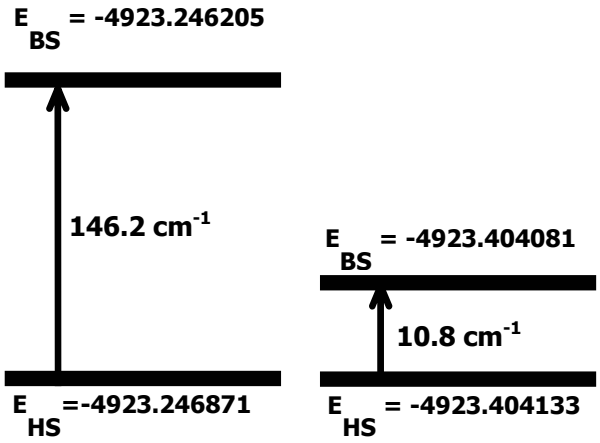
Supplementary Material (ESI) for Chemical Communications

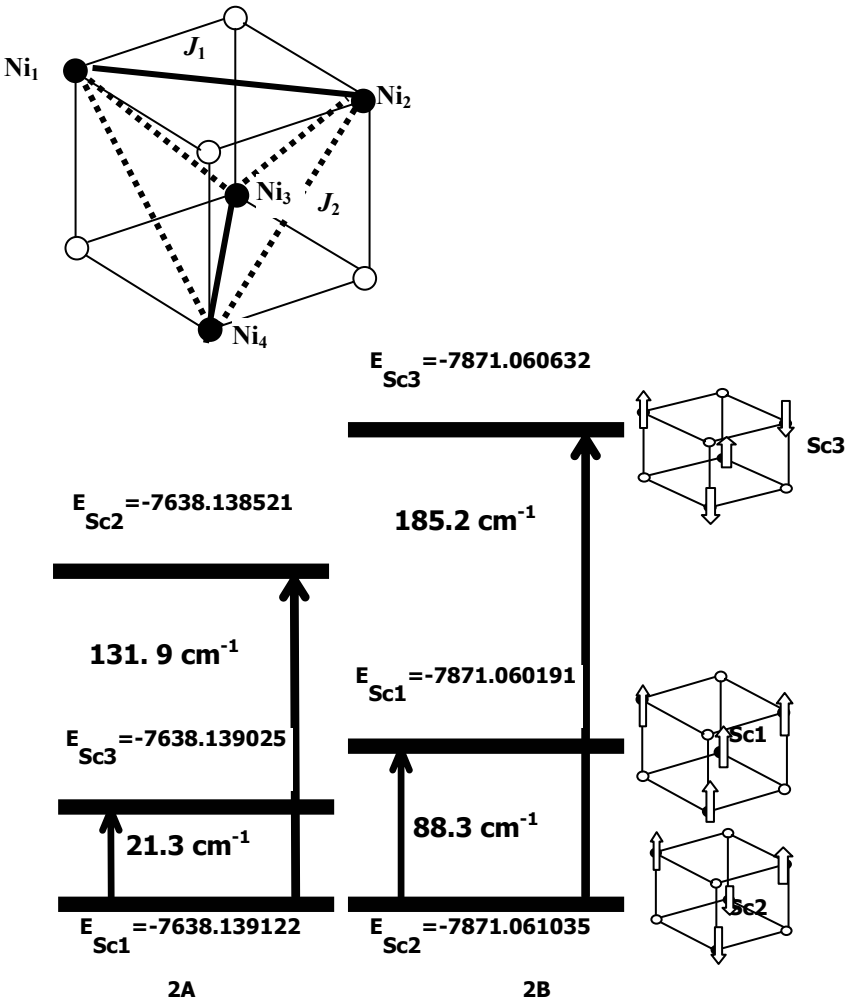
Electronic supplementary information:

Theoretical Studies on Di- and Tetra-nuclear Ni Pivalate Complexes

Gopalan Rajaraman,* Kirsten E. Christensen, Finn K. Larsen, Grigore A. Timco and R. E. P. Winpenny *



ESI-Figure 1. The absolute energies of the high spin and broken symmetry state (in Hartree) of 1A and 1B and the energy difference between the states (in cm^{-1}) are shown in ESI-Figure 1. The chosen spin configurations and their relative energy to calculate the *J*-values for 2 is given ESI-Figure 2.



