

A novel tridentate co-ordination mode for the carbonatonicel system exhibited in an unusual hexanuclear nickel(II) μ_3 -carbonato-bridged complex

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Single crystals suitable for X-ray analysis were obtained by crystallisation (CH_2Cl_2 , slow evaporation) to yield a green solid $[\text{Ni}_6(\mu_3\text{-CO}_3)_4(\text{TMEDA})_6(\text{H}_2\text{O})_{12}]\text{Cl}_4\cdot\text{CH}_2\text{Cl}_2$ (**9**) with identical spectroscopic data to **10**. There are 200 H atoms per unit cell which could not be located: 192 of these are water H atoms, the other 8 belong to the disordered CH_2Cl_2 solvent molecules. Of the 92 restraints, 3 were geometric restraints applied to the solvent molecule. The remaining 89 were applied to anisotropic displacement parameters for the entire structure.

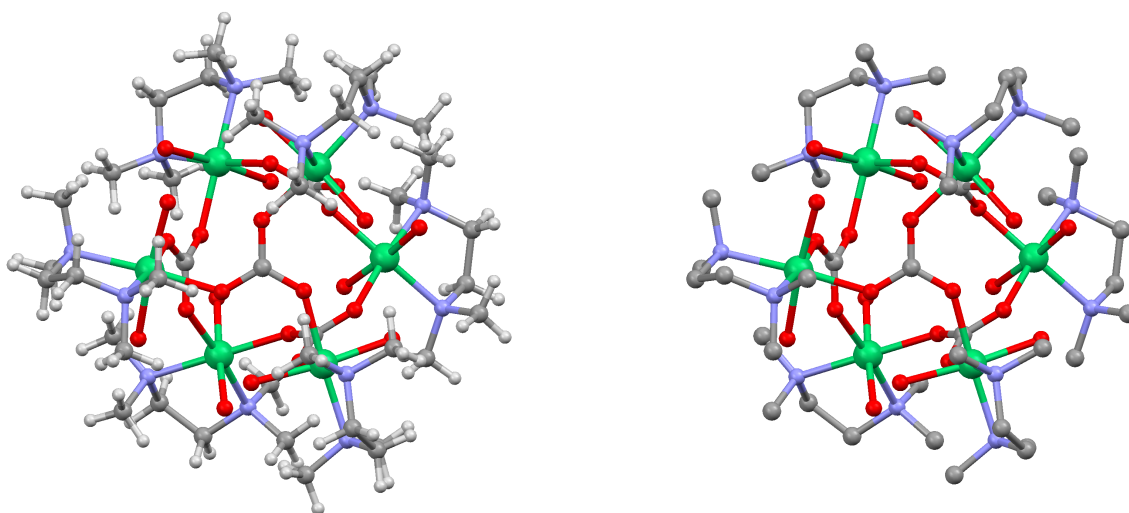


Figure S1. Two views of the hexanuclear cation with and without H atoms.

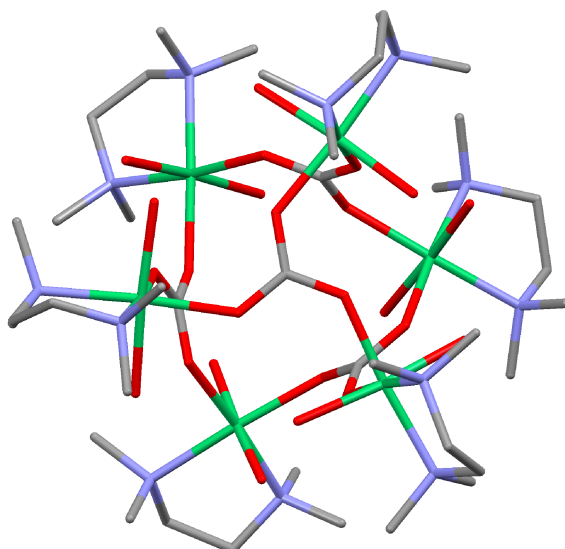


Figure S2. A view of the cation along the crystallographic three-fold axis. This axis passes through the carbon atom at the centre of the picture.

