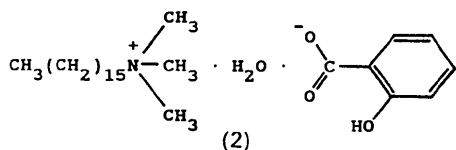
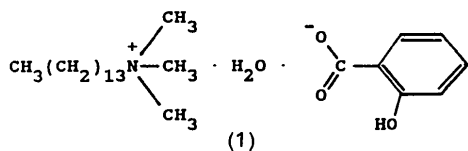
**Abstract**

(1)  $[(\text{C}_{14}\text{H}_{29})(\text{CH}_3)_3\text{N}]^+ \cdot \text{C}_7\text{H}_5\text{O}_3^- \cdot \text{H}_2\text{O}$ : the tetradecyl chain is fully extended in a zigzag form; the cation, anion and the water molecule are packed in layers with the tetradecyl chains parallel within a layer and antiparallel in alternate layers; the water molecule is hydrogen bonded to one of the carboxylate O atoms of the anion. (2)  $[(\text{C}_{16}\text{H}_{33})(\text{CH}_3)_3\text{N}]^+ \cdot \text{C}_7\text{H}_5\text{O}_3^- \cdot \text{H}_2\text{O}$ : the crystal packing, bond lengths and bond angles are all very similar to those of (1).

**Comment**

It has been reported recently that aqueous solutions of (1) and (2) show interesting viscoelastic and spinable properties (Imae, Hashimoto & Ikeda, 1990;

Imae, 1990). It was assumed that a pseudo-network structure composed of rod-like miscelles was formed in these viscoelastic and spinnable surfactant solutions. This tempted us to determine the crystal structures of (1) and (2) to find out the structures in the solid phase.



**Structure of (1).** The asymmetric unit contains one tetradecyltrimethylammonium cation, one salicylate anion and one water molecule (Fig. 1). The tetradecyl chain of the cation is fully extended. All C atoms of the chain, from C(1) to C(14), are coplanar to within a mean deviation of 0.025 Å. The average torsion angle along the chain is 179 (1)°. The thermal displacement coefficients  $U_{eq}$  increase markedly from C(1) to C(14), ranging from 0.057 to 0.172 Å<sup>2</sup>. This increased thermal motion probably accounts for the C—C bonds tending to be shorter towards the end of the chain, and the C—C—C angles tending to be larger. The average C—C bond length is 1.50 (2) Å and the average C—C—C angle 115.6 (2.4)°. These values are not significantly different from 1.523 (8) Å and 113.2 (5)° found in hexadecyltrimethylammonium bromide (Campanelli & Scaramuzza, 1986), or 1.516 (8) Å and 113 (1)° in dodecyldimethylpropylammonium bromide monohydrate (Taga, Machida, Kimura, Hayashi, Umemura & Takenaka, 1986). The geometry around the N atom N(1) is normal with an average N—C bond length of 1.496 (5) Å and C—N—C angle of 109.4 (1.0)°. The salicylate anion is planar and the bond lengths and angles are in close agreement with those in other salicylates (Gellert & Hsu, 1988). C atoms deviate from planarity by an average of 0.007 Å, while O atoms deviate by 0.04 Å. All C—C and C—O bond lengths are within the usual ranges. The C(22)—C(21)—C(26) angle is slightly smaller than the other C—C—C angles. The intramolecular hydrogen bond between O(1) and O(2) has a distance of 2.493 (5) Å. There is an intermolecular hydrogen bond between O(3) of the salicylate anion and O(4) of the water molecule with an O···O distance of 2.754 (5) Å.

The cation, the anion and the water molecule are packed in approximately planar layers which are

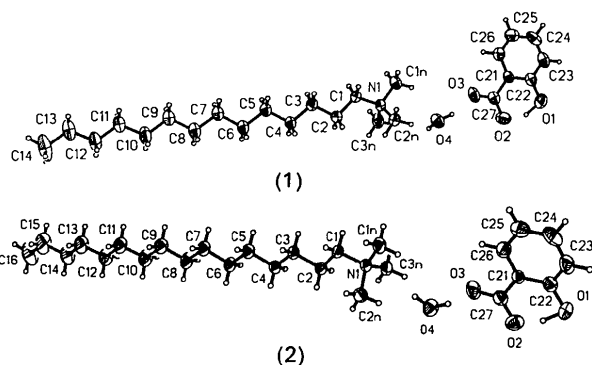


Fig. 1. Perspective views and atomic numbering of (1) and (2).

perpendicular to the *b* axis. The water molecule is held between the CO<sub>2</sub> group and the N(CH<sub>3</sub>)<sub>3</sub> group of the cation. The tetradecyl chains are arranged parallel within the same layer and antiparallel in alternate layers. The packing of the crystal viewed along the *a* axis is shown in Fig. 2.

