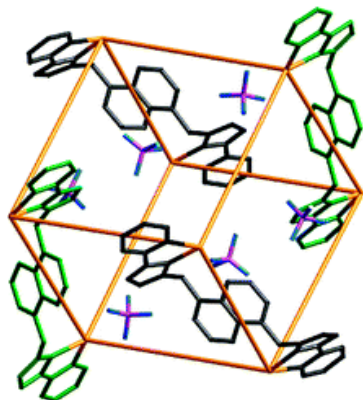
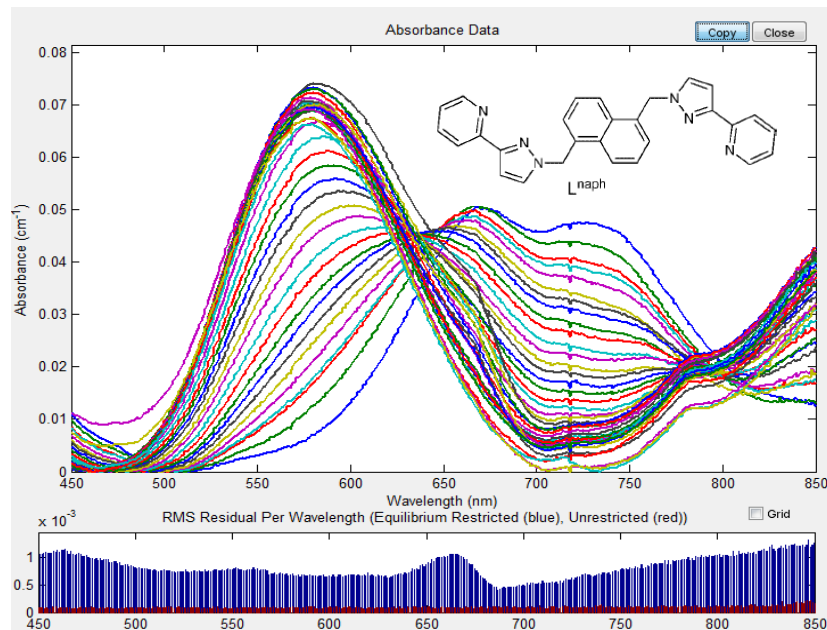


Equilibrium Studies of Self-Assembly Events



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I.S. Tidmarsh,
T.B. Faust,
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J. Am. Chem. Soc.
2008, 130,
15167-15173.

Twelve ligand molecules and eight nickel dications can form a cubic nanocage (bottom left). But what happens as nickel(II) is slowly added to the ligand solution? From spectroscopic 'snapshots' taken throughout the process (left), we have modeled and identified at least 12 additional partial structures (green boxes below). Initial mass spec evidences all of these species and more (green and yellow boxes below; X marks unambiguous identification in mass spec data).

And all this without chemically isolating anything!

		Ligand											
	0	1	2	3	4	5	6	7	8	9	10	11	12
Nickel	1			X									
	2			X									
	3			X	X				X	X			
	4							X		X			
	5						X		X	X		X	X
	6							X	X	X		X	X
	7								X	X	X	X	X
	8									X		X	X