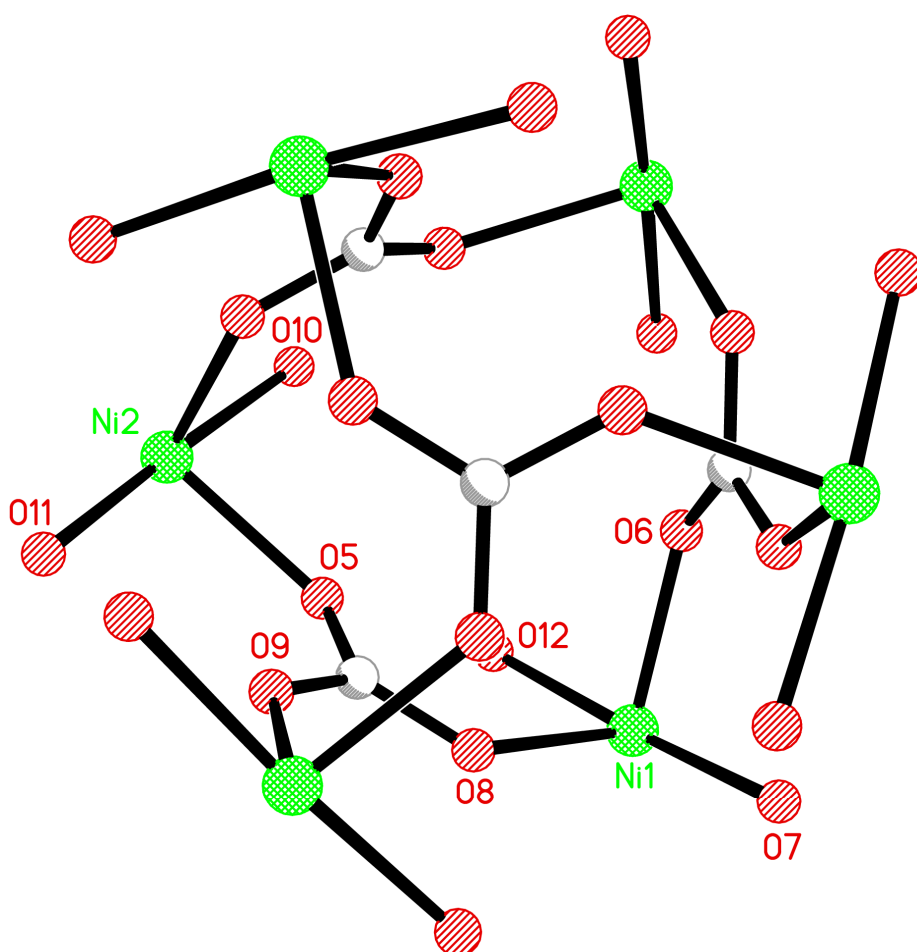


Figure S3. A view of the complex cation showing only the metal centres, carbonate anions and water oxygen atoms.

