Supporting Information

A rare example of nickel(II) chain based on an heteroscorpionate-like ligand with quadruple imidazolyl interactions

Carlos J. Gómez-García,[a]* Emilio Escrivà[b]*, Guillermo Mínguez Espallargas,[a] Juan José Borrás-Almenar,[b] Lucwía Soto,[b] Amparo Sancho,[b] Julia García-Lozano,[b] and Carmen Ramírez de Arellano[c]

[a] *Instituto de Ciencia Molecular (ICMol), Parque Científico, Universidad de Valencia, C/ Catedrático José Beltrán, 2, 46980 Paterna, Valencia, Spain.*

[b] *Departament de Química Inorgànica, Universitat de València, c/ Vicent Andrés Estellés, s/n and c/Dr. Moliner, 50, 46100 Burjassot (València) Spain.*

[c]*Departament de Química Orgànica, Universitat de València, c/ Vicent Andrés Estellés, s/n, 46100 Burjassot (València) Spain.*

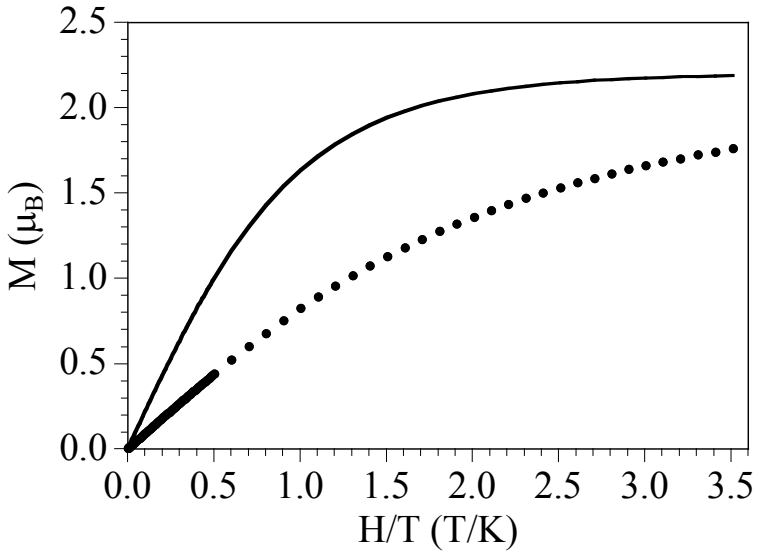

Figure S1. Isothermal magnetization for compound **1** at 2 K. Solid line shows the Brillouin function for a S = 1 ions with g = 2.2

X-Ray powder diffraction studies

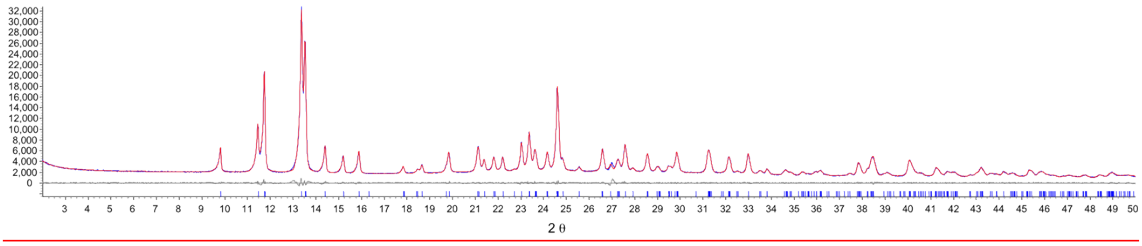

Figure S2. Observed (blue) and calculated (red) profiles and difference plot [(I_{obs} – I_{calcd})] (grey) of the Pawley refinements for compound **1** (2θ range 2.0–50.0 °)

Table S1. Crystallographic data for compound **1**.

Compound	**1**
Empirical formula	$C_{10}H_{18}N_4NiO_9$
Formula weight	396.99
Crystal colour	light blue
Crystal size (mm^3)	0.20 × 0.16 × 0.06
Temperature (K)	120(2)
Crystal system, Z	Triclinic, 4
Space group	$P2_1/n$
a (Å)	9.4748(3)
b (Å)	13.1587(3)
c (Å)	12.2363(4)
α □°□	90
β□ □°□	90.169(3)
γ □°□	90
V ($Å^3$)	1525.57(8)
ρ_{calc} (Mg/m^3)	1.728
$\mu(Mo_{K\alpha})$ (mm^{-1})	1.329
θ range (°)	3.13-32.05
Reflns collected	30625
Independent reflns	5060
(R_{int})	(0.0329)
Reflns used in refinement, n	5060
L. S. parameters, p/ restraints, r	265/21
$R1(F)$,[a] $I>2\sigma(I)$	0.0269
$wR2(F^2)$,[b] all data	0.0670
$S(F^2)$,[c] all data	1.055

[a] $R1(F) = \Sigma(|F_O| - |F_C|)/\Sigma|F_O|$;

[b] $\omega R2(F^2) = [\Sigma\omega(F_O^2 - F_C^2)^2/\Sigma\omega F_O^4]^{½}$;

[c] $\Sigma(F^2) = [\Sigma\omega(F_O^2 - F_C^2)^2/\square(n + r - p)]^{½}$

Table S2. Hydrogen bond parameters (in Å and º) in compound **1**

D-H···A	**D-H**	**H···A**	**D···A**	**<(DHA) (º)**
N11-H11...O8$^{\$1}$	0.88	1.98	2.8414(14)	166.2
N21-H21...O2	0.88	2.56	3.0666(14)	117.7
N21-H21...O7$^{\$2}$	0.88	2.22	2.8830(14)	131.9
O5-H51...O9$^{\$3}$	0.827(14)	2.311(17)	3.0493(15)	149(2)
O5-H52...O9$^{\$4}$	0.831(14)	1.998(14)	2.8276(15)	177(2)
O6-H61...O1$^{\$5}$	0.820(13)	1.791(13)	2.6067(13)	173(2)
O6-H62...O8$^{\$6}$	0.811(14)	1.963(14)	2.7713(14)	175(2)
O7-H71...O4	0.825(14)	1.788(14)	2.5862(14)	162(2)
O7-H72...O2$^{\$5}$	0.825(14)	1.948(14)	2.7675(13)	172(2)
O8-H81...O1	0.810(15)	1.874(15)	2.6806(13)	174(2)
O8-H82...O9$^{\$3}$	0.804(15)	2.052(15)	2.8528(15)	174(2)
O9-H92...O4	0.843(16)	1.850(17)	2.6765(15)	166(2)
O9-H91...O2$^{\$2}$	0.831(16)	2.020(16)	2.8326(14)	166(2)

$1 = -x+1/2, y-1/2, -z+1/2; $2 = -x+1, -y, -z+1; $3 = x-1/2, -y+1/2, z-1/2; $4 = -x+3/2, y+1/2, -z+3/2; $5 = x+1, y, z; $6 = -x+1, -y+1, -z+1.