**Structure of (2).** The structure of (2) is very similar to that of (1) (Fig. 1). Corresponding bond lengths and angles are almost identical to those of (1), and the crystal packing is essentially the same. The average bond lengths and angles are: 1.50 (2) Å for the alkyl C—C bond, 115.6 (2.5)° for the alkyl C—C—C angle, 179 (1)° for the torsion angles of the alkyl chain, 1.499 (7) Å for N—C, and 109.4 (1.0)° for C—N—C. Hydrogen-bond distances are 2.497 (6) Å for O(1)···O(2) and 2.752 (6) Å for O(3)···O(4).

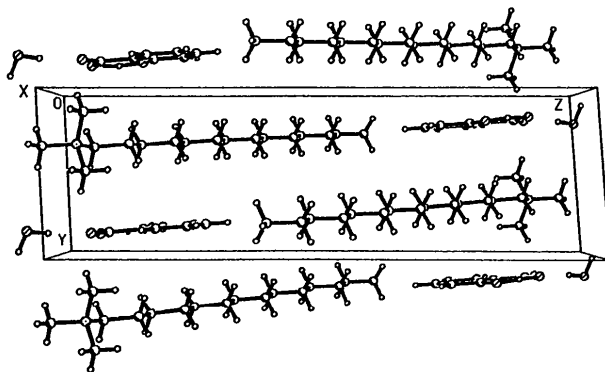


Fig. 2. Packing of (1) viewed along the *a* axis.

## Experimental

### Compound (1)

#### Crystal data

C<sub>17</sub>H<sub>38</sub>N<sup>+</sup>·C<sub>7</sub>H<sub>5</sub>O<sub>3</sub><sup>-</sup>·H<sub>2</sub>O

$M_r = 411.6$

Mo K $\alpha$  radiation

$\lambda = 0.71073$  Å

## Triclinic

$P\bar{1}$   
 $a = 7.059$  (1) Å  
 $b = 7.436$  (2) Å  
 $c = 24.572$  (7) Å  
 $\alpha = 86.25$  (2)°  
 $\beta = 88.85$  (2)°  
 $\gamma = 88.62$  (2)°  
 $V = 1284.6$  (5) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.064$  Mg m<sup>-3</sup>

## Data collection

Siemens R3m/V diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 3707 measured reflections  
 3378 independent reflections  
 1696 observed reflections  
 $[I > 2.0\sigma(I)]$

## Refinement

Refinement on  $F$   
 Final  $R = 0.042$   
 $wR = 0.061$   
 $S = 0.77$   
 1696 reflections  
 263 parameters  
 H-atom parameters not refined

## Compound (2)

## Crystal data

$C_{19}H_{42}N^+ \cdot C_7H_5O_3^- \cdot H_2O$   
 $M_r = 439.7$

## Triclinic

$P\bar{1}$   
 $a = 7.055$  (1) Å  
 $b = 7.450$  (1) Å  
 $c = 26.389$  (7) Å  
 $\alpha = 93.29$  (3)°  
 $\beta = 92.92$  (2)°  
 $\gamma = 93.35$  (2)°  
 $V = 1380.2$  (7) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.058$  Mg m<sup>-3</sup>

## Data collection

Siemens R3m/V diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 4941 measured reflections  
 4825 independent reflections  
 2065 observed reflections  
 $[I > 2.0\sigma(I)]$

## Cell parameters from 16 reflections

$\theta = 3.0$ – $12.6$ °  
 $\mu = 0.071$  mm<sup>-1</sup>  
 $T = 298$  K  
 Prism  
 $0.4 \times 0.4 \times 0.2$  mm  
 Colourless  
 Crystal source: recrystallization from acetone/ethyl acetate

$R_{int} = 0.012$   
 $\theta_{max} = 25$ °  
 $h = 0 \rightarrow 7$   
 $k = -8 \rightarrow 8$   
 $l = -26 \rightarrow 26$   
 3 standard reflections monitored every 97 reflections  
 intensity variation:  $\pm 1.5\%$

