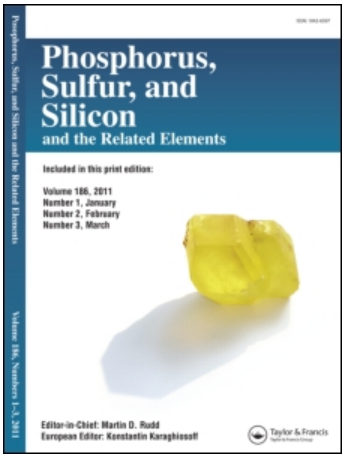

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The Structure of 1-(Arylthio)naphthalenes, Together with the Selenium and Oxygen Derivatives in Crystals and Solutions

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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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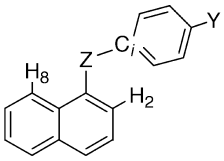
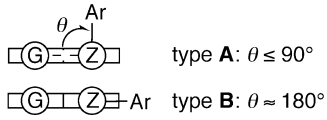
The structures are determined for some members of 1-(p-YC_6H_4Z) $C_{10}H_7$ (**1** (Z = S), **2** (Z = Se), and **3** (Z = O) by the X-ray crystallographic analysis if they give suitable crystals for measurements. They are type



	1	2	3
Z =	S	Se	O

	a	b	c	d	e	f	g
Y =	H	OMe	Me	Cl	Br	COOEt	NO_2

g(**m**): Y = H, OMe, and Me.
g(**n**): Y = Cl, Br, COOEt, and NO_2.



A for g(**n**) and are mainly type **B** for g(**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 $CDCl_3$ solution for **2g** with Y = NO_2. The fraction

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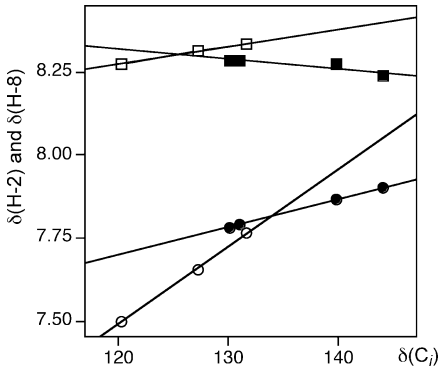

FIGURE 1 Pots of δ(H-2) and δ(H-8) *versus* δ(C*i*) in **2**: ○, ●, □, and ■ stand for g(**m**) of δ(H-2), g(**n**) of δ(H-2), g(**m**) of δ(H-8), and g(**n**) of δ(H-8), respectively.

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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[1] W. Nakanishi, S. Hayashi, and T. Uehara, *Eur. J. Org. Chem.*, 3933–3943 (2001). See also W. Nakanishi, S. Hayashi, and T. Nakai, ISOCS-XXI, Madrid, Spain, July 4–9, 2004, Abstracts, p. 119.