LINEAR TRINUCLEAR COBALT(II) ISOBUTYRATE WITH 1,10-PHENANTHROLINE

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INTRODUCTION

The polynuclear cobalt complexes are of great current interest due to their great potential as catalysts, electron transfer mediators in dye-sensitized solar cells, antiviral agents and nanomagnet molecules.

A new trinuclear cobalt(II) - containing compound **$[Co_3(is)_6(phen)_2]$ (1)** was obtained from the reaction of $Co(is)_2$ (His = isobutyric acid) with 1,10`-phenanthroline (phen) in acetone/dmso (1:1) mixture under ultrasonic treatment (Fig. 1). The compound has been characterized by elemental and TG analyses, IR spectroscopy, ESI mass spectrometry, single-crystal and powder X-ray diffraction study.

SYNTHESIS

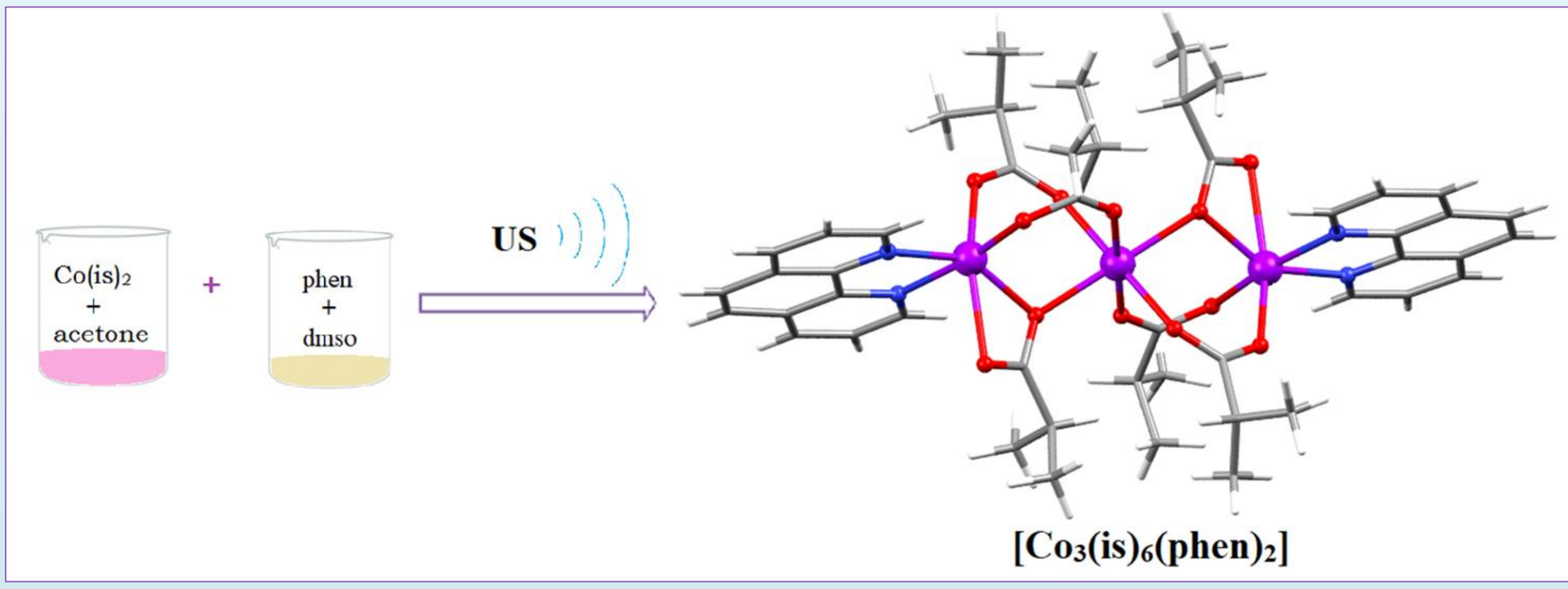

Fig. 1. Synthesis of 1.

RESULTS

X-ray analysis shows that **1** crystalizes in the orthorhombic *Pbca* space group. The trinuclear cluster consists of three Co(II) atoms, six isobutyrate anions and two phen ligands.

In the crystal structure trinuclear clusters form a supramolecular chain along the *b* axis due to stacking interactions between phen ligands (π···π separations are 3.397 Å). Additionally, the clusters are joint through C-H...O hydrogen bonds of 2.525-3.043 Å between phen and oxygen from isobutyrates (Fig. 2).

The experimental PXRD pattern of **1** matches the pattern simulated for the single-crystal diffraction-derived structure (Fig. 3).