ESI-Figure 2. The two exchange interaction J_1 and J_2 in **2**. The absolute energies of the chosen spin configuration (in Hartree) and the relative energies (in cm^{-1}) of the spin configurations of **2A** and **2B**.

The equations used to calculate the *J*-values is given in as follows,

$$\frac{\left(E_{Sc_1} - E_{Sc_2}\right)}{2S_1S_2 + S_2} = -2J_1 - 2J_2$$

$$\frac{\left(E_{Sc_1} - E_{Sc_3}\right)}{2S_1S_2 + S_2} = -4J_2$$

Where S_1 and S_2 are the spin on the metal centre.

The XYZ coordinates of the optimised structure of 2B is as follows,

Ni	10.28200	1.57300	6.70700
Ni	10.47700	1.50600	3.80700
Ni	8.09100	2.95500	5.24000
Ni	8.01800	0.17000	5.07300
O	10.07500	2.93100	5.21500
C	10.88500	4.13400	5.20400
H	11.71300	4.01400	4.48400
H	11.29300	4.32700	6.21300
H	10.27200	5.00300	4.89500
O	10.01500	0.09000	5.25300
C	10.78900	-1.13100	5.21700
H	10.30100	-1.88100	4.56200
H	10.90500	-1.55400	6.23700
H	11.79400	-0.93200	4.80500
O	8.21700	1.46100	6.57100
C	7.35400	1.34700	7.71700
H	7.46300	2.23500	8.36300
H	7.63300	0.45600	8.30900
H	6.29600	1.26200	7.41000
O	8.39100	1.61900	3.73200
C	7.75800	1.70700	2.43400
H	6.66200	1.82200	2.52500
H	7.97900	0.79500	1.84800
H	8.17200	2.57300	1.88500
O	8.17300	4.32600	6.72100
H	8.88100	4.03000	7.39000
C	7.14100	5.17900	7.27200
H	7.56200	6.16100	7.55500
H	6.66300	4.71400	8.15600
H	6.37700	5.31700	6.49100
O	7.76700	-1.54100	6.12300
H	8.53800	-1.82700	6.65800
C	6.51800	-2.22400	6.45900
H	6.28100	-2.09100	7.53000
H	6.59400	-3.29900	6.21400
H	5.74500	-1.74100	5.84500
O	10.00900	3.10400	8.22400
O	10.31500	0.96400	8.77500
C	10.16100	2.18500	9.14700
C	10.23400	2.56800	10.59900
O	12.26500	1.61300	6.59300
O	12.44500	1.45200	4.32100
C	12.95500	1.54500	5.49900
C	14.46200	1.60600	5.62700
O	10.86300	2.57300	2.02000
O	10.76000	0.34800	2.07100
C	10.98800	1.43900	1.40400
C	11.43500	1.38100	-0.03100
O	6.09900	2.75600	5.08100
O	6.04300	0.47600	4.86900
C	5.47400	1.64300	4.88500
C	3.98100	1.69100	4.65800
H	14.76800	2.64900	5.83800
H	14.79800	0.98800	6.47800
H	14.94300	1.27700	4.69300
H	9.78500	3.56000	10.76900
H	9.73800	1.80500	11.22300
H	11.29600	2.61000	10.91000
H	11.27400	2.35200	-0.52700
H	12.51600	1.14300	-0.06900
H	10.90100	0.57800	-0.56800
H	3.61600	2.72900	4.68000
H	3.73700	1.22900	3.68300
H	3.46200	1.09600	5.43400