Insights into Antiradical Behavior: Crystal Structures and DFT Analysis of 2-Formylpyridine N^4-Allylthiosemicarbazone Salts

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Table S1. Selected bond lengths and angles in **1**–**5**. For compound **3** the selected data are shown for one independent molecule.

Bond	**d,** Å				
	1	**2**	**3**	**4**	**5**
S1–C1	1.678(6)	1.674(8)	1.667(4)	1.672(3)	1.669(2)
N1–N2	1.325(6)	1.370(7)	1.352(3)	1.349(4)	1.346(2)
N2–C2	1.280(7)	1.263(8)	1.276(4)	1.274(5)	1.277(3)
N1–C1	1.346(7)	1.354(9)	1.371(4)	1.356(5)	1.367(3)
N3–C1	1.339(7)	1.335(8)	1.327(4)	1.326(5)	1.329(3)
N4–C3	1.353(7)	1.362(8)	1.368(4)	1.338(5)	1.350(3)
N4–C7	1.340(7)	1.323(9)	1.335(4)	1.338(5)	1.337(3)
C2–C3	1.449(8)	1.444(10)	1.435(4)	1.457(5)	1.450(3)
Angle	**ω°**				
N2–N1–C1	122.0(5)	119.7(6)	120.4(3)	120.1(3)	118.97(17)
N1–N2–C2	118.4(5)	118.0(6)	118.9(3)	118.8(3)	118.95(17)
S1–C1–N1	119.1(5)	118.1(6)	118.9(3)	119.0(3)	119.14(16)
S1–C1–N3	124.6(5)	125.2(6)	126.1(3)	125.0(3)	125.05(16)
N1–C1–N3	116.3(6)	116.7(7)	115.0(3)	116.1(3)	116.3(6)
N2–C2–C3	120.9(6)	118.4(7)	118.5(3)	118.1(3)	116.88(18)

