

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]

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*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*

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#### 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-

clinic unit cell, space group  $I2/a$ ,  $a = 13.885$  (2),  $b = 5.8864$  (6),  $c = 21.624$  (2) Å,  $\beta = 93.250$  (8)°,  $V = 1764.5$  (7) Å<sup>3</sup>,  $Z = 8$ ,  $F(000) = 1184$ . Updated experimental data and revised atomic coordinates and geometrical data are given.

Updated experimental data: 14 959 reflections measured, 8107 independent ( $R_{\text{merge}} = 0.036$ ), 5473 with  $I \geq 3\sigma(I)$ ,  $\sigma^2(F_o^2) = [S^2(C + 4B)]/Lp^2$ ,  $S = \text{scan speed}$ ,  $C = \text{scan count}$ ,  $B = \text{background count}$ . Final  $R = 0.023$ ,  $wR = 0.024$  for 5473 reflections,  $S = 1.51$ , for 124 parameters,  $R = 0.054$  for all 8107 reflections,  $(\Delta/\sigma)_{\text{max}} = 0.005$ , maximum final difference density  $-0.84$  to  $0.96$  e Å<sup>-3</sup>. Revised atomic coordinates and geometrical data are given in Tables 1 and 2.\* Atom labeling in the asymmetric unit is

\* Lists of H-atom parameters, anisotropic thermal parameters, bond lengths and angles involving H atoms, torsion angles, least-squares-planes data, intermolecular contacts, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55895 (38 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH1056]

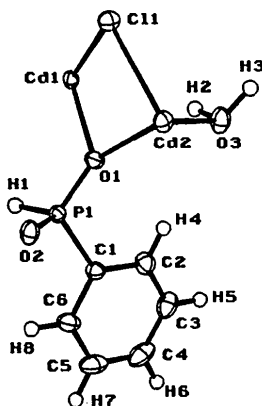


Fig. 1. A view of the asymmetric unit of  $[\text{Cd}(\text{C}_6\text{H}_6\text{O}_2\text{P})(\text{Cl})(\text{H}_2\text{O})]_x$ , showing the atom-labeling scheme and 50% probability thermal ellipsoids.

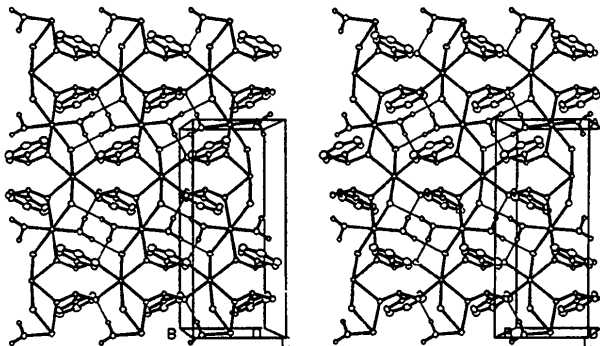


Fig. 2. A view of one layer of the polymeric  $[\text{Cd}(\text{C}_6\text{H}_6\text{O}_2\text{P})(\text{Cl})(\text{H}_2\text{O})]_x$  structure along  $c$ .

Table 1. Final atomic coordinates (fractional) and  $B_{\text{eq}}$  values (Å<sup>2</sup>)

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	$x$	$y$	$z$	$B_{\text{eq}}$
Cd(1)	$\frac{1}{2}$	0.27041 (2)	$\frac{1}{2}$	1.337 (4)
Cd(2)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1.583 (4)
Cl(1)	0.61937 (2)	0.28768 (5)	0.580156 (15)	1.77 (1)
P(1)	0.68604 (2)	0.76559 (5)	0.421381 (15)	1.255 (9)
O(1)	0.64794 (7)	0.5540 (2)	0.45277 (4)	1.58 (3)
O(2)	0.66020 (8)	0.9906 (2)	0.45068 (5)	1.88 (3)
O(3)	0.48790 (9)	0.1898 (2)	0.43900 (6)	2.33 (4)
C(1)	0.64961 (10)	0.7703 (2)	0.34078 (6)	1.59 (4)
C(2)	0.60592 (12)	0.5861 (3)	0.31080 (7)	2.18 (5)
C(3)	0.58672 (13)	0.5922 (3)	0.24678 (7)	2.70 (6)
C(4)	0.61175 (13)	0.7843 (4)	0.21354 (7)	2.95 (6)
C(5)	0.65410 (14)	0.9679 (3)	0.24299 (8)	2.85 (6)
C(6)	0.67390 (12)	0.9630 (3)	0.30691 (7)	2.26 (5)

