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catena-Poly[[diaqua(1,4,7,10,13,16-hexaoxacyclooctadecane)barium(II)]-μ-cyano-[dicyanoplatinum(II)]-μ-cyano]

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The title compound, $[BaPt(CN)_4(C_{12}H_{24}O_6)(H_2O)_2]$, contains a polymeric chain of alternating complexes of Ba^{2+} and Pt^{2+}. A ten-coordinate Ba^{2+} complex results from coordination of the metal by 18-crown-6 and two water molecules, and N-atom coordination by a cyano group of $[Pt(CN)_4]^{2-}$ and by a second *cis*-related cyano group of a second $[Pt(CN)_4]^{2-}$ generated by a crystallographic *b*-glide. Crosslinking *via* hydrogen bonds involving the remaining two cyano N atoms completes the crystal structure in the *a* and *c* directions.

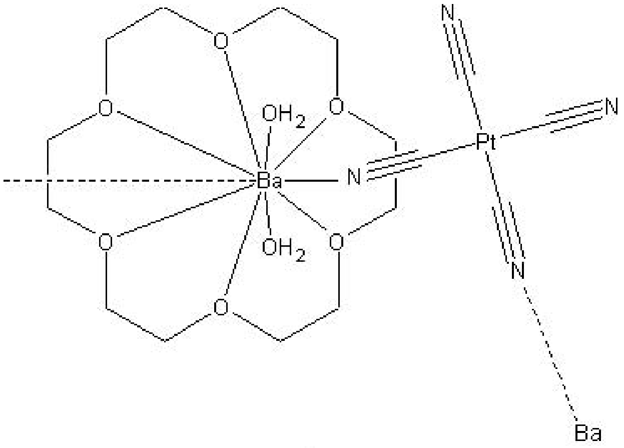
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.004 Å
R factor = 0.018
wR factor = 0.039
Data-to-parameter ratio = 25.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The propensity of Ba^{2+} to achieve high coordination numbers has enabled a number of salts of $[Ba(18\text{-crown-}6)(H_2O)_x]^{2+}$ (x = 2 and 3; 18-crown-6 is 1,4,7,10,13,16-hexaoxacyclooctadecane) to crystallize with coordinating anions, namely $[Co(NCS)_4]^{2-}$ (Fan *et al.*, 1987), $[Fe(NCS)_4]^{2-}$ (Fan *et al.*, 1989), $[CoCl_4]^{2-}$ (Fender *et al.*, 1994) and $[CuCl_4]^{2-}$ (Kahwa *et al.*, 1992). In these structures, the ligands of the tetrahedral anions coordinate to the Ba^{2+} ion in either a κ^2Cl or a κ^1S fashion. None of the structures is polymeric. We report here the structure of a salt utilizing the planar dianion, $[Pt(CN)_4]^{2-}$, which exhibits κ^1N coordination to Ba^{2+} *via* two cyano ligands of the $[Pt(CN)_4]^{2-}$ ion and forms a polymer of alternating complexes of Ba^{2+} and Pt^{2+}.



(I)

The asymmetric unit consists of $[Ba(18\text{-crown-}6)(H_2O)_2]$-$[Pt(CN)_4]$, (I). As shown in Fig. 1, the crown ether is slightly domed, the Ba^{2+} ion lying 0.654 (1) Å out of the plane of the six O atoms. The two water molecules cap the *exo* side of Ba(18-crown-6). In addition, atom N4 from the $[Pt(CN)_4]^{2-}$ ion is found on the *exo* side and forms a Ba1—N4—C4 angle of 155.0 (2)°. In order to form the polymer, a *cis*-related cyano

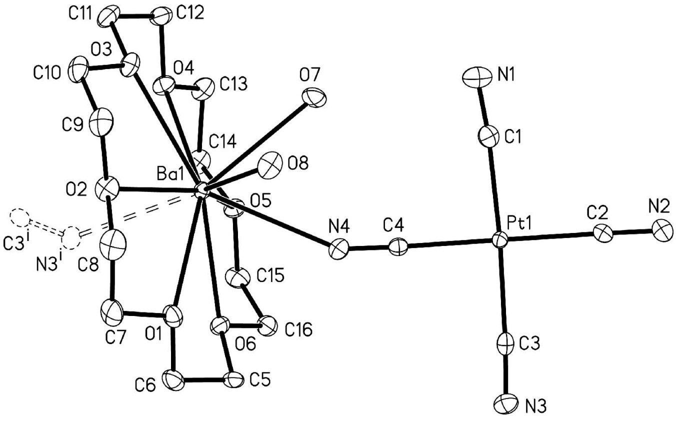


Figure 1

A view of (I). Displacement ellipsoids are drawn at the 50% probability level. A portion of the coordinated $[Pt(CN)_4]^{2-}$ ion generated by symmetry [symmetry code: (i) $\frac{1}{2} - x, -\frac{1}{2} + y, z$] is indicated with dashed lines. H atoms have been omitted for clarity.

group from a second $[Pt(CN)_4]^{2-}$ ion, related by a crystallographic *b*-glide, is N-bound ($N3^i$) to the *endo* side, giving angles $Ba—N3^i—C3^i$ = 118.2 (2)° and $N3^i—Ba1—N4$ = 136.50 (6)° [symmetry code: (i) $\frac{1}{2} - x, -\frac{1}{2} + y, z$]. The polymeric chain is also bent at the Pt atom by virtue of the square-planar geometry [C4—Pt1—C3 = 89.06 (10)°]. The ten-coordinate geometry of Ba^{2+} has no regular polyhedral shape as it is dictated by the constraints of the crown ether. The remainder of the structure consists of hydrogen bonding through the two remaining N atoms (N1 and N2). These motifs propagate orthogonally to the basic Ba···Pt···Ba···Pt chain. Fig. 2 depicts the hydrogen-bonding portion involving atom N1, as well as the chain propagation.

