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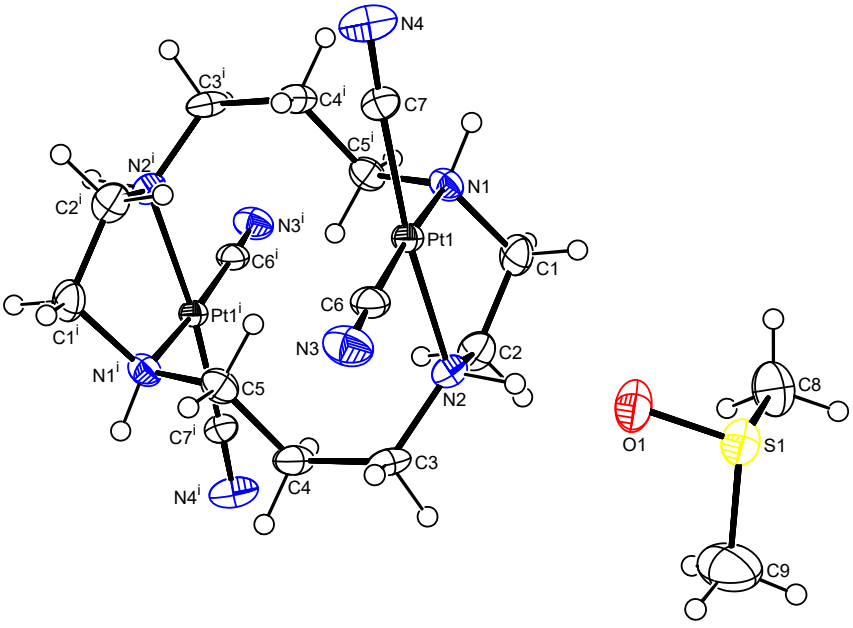
# Crystal structure of [(1,4,8,11-tetraazacyclotetradecane-$\kappa^4N,N',N'',N'''$) tetracyanidodiplatinum(II)] dimethyl sulfoxide solvate, $C_{18}H_{36}N_8O_2Pt_2S_2$

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**Abstract**

$C_{18}H_{36}N_8O_2Pt_2S_2$, monoclinic, $P2_1/c$ (no. 14), $a$ = 12.0848(16) Å, $b$ = 14.1725(18) Å, $c$ = 8.1065(9) Å, $\beta$ = 97.603(4)°, $V$ = 1376.2 Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0279, $wR_{ref}(F^2)$ = 0.0749, T = 223 K.

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The title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colorless block |
| Size: | 0.16 × 0.13 × 0.07 mm |
| Wavelength: | Mo $K\alpha$ radiation (0.71073 Å) |
| $\mu$: | 10.3 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II CCD, $\varphi$ and $\omega$ scans |
| $\theta_{max}$, completeness: | 28.4°, 100 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 26775, 3439, 0.053 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2,962 |
| $N(param)_{refined}$: | 155 |
| Programs: | Bruker,[1] SHELX[2], PLATON[3] |

## 1 Source of materials

To a solution of [Pt(cyclam)]$Cl_2$ (cyclam = 1,4,8,11-tetraazacyclotetradecane; 0.1053 g, 0.226 mmol) in methanol (10 ml) was added $K_2Pt(CN)_4$ (0.0852 g, 0.226 mmol) and refluxed for 1 h. After cooling, the formed precipitate was separated by filtration, washed with methanol and

