nitrogen ligands. In the present paper the study of Pd(II) complexes with N-methylimidazole ligands is continued and crystal data of the cis and trans isomers [Pd(NMeIm)2Cl2] are reported; i.e. of those compounds where the palladium is surrounded by two nitrogen ligands and two chlorine atoms.

Origin of specimens
The cis isomer was obtained by the reaction of PdCl2 with N-methylimidazole (NMeIm) in absolute methanol with a ratio Pd/NMeIm = 1/2.3. The trans isomer was obtained by the same method but the ratio Pd/NMeIm was 1/4.3. The latter compound, was also obtained by reaction of K2PdCl6 with NMeIm in ratios Pd/NMeIm = 1/3, 1/4, 1/5, with production of KCl.

The synthesis and characterization of these complexes by analytical methods and infrared spectroscopy are given in detail by Navarro & Gayoso (1978).

Cell data
Triclinic; space groups P1 or P1.

<table>
<thead>
<tr>
<th>cis-[Pd(NMeIm)2Cl2]</th>
<th>trans-[Pd(NMeIm)2Cl2]</th>
</tr>
</thead>
<tbody>
<tr>
<td>a = 16.594 (2) Å</td>
<td>a = 11.030 (9) Å</td>
</tr>
<tr>
<td>b = 10.440 (4) Å</td>
<td>b = 9.393 (7) Å</td>
</tr>
<tr>
<td>c = 8.7577 (1) Å</td>
<td>c = 7.239 (5) Å</td>
</tr>
<tr>
<td>α = 64.99 (1) °</td>
<td>α = 101.14 (1) °</td>
</tr>
<tr>
<td>β = 83.73 (1) °</td>
<td>β = 94.43 (1) °</td>
</tr>
<tr>
<td>γ = 80.41 (1) °</td>
<td>γ = 98.39 (1) °</td>
</tr>
<tr>
<td>V = 1354.4 (3) Å</td>
<td>V = 723.7 (6) Å</td>
</tr>
<tr>
<td>Dv = 1.67</td>
<td>Dv = 1.57 Mg m-3</td>
</tr>
<tr>
<td>Z = 4</td>
<td>Z = 2</td>
</tr>
</tbody>
</table>

Powder data
The X-ray powder diffractograms for the crystalline cis and trans-[Pd(NMeIm)2Cl2] were recorded with a Philips PM-8000 and nickel-filtered Cu Kα radiation (mean λ = 1.5418 Å). The powder data are given in Tables 1 and 2.

Both cis and trans isomers showed stable crystalline forms and were studied by electron microscopy but no single crystals suitable for X-ray analysis were obtained. However, unit-cell parameters were determined from X-ray powder patterns. The computations were carried out with the programs INDEX 1 (Kohlbeck & Hörl, 1976) and L-SUCRE (Appleman, 1973).

Comparison with other results
A similar study on the cis and trans isomers of [Pd(ImH)2Cl2] is in progress. The powder patterns of the cis isomers of both compounds must be obtained with freshly prepared samples because the crystals slowly convert to the trans isomers particularly when exposed to light.

I am very grateful to Professor Dr J. R. Masaguér Fernández, Director del Departamento de Quimica Inorgánica de la Universidad Autónoma de Madrid, for his help; also I am indebted to Professor Dr J. Rodriguez Martinez and Dr M. T. Martin Patino for useful discussions. The calculations were preformed on the Univac 1108 (Ministerio de Educación y Ciencia, Madrid, Spain) for which I am grateful. Thanks are also due to Professor Dr S. Garcia Blanco, Jefe del Departamento de Rayos X del CSIC, Madrid, whose interest made this work possible.

References
Crystal geometry

Precession and Weissenberg photographs showed monoclinic symmetry with systematic absences of $hkl$ with $h + k = 2n + 1$ and $h0l$ with $l = 2n + 1$ indicating that the space group is $C2/c$. The unit-cell parameters were refined by least-squares using 12 reflections with $2\theta > 45^\circ$ centered on a Picker FACS-I automatic diffractometer using monochromatized Cu K$\alpha$ radiation ($\lambda = 1.5405 \ \text{Å}$). The experimental density was determined by the flotation method in CCl$_4$–hexane.

The crystal data are:

$$C_{30}H_{14}N_5S_2, \ M_\text{s} = 494.60$$

$$a = 19.252 \ (7), \ b = 8.656 \ (3), \ c = 13.879 \ (5) \ \text{Å}, \ \beta = 90.28 \ (3)^\circ$$

$$V = 2313 \ \text{Å}^3, \ Z = 4, \ D_m = 1.43 \ (2) \ \text{mg} \ \text{m}^{-3}, \ D_x = 1.42 \ \text{Mg} \ \text{m}^{-3}.$$  

Powder diffraction data

The powder pattern was obtained with a 114.6 mm diameter Debye–Scherrer camera using Ni-filtered Cu K$\alpha$ radiation ($\lambda = 1.5418 \ \text{Å}$). Intensities were estimated visually. The indexed powder diffraction data are given in Table 1.

Crystal physics

Single crystals of DTT–TCNQ appear yellow under optical transmission microscopy and extinguish polarized light along the c needle axis. The four-probe room-temperature electrical conductivity measured on single crystals of DTT–TCNQ was $3 \times 10^{-4} \ (\Omega \text{m})^{-1}$ characteristic of an organic semiconductor. The single crystal ESR spectrum of DTT–TCNQ shows a single line spectrum with $g = 2.0014$.

Reference