According to Scheme I,[9] selenocyanates **3a–d** were prepared by treatment of the corresponding *o*-iodobenzoic acids[10] with freshly prepared NaSeCN in DMA.[11] Reductive coupling with 2,4-dichloronitrobenzene afforded the biarylselenides in excellent yield. Little, if any, of the alternate para isomer was detected. Cyclization of these 2-(phenylseleno)benzoic acids by brief treatment in neat PPSE with excess P_2O_5 at 210 °C proceeded in good yield (Table I).[12] Only in the case of the methylenedioxy compound (entry e) was cyclization with a mixture of TFA/TFAA with catalytic H_3PO_4 found to be superior.

In the sulfur series, PPSE was generally superior to $SOCl_2/AlCl_3$ (entries g–i). In the oxygen series (entries j, k), however, PPA cyclizations were higher yielding.

Since reagents for Friedel–Crafts cyclizations occasionally show substrate specificity, new alternatives are important additions to the chemist's armamentarium. We have found PPSE to be the reagent of choice for the preparation of deactivated 9*H*-selenoxanth-9-ones from their corresponding benzoic acid precursors. Given the convenience of preparation and the effectiveness of PPSE as an aprotic cyclization medium, it may prove to be the reagent of choice when other more routine methods fail.

Experimental Section

Melting points were taken on a Thomas-Hoover Unimelt capillary melting point apparatus and are uncorrected. ^1H NMR spectra were measured in $CDCl_3$ or DMSO-d_6 solutions and recorded at 100 MHz on a Bruker WP100SY instrument or at 200 MHz on a Varian XL-200 instrument. IR spectra were recorded on a Nicolet MX-1 FT-IR spectrometer system. Combustion analyses were performed on a Perkin-Elmer 240 elemental analyzer.

General Procedure for Friedel–Crafts Cyclizations with PPSE. Preparation of 1-Chloro-7-methoxy-4-nitro-9*H*-selenoxanthen-9-one (5d). To a mechanically stirred mixture of 200 g of PPSE syrup[3] and 24 g of P_2O_5 at 210 °C was added 6.0 g of 2-[(5-chloro-2-nitrophenyl)seleno]-5-methoxybenzoic acid. After 20 min, the reaction was poured into an ice-cold solution of 6 N HCl. After the mixture was stirred for 3 h, the orange precipitate was collected and recrystallized from acetonitrile to give 3.58 g (68%) of the selenoxanthenone, mp 222–224 °C. Anal. Calcd for $C_{14}H_8NClSeO_4$: C, 45.62; H, 2.19; N, 3.80; Cl, 9.62. Found: C, 45.34; H, 2.31; N, 3.68; Cl, 9.32.

Registry No. **2a**, 88-67-5; **2b**, 54435-09-5; **2c**, 54413-93-3; **2d**, 123239-80-5; **3a**, 104101-90-8; **3b**, 104101-95-3; **3c**, 104101-92-0; **3d**, 123239-79-2; **4a**, 104101-87-3; **4b**, 123239-71-4; **4c**, 123239-72-5; **4d**, 123239-73-6; **4e**, 123239-74-7; **4f**, 54920-86-4; **4g**, 94636-18-7; **4h**, 94636-20-1; **4i**, 123239-75-8; **4j**, 101709-75-5; **4k**, 123239-76-9; **5a**, 104101-88-4; **5c**, 104101-94-2; **5d**, 104101-91-9; **5e**, 123239-77-0; **5f**, 41215-88-7; **5g**, 94636-19-8; **5i**, 123239-78-1; **5j**, 101709-74-4; **5k**, 101709-79-9.

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[9] A full paper including all experimental details is in preparation for *J. Med. Chem.*

[10] The *o*-iodo acids were conveniently prepared from commercially available benzoic acids via ortholithiation and iodination of the corresponding oxazoline according to the work of A. I. Meyers; see for example: *Tetrahedron Lett.* **1980**, *21*, 3335 and references cited therein.

[11] Hori, T.; Sharpless, K. B. *J. Org. Chem.* **1978**, *43*, 1689.

[12] The addition of excess P_2O_5 to PPSE prepared according to ref 3 improved yields slightly. Changes if any, in the composition and structure of the resulting reagent were not investigated.

Additions and Corrections

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Dieter Cremer,* Thomas Schmidt, Wolfram Sander,* and Peter Bischof. Electronic Structure of Carbonyl Oxides: Semiempirical Calculation of Ground-State Properties and UV-Vis Spectra.

Page 2519, right column. During the printing process Figures 3 and 4 were reversed (the captions are correct). Figure 4 (top right) is a valence spin density distribution for 13 and Figure 3 (bottom right) is a valence charge density distribution for 13.