# Crystallochemistry of Ni(II) complexes based on halogen derivatives of 8-hydroxyquinoline with different bridging of central atoms

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High-spin Ni(II) complexes have been a very important class of molecules due to their potential application as a new type of magnetic materials. In general, multinuclear Ni(II) complexes, such as $Ni_4O_4$ cubane, may exhibit either ferromagnetic or antiferromagnetic interactions between the nickel ions, as well as the slow magnetic relaxation characteristic for single molecule magnets (SMM) [1].

In this work we describe the preparation of four new multinuclear Ni(II) complexes: $[Ni_2(BrQ)_3(HBrQ)_3]ClO_4$ (**1**), $[Ni_2(dBrQ)_4(MeOH)_2]$ (**2**), $NH_2(CH_3)_2[Ni_2(\mu\text{-}Cl)_2(BrQ)_3(DMF)(H_2O)]\cdot DMF$ (**3**) and $[Ni_4(ClQ)_6Cl_2(H_2O)_2]\cdot 2DMF$ (**4**), containing molecules of halogen derivatives of 8-hydroxyquinoline: 5-chloro-8-hydroxyquinoline (HClQ), 7-bromo-8-hydroxyquinoline (HBrQ) and 5,7-dibromo-8-hydroxyquinoline (HdBrQ) (Fig. 1). The complexes were studied by infrared spectroscopy, CHN elemental analysis and single crystal X-ray analysis.

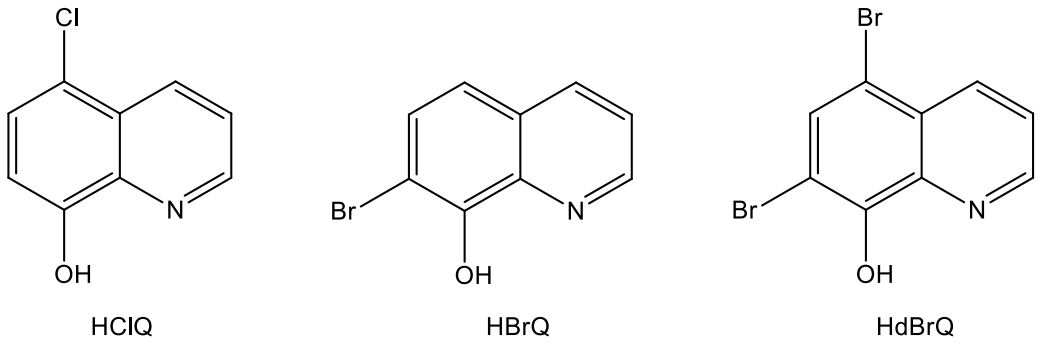


**Figure 1.** Structural formulas of different halogen derivatives of 8-hydroxyquinoline.

Using infrared spectroscopy, we identified individual characteristic vibrations in the measured spectra of complexes **1** – **4**, which confirmed the presence of coordinated molecules of anionic ligands ClQ, BrQ or dBrQ, as well as perchlorate anion in sample **1** and solvent water and dimethylformamide molecules in samples **3** and **4**.

Structural analysis revealed different bridges between the central nickel atoms in the structures of these multinuclear complexes. Nickel atoms are bridged by the hydrogen atom connecting the opposite oxygen atoms in the HBrQ molecules (**1**), by two oxygen atoms of the dBrQ ligands (**2**), by two chlorine atoms (**3**) and by six oxygen atoms of the ClQ ligands; four of them bridge two nickel atoms while remaining two bridge three nickel atoms (**4**). As a result, complexes **1**, **2** and **3** are dinuclear, while complex **4** forms a tetranuclear structure. We observed the stabilization of these complexes through intermolecular interactions, such as hydrogen bonds (**1** – **4**) and $\pi - \pi$ interactions (**2** and **4**).

[1] Gusev, A. N., Nemec, I., Herchel, R., Baluda, Y. I., Kryukova, M. A., Efimov, N. N. & Kiskin, M. A. (2021). *Polyhedron.* **196**, 115017.

**Keywords: halogen derivates of 8-hydroxyquinoline; multinuclear Ni(II) complexes; single molecule magnets**

*Slovak Grant Agencies (VEGA 1/0148/19 and VVGS-PF-2021-1769) are acknowledged for financial support.*