# Crystal structure of bis(aza-15-crown-5-dithiocarbamato)platinum(II)—dichloromethane (1/2), $((CH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2)NCS_2)_2Pt \cdot 2CH_2Cl_2$

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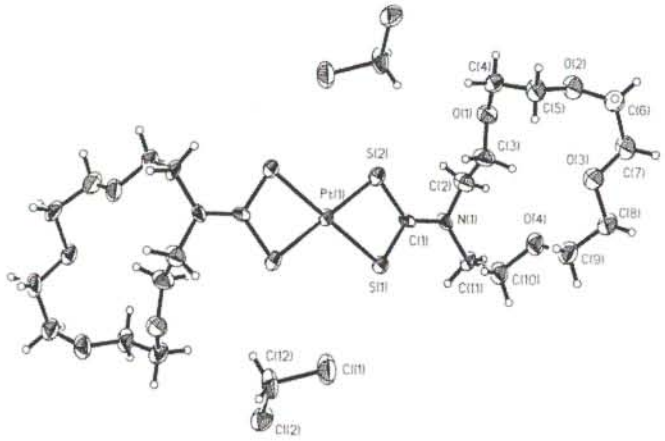
Received May 7, 1999, CCDC-No. 1267/182




**Abstract**

$C_{24}H_{44}Cl_4N_2O_8PtS_4$, triclinic, $P\bar{1}$ (No. 2), $a = 11.822(3)$ Å, $b = 10.004(4)$ Å, $c = 8.412(4)$ Å, $\alpha = 94.83(3)°$, $\beta = 107.29(4)°$, $\gamma = 109.82(4)°$, $V = 874.5$ Å$^3$, $Z = 1$, $R_{gt}(F) = 0.089$, $wR(F) = 0.089$, $T = 293$ K.

**Source of material**

Samples of the complex were kindly supplied by Dr. Fracasso. The compound was prepared in heterogeneous phase by adding $PtCl_2$ to the dithiocarbamate ligand in $CH_2Cl_2$. Orange-yellow crystals were separated slowly from the $CH_2Cl_2$ solution after addition of n-hexane.

**Discussion**

The square planar complex consists of discrete centrosymmetric $PtL_2$ molecules, where the bidentate ligand forms a bite S–Pt–S angle of 75.1(1)°. Relevant bond distances are: Pt–S 2.311(4) Å and 2.299(5) Å, C–S 1.72(2) Å and 1.69(2) Å, N–C(1) (partial double) 1.33(2) Å, N–C(2) and N–C(11) (single covalent) 1.46(2) Å and 1.47(2) Å, respectively. Bond lengths in the crown ring are normal. Two $CH_2Cl_2$ molecules are associated to each complex molecule as clathrate solvent. The high fraction of unobserved or low intensities seems to indicate a poor crystal quality, which could also explain the relatively high standard deviations at convergence. However, no anomaly was observed in bond lengths or bond angles, which have the expected values. The H atoms were introduced in calculated positions.

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

| | |
|---|---|
| Crystal: | orange-yellow prism, size 0.2 × 0.15 × 0.2 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| μ: | 84.1 cm$^{-1}$ |
| Diffractometer, scan mode: | Philips PW 1100 (FEBO SYSTEM), 2θ |
| $2\theta_{max}$: | 60° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 4101, 3411 |
| Criterion for $F_{obs}$, $N(hkl)_{gt}$: | $F_{obs} > 3\ \sigma(F_{obs})$, 2862 |
| $N(param)_{refined}$: | 196 |
| Program: | SHELX-76 [1] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(2A) | 2*i* | 0.169(2) | –0.091(2) | 0.712(2) | 0.08 |
| H(2B) | 2*i* | 0.036(2) | –0.178(2) | 0.522(2) | 0.08 |
| H(3A) | 2*i* | 0.306(2) | –0.171(2) | 0.607(2) | 0.08 |
| H(3B) | 2*i* | 0.205(2) | –0.205(2) | 0.393(2) | 0.08 |
| H(4A) | 2*i* | 0.114(2) | –0.563(2) | 0.459(2) | 0.08 |
| H(4B) | 2*i* | 0.139(2) | –0.451(2) | 0.311(2) | 0.08 |
| H(5A) | 2*i* | 0.361(2) | –0.328(2) | 0.494(2) | 0.08 |
| H(5B) | 2*i* | 0.320(2) | –0.515(2) | 0.427(2) | 0.08 |
| H(6A) | 2*i* | 0.497(2) | –0.478(2) | 0.842(2) | 0.08 |
| H(6B) | 2*i* | 0.524(2) | –0.409(2) | 0.664(2) | 0.08 |
| H(7A) | 2*i* | 0.643(2) | –0.229(2) | 0.923(2) | 0.08 |
| H(7B) | 2*i* | 0.499(2) | –0.244(2) | 0.955(2) | 0.08 |
| H(8A) | 2*i* | 0.595(2) | –0.014(2) | 0.969(2) | 0.08 |
| H(8B) | 2*i* | 0.706(2) | 0.018(2) | 0.867(2) | 0.08 |
| H(9A) | 2*i* | 0.571(2) | 0.069(2) | 0.617(2) | 0.08 |
| H(9B) | 2*i* | 0.630(2) | 0.205(2) | 0.802(2) | 0.08 |
| H(10A) | 2*i* | 0.463(2) | 0.288(2) | 0.704(2) | 0.08 |
| H(10B) | 2*i* | 0.404(2) | 0.163(2) | 0.510(2) | 0.08 |
| H(11A) | 2*i* | 0.243(2) | 0.242(2) | 0.579(2) | 0.08 |
| H(11B) | 2*i* | 0.261(2) | 0.151(2) | 0.750(2) | 0.08 |
| H(12A) | 2*i* | 0.059(2) | 0.438(2) | –0.194(2) | 0.08 |
| H(12B) | 2*i* | 0.195(2) | 0.567(2) | –0.218(2) | 0.08 |

