**Coordination Isomers of Phenyl Substituted Thiourea Ligands**

Jason Hurst and Lee Roecker
Department of Chemistry
Berea College

**Introduction**

In this work, we report on the preparation and characterization of two coordination isomers of cobalt(III) complexes for a series of diphenyl substituted thiourea ligands. These complexes crystallize together and so far we have been unable to separate the isomers. In contrast, when N-methyl-N'-phenyl thiourea ligands are used the isomers can be resolved. Characterization has been by NMR.

What isomer is formed depends on the electron withdrawing or electron donating properties of the thiourea ligand. When X is a strong EWG, only isomer A is formed. As X becomes less electron withdrawing, both isomers are formed.

**Preparation of Complexes**

**C-13 NMR**

**PROTON NMR**

**Conclusions**

1. The coordination of unsymmetrical thiourea ligands depends on the electron donating ability of the substituted phenyl group.

2. The red isomer is favored when X is a good electron withdrawing group such as nitro. With the methyl substituted series, both isomers are formed when X is not nitro.

3. Perhaps these isomers can be separated with longer columns, or different chromatography resins, or selective crystallization.

---

**Distribution of Isomers**

<table>
<thead>
<tr>
<th>X</th>
<th>YES</th>
<th>YES</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₃O⁻</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H⁻</td>
<td>YES</td>
<td>YES</td>
</tr>
<tr>
<td>NO₂⁻</td>
<td>YES</td>
<td>NO</td>
</tr>
</tbody>
</table>

Isomers do NOT separate on Sephadex-SPC-25.

Sephadex-SPC-25 is a cation exchange resin. It separates molecules based on their charge. The diphenyl substituted thiourea isomers do not separate on this resin.