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**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pt1 | 0.19549 (2) | 0.52653 (2) | 0.64789 (2) | 0.02312 (7) |
| N1 | 0.1502 (4) | 0.6092 (3) | 0.4349 (5) | 0.0288 (9) |
| H1 | 0.180 (6) | 0.671 (5) | 0.455 (9) | 0.06 (2)* |
| N2 | 0.2000 (4) | 0.4181 (3) | 0.4729 (5) | 0.0293 (8) |
| H2 | 0.281 (7) | 0.410 (6) | 0.472 (10) | 0.09 (3)* |
| N3 | 0.2630 (4) | 0.3894 (3) | 0.9427 (6) | 0.0407 (11) |
| N4 | 0.2144 (5) | 0.6937 (3) | 0.8960 (7) | 0.0484 (13) |
| C1 | 0.1989 (5) | 0.5578 (4) | 0.2983 (7) | 0.0369 (12) |
| H1A | 0.1704 | 0.5851 | 0.1898 | 0.044* |
| H1B | 0.2804 | 0.5636 | 0.3146 | 0.044* |
| C2 | 0.1662 (5) | 0.4567 (4) | 0.3038 (7) | 0.0370 (12) |
| H2A | 0.0851 | 0.4508 | 0.2746 | 0.044* |
| H2B | 0.2023 | 0.4207 | 0.2225 | 0.044* |
| C3 | 0.1508 (4) | 0.3232 (3) | 0.4998 (7) | 0.0336 (11) |
| H3A | 0.1803 | 0.3015 | 0.6118 | 0.040* |
| H3B | 0.1765 | 0.2788 | 0.4203 | 0.040* |
| C4 | 0.0238 (4) | 0.3186 (3) | 0.4820 (7) | 0.0349 (11) |
| H4A | −0.0062 | 0.3408 | 0.3705 | 0.042* |
| H4B | 0.0015 | 0.2525 | 0.4907 | 0.042* |
| C5 | −0.0287 (4) | 0.3760 (3) | 0.6095 (6) | 0.0309 (10) |
| H5A | −0.0154 | 0.3437 | 0.7172 | 0.037* |
| H5B | 0.0083 | 0.4376 | 0.6222 | 0.037* |
| C6 | 0.2382 (4) | 0.4413 (3) | 0.8371 (6) | 0.0294 (10) |
| C7 | 0.2044 (4) | 0.6327 (3) | 0.8043 (6) | 0.0299 (10) |
| S1 | 0.52466 (12) | 0.37642 (11) | 0.38997 (18) | 0.0414 (3) |
| O1 | 0.4279 (3) | 0.3953 (3) | 0.4853 (5) | 0.0498 (10) |
| C8 | 0.5019 (6) | 0.4465 (5) | 0.2090 (8) | 0.0537 (16) |
| H8A | 0.5609 | 0.4352 | 0.1411 | 0.081* |
| H8B | 0.5018 | 0.5126 | 0.2400 | 0.081* |
| H8C | 0.4305 | 0.4303 | 0.1462 | 0.081* |
| C9 | 0.4997 (8) | 0.2644 (6) | 0.2945 (12) | 0.090 (3) |
| H9A | 0.5618 | 0.2478 | 0.2356 | 0.134* |
| H9B | 0.4315 | 0.2668 | 0.2165 | 0.134* |
| H9C | 0.4921 | 0.2173 | 0.3791 | 0.134* |

acetone, and dried at 50 °C, to give a white powder (0.0902 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a dimethyl sulfoxide (DMSO) solution at 90 °C.

## 2 Experimental details

Hydrogen atoms on C atoms were positioned geometrically and allowed to ride on their parent atoms with *d*(C–H) = 0.98 or 0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C) with the help of the SHELXL program (AFIX 23 or 137 options).[2] Hydrogen atoms bonded to N atoms were located from Fourier difference maps and refined isotropically; *d*(N–H) = 0.95(8) and 0.99(8) Å.

## 3 Comment

The crystal structures of the related heterometallic complexes $[Ag(cyclam)M1(CN)_4]_n$ (cyclam = 1,4,8,11-tetraazacyclotetradecane; M1 = Pd, Pt)[5] and $[Cu(cyclam)M2(CN)_4]_n$ (M2 = Ni, Pd, Pt)[6] have been determined previously. The structures are formed by one-dimensional cyanido-bridged chains. On the contrary, in the reported bimetallic compounds $[Pd(cyclam)][M3(CN)_4]$ (M3 = Pd, Pt, Ni),[7–9] the compounds consist of a cationic Pd(II) complex $[Pd(cyclam)]^{2+}$ and an anionic M3(II) complex $[M3(CN)_4]^{2-}$, respectively.

The title compound consists of a dinuclear Pt(II) complex $[Pt_2(cyclam)(CN)_4]$ and two solvent DMSO molecules. In the complex, each Pt(II) ion is four-coordinated in a distorted square-planar environment by two N atoms of a tetradentate cyclam ligand and two C atoms derived from two mutually cis-positioned $CN^-$ ligands, and an inversion center is located at the centroid of the complex; the asymmetric unit contains one half of the compound. The tight N–Pt–N chelating angles of <N1–Pt1–N2 = 83.09(16)° contribute the distortion of the square-plane. The Pt–N(cyclam) bonds [Pt1–N1/2 = 2.099(4) and 2.097(4) Å] are slightly longer than the Pt–C(cyanido) bonds [Pt1–C6/7 = 1.967(5) and 1.961(5) Å]. The C≡N bond lengths are almost equal with *d*(C≡N) = 1.136(7) and 1.138(7) Å. In the crystal structure, the complex and solvent DMSO molecules are linked by extensive intermolecular N–H···O, N–H···N and C–H···N hydrogen bonds with distances of 2.762(6)–3.464(8) Å between the donor and acceptor atoms, forming a three-dimensional network.[4]

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**Conflict of interest:** The authors declare no conflicts of interest regarding this article.

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