Bond distances and angles involving the central atoms of the cationic and anionic species are typical. For Ba—O(crown), the average distance is 2.858 (17) Å, while the two $Ba—O(H_2O)$ distances average 2.833 (13) Å. The cyano coordination shows distances of Ba1—N4 = 2.889 (2) Å for the *exo* group and $Ba1—N3^i$ = 2.901 (2) Å for the *endo* group.

Experimental

To a mixture of $Ba[Pt(CN)_4]\cdot 4H_2O$ (0.0426 g, 0.0838 mmol) and 18-crown-6 (0.0210 g, 0.079 mmol) in a beaker was added sufficient methanol to dissolve the solids. The solution gradually changed from yellow to colorless. After brief warming, the solution was allowed to evaporate to dryness, yielding a white powder. The powder was dissolved in 90% ethanol with warming, and the solution was placed in a 5 mm tube. An equal amount of 100% ethanol was carefully layered on top and the tube was capped. After one week at room temperature, well formed crystals were harvested for data collection.

Crystal data

$[BaPt(CN)_4(C_{12}H_{24}O_6)(H_2O)_2]$
M_r = 736.85
Orthorhombic, *Pbca*
a = 10.8458 (6) Å
b = 17.0539 (9) Å
c = 25.9179 (13) Å
V = 4793.9 (4) Å^3
Z = 8
D_x = 2.042 Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 7898 reflections
θ = 2.4–31.5°
μ = 7.51 mm^{-1}
T = 100 (2) K
Plate, colorless
0.34 × 0.20 × 0.004 mm

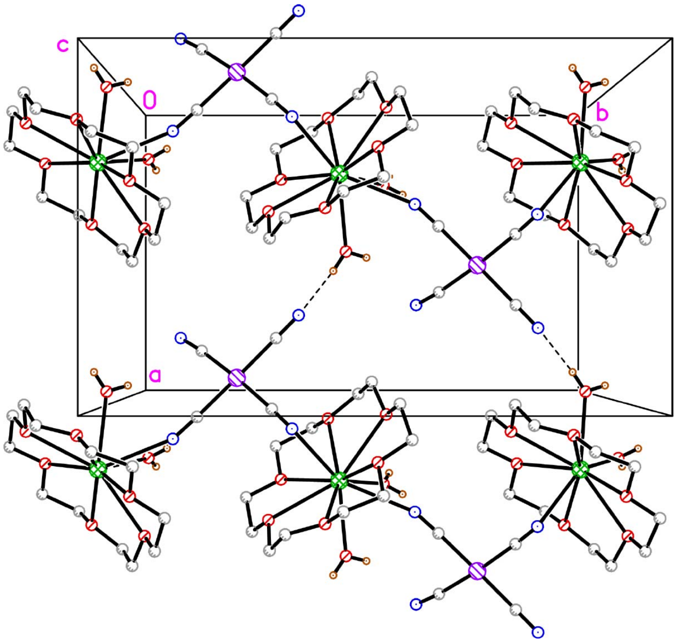


Figure 2

A portion of the polymeric chain propagated by the *b* glide and hydrogen bonding (dashed lines) between chains in the *ab* plane. H atoms have been omitted.

Data collection

Bruker SMART APEX diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.21, T_{max} = 0.97
62 537 measured reflections

7316 independent reflections
6160 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 30.5°
$h = -15 \rightarrow 15$
$k = -24 \rightarrow 23$
$l = -37 \rightarrow 37$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.039
S = 1.06
7316 reflections
287 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0044P)^2 + 6.6164P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1

Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*D*···N2^{ii}	0.83 (3)	2.00 (2)	2.827 (3)	173 (4)
O8—H8*D*···N1^{iii}	0.82 (3)	2.04 (2)	2.853 (3)	168 (4)

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

H atoms on water molecules were located in a difference Fourier map and refined with a distance constraint of 0.84 (2) Å. All other H atoms were treated as riding on their parent C atoms, with C—H distances of 0.99 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The largest peak in a final difference map was 0.79 Å from Pt1.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1994); software used to prepare material for publication: *SHELXL97*.

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References

Bruker (2005). *APEX2* and *SAINT* (Version 7.15). Bruker AXS Inc., Madison, Wisconsin, USA.

Fan, Y.-P., Du, G.-Y. & Zhang, W.-X. (1989). *Acta Chim. Sinica*, **47**, 276–278.

Fan, Y.-P., Zhang, W.-X. & Wang, X.-W. (1987). *Chem. J. Chin. Univ.* **8**, 297–299.

Fender, N. S., Finegan, S. S., Miller, D., Mitchell, M., Kahwa, I. A. & Fronczek, F. R. (1994). *Inorg. Chem.* **33**, 4002–4008.

Kahwa, I. A., Miller, D., Mitchel, M., Fronczek, F. R., Goodrich, R. G., Williams, D. J., O'Mahoney, C. A., Slawin, A. M., Ley, S. V. & Groombridge, C. J. (1992). *Inorg. Chem.* **31**, 3963–3970.

Sheldrick, G. M. (1994). *XP* in *SHELXTL*. Version 5.1. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.

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