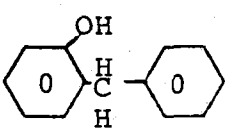
Spectroscopy
Method 70-24
Job No. 8903209

DETERMINATION OF THE RATIO OF ORTHO AND PARA ISOMERS IN SANTOPHEN 7

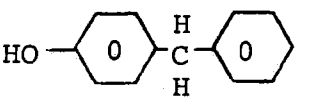
PRINCIPLE

Santophen 7 is a mixture of ortho and para benzylphenols. The CH_2, benzyl protons, are separated in chemical shift by 0.10 ppm. This separation allows integration of the individual peaks. Since the peak areas of the benzyl protons are directly proportional to the concentration of the corresponding isomer in solution, the ratio of ortho to para benzylphenol can easily be determined.

Structure of components:



ortho



para

Concentration/Solvent: A 20 to 40 percent solution of Santophen 7 in deutero chloroform is useful.

Accuracy and/or Precision: ±1 percent of the O/P ratio.

Interferences: None likely.

Peaks Used in Analysis: CH_2 (benzyl) peaks at 3.81 ppm (para) and 3.91 ppm (ortho).

Special Reagents: None.

NMR Equipment: A-60.

PROCEDURE

1. Sample Preparation: Make up a 20 to 40 percent solution of Santophen 7 in $CDCl_3$.

2. Instrument Settings: For maximum signal.

3. Spectrum:

   a) Record spectrum of Santophen 7 solution.

   b) Identify benzyl protons from ortho and para isomers. See NMR file number 16-609.

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c) Quantitatively measure the area of the benzyl protons with the electronic integrator.

CALCULATION

O/P ratio = area of the ortho benzyl peak (A_o)/area of para benzyl peak (A_p) or -

$$\% \text{ Ortho} = \frac{A_o}{A_o + A_p} \times 100$$

db

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