

A family of [Ni₈] cages templated by μ_6 -peroxide from dioxygen activation

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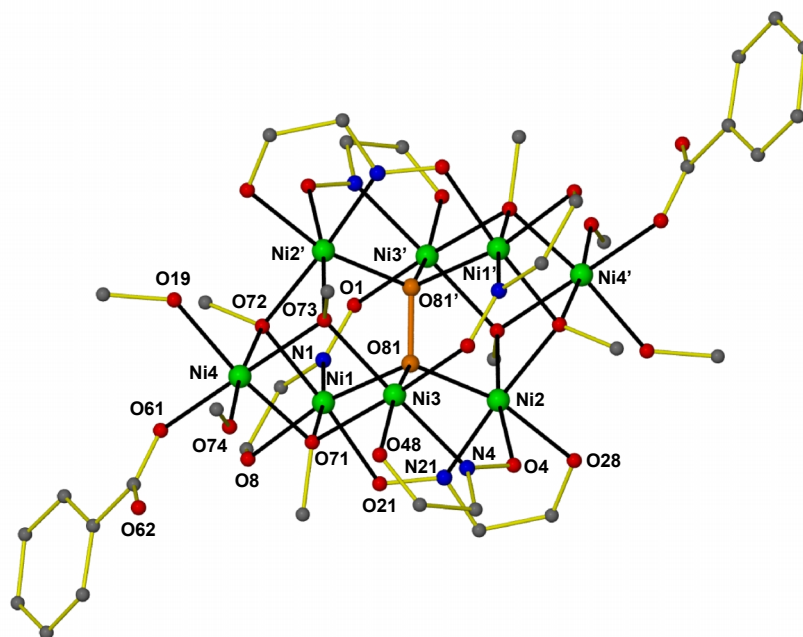


Fig. S1. The structure of $[\text{Ni}_8(\text{O}_2)(\text{abmo})_6(\text{PhCO}_2)_2(\text{MeO})_6(\text{MeOH})_4]$ **2**. All hydrogen atoms and most carbon atoms have been omitted for clarity. Color code: Ni green, C grey, N blue, O red. The $\eta^3:\eta^3:\mu_6\text{-O}_2^{2-}$ has been highlighted in orange. Symmetry code: (') 1-x, 1-y, 2-z.

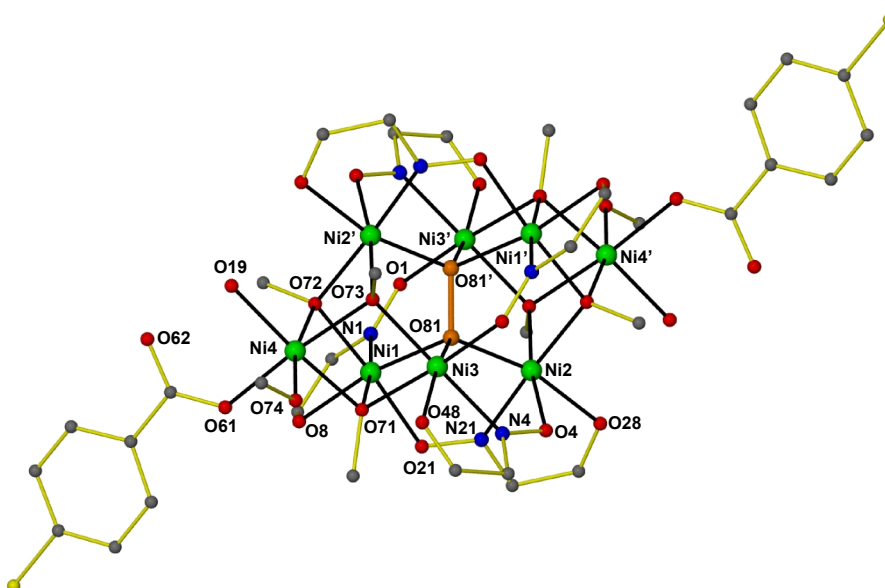


Fig. S2. The structure of $[\text{Ni}_8(\text{O}_2)(\text{abmo})_6(4\text{ClPhCO}_2)_2(\text{MeO})_6(\text{MeOH})_2(\text{H}_2\text{O})_2]$ **3**. All hydrogen atoms and most carbon atoms have been omitted for clarity. Color code: Ni green, C grey, N blue, O red, Cl yellow. The $\eta^3:\eta^3:\mu_6\text{-O}_2^{2-}$ has been highlighted in orange. Symmetry code: (') -x, 1-y, 1-z.

