Supporting information

Origin of the Relaxation Barriers in a Family of MRe\textsuperscript{IV}(CN)\textsubscript{2} Single-Chain Magnets (M = Mn\textsuperscript{II}, Ni\textsuperscript{II}, Co\textsuperscript{II}): A Theoretical Investigation

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Figure S1. Magnetic orbitals on the Re\textsuperscript{IV} (left) and Ni\textsuperscript{II} (right) of 2 in the low-spin state.
Figure S2. Magnetic orbitals on the ReIV (left) and CoII (right) of 3 in the low-spin state.