

FOURIER-TRANSFORM RAMAN ANALYSIS AND FUNGICIDAL ACTIVITY OF A NOVEL SERIES OF SELENIUM CONTAINING COMPOUNDS

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Abstract: A novel series of selenium containing compounds, (3-(Ar¹)-2-(4'-selenomorpholynyl)-5-(Ar²)-vinyl-4-imidazolin-4-one), had been synthesized. The Fourier-transform Raman spectra of these compounds were acquired for the first time and carefully assigned and discussed. The effects of the substituted group on the molecular symmetry and vibrational spectra were also examined. All investigated compounds showed fungicidal activity.

Selenium-containing compounds have been shown to display diverse and useful biological properties. Some of them have been developed as fungicides, herbicides or plant growth regulators. It has been also known that a wide variety of derivatives of imidazoline-one have potential biological activity. We are interested in compounds which have both active chemical moieties. So we synthesised a novel series of selenium containing compounds, XMZ1 (Ar¹= C₆H₅, Ar²= C₆H₅), XMZ6 (Ar¹= C₆H₅, Ar²= 3-ClC₆H₄), XMZ8 (Ar¹=4-ClC₆H₄, Ar²= 3-ClC₆H₄), XMZ11 (Ar¹= C₆H₅, Ar²= 4-ClC₆H₄), XMZ13 (Ar¹=4-ClC₆H₄, Ar²= 4-ClC₆H₄). The synthesis routine of the compounds is shown in Fig. 1.

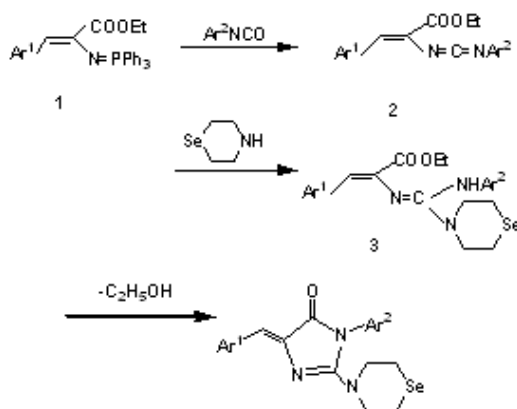


Fig. 1. The synthesis routine of the compounds

All these compounds have been characterized by elemental analysis, ¹H NMR, MS, IR spectra, and FT-Raman spectra. The compounds' FT-Raman spectra were measured in their solid state with a Bruker IFS 120HR spectrometer equipped with an integrated FRA 106 Raman module. The

spectral regions were 150-3600 cm^{-1} . The 1064 nm radiation from a Nd: YAG laser with an output of about 800 mW was used for excitation. Figure 2 shows the 1000-2000 cm^{-1} region of the XMZ6 FT-Raman spectra.

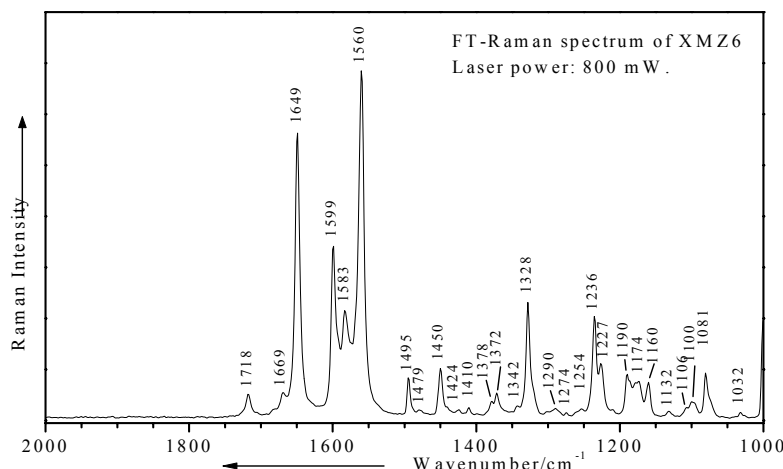


Fig. 2. The FT-Raman spectrum of XMZ6

In the FT-Raman spectra, we can easily distinguish the C=O, C=N, C-C, C-Cl vibrational modes. The 1641–1649 cm^{-1} bands are attributed to the stretching vibration of C=O, and the 1587–1600 cm^{-1} bands are assigned to the stretching vibration of C=N. The 1549–1562 cm^{-1} and 1446-1458 cm^{-1} bands are assigned to the skeleton vibration of the benzene ring. The bands at 843–862 cm^{-1} are identified as C–Cl stretching vibrational modes, etc.

The fungicidal activity of the compounds was evaluated against *Gibberella Zeae*, *Cercospora beticola*, *Fusarium oxysporium*, *Rhizoctonia solani* and *Botryosphaeria berengeriana* at 0.005% concentration. The results shown in Table 1 indicate that all compounds have significant toxicity at 0.005% concentration against three fungi (*Gibberella Zeae*, *Cercospora beticola* and *Botryosphaeria berengeriana*).

Table 1. Fungicidal activity of the compounds (0.005% inhibition %)

compound	<i>Gibberella Zeae</i>	<i>Cercospora beticola</i>	<i>Fusarium oxysporium</i>	<i>Rhizoctonia solani</i>	<i>Botryosphaeria berengeriana</i>
XMZ1	60.0	75.0	44.4	2.9	88.9
XMZ6	33.3	45.0	0	0	55.6
XMZ8	53.3	25.0	0	0	72.2
XMZ11	33.3	45.0	44.4	28.6	83.3
XMZ13	46.7	50.0	38.9	54.3	72.2

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