The X-ray structures, vibrational spectroscopy and antimicrobial activity of nickel(II) complexes with 4-hydroxybenzhydrazide.

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Two novel nickel(II) complexes, *[Ni(4hbah)$_3$]SO$_4$·CH$_3$OH·5H$_2$O* (**I**) and *[Ni(4hbah)$_3$](SO$_4$)·6H$_2$O* (**II**), have been synthesized and characterized by single-crystal X-ray crystallography. The nickel(II) coordinates three 4-hydroxybenzhydrazide (4hbah) ligands with the donor oxygen and nitrogen atoms arranged in *fac* configuration. Both compounds spontaneously decompose on air losing some water molecules and forming *[Ni(4hbah)$_3$]SO$_4$·CH$_3$OH·2H$_2$O* (**Ia**) and *[Ni(4hbah)$_3$]SO$_4$·2H$_2$O* (**IIa**), respectively. The **Ia** and **IIa** were used for measurement of IR and Raman spectra, which have been interpreted with help of DFT calculations and special experimental techniques, such as O,N-deuteration and ^{58}Ni/^{64}Ni isotope substitution. The combination of these experimental and theoretical attempts allowed us to make reliable assignment of the observed bands, including the strongly coupled nickel(II)–ligand vibrations. The **Ia** complex shows better antibacterial activity than the 4hbah ligand.

Słowa kluczowe

4-Hydroxybenzhydrazide nickel(II) complexes, IR and Raman spectra, Deuteration, Metal isotope effect, biological activity

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