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Supporting information

Origin of the Relaxation Barriers in a Family of $MRe^{IV}(CN)_2$ Single-Chain Magnets (M = Mn^{II}, Ni^{II}, Co^{II}): A Theoretical Investigation

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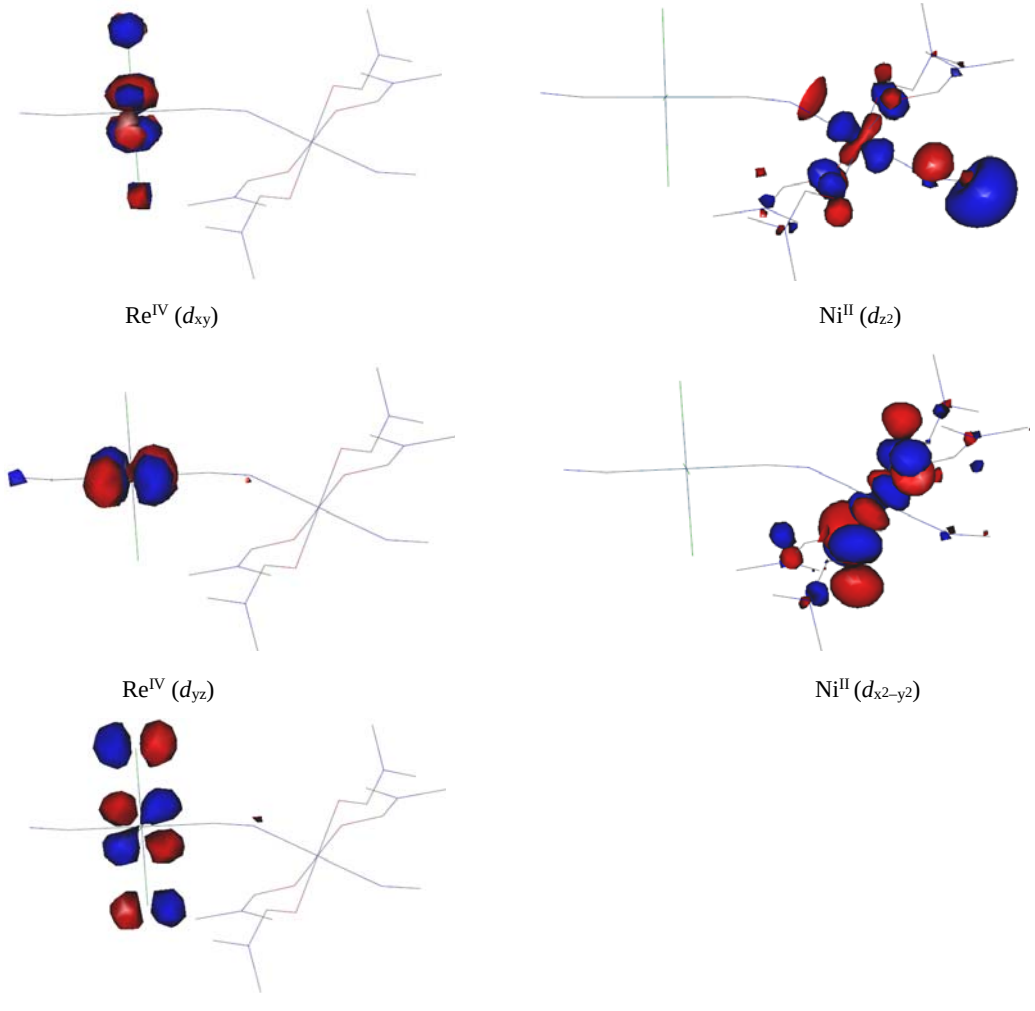
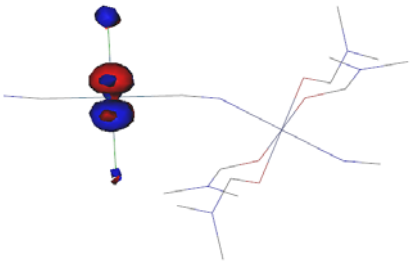
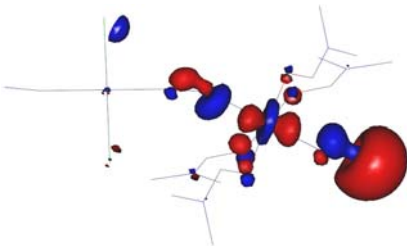


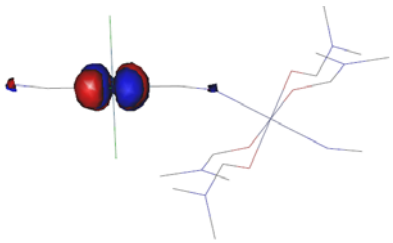
Figure S1. Magnetic orbitals on the Re^{IV} (left) and Ni^{II} (right) of **2** in the low-spin state.



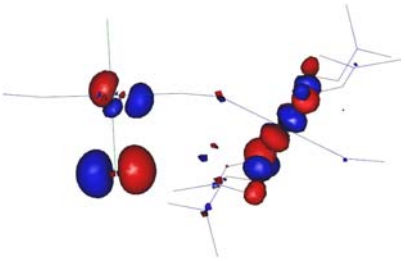
Re^{IV} (d_{xy})



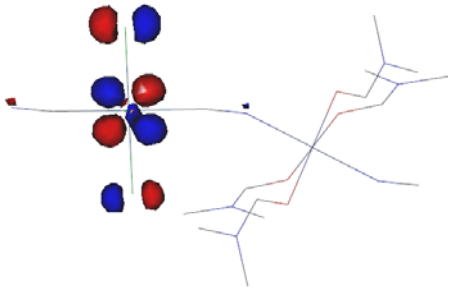
Co^{II} (d_{z2})



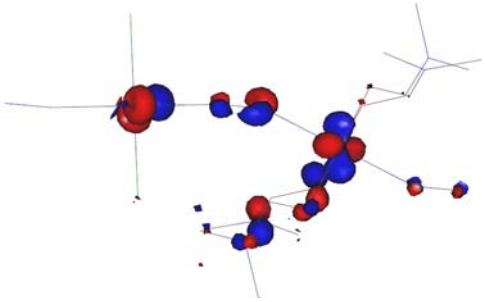
Re^{IV} (d_{yz})



Co^{II} ($d_{x2–y2}$)



Re^{IV} (d_{zx})



Co^{II} (d_{zx})

Figure S2. Magnetic orbitals on the Re^{IV} (left) and Co^{II} (right) of **3** in the low-spin state.