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SUPPLEMENTARY MATERIAL TO

Introducing a novel crystal form of pyruvic acid thiosemicarbazone and its sodium salt

SVETLANA K. BELOŠEVIĆ[1], SLAĐANA B. NOVAKOVIĆ[2]*, MARKO V. RODIĆ[3], VUKADIN M. LEOVAC[3], LJILJANA S. VOJINOVIĆ-JEŠIĆ[3], GORAN A. BOGDANOVIĆ[2] and MIRJANA M. RADANOVIĆ[3]**

[1]Faculty of Technical Sciences, University of Priština, Knjaza Miloša 7, 38220 Kosovska Mitrovica, Serbia, [2]"Vinča" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, P. O. Box 522, 11001 Belgrade, Serbia and [3]University of Novi Sad, Faculty of Sciences, Trg Dositeja Obradovića 3, 21000, Novi Sad

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ANALYTICAL AND SPECTRAL DATA

*$H_2pt{\cdot}0.5H_2O$ (**1**)*

Anal. Calc. for $C_4H_7N_3O_2S{\cdot}0.5H_2O$ ($H_2pt{\cdot}0.5H_2O$): C, 28.23; H, 4.71; N, 24.71; S, 18,82 %. Found: C, 28.52; H, 4.60; N, 24.58; S, 18.74 %. M. p. 216 °C. Selected IR bands (cm^{-1}): 3414_m, $\nu_a(H_2O)$; 3293_m, 3182_m, $\nu_s(NH_2/NH)$; 1727_s, 1699_{vs}, ν(CO) of COOH; 1614_{vs}, ν(CN); 802_m, ν(CS).

*Sodium pyruvate thiosemicarbazone $\{[Na(Hpt)(H_2O)_3]{\cdot}H_2O\}_n$ (**2**)*

Anal. Calc. for $NaC_4H_8N_3O_3S{\cdot}3H_2O$: C, 20.70; H, 6.03; N, 18.10 %. Found: C, 20.55; H, 5.89; N, 18.01 %. M. p. 208 °C; λ_M [Scm^2mol^{-1}]: 87 (H_2O), 98 (MeOH). Selected IR bands (cm^{-1}): 3458_m $\nu(H_2O)$; 3366_m, 3315_m, 3141_m, $\nu(NH_2/NH)$; 1622_m, ν(CN); 1571_{vs}, $\nu_a(CO_2^-)$; 1381_{vs}, $\nu_s(CO_2^-)$; 789_m, ν(CS).

* Corresponding authors. E-mail: (*)snovak@vin.bg.ac.rs; (**)mirjana.lalovic@dh.uns.ac.rs

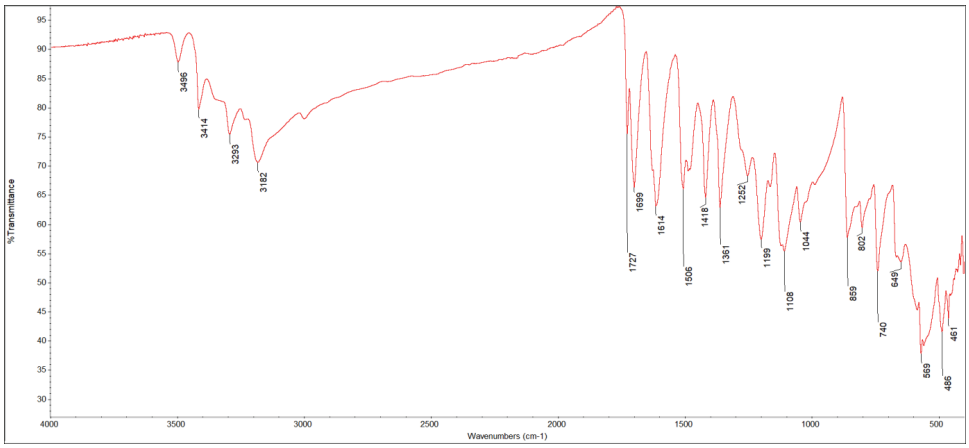

Fig. S-1. IR spectra of compound **1**.

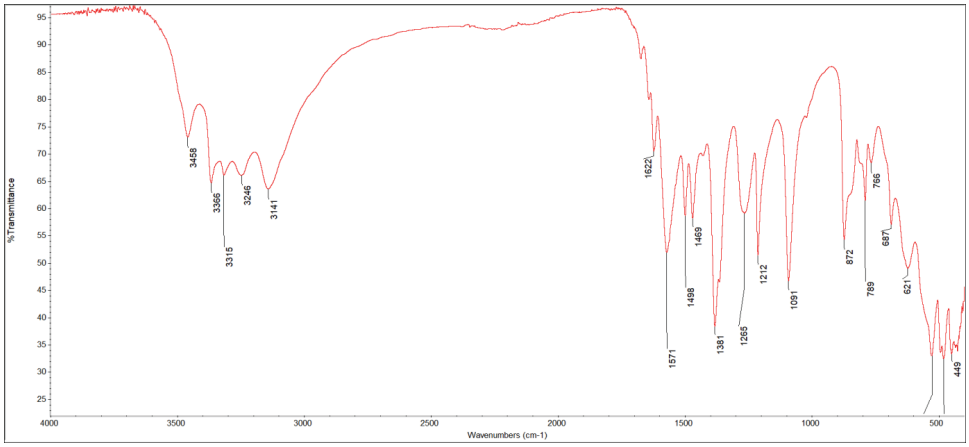

Fig. S-2. IR spectra of compound **2**.

TABLE S-I. Crystallographic data

	1	**2**
Empirical formula	$C_8H_{16}N_6O_5S_2$	$C_4H_{14}N_3NaO_6S$
Formula weight	340.39	255.23
Temperature (K)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
Unit cell dimensions		
a (Å)	7.3991(6)	5.2792(5)
b (Å)	8.8745(5)	8.5201(7)
c (Å)	12.2109(7)	13.1342(10)
α (°)	75.274(5)	86.131(6)
β (°)	79.180(6)	87.338(7)
γ (°)	82.915(6)	74.253(8)
V (Å^3)	759.27(9	567.06(9)
Z	2	2
D_{calc} (Mg/m^3)	1.489	1.495
μ (mm^{-1})	0.381	0.337
θ range for data collection (°)	2.6–29.1	2.5–29.1
Reflections collected	13178	4043
Independent reflections, R_{int}	3584, 0.0215	2557, 0.0162
Data / restraints/parameters	3584/10/225	2557/0/181
Goodness-of-fit	1.028	1.040
Final R_1/wR_2 indices [$I>2\sigma(I)$]	0.035/0.089	0.034/0.083
Final R_1/wR_2 indices (all data)	0.046/0.096	0.044/0.089
Largest diff. peak and hole (e Å^{-3})	0.27/−0.24	0.22/−0.23