Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2014



Fig. S1 Molecular structure of an hexanuclear $[Fe_6(\mu-L_1)_6(\mu-O)_3(NCS)_6]^{6+}$ complex of $[Fe_6(\mu-L_1)_6(\mu-O)_3(NCS)_6](NO_3)_6(CH_3OH)_3(H_2O)$ (4) (iron (brown), sulfur (yellow), oxygen (red), nitrogen (blue), carbon (black)). The complex is generated from half of the molecule, which is crystallographically independent, through a 2-fold axis.



Fig. S2 Molecular structure of an hexanuclear $[Fe_6(\mu-L_2)_6(\mu-O)_3(NCS)_6]^{6+}$ complex with a $[FeF_6]^-$ anion close to the center of the ring of $[Fe_6(\mu-L_2)_6(\mu-O)_3(NCS)_6](FeF_6)_{0.5}(NCS)_{4.5}(CH_3OH)_2_(solvate)$ (**5**) (iron (brown), sulfur (yellow), oxygen (red), nitrogen (blue), carbon (black), fluoride (green)). The FeF₆³⁻ complex is generated from half of the molecule, which is crystallographically independent, through a 2-fold axis linking F3, F4 and Fe7 atoms.



Fig. S3 Powder X-ray diffraction patterns (blue) and simulated patterns (red) of 2 (top) and 3 (bottom).



Fig. S4 ES-MS of 2 in methanol.



Fig. S5 ES-MS of 2 in methanol (isotopic resolution of the most intense peaks).