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## Key indicators

Single-crystal X-ray study  
 $T = 273\text{ K}$   
Mean  $\sigma(\text{C}–\text{C}) = 0.008\text{ \AA}$   
 $R$  factor = 0.049  
 $wR$  factor = 0.144  
Data-to-parameter ratio = 15.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

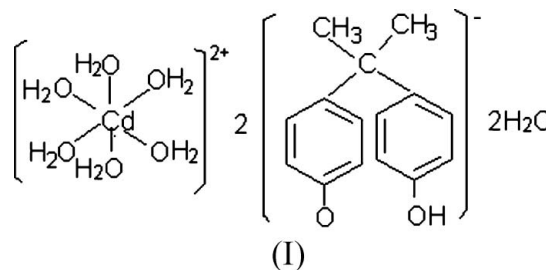
## Hexaaquacadmium(II) bis{4-[2-(4-hydroxyphenyl)-2-propyl]phenolate} dihydrate

In the title compound,  $[\text{Cd}(\text{H}_2\text{O})_6](\text{C}_{15}\text{H}_{15}\text{O}_2)_2 \cdot 2\text{H}_2\text{O}$ , the hexaaquacadmium(II) cation possesses a crystallographically imposed centre of symmetry. In the crystal structure, the  $[\text{Cd}(\text{H}_2\text{O})_6]^{2+}$  cations, 4-[2-(4-hydroxyphenyl)-2-propyl]phenolate anions and solvent water molecules are connected through a complex pattern of  $\text{O}–\text{H} \cdots \text{O}$  hydrogen bonds.

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## Comment

The  $\text{Cd}^{\text{II}}$  atom of the title compound, (I) (Fig. 1), coordinated by six water molecules, is situated on an inversion centre. The  $\text{Cd}–\text{O}$  bond lengths [2.301 (5)–2.369 (4) Å; Table 1] are normal. The three *trans* angles of the  $\text{CdO}_6$  octahedron are all  $180^\circ$  by symmetry. The other  $\text{O}–\text{Cd}–\text{O}$  angles vary from  $86.28(17)$  to  $93.72(17)^\circ$ , indicating a slightly distorted octahedral environment.



The 4-[2-(4-hydroxyphenyl)-2-propyl]phenolate anions do not coordinate to the  $\text{Cd}^{\text{II}}$  atom but act as counter-anions. The crystal structure is composed of alternating layers of  $[\text{Cd}(\text{H}_2\text{O})_6]^{2+}$  cations and  $\text{C}_{15}\text{H}_{15}\text{O}_2^-$  anions, and the uncoordinated water molecules fit into these alternating layers of cations. All the coordinated and uncoordinated water molecules and the O atoms of the anions contribute to intermolecular  $\text{O}–\text{H} \cdots \text{O}$  hydrogen bonds (Table 2), which lead to the formation of two-dimensional networks parallel to the *bc* plane (Fig. 2).

## Experimental

2,2-Bis(4-hydroxyphenyl)propane (2.0 mmol) and NaOH (1.0 mmol) were dissolved in water (10 ml) and stirred for 10 min to obtain a clear purple solution. To this solution was added an aqueous solution (10 ml) of  $\text{Cd}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  (1.0 mmol). After keeping the resulting solution in air for 6 d, large colourless crystals of (I) were formed. The crystals were isolated, washed three times with water and dried in a vacuum desiccator using  $\text{CaCl}_2$  (yield 75%). Elemental analysis, found: C 50.55, H 6.46%; calculated for  $\text{C}_{30}\text{H}_{46}\text{CdO}_{12}$ : C 50.67, H 6.52%.

Crystal data

[Cd(H<sub>2</sub>O)<sub>6</sub>](C<sub>15</sub>H<sub>15</sub>O<sub>2</sub>)<sub>2</sub>·2H<sub>2</sub>O  
*M<sub>r</sub>* = 711.07  
 Orthorhombic, *Pbca*  
*a* = 10.4207 (18) Å  
*b* = 10.976 (2) Å  
*c* = 28.962 (4) Å  
*V* = 3312.6 (9) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.426 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 3183 reflections  
 $\theta = 2.8\text{--}22.4^\circ$   
 $\mu = 0.72\text{ mm}^{-1}$   
*T* = 273 (2) K  
 Block, colourless  
 0.46 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Bruker, 1997)  
*T<sub>min</sub>* = 0.734, *T<sub>max</sub>* = 0.803  
 16112 measured reflections