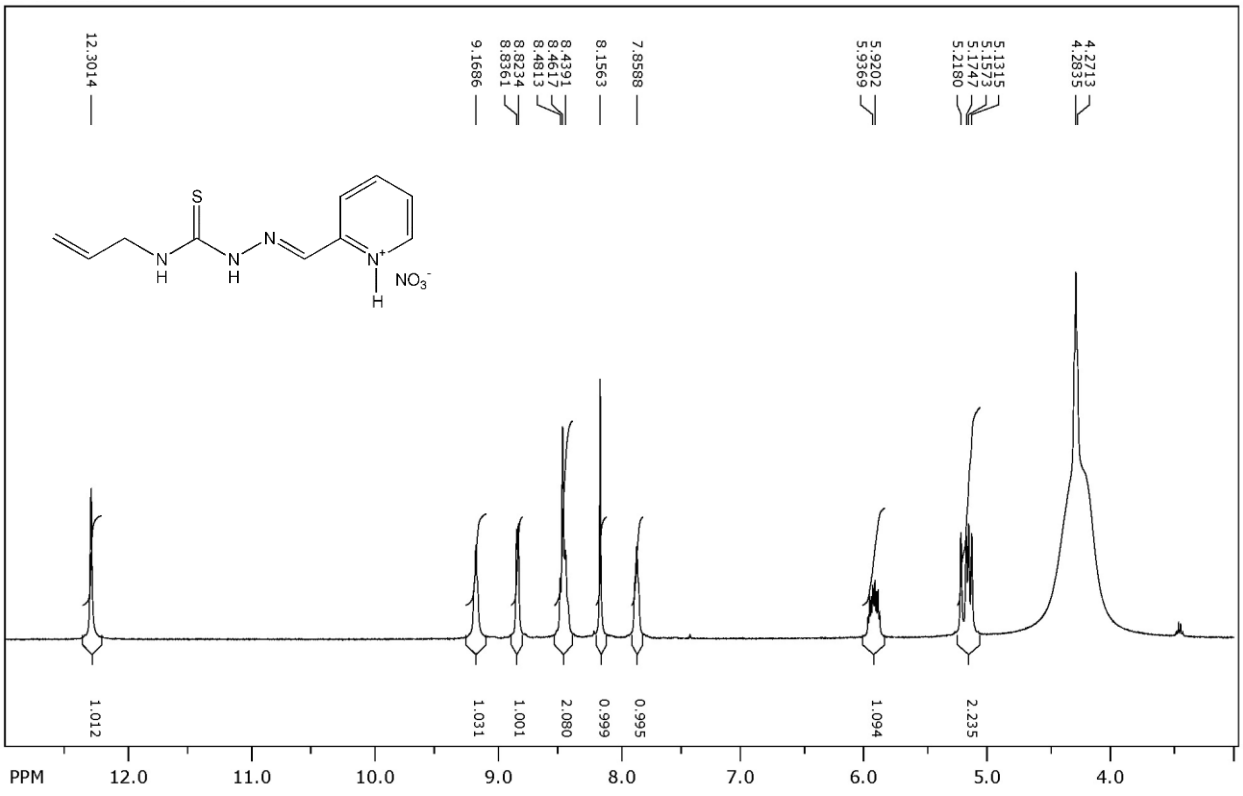

Figure S2. ^{1}H NMR spectrum of 2-({2-[(prop-2-en-1-yl)carbamothioyl]hydrazinylidene}methyl)pyridin-1-ium nitrate **[H$_2$L]NO$_3$ (1)**.

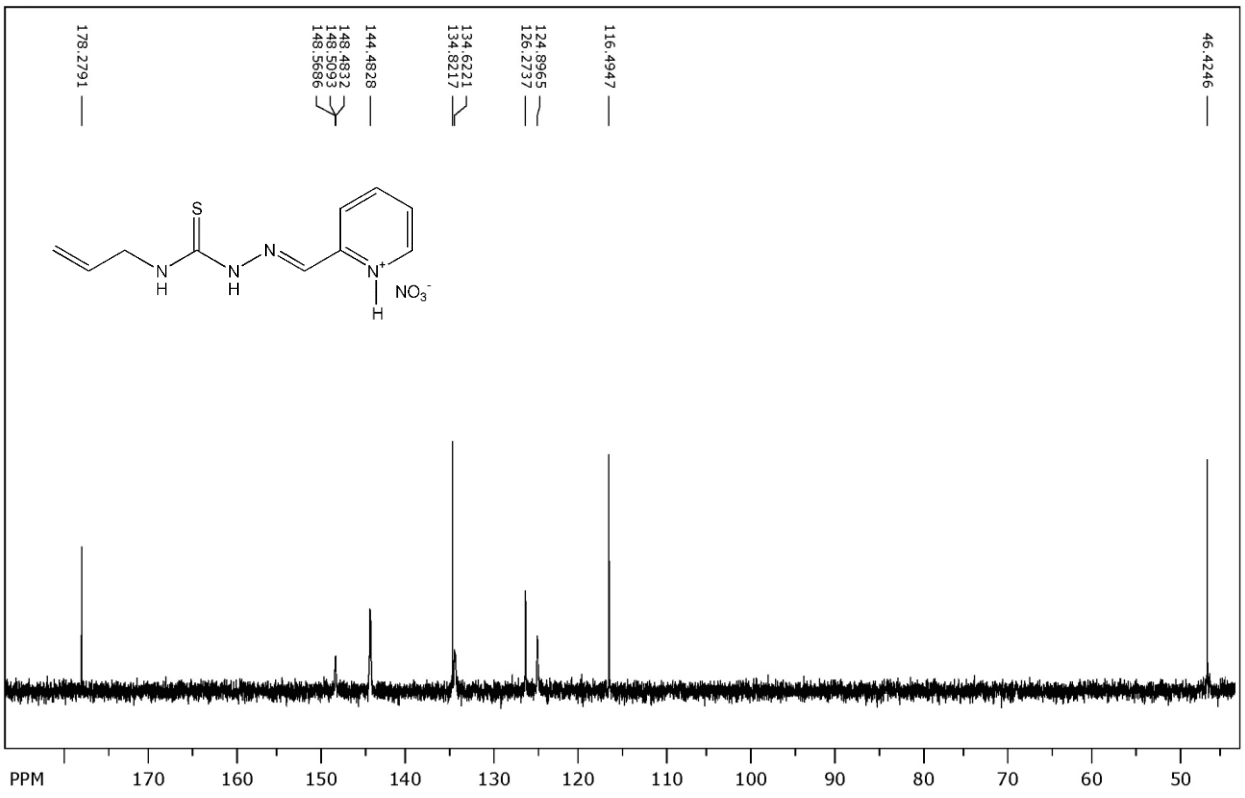

Figure S3. ^{13}C NMR spectrum of 2-({2-[(prop-2-en-1-yl)carbamothioyl]hydrazinylidene}methyl)pyridin-1-ium nitrate **[H_2L]NO_3 (1)**.