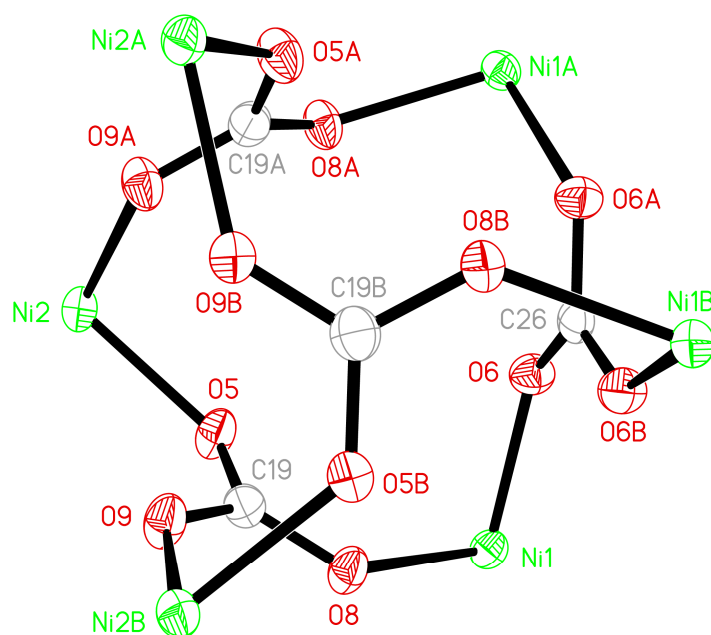


Figure S4. A view showing the μ_3 -carbonato ligands linking the Ni(II) centres. All other ligands, chloride anions and solvent molecules are omitted for clarity.

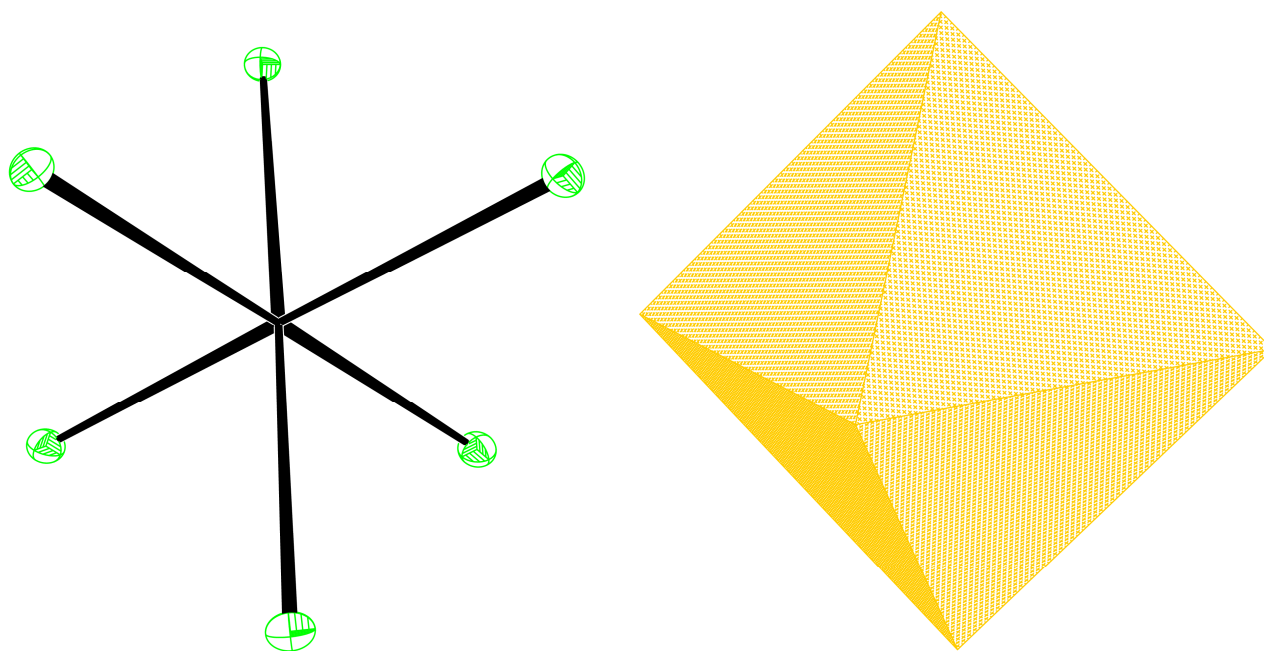


Figure S5. Two views of the octahedron defined by the six vertex Ni(II) cations. The centroid visible on the left-hand view represents a calculated position and does not coincide with any atom.