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The Structure of 1-(Arylthio)naphthalenes, Together with the Selenium and Oxygen Derivatives in Crystals and Solutions

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The Structure of 1-(Arylthio)naphthalenes, Together with the Selenium and Oxygen Derivatives in Crystals and Solutions

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The structures are determined for some members of 1-(p-YC₆H₄Z) C₁₀H₇ (1 (Z = S), 2 (Z = Se), and 3 (Z = O) by the X-ray crystallographic analysis if they give suitable crystals for measurements. They are type

$$\frac{1}{Z} = \frac{3}{S}$$

$$\frac{1}{Z} = \frac{3}{S} = \frac{1}{S}$$

$$\frac{1}{Z} = \frac{1}{S} = \frac{1}{S}$$

$$\frac{1}{Z} = \frac{1}{S} = \frac{1}{S}$$

$$\frac{1}{Z} = \frac{1}{S} = \frac{1}$$

A for $g(\mathbf{n})$ and are mainly type **B** for $g(\mathbf{m})$.¹ The structures of **1–3** are also investigated in solutions based on the NMR data. Figure 1 shows the results for **2**, for an example.¹ The results demonstrate that type **A** is predominant in the CDCl₃ solution for **2g** with $Y = NO_2$. The fraction

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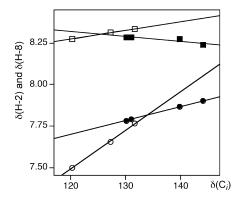


FIGURE 1 Pots of $\delta(\text{H-2})$ and $\delta(\text{H-8})$ *versus* $\delta(\text{C}i)$ in **2**: \bigcirc , \bullet , \square , and \blacksquare stand for $g(\mathbf{m})$ of $\delta(\text{H-2})$, $g(\mathbf{n})$ of $\delta(\text{H-2})$, $g(\mathbf{m})$ of $\delta(\text{H-8})$, and $g(\mathbf{n})$ of $\delta(\text{H-8})$, respectively.

of type **B** gradually increases when 2g goes to 2b of $Y = OMe \ via \ Y = COOEt$, Br, Cl, H, and/or Me. Similar results are obtained for 1 and 3.

Dedicated to Prof. Michinori Ōki on occasion of his 77th birthday.

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