

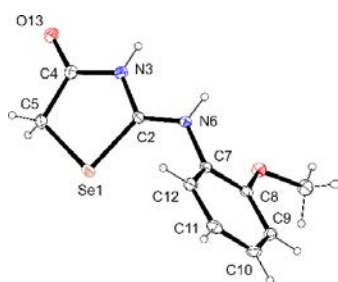
## 4-Selenazolidinones: tautomerism and stereoisomerism in the solid state

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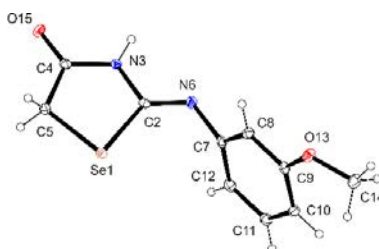
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Selenium-based organic compounds, and in particular selenium-containing heterocycles, have recently gained interest as perspective components of a medicinal chemistry toolkit, due to the unique properties that this element can endow on the parent molecules. Thus, thorough structural studies of selenoheterocycles are of high importance for this emerging field.

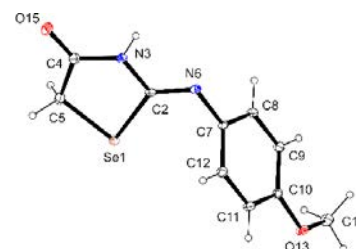
In this work, we report the synthesis of 2-phenylimino-1,3-selenazol-(2*H*)-ones with focus on their prototropic tautomerism. Three isomers, namely *ortho*-, *meta*- and *para*- (**I**, **II**, **III**) bearing a methoxy substituent at the phenyl ring, were studied by single-crystal X-ray diffractometry in order to investigate the influence of the substituent's proximity to the amidine system on the tautomeric equilibrium. In contrast to their sulfur-containing counterparts, molecules of compound **I** were found to coexist as imino/amino tautomers in the same crystalline sample, i.e. with the N-H hydrogen atom residing partially at the endocyclic N3 and exocyclic N7 atoms with approximately equal occupancy. Surprisingly, compounds **II** and **III** were found to exist exclusively in the imino tautomeric form in the solid state. In all three molecules, the Se1–C2 and N6–C7 bonds assume synperiplanar conformation, with the following Se1–C2–N6–C7 torsion angle:  $-2.41(16)^\circ$  (**I**),  $1.6(3)^\circ$  (**II**), and  $-0.1(2)^\circ$  (**III**).



2-(2-methoxyphenyl)-amino-1,3-selenazol-4(5*H*)-one (**I**)



2-(3-methoxyphenyl)-imino-1,3-selenazol-4(5*H*)-one (**II**)



2-(4-methoxyphenyl)-imino-1,3-selenazol-4(5*H*)-one (**III**)