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

Cd(1)—Cl(1)	2.5809 (4)	P(1)—C(1)	1.787 (1)
Cd(1)—O(1)	2.3821 (9)	C(1)—C(2)	1.386 (2)
Cd(1)—O(2)	2.292 (1)	C(1)—C(6)	1.402 (2)
Cd(2)—Cl(1)	2.6434 (4)	C(2)—C(3)	1.395 (2)
Cd(2)—O(1)	2.367 (1)	C(3)—C(4)	1.395 (3)
Cd(2)—O(3)	2.253 (1)	C(4)—C(5)	1.370 (3)
P(1)—O(1)	1.5272 (9)	C(5)—C(6)	1.394 (2)
P(1)—O(2)	1.520 (1)		
Cl(1)—Cd(1)—Cl(1 <sup>ii</sup> )	175.48 (2)	O(3)—Cd(2)—O(3 <sup>iv</sup> )	180.00
Cl(1)—Cd(1)—O(1)	80.60 (2)	Cd(1)—Cl(1)—Cd(2)	90.95 (1)
Cl(1)—Cd(1)—O(1 <sup>ii</sup> )	96.21 (2)	O(1)—P(1)—O(2)	115.43 (6)
Cl(1)—Cd(1)—O(2)	87.50 (3)	O(1)—P(1)—C(1)	111.10 (6)
Cl(1)—Cd(1)—O(2 <sup>iii</sup> )	95.76 (3)	O(2)—P(1)—C(1)	109.42 (6)
O(1)—Cd(1)—O(1 <sup>ii</sup> )	91.01 (5)	Cd(1)—O(1)—Cd(2)	103.33 (3)
O(1)—Cd(1)—O(2)	90.54 (4)	Cd(1)—O(1)—P(1)	123.32 (5)
O(1)—Cd(1)—O(2 <sup>iii</sup> )	176.18 (4)	Cd(2)—O(1)—P(1)	129.23 (5)
O(2)—Cd(1)—O(2 <sup>iii</sup> )	88.14 (5)	Cd(1 <sup>v</sup> )—O(2)—P(1)	133.23 (6)
Cl(1)—Cd(2)—Cl(1 <sup>ii</sup> )	180.00	P(1)—C(1)—C(2)	122.4 (1)
Cl(1)—Cd(2)—O(1)	79.58 (2)	P(1)—C(1)—C(6)	117.3 (1)
Cl(1)—Cd(2)—O(1 <sup>iv</sup> )	100.42 (2)	C(2)—C(1)—C(6)	120.1 (1)
Cl(1)—Cd(2)—O(3)	91.37 (3)	C(1)—C(2)—C(3)	119.9 (1)
Cl(1)—Cd(2)—O(3 <sup>iv</sup> )	88.63 (3)	C(2)—C(3)—C(4)	119.5 (2)
O(1)—Cd(2)—O(1 <sup>iv</sup> )	180.00	C(3)—C(4)—C(5)	120.9 (1)
O(1)—Cd(2)—O(3)	83.91 (4)	C(4)—C(5)—C(6)	120.0 (2)
O(1)—Cd(2)—O(3 <sup>iv</sup> )	96.09 (4)	C(1)—C(6)—C(5)	119.7 (2)

Symmetry code: (i)  $x, y - 1, z$ ; (ii)  $\frac{1}{2} - x, y, 1 - z$ ; (iii)  $\frac{1}{2} - x, y - 1, 1 - z$ ; (iv)  $1 - x, 1 - y, 1 - z$ ; (v)  $x, 1 + y, z$ .

shown in Fig. 1 and a layer of the sheet structure (with the new unit cell outlined) is shown in Fig. 2. Both Cd atoms lie on symmetry elements: Cd(1) on a twofold axis and Cd(2) at a centre of symmetry. Other aspects of the structure are as discussed previously (Du, Rettig, Thompson & Trotter, 1992).

The authors thank Professor R. E. Marsh for pointing out the transformation to the higher symmetry unit cell.

#### Reference

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