$w = [\sigma^2(F) + 0.0044F^2]^{-1}$   
 $(\Delta/\sigma)_{max} = 0.010$   
 $\Delta\rho_{max} = 0.18$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.12$  e Å<sup>-3</sup>  
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å  
 Cell parameters from 20 reflections  
 $\theta = 3.3$ – $11.8$ °  
 $\mu = 0.069$  mm<sup>-1</sup>  
 $T = 298$  K  
 Prism  
 $0.5 \times 0.4 \times 0.25$  mm  
 Colourless  
 Crystal source: recrystallization from acetone

$R_{int} = 0.013$   
 $\theta_{max} = 25$ °  
 $h = -8 \rightarrow 8$   
 $k = -8 \rightarrow 8$   
 $l = 0 \rightarrow 30$   
 3 standard reflections monitored every 97 reflections  
 intensity variation:  $\pm 1.5\%$

## Refinement

Refinement on  $F$   
 Final  $R = 0.059$   
 $wR = 0.067$   
 $S = 1.60$   
 2065 reflections  
 281 parameters  
 H-atom parameters not refined

$w = [\sigma^2(F) + 0.0006F^2]^{-1}$   
 $(\Delta/\sigma)_{max} = 0.011$   
 $\Delta\rho_{max} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.16$  e Å<sup>-3</sup>  
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (Å<sup>2</sup>) for compound (1) and compound (2)

$U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U_{eq}$
(1)				
N(1)	0.2900 (3)	0.3334 (3)	0.0828 (1)	0.056 (1)
C(1N)	0.2855 (5)	0.3451 (5)	0.0217 (1)	0.083 (2)
C(2N)	0.4008 (4)	0.4829 (5)	0.1005 (1)	0.074 (1)
C(3N)	0.3874 (5)	0.1571 (5)	0.1015 (2)	0.080 (1)
C(1)	0.0893 (4)	0.3476 (4)	0.1043 (1)	0.057 (1)
C(2)	0.0608 (4)	0.3271 (4)	0.1652 (1)	0.059 (1)
C(3)	-0.1492 (4)	0.3307 (4)	0.1790 (1)	0.059 (1)
C(4)	-0.1973 (4)	0.3103 (4)	0.2392 (1)	0.064 (1)
C(5)	-0.4085 (4)	0.3104 (5)	0.2508 (1)	0.069 (1)
C(6)	-0.4656 (5)	0.2939 (5)	0.3105 (1)	0.079 (1)
C(7)	-0.6785 (5)	0.2899 (5)	0.3204 (1)	0.079 (1)
C(8)	-0.7389 (5)	0.2806 (6)	0.3795 (2)	0.102 (2)
C(9)	-0.9471 (5)	0.2713 (6)	0.3913 (1)	0.092 (2)
C(10)	-1.0049 (6)	0.2661 (7)	0.4505 (2)	0.113 (2)
C(11)	-1.2053 (6)	0.2508 (7)	0.4645 (2)	0.109 (2)
C(12)	-1.2654 (7)	0.2469 (7)	0.5233 (2)	0.114 (2)
C(13)	-1.4640 (8)	0.2348 (9)	0.5372 (2)	0.156 (3)
C(14)	-1.5229 (10)	0.2304 (8)	0.5956 (2)	0.172 (3)
C(21)	1.0721 (5)	0.1774 (4)	-0.1767 (1)	0.057 (1)
C(22)	1.2412 (5)	0.1835 (4)	-0.2071 (2)	0.068 (1)
C(23)	1.2370 (7)	0.1971 (5)	-0.2631 (2)	0.091 (2)
C(24)	1.0681 (9)	0.2062 (5)	-0.2894 (2)	0.102 (2)
C(25)	0.9010 (7)	0.2008 (5)	-0.2603 (2)	0.094 (2)
C(26)	0.9022 (5)	0.1861 (4)	-0.2045 (2)	0.072 (2)
C(27)	1.0734 (6)	0.1590 (4)	-0.1156 (1)	0.069 (1)
O(1)	1.4100 (3)	0.1760 (3)	-0.1816 (1)	0.093 (1)
O(2)	1.2330 (4)	0.1435 (4)	-0.0931 (1)	0.097 (1)
O(3)	0.9185 (4)	0.1590 (3)	-0.0905 (1)	0.097 (1)
O(4)	0.7824 (3)	0.1733 (3)	0.0150 (1)	0.088 (1)
(2)				
N(1)	0.3105 (4)	0.1663 (4)	0.0774 (1)	0.055 (1)
C(1N)	0.2899 (6)	0.1555 (6)	0.0204 (1)	0.080 (2)
C(2N)	0.4114 (5)	0.3429 (5)	0.0944 (2)	0.078 (2)
C(3N)	0.4252 (5)	0.0162 (5)	0.0936 (1)	0.072 (2)
C(1)	0.1130 (5)	0.1516 (5)	0.0974 (1)	0.056 (1)
C(2)	0.1022 (5)	0.1710 (5)	0.1544 (1)	0.055 (1)
C(3)	-0.1068 (5)	0.1665 (5)	0.1669 (1)	0.059 (1)
C(4)	-0.1392 (5)	0.1864 (5)	0.2234 (1)	0.062 (2)
C(5)	-0.3485 (5)	0.1859 (6)	0.2339 (1)	0.070 (2)
C(6)	-0.3900 (5)	0.2016 (6)	0.2898 (1)	0.077 (2)
C(7)	-0.6013 (6)	0.2066 (6)	0.2986 (2)	0.078 (2)
C(8)	-0.6458 (6)	0.2136 (7)	0.3542 (2)	0.100 (2)
C(9)	-0.8518 (6)	0.2225 (7)	0.3648 (2)	0.088 (2)
C(10)	-0.8934 (7)	0.2269 (7)	0.4200 (2)	0.108 (2)
C(11)	-1.0935 (6)	0.2414 (7)	0.4333 (2)	0.098 (2)
C(12)	-1.1346 (7)	0.2445 (7)	0.4886 (2)	0.105 (2)
C(13)	-1.3331 (7)	0.2568 (8)	0.5026 (2)	0.117 (3)
C(14)	-1.3779 (8)	0.2601 (7)	0.5569 (2)	0.115 (3)
C(15)	-1.5761 (9)	0.2734 (10)	0.5697 (2)	0.162 (4)
C(16)	-1.6235 (10)	0.2758 (8)	0.6237 (2)	0.168 (4)
C(21)	1.0275 (5)	0.3251 (4)	-0.1643 (2)	0.054 (2)
C(22)	1.1894 (7)	0.3199 (5)	-0.1927 (2)	0.066 (2)
C(23)	1.1705 (8)	0.3075 (6)	-0.2449 (2)	0.092 (2)
C(24)	0.9972 (10)	0.2975 (7)	-0.2697 (2)	0.103 (3)
C(25)	0.8352 (8)	0.3033 (6)	-0.2424 (2)	0.092 (2)

