



SUPPLEMENTARY MATERIAL TO
**2-Acetylpyridine-aminoguanidine Schiff base – Novel ligand salt
and zinc(II) complex containing thiocyanate**

MIRJANA M. RADANOVIĆ^{1*#}, SLAĐANA B. NOVAKOVIĆ^{2#}, LJILJANA S.
VOJINOVIĆ-JEŠIĆ^{1#}, MARKO V. RODIĆ^{1#} and VUKADIN M. LEOVAC^{1#}

¹Faculty of Sciences, University of Novi Sad, Trg D. Obradovića 3, 21000 Novi Sad, Serbia
and ²Vinča Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed
Matter Physics, P. O. Box 522, 11001 Belgrade, Serbia

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CHARACTERISATION DATA FOR THE LIGAND AND COMPLEX

(2E)-2-[1-(2-pyridinyl)-ethylidene]-hydrazinecarboximidamide dihydrothiocyanate dihydrothiocyanate (*L*-2HNCS). Yield: 0.36 g (61 %); Anal. Calcd. for C₁₀H₁₃N₇S₂: C, 40.66; H, 4.43; N, 33.20; S, 21.71 %. Found: C, 40.38; H, 4.57; N, 33.51; S, 21.36 %; IR (KBr, cm⁻¹): 3092(w), 2820(w), 2058(vs), 1680(s), 1628(s), 1592(s), 1532(m), 1452(m), 1295(w), 1236(w), 1164(m), 1096(w), 956(w), 781(m), 618(w), 601(w), 557(w); Conductivity (DMF, $\Lambda_M/\Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$): 157.

[ZnL(NCS)₂]. Yield: 0.12 g (67 %); Anal. Calcd. for C₁₀H₁₁N₇S₂Zn: C, 33.48; H, 3.09; N, 27.33; S, 17.87 %. Found: C, 33.20; H, 2.72; N, 27.34; S, 17.50 %; IR (KBr, cm⁻¹): 3464(w), 3357(m), 3224(w), 2922(w), 2109(vs), 2084(vs), 1659(s), 1595(m), 1542(m), 1471(m), 1262(w), 1193(m), 1182(m), 1159(w), 1115(w), 780(w), 745(w), 633(w), 477(w); Conductivity (DMF, $\Lambda_M/\Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$): 36.

TABLE S-I. Pertinent crystallographic and refinement details

	C ₁₀ H ₁₃ N ₇ S ₂	C ₁₀ H ₁₁ N ₇ S ₂ Zn
Empirical formula	C ₁₀ H ₁₃ N ₇ S ₂	C ₁₀ H ₁₁ N ₇ S ₂ Zn
Formula weight	295.39	358.75
Colour, crystal shape	colourless, prism	colourless, prism
Crystal size, mm ³	0.158 × 0.40 × 0.54	0.25 × 0.26 × 0.60
Temperature, K	293(2)	293(2)
Wavelength, Å	0.71073	0.71073
Crystal system	triclinic	tetragonal
Space group	<i>P</i> 1	<i>P</i> 4 ₃
Unit cell dimensions		

* Corresponding author. E-mail: mirjana.lalovic@dh.uns.ac.rs

TABLE S-I. Continued

$a / \text{\AA}$	6.6021(5)	10.81504(14)
$b / \text{\AA}$	7.5617(7)	10.81504(14)
$c / \text{\AA}$	8.1001(7)	12.7901(3)
$\alpha / ^\circ$	110.521(8)	90
$\beta / ^\circ$	100.869(7)	90
$\gamma / ^\circ$	99.006(7)	90
$V / \text{\AA}^3$	360.87(6)	1495.99(5)
Z	1	4
$D_{\text{calc}} / \text{Mg m}^{-3}$	1.359	1.593
μ / mm^{-1}	0.367	1.921
θ range for data collection, $^\circ$	2.783 – 28.911	2.466 – 29.016
Reflections collected	4299	10498
Independent reflections, R_{int}	2846, 0.0235	3528, 0.0201
Data /parameters	2846/1193	3528/195
Goodness-of-fit	1.027	1.093
Final R_1/wR_2 indices [$I > 2\sigma(I)$]	0.0348/0.0841	0.0305/0.0727
Final R_1/wR_2 indices (all data)	0.0400/0.0887	0.0344/0.0744
Largest diff. peak and hole, e \AA^{-3}	0.257 / -0.252	0.467 / -0.187