

Supporting Information

Magnetic anisotropy in Ni^{II}-Y^{III} binuclear complexes: on the importance of both the first coordination sphere of the Ni^{II} ion and of the Y^{III} ion belonging to the second coordination sphere

Rémi Maurice,^{a,b,*} Laure Vendier^{c,d} and Jean-Pierre Costes^{c,d,*}

^a Laboratoire de Chimie et de Physique Quantique ; IRSAMC/UMR5626 ; Université de Toulouse III ; 118 route de Narbonne, F-31062 Toulouse Cedex 4, France

^b Departament de Química Física i Inorganica ; Universitat Rovira i Virgili ; Marcel·lí Domingo s/n, 43007 Tarragona, Spain

^c CNRS ; LCC (Laboratoire de Chimie de Coordination) ; 205, route de Narbonne, F-31077 Toulouse, France

^d Université de Toulouse ; UPS, INPT ; LCC ; F-31077 Toulouse, France

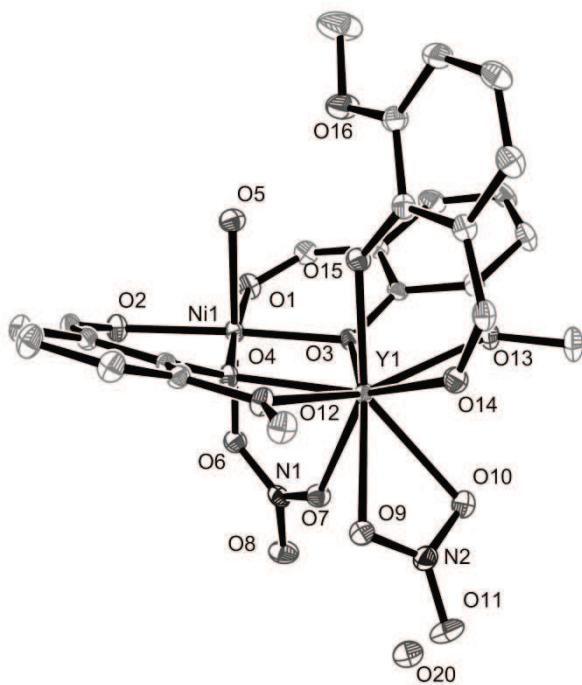


Figure S1. Plot of complex (2) with ellipsoids drawn at the 30 % probability level and with atom numbering. Hydrogen atoms have been omitted for clarity. Selected bond lengths [Å] and angles [°]: Ni O1 2.0209(14), Ni O2 2.0210(14), Ni O3 1.9919(13), Ni O4 2.0027(13), Ni O5 2.0433(15), Ni O6 2.0838(14), Y O3 2.2864(13), Y O4 2.2832(13), Y O7 2.5423(14), Y O9 2.4358(14), Y O10 2.4500(14), Y O12 2.6035(14), Y O13 2.5418(14), Y O14 2.3143(14), Y O15 2.2222(14), O3 Ni1 O4 84.61(5), O4 Y1 O3 72.09(5), Ni1 O3 Y1 101.76(5), Ni1 O4 Y1 101.53(5).

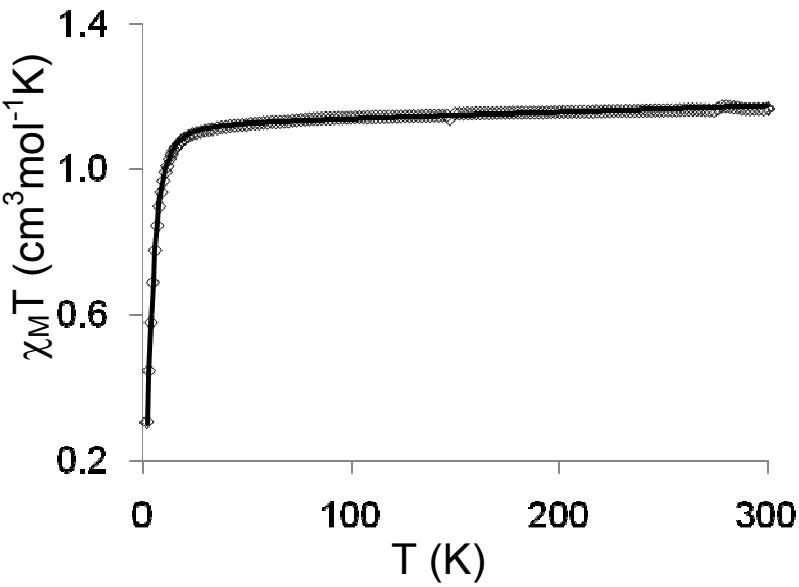


Figure S2. Temperature dependence of the $\chi_M T$ product for (1) from 300 to 2 K. The solid line corresponds to the best data fit ($D_{Ni} = 10.4 \text{ cm}^{-1}$, and $g = 2.12$).

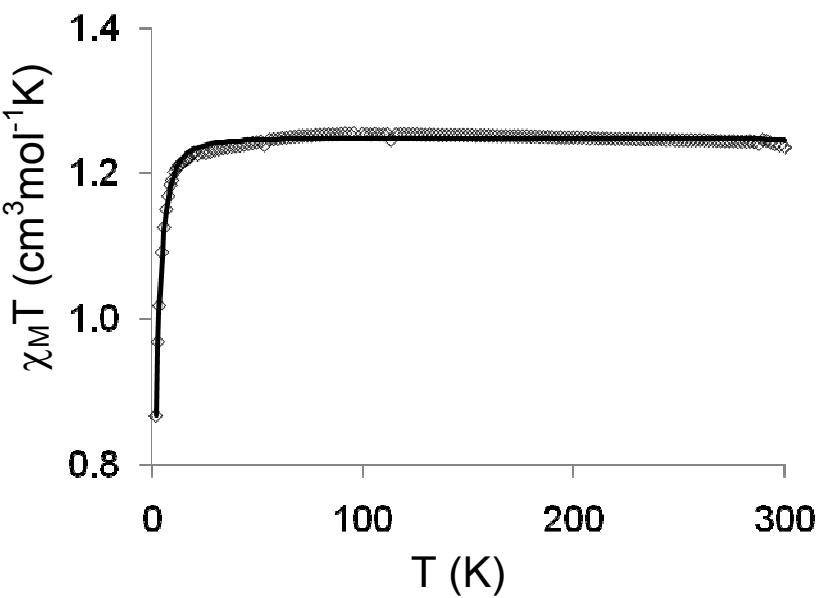


Figure S3. Temperature dependence of the $\chi_M T$ product for (2) from 300 to 2 K. The solid line corresponds to the best data fit ($D_{Ni} = -6.6 \text{ cm}^{-1}$, and $g = 2.23$).