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Hydrogen bonding interactions of tris, bis urea and thioureas with cyanide ligand in an analogue of the sub-site of [FeFe]-hydrogenase

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Second coordination sphere interactions of metal centers involving hydrogen bonding, ion-pairing or dipolar bonding can play a significant role in determining the physical and chemical properties of molecular and biomolecular systems. The second coordination sphere interactions of coordinated cyanide in a model for the diiron subsite of [FeFe]-hydrogenase has been examined. The natural subsite in its protein environment catalyzes hydrogen evolution (or uptake) at very fast rates ca 10^4 s⁻¹ near the reversible potential of the H⁺ / 1/2 H₂ couple but such rates have yet to be attained in model systems. Controlling the electronic and geometric properties of synthetic diiron subsites by hydrogen bonding or other interactions might provide a means of attaining the turnover rates of the natural system. The specific approach taken in this work was to explore the potential binding properties of certain bis- and tris-(thio) ureas to the synthetic subsite analogue [Fe²(CO)₄(CN)₂pdt]²⁻. It is shown that hydrogen bonding interactions with the ligated cyanide using certain activated amides also perturbs spectroscopic and redox properties and importantly, the rate of protonation at the metal-metal bond and the stability of the resulting μ -hydride.

Biography

Faizah S Aljohani has completed her PhD from University of East Anglia. She is working under the supervision of Professor Chris Pickett. She has published two papers and three papers, now, she works as Assistant Professor of Inorganic Chemistry at Taibah University in Saudi Arabia.

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