



SUPPLEMENTARY MATERIAL TO  
**Introducing a novel crystal form of pyruvic acid thiosemicarbazone  
and its sodium salt**

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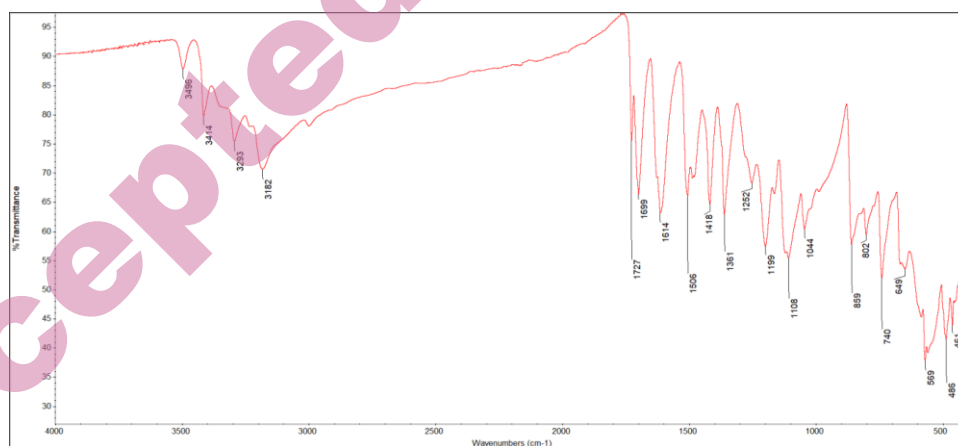


Fig. S1 IR spectra of compound 1.

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#Serbian Chemical Society member

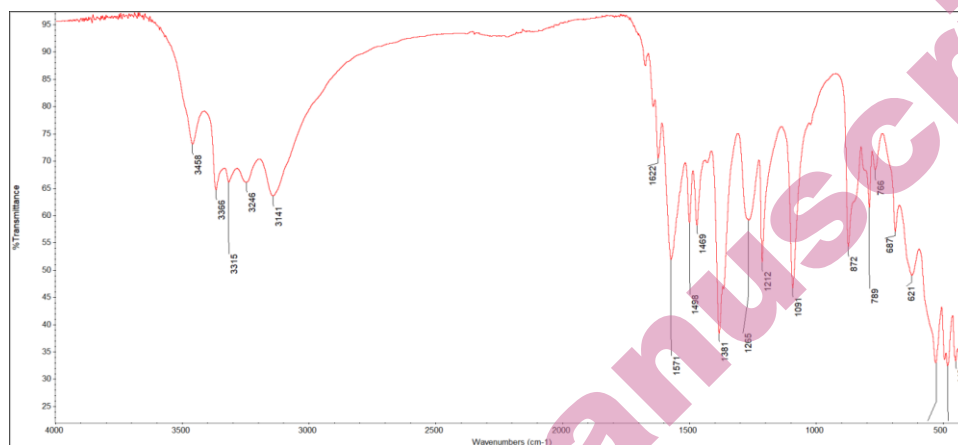


Fig. S2 IR spectra of compound 2.

TABLE SI. Crystallographic data

	1	2
Empirical formula	C <sub>8</sub> H <sub>16</sub> N <sub>6</sub> O <sub>5</sub> S <sub>2</sub>	C <sub>4</sub> H <sub>14</sub> N <sub>3</sub> NaO <sub>6</sub> S
Formula weight	340.39	255.23
Temperature (K)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
Unit cell dimensions		
<i>a</i> (Å)	7.3991(6)	5.2792(5)
<i>b</i> (Å)	8.8745(5)	8.5201(7)
<i>c</i> (Å)	12.2109(7)	13.1342(10)
$\alpha$ (°)	75.274(5)	86.131(6)
$\beta$ (°)	79.180(6)	87.338(7)
$\gamma$ (°)	82.915(6)	74.253(8)
<i>V</i> (Å <sup>3</sup> )	759.27(9)	567.06(9)
<i>Z</i>	2	2
<i>D</i> <sub>calc</sub> (Mg/m <sup>3</sup> )	1.489	1.495
$\mu$ (mm <sup>-1</sup> )	0.381	0.337
$\theta$ range for data collection (°)	2.6–29.1	2.5–29.1
Reflections collected	13178	4043
Independent reflections, <i>R</i> <sub>int</sub>	3584, 0.0215	2557, 0.0162
Data / restraints/parameters	3584/10/225	2557/0/181
Goodness-of-fit	1.028	1.040
Final <i>R</i> <sub>1</sub> / <i>wR</i> <sub>2</sub> indices [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	0.035/0.089	0.034/0.083
Final <i>R</i> <sub>1</sub> / <i>wR</i> <sub>2</sub> indices (all data)	0.046/0.096	0.044/0.089
Largest diff. peak and hole (e Å <sup>-3</sup> )	0.27/–0.24	0.22/–0.23