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**Table 3.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Pt(1) | 1*a* | 0 | 0 | 0 | 0.0399(6) | 0.0281(5) | 0.0138(5) | 0.0150(4) | 0.0003(4) | –0.0039(3) |
| S(1) | 2*i* | 0.1431(4) | 0.1604(5) | 0.2502(5) | 0.045(3) | 0.031(2) | 0.022(2) | 0.013(2) | –0.002(2) | –0.003(2) |
| S(2) | 2*i* | –0.0041(4) | –0.1360(5) | 0.2069(5) | 0.044(3) | 0.040(2) | 0.020(2) | 0.013(2) | –0.002(2) | –0.003(2) |
| C(l) | 2*i* | 0.113(2) | 0.014(2) | 0.347(2) | 0.05(1) | 0.026(8) | 0.032(9) | 0.022(7) | 0.008(7) | 0.003(7) |
| N(1) | 2*i* | 0.168(1) | 0.017(2) | 0.510(2) | 0.048(9) | 0.042(8) | 0.012(6) | 0.028(7) | 0.003(6) | 0.006(5) |
| C(2) | 2*i* | 0.138(2) | –0.117(2) | 0.574(2) | 0.05(1) | 0.05(1) | 0.024(8) | 0.02(1) | 0.012(8) | 0.009(8) |
| C(3) | 2*i* | 0.207(2) | –0.210(2) | 0.522(2) | 0.06(1) | 0.030(9) | 0.04(1) | 0.019(9) | 0.017(9) | 0.006(8) |
| O(1) | 2*i* | 0.140(1) | –0.353(1) | 0.535(2) | 0.050(8) | 0.034(6) | 0.033(6) | 0.017(6) | 0.012(6) | 0.006(5) |
| C(4) | 2*i* | 0.168(2) | –0.457(2) | 0.444(2) | 0.04(1) | 0.029(8) | 0.034(9) | 0.009(7) | –0.001(8) | –0.003(7) |
| C(5) | 2*i* | 0.306(2) | –0.436(2) | 0.504(2) | 0.05(1) | 0.04(1) | 0.024(8) | 0.016(8) | 0.006(8) | 0.001(7) |
| O(2) | 2*i* | 0.346(1) | –0.450(2) | 0.677(1) | 0.059(9) | 0.059(8) | 0.022(6) | 0.024(7) | 0.010(6) | 0.008(6) |
| C(6) | 2*i* | 0.481(2) | –0.404(2) | 0.760(2) | 0.06(1) | 0.05(1) | 0.030(9) | 0.024(9) | 0.002(8) | –0.003(8) |
| C(7) | 2*i* | 0.543(2) | –0.253(2) | 0.861(2) | 0.05(1) | 0.07(1) | 0.018(8) | 0.03(1) | –0.006(8) | –0.002(9) |
| O(3) | 2*i* | 0.530(1) | –0.151(1) | 0.757(1) | 0.057(8) | 0.043(7) | 0.019(6) | 0.018(6) | –0.002(5) | –0.002(5) |
| C(8) | 2*i* | 0.606(2) | –0.003(2) | 0.847(2) | 0.04(1) | 0.04(1) | 0.030(9) | 0.016(8) | –0.007(8) | –0.015(8) |
| C(9) | 2*i* | 0.566(2) | 0.094(2) | 0.742(2) | 0.05(1) | 0.04(1) | 0.04(1) | 0.016(9) | –0.004(8) | –0.039(8) |
| O(4) | 2*i* | 0.439(1) | 0.078(1) | 0.726(1) | 0.039(7) | 0.046(7) | 0.025(6) | 0.014(6) | –0.000(5) | 0.003(5) |
| C(10) | 2*i* | 0.400(2) | 0.179(2) | 0.637(2) | 0.04(1) | 0.05(1) | 0.023(8) | 0.016(8) | 0.000(7) | –0.000(8) |
| C(11) | 2*i* | 0.266(1) | 0.153(2) | 0.624(2) | 0.04(1) | 0.05(1) | 0.012(7) | 0.022(8) | –0.003(7) | –0.007(7) |
| Cl(1) | 2*i* | 0.2471(6) | 0.4777(7) | 0.0339(7) | 0.073(4) | 0.076(4) | 0.039(3) | 0.039(3) | –0.004(3) | 0.009(3) |
| Cl(2) | 2*i* | 0.1106(5) | 0.6707(6) | –0.0447(7) | 0.056(3) | 0.050(3) | 0.050(3) | 0.024(2) | 0.001(2) | –0.014(2) |
| C(12) | 2*i* | 0.148(2) | 0.531(2) | –0.129(2) | 0.07(1) | 0.06(1) | 0.023(9) | 0.04(1) | 0.004(9) | 0.003(8) |

## Reference

1. Sheldrick, G. M.: SHELX-76, Program for Crystal Structures Determination, Cambridge 1976.