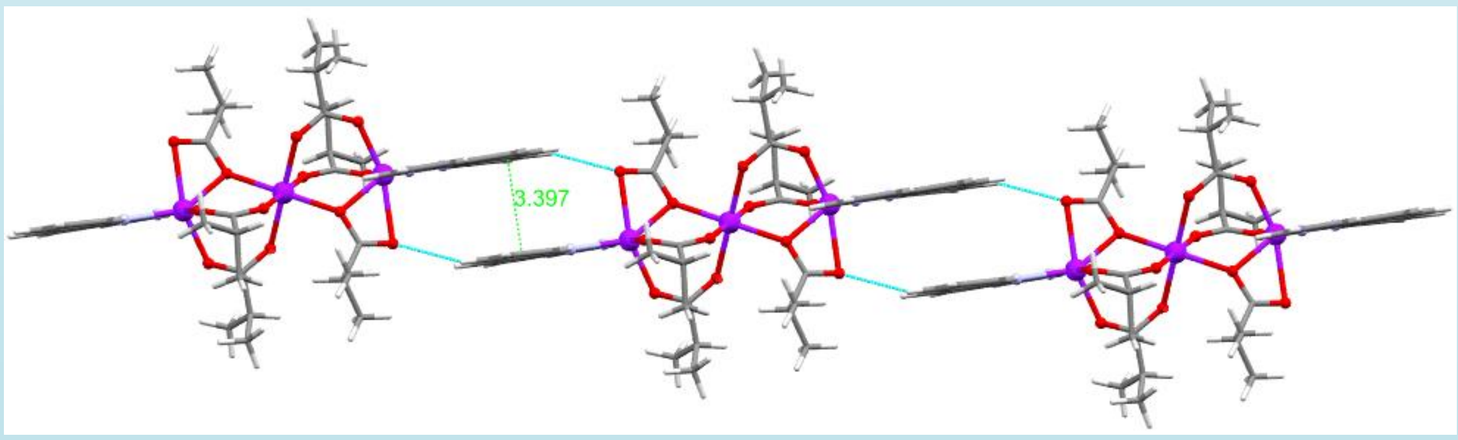

Fig. 2. A supramolecular chain formed due to π···π stacking interactions and hydrogen bonds in 1.

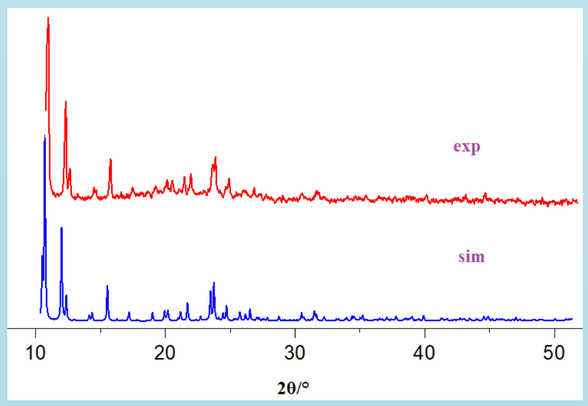

Fig. 3. Experimental and simulated powder X-ray diffraction patterns for 1.

THERMAL ANALYSIS

TG analysis indicated that **1** is thermally stable up to 170°C and then it decomposes to Co-oxides. The process is accompanied by two endothermic effects at 230 and 360°C (Fig. 5).

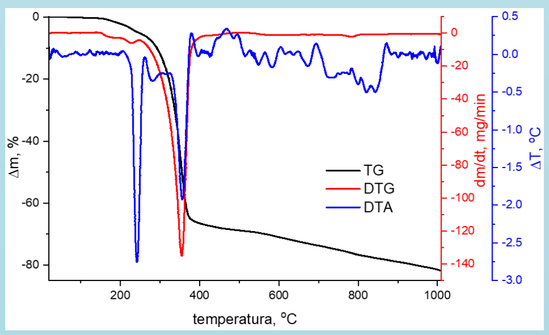

Fig. 5. TGA/DTG/DTA curves for 1.

IR-SPECTROSCOPY

The IR spectrum displays the asymmetric and symmetric C–H stretching vibrations of $–CH_3$ and –CH groups of isobutyrates and phen in the range of 2963–2869 cm^{-1} and asymmetric and symmetric bending vibrations at 1513 and 1469 cm^{-1} and a doublet at 1368 and 1354 cm^{-1}, respectively. The characteristic strong peaks observed at 1584 and 1415 cm^{-1} corespond to vibrations of the coordinated carboxylate groups (Fig. 4).

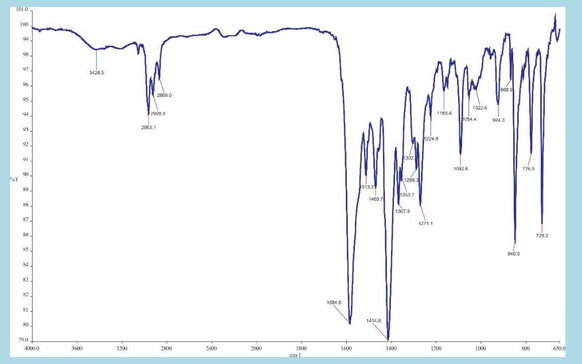

Fig. 4. IR spectrum for 1.

ESI MASS SPECTROMETRY

Table 1. Fragments observed in positive/negative mode ESI MS of 1.

	ESI^+	ESI^-
m/z	326,045 → $[Co(is)(phen)]^+$	469,032 → $[Co(is)_3(His)\ (CH_3COOH)]^-$
	506,114 → $[Co(is)(phen)_2]^+$	497,063 → $[Co\ (is)_3(phen)]^-$
	559,068 → $[Co_2(is)_3(phen)]^+$	**553,089 → $[Co_2(is)_5]^-$ (100%)**
	739,137 → $[Co_2(is)_3(phen)_2]^+$ (100%)	1038,036 → $[Co_3(is)_5(phen)_2(CH_3O)_2]^-$

The ESI mass pattern of **1**, recorded in positive/negative mode reveals several peaks (Table 1) suggesting that trinuclear core of **1** is stable in solution
m/z = 1038,036 ;
$\{[Co_3(is)_5(phen)_2(CH_3O)_2]^-\}$

CONCLUSION

The new trinuclear compound of the formula $[Co_3(is)_6(phen)_2$ was synthesized and studied by different physico-chemical methods, as the next purpose is the magnetic analysis due to the presence in the structure of **Co^{II}** ions**.**

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