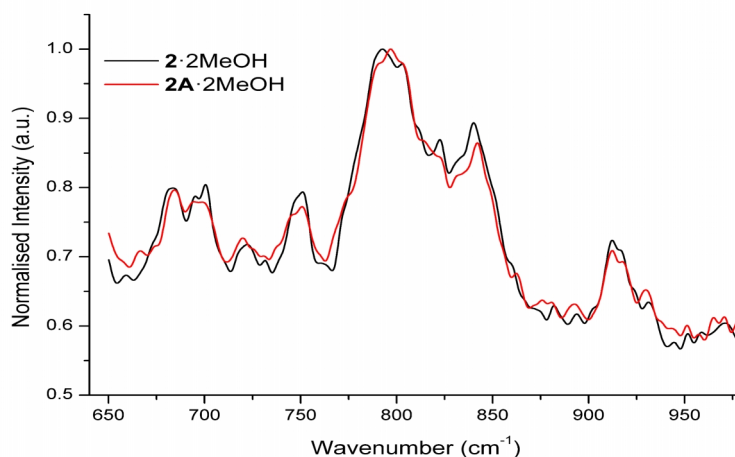


Fig. S3. Overlaid normalized Raman spectra of $[\text{Ni}_8(\text{O}_2)(\text{abmo})_6(\text{PhCO}_2)_2(\text{MeO})_6(\text{MeOH})_4] \cdot 2\text{MeOH}$ ($2 \cdot 2\text{MeOH}$) and $[\text{Ni}_8(^{18}\text{O}_2)(\text{abmo})_6(\text{PhCO}_2)_2(\text{MeO})_6(\text{MeOH})_4] \cdot 2\text{MeOH}$ ($2\text{A} \cdot 2\text{MeOH}$) collected using the WorkStationTM (Kaiser Optical Systems Inc.) Raman spectrometer.

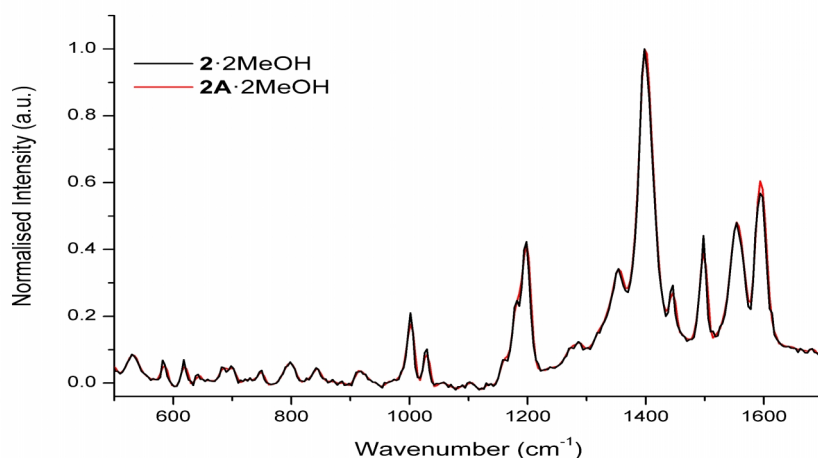


Fig. S4. Overlaid normalized Raman spectra of $[\text{Ni}_8(\text{O}_2)(\text{abmo})_6(\text{PhCO}_2)_2(\text{MeO})_6(\text{MeOH})_4] \cdot 2\text{MeOH}$ ($2 \cdot 2\text{MeOH}$) and $[\text{Ni}_8(^{18}\text{O}_2)(\text{abmo})_6(\text{PhCO}_2)_2(\text{MeO})_6(\text{MeOH})_4] \cdot 2\text{MeOH}$ ($2\text{A} \cdot 2\text{MeOH}$) collected using the RamanStation spectrometer (AVALON Instruments).