Electronic Supplementary Information for Dalton Transactions

Supporting information for

A deliberate approach for the syntheses of heterometallic supramolecules containing dimolybdenum Mo_2^{4+} species coordinated to other metal units

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Preparation of $\{[cis\text{-}Mo_2(DAniF)_2(O_2CC_5H_4N)_2][Ni(C_5H_7O_2)_2]\}_n$

A solution prepared by dissolving the dimolybdenum building block *cis*-$Mo_2(DAniF)_2(O_2CC_5H_4N)_2$ **(2)** (0.095 g, 0.100 mmol) in 20 mL of THF was transferred, with stirring, into a flask that contained $Ni(acac)_2$ (0.026 g, 0.100 mmol), giving a bright red solution. This solution was stirred for 1 h, and then the solvent was removed under reduced pressure, leaving a red solid, which was washed with ethanol (ca. 15 mL) and hexanes (ca. 15 mL). After adding dichloromethane (5 mL) and tetrahydrofuran (15 mL) to the solid, the mixture was filtered through a Celite-packed frit. The filtrate was carefully layered first with 5 mL of toluene and then with 25 mL of hexanes. Red block-shaped crystals were obtained after one week of diffusion.

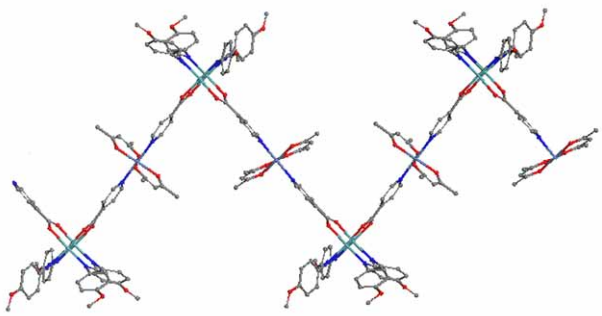

Fig. S1 Structure of $\{[cis\text{-}Mo_2(DAniF)_2(O_2CC_5H_4N)_2][Ni(acac)_2]\}_n$ showing the zig-zag chain. Crystallographic data: space group = $P\bar{1}$, a =14.321(16), b = 14.331(16), c = 18.22(2) Å, α = 92.88(2), β = 110.84(2), γ = 97.32(2) (deg), V = 3447(7) Å^3.