C(26)	0.8512 (6)	0.3167 (5)	-0.1901 (2)	0.071 (2)	C(13)—C(14)—C(15)	118.4 (4)
C(27)	1.0439 (7)	0.3427 (5)	-0.1074 (2)	0.067 (2)	C(14)—C(15)—C(16)	119.2 (5)
O(1)	1.3659 (4)	0.3255 (4)	-0.1693 (1)	0.094 (1)	C(22)—C(21)—C(26)	118.2 (3)
O(2)	1.2098 (5)	0.3576 (4)	-0.0867 (1)	0.095 (1)	C(22)—C(21)—C(27)	121.1 (3)
O(3)	0.8959 (5)	0.3419 (4)	-0.0838 (1)	0.093 (1)	C(26)—C(21)—C(27)	120.6 (3)
O(4)	0.7890 (4)	0.3292 (4)	0.0148 (1)	0.087 (1)	C(21)—C(22)—C(23)	120.2 (4)
					C(21)—C(22)—O(1)	120.2 (3)
					C(23)—C(22)—O(1)	119.7 (4)
					C(22)—C(23)—C(24)	120.4 (4)
					C(23)—C(24)—C(25)	120.3 (4)
					C(24)—C(25)—C(26)	120.2 (4)
					C(21)—C(26)—C(25)	120.7 (4)
					C(21)—C(27)—O(2)	117.2 (3)
					C(21)—C(27)—O(3)	118.4 (3)
					O(2)—C(27)—O(3)	124.4 (3)
						118.7 (4)
						124.5 (4)

Table 2. Selected bond lengths (Å) and angles (°) for compound (1) and compound (2)

