s13.m35.p26 **Synthesis and Structure of Selenium-based Compounds as Therapeutic and Chemopreventive Agents: Se-(phenacyl)-2-selenobenzoic Acid.** Manuel Soriano-Garcia[1] and Federico Martinez-Ramos[2]. [1]*Instituto de Química, Universidad Nacional Autonoma de Mexico, Circuito Exterior, Ciudad Universitaria, 04510, Mexico D. F. MEXICO, and* [2]*Departamento de Quimica Inorganica, E. N. C. B. del IPN, Prolongacion de Carpio y Plan de Ayala, 11340, Mexico, D. F. Mexico. E-mail: soriano@servidor.unam.mx*

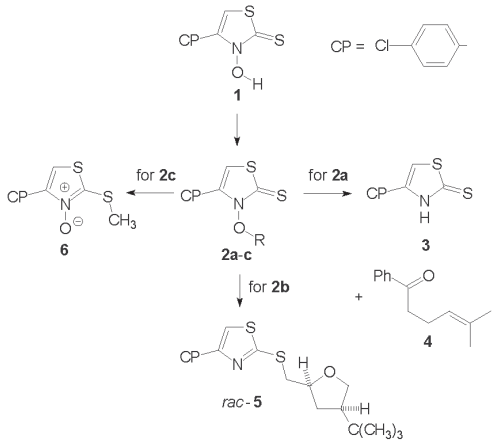
Keywords: Synthesis; Organoselenium compounds; Therapeutic and chemopreventive agents

Selenium is known to be as an important dietary antioxidant and essential component of the active sites of a number of enzymes, and several additional mammalian selenoproteins. Dietary selenium deficiency has been linked to diseases as diverse as cancer, hearth disease and arthritis. Thus, the pharmacology, biology and biochemistry of selenium metabolism have become subjects of considerable interest, which are spurring efforts to develop synthetic selenium-containing compounds as possible therapeutic and chemopreventive agents. We are currently working on the synthesis of selenium-based compounds as possible therapeutic and chemopreventive agents, such as Se-(phenacyl)-2-selenobenzoic acid (I). Crystals of (I) belong to monoclinic system and space group $P2_1/n$ with cell dimensions: a = 5.080(1), b = 10.709(1), c = 24.102(3)A, β = 91.272(3)° and Z = 4. The structure was solved by direct methods and refined by full-matrix least-squares method to a final R = 0.038. The dihedral angle between the benzoic and phenacyl rings is 68.8(1)°. This conformation keeps the Se atom's unshared electron pairs in a more stable conformation. A part from the intermolecular hydrogen bond between two symmetry-related molecules, O2-H2·····O1, the molecules in the crystal are stabilized by van der Waals forces.

s13.m35.p27 **On the Modes of Decomposition of *N*-(Alkoxy)-*p*-(chlorophenyl)thiazole-2(3*H*)-thiones on Prolonged Storage.** Ingrid Svoboda[a], Hartmut Fuess[a], Michaela Schwarz[b], Kristina Spehar[b], Jens Hartung[b], [a]*Fachbereich Materialwissenschaft, TU Darmstadt, Petersenstrasse 23, D-64287 Darmstadt, Germany,* [b]*Fachbereich Chemie, TU Kaiserslautern, Erwin-Schrödinger Strasse, D-67663 Kaiserslautern, Germany. E-mail: svoboda@tu-darmstadt.de*

Keywords: Thiazolethione; Thiohydroxamic acid; Fragmentation and rearrangement

N-(Hydroxy)-4-(*p*-chlorophenyl)thiazole-2(3*H*)-thione (1) serves as reagent for the synthesis of efficient oxyl radical precursors [1]. The utility of this compound originates from a fortunate balance between the stability of the corresponding *N*-(alkoxy) derivatives **2** and their ability to undergo selective N,O homolysis upon UV-excitation. The majority of *N*-(alkoxy)thiazole-2(3*H*)-thiones **2** have been applied in terms of weeks or months after their preparation. Based on the growing importance of *N*-(alkoxy)-4-(*p*-chlorophenyl)-thiazole-2(3*H*)-thiones (**2**) in photobiological, mechanistic and synthetic investigations [2], it has been essential to investigate the stability of these compounds, if stored for a longer period of time in the absence of light at 5 °C. Surprisingly, only three instances of *N*-(alkoxy)-4-(*p*-chlorophenyl)thiazole- 2(3*H*)-thione decompositions have been observed after in a timeframe of four years. These reactions follow three different mechanisms: (i) β-fragmenation [**2a**→**3**+**4**, for R = $PhCH(CH_2)_2CH{=}CMe_2$], (ii) N,O homolysis [**2b**→**5** for R = CH_2CH(*tert*-Bu)-$CH_2CH{=}CH_2$], and (iii) O,S alkyl shift [**2c**→**6**, for R = Me]. The structural characteristics of *N*-(hydroxy)-4-(*p*-chlorophenyl)thiazole-2(3*H*)-thione (**1**), selected *N*-(alkoxy) derivatives **2**, and decomposition products **4** and **6** are discussed in detail in the present contribution.



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