

The 90-year-old story of nickel benzoate

Anna Vráblová¹, Milagros Tomás², Javier Campo³, Juraj Černák¹, and Larry R. Falvello⁴

¹*P. J. Šafárik Univ. in Košice, Fac. Sci., Inst. Chem., Dep. Inorg. Chem., Moyzesova 11, 041 54 Košice, Slovakia*

²*Dep. Quím. Inorg., Inst. Sínt. Quím. y Catál. Homog. (ISQCH), Univ. Zaragoza-CSIC, Pedro Cerbuna 12, E-50009, Zaragoza, Spain*

³*Dep. Física, Inst. Cien. Mater. de Aragón (ICMA), Univ. Zaragoza-CSIC, Pedro Cerbuna 12, E-50009 Zaragoza, Spain*

⁴*Dep. Quím. Inorg., Inst. Cien. Mater. Aragón (ICMA), Univ. Zaragoza-CSIC, Pedro Cerbuna 12, E-50009 Zaragoza, Spain*

The synthesis of nickel benzoate trihydrate, $\text{Ni}(\text{Bz})_2 \cdot 3\text{H}_2\text{O}$ was first published by Ephraim and Pfister [1] and by Pfeiffer and Müllenheim [2] in 1925 and 1933, respectively. Later, in 1971 Pavkovic studied its IR spectrum and suggested the presence of coordinated and uncoordinated benzoate groups in the structure [3]. The anhydrous complex $\text{Ni}(\text{Bz})_2$ was synthesized in microcrystalline form [4] and Balarew et al. studied the thermal properties of the nickel benzoate tetrahydrate [5]. In 2009 the crystal structure of the dinuclear “paddle wheel” type complex $[\text{Ni}_2(\mu_2\text{-Bz})_4(\text{HBz})_2]$, formed incidentally under solvothermal conditions beginning with nickel(II) nitrate, sodium benzoate and bipyridine, was reported [6]. More recently, we were successful in preparing $\text{Ni}(\text{Bz})_2 \cdot 3\text{H}_2\text{O}$ in single crystal form. The results of a crystal structure analysis led to the reformulation of the trihydrate as $([\text{Ni}(\text{Bz})(\text{H}_2\text{O})_2](\text{Bz}) \cdot \text{H}_2\text{O})_n$; its crystal structure is comprised of positively charged chains $[\text{Ni}(\text{Bz})(\text{H}_2\text{O})_2]_n^{n+}$, benzoate anions and one water solvate molecule per formula unit. Within the chains hexacoordinated Ni(II) atoms are triply bridged by two aqua ligands and one syn-syn benzoato ligand. The results will be discussed.

This work was supported by the Projects VEGA 1/0075/13, APVV-0132-11 and MAT2011-27233-C02-01 (Spain).

- [1] F. Ephraim, A. Pfister, *Helv. Chim. Acta*, 1925, 8, 369.
- [2] P. Pfeiffer and S. V. Müllenheim, *J. Prak. Chem.* 137 (1933) 9.
- [3] S. F. Pavkovic, *J. Inorg. Nucl. Chem.*, 33 (1971) 1475.
- [4] A. B. Siqueira, E. Y. Ionashiro, C. T. de Carvalho, G. Bannach, E. C. Rodrigues, M. Ionashiro, *Quim. Nova* 30 (2007) 318.
- [5] C. Balarew, D. Stoilova, R. Krasteva, *Thermochim. Acta* 92 (1985) 719.
- [6] J. H. Deng, Y. P. Yi, Z. X. Xiong, L. Yuan, G. Q. Mei, *Acta Crystallogr.* E65 (2009) m1484.