	Compound (1)	Compound (2)
N(1)—C(1 <i>N</i> )	1.499 (4)	1.500 (5)
N(1)—C(2 <i>N</i> )	1.488 (4)	1.493 (5)
N(1)—C(3 <i>N</i> )	1.494 (4)	1.487 (5)
N(1)—C(1)	1.502 (4)	1.515 (4)
C(1)—C(2)	1.507 (4)	1.509 (5)
C(2)—C(3)	1.513 (4)	1.526 (5)
C(3)—C(4)	1.511 (4)	1.518 (5)
C(4)—C(5)	1.512 (4)	1.516 (5)
C(5)—C(6)	1.514 (4)	1.519 (5)
C(6)—C(7)	1.519 (5)	1.522 (6)
C(7)—C(8)	1.504 (5)	1.515 (6)
C(8)—C(9)	1.497 (5)	1.499 (6)
C(9)—C(10)	1.501 (5)	1.500 (6)
C(10)—C(11)	1.458 (6)	1.480 (7)
C(11)—C(12)	1.497 (6)	1.503 (6)
C(12)—C(13)	1.443 (7)	1.473 (7)
C(13)—C(14)	1.484 (7)	1.482 (7)
C(14)—C(15)		1.463 (8)
C(15)—C(16)		1.480 (9)
C(21)—C(22)	1.397 (5)	1.399 (6)
C(21)—C(26)	1.389 (5)	1.384 (6)
C(22)—C(23)	1.372 (6)	1.374 (7)
C(23)—C(24)	1.364 (7)	1.354 (9)
C(24)—C(25)	1.368 (7)	1.384 (9)
C(25)—C(26)	1.369 (6)	1.376 (7)
C(21)—C(27)	1.498 (5)	1.497 (6)
C(22)—O(1)	1.354 (5)	1.360 (5)
C(27)—O(2)	1.260 (5)	1.263 (6)
C(27)—O(3)	1.245 (5)	1.242 (6)
N(1)—C(1)—C(2)	117.1 (2)	116.2 (3)
C(1)—C(2)—C(3)	109.7 (2)	108.5 (3)
C(2)—C(3)—C(4)	115.0 (2)	114.3 (3)
C(3)—C(4)—C(5)	112.9 (2)	112.3 (3)
C(4)—C(5)—C(6)	115.3 (3)	114.8 (3)
C(5)—C(6)—C(7)	113.7 (3)	113.1 (3)
C(6)—C(7)—C(8)	114.7 (3)	113.7 (3)
C(7)—C(8)—C(9)	116.6 (3)	115.7 (3)
C(8)—C(9)—C(10)	115.7 (3)	114.9 (4)
C(9)—C(10)—C(11)	118.1 (3)	117.7 (4)
C(10)—C(11)—C(12)	118.7 (4)	117.5 (4)
C(11)—C(12)—C(13)	118.9 (4)	118.3 (4)
C(12)—C(13)—C(14)	118.7 (5)	119.5 (4)

(1) and (2) were prepared as described by Imae, Hashimoto & Ikeda (1990). Both structures were solved by direct methods and refined anisotropically by full-matrix least squares for all non-H atoms. H atoms bonded to C atoms were placed in calculated positions. H atoms bonded to O atoms were located from a difference map. All H atoms were given fixed isotropic thermal parameters. Data processing, computation and preparation of graphics were performed with programs from *SHELXTL-Plus* (Sheldrick, 1990).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55918 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HL1018]

## References

- Campanelli, A. R. & Scaramuzza, L. (1986). *Acta Cryst.* **C42**, 1380–1383.
- Gellert, R. W. & Hsu, I.-N. (1988). *Acta Cryst.* **C44**, 311–313.
- Imae, T. (1990). *J. Phys. Chem.* **94**, 5953–5959.
- Imae, T., Hashimoto, K. & Ikeda, I. (1990). *Colloid Polym. Sci.* **268**, 460–468.
- Sheldrick, G. M. (1990). *SHELXTL-Plus*. Version 4.0. Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.
- Taga, T., Machida, K., Kimura, N., Hayashi, S., Umemura, J. & Takenaka, T. (1986). *Acta Cryst.* **C42**, 608–610.

## SHORT COMMUNICATION

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.* (1993). **C49**, 1035–1036

### Structure of a polymeric cadmium complex containing triply bridging monophenylphosphinate ligands.

**Erratum.** By JING-LONG DU, STEVEN J. RETTIG, ROBERT C. THOMPSON and JAMES TROTTER, *Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, BC, Canada V6T 1Z1*

(Received 6 November 1992; accepted 2 February 1993)

#### Abstract

Due to a now-corrected error in a Delaunay reduction program, the structure of  $[\text{Cd}(\text{C}_6\text{H}_5\text{O}_2\text{P})(\text{Cl})(\text{H}_2\text{O})_x]$  was

incorrectly reported as triclinic, space group  $P\bar{1}$  [Du, Rettig, Thompson & Trotter (1992). *Acta Cryst.* **C48**, 1394–1397]. The matrix (111/001/1–10) transforms the previously reported triclinic cell to a body-centred mono-