2944 independent reflections  
 1681 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.052  
 $\theta_{\text{max}} = 25.2^\circ$   
*h* = -12 → 12  
*k* = -13 → 13  
*l* = -24 → 34

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.049  
*wR* (*F*<sup>2</sup>) = 0.144  
*S* = 1.00  
 2944 reflections  
 196 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 10.4291P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.49\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.44\text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cd1—O3	2.301 (5)	O1—C5	1.364 (6)
Cd1—O5	2.368 (4)	O2—C11	1.357 (6)
Cd1—O4	2.369 (4)		
O3—Cd1—O5	90.67 (16)	O5—Cd1—O4 <sup>i</sup>	93.72 (17)
O3—Cd1—O5 <sup>i</sup>	89.33 (16)	O3—Cd1—O4	89.16 (18)
O3—Cd1—O4 <sup>i</sup>	90.84 (18)	O5—Cd1—O4	86.28 (17)

Symmetry code: (i) -x + 1, -y + 1, -z + 1.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2...O1 <sup>ii</sup>	0.82	1.62	2.434 (5)	170
O4—H18...O1 <sup>iii</sup>	0.76	2.43	2.893 (6)	121
O5—H20...O6	0.84	1.85	2.686 (6)	171
O5—H21...O1 <sup>iv</sup>	0.85	1.97	2.801 (5)	168
O6—H22...O2 <sup>v</sup>	0.84	1.99	2.822 (6)	171
O6—H23...O2 <sup>vi</sup>	0.85	1.93	2.778 (6)	178

Symmetry codes: (ii) *x* - 1, *y*, *z*; (iii) -*x* + 2, *y* +  $\frac{1}{2}$ , -*z* +  $\frac{3}{2}$ ; (iv) -*x* +  $\frac{3}{2}$ , -*y* + 1, *z* -  $\frac{1}{2}$ ; (v) -*x* + 1, *y* +  $\frac{1}{2}$ , -*z* +  $\frac{3}{2}$ ; (vi) *x*, -*y* +  $\frac{3}{2}$ , *z* -  $\frac{1}{2}$ .

All H atoms were placed in idealized positions and constrained to ride on their parent atoms [O—H = 0.765–1.008 Å and *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(O); aromatic C—H = 0.93 Å and *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C); methyl C—H = 0.96 Å and *U<sub>iso</sub>*(H) = 1.5*U<sub>eq</sub>*(C)].

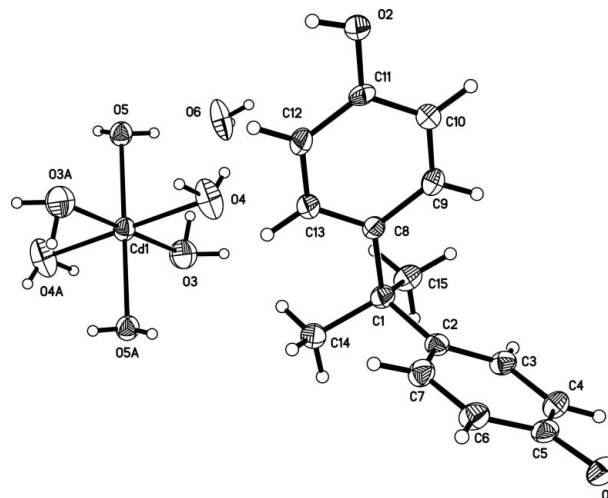


Figure 1

A view of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. The suffix A corresponds to symmetry code (i) in Table 1.

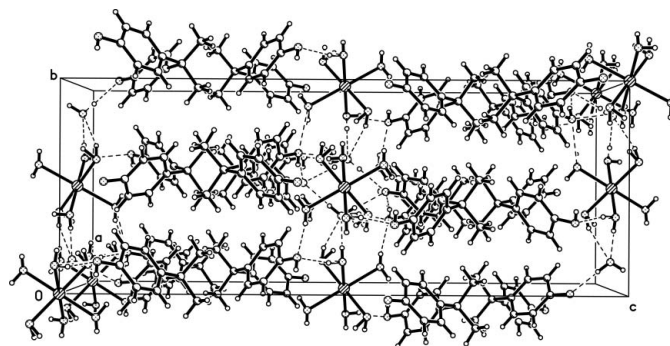


Figure 2

A perspective view of the crystal packing, along the *a* axis. Intermolecular O—H...O hydrogen bonds are shown as dashed lines.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SMART, SAINT, SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.  
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