

## Poster Presentation

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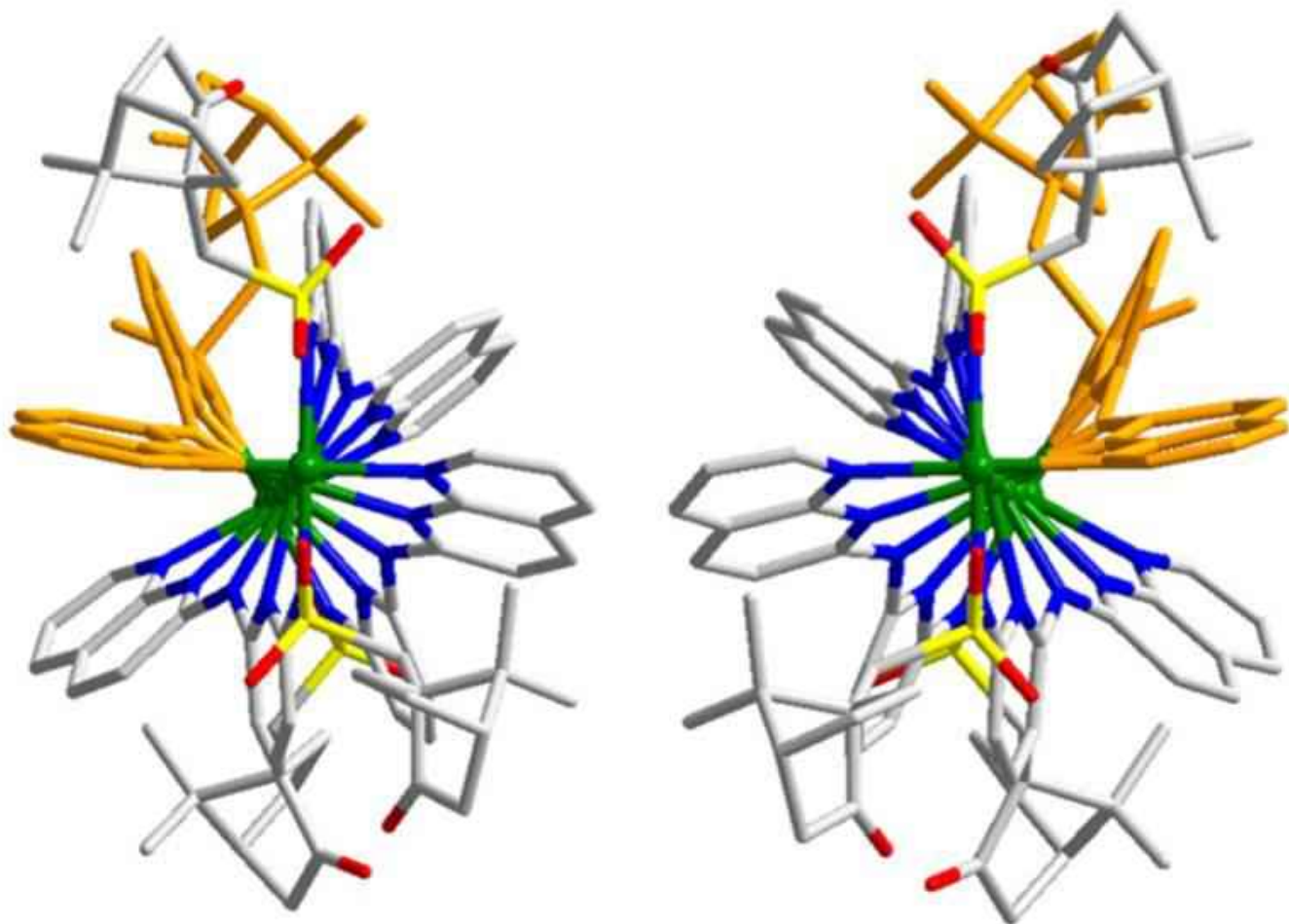
### Chirality control of the Quadruple helixes of the metal strings

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Novel chiral pentadentate ligands with naphthyridine and camphorsulfonyl groups have been designed and used to control the chirality of quadruple helices of metal strings directly:  $\Delta$ -Ni<sub>5</sub>(-)-camnpda)<sub>4</sub> (1) and  $\Lambda$ -Ni<sub>5</sub>(+)-camnpda)<sub>4</sub> (2). Compound 1 is a  $\Delta$  form metal string complex with H<sub>2</sub>(-)-camnpda and 2 is  $\Lambda$  form one with H<sub>2</sub>(+)-camnpda. By X-ray single-crystal diffraction, The structures of the compound 1 and 2 are both 2,2-trans form in the same monoclinic space group C<sub>2</sub> and have the similar unit cell. Further, it demonstrates that two metal strings are chiral isomers each other by CD spectra. In theoretical computation, the local minimum ( $\Lambda$ -Ni<sub>5</sub>(+)-camnpda)<sub>4</sub> with the  $\Delta$  form) becomes energetically unfavourable by about 100 kcal/mol due to the strong steric repulsion introduced by the camphor groups. Finally, the racemic crystal is obtained with a 1:1 mixture of compounds 1 and 2 in triclinic space group P-1. Both the external dinickel distance in 1 and 2, about 2.280 Å, and the SQUID experiment reveal mixed valence [Ni<sub>2</sub>]<sup>3+</sup> characters and the magnetic behaviors are anti-ferromagnetic ( $J = -55.0$  cm<sup>-1</sup> for 1 and  $-63.3$  cm<sup>-1</sup> for 2). In the electrochemistry, the three reversible oxidation waves in 1 and 2 are  $-0.13$ ,  $0.20$  and  $0.97$  V.

[1] B. R. Groves, D. I. Arbuckle, E. Essoun, T. L. Lundrigan, R. Wang, M. A. S. Aquino, *Inorg. Chem.* 2013, 52, 11563-11572, [2] C.-W. Yeh, I. P.-C. Liu, R.-R. Wang, C.-Y. Yeh, G.-H. Lee, S.-M. Peng, *Eur. J. Inorg. Chem.* 2010, 2010, 3153-3159., [3] I. P.-C. Liu, M. Bénard, H. Hasanov, I. W. P. Chen, W.-H. Tseng, M.-D. Fu, M.-M. Rohmer, C.-h. Chen, G.-H. Lee, S.-M. Peng, *Chem. Eur. J.* 2007, 13, 8667-8677.



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