Supporting Information for

Electronic structure and solution behavior of a tris(*N,N'*-diphenylhydrazido)manganese(IV) propeller complex.

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Contents

Determination of multinuclear cluster equilibrium.

Dimerization and tetramerization were considered as the causes of speciation to S = 0 species in solution. Assuming no magnetic moment for the multinuclear species, the concentration of monomer is calculated from Equation (7) in the main text.

$$[\mathbf{1}] = \frac{[\mathbf{1}]_0(\mu_{calc})^2}{(3.87)^2} \qquad (7)$$

With the concentration of **1** determined from Equation 7, the concentration of the cluster species may be determined from mass balance. For instance, for the formation of dimers:

$$[\mathbf{1}]_0 = [\mathbf{1}] + 2[\mathbf{1}_2] \qquad (8)$$

or

$$[\mathbf{1}_2] = ([\mathbf{1}]_0 - [\mathbf{1}])/2 \qquad (9)$$

Or, for the formation of tetramers,

$$[\mathbf{1}]_0 = [\mathbf{1}] + 4[\mathbf{1}_4] \qquad (S1)$$

or

$$[\mathbf{1}_4] = ([\mathbf{1}]_0 - [\mathbf{1}])/4 \qquad (S2)$$

The equilibrium constant for these two hypothetical situations is determined by plotting, for dimers:

$$[\mathbf{1}]^2 = K_{dim}[\mathbf{1}_2] \qquad (10)$$

and for monomers:

$$[\mathbf{1}]^4 = K_{dim}[\mathbf{1}_4] \qquad (10)$$

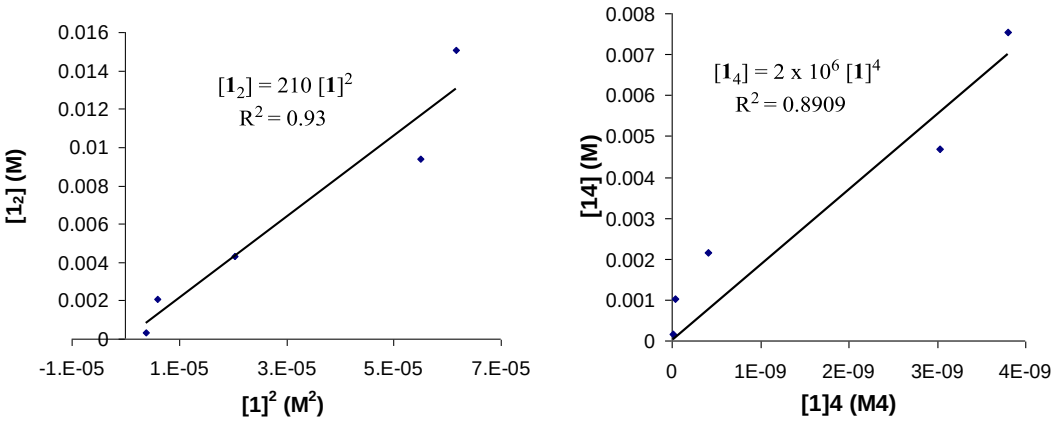

Figure S1. Plots of concentration of multinuclear complexes vs. [**1**] for the determination of K_{dim} and $K_{tet.}$ (slope of the plot). Dimer formation plot gives the superior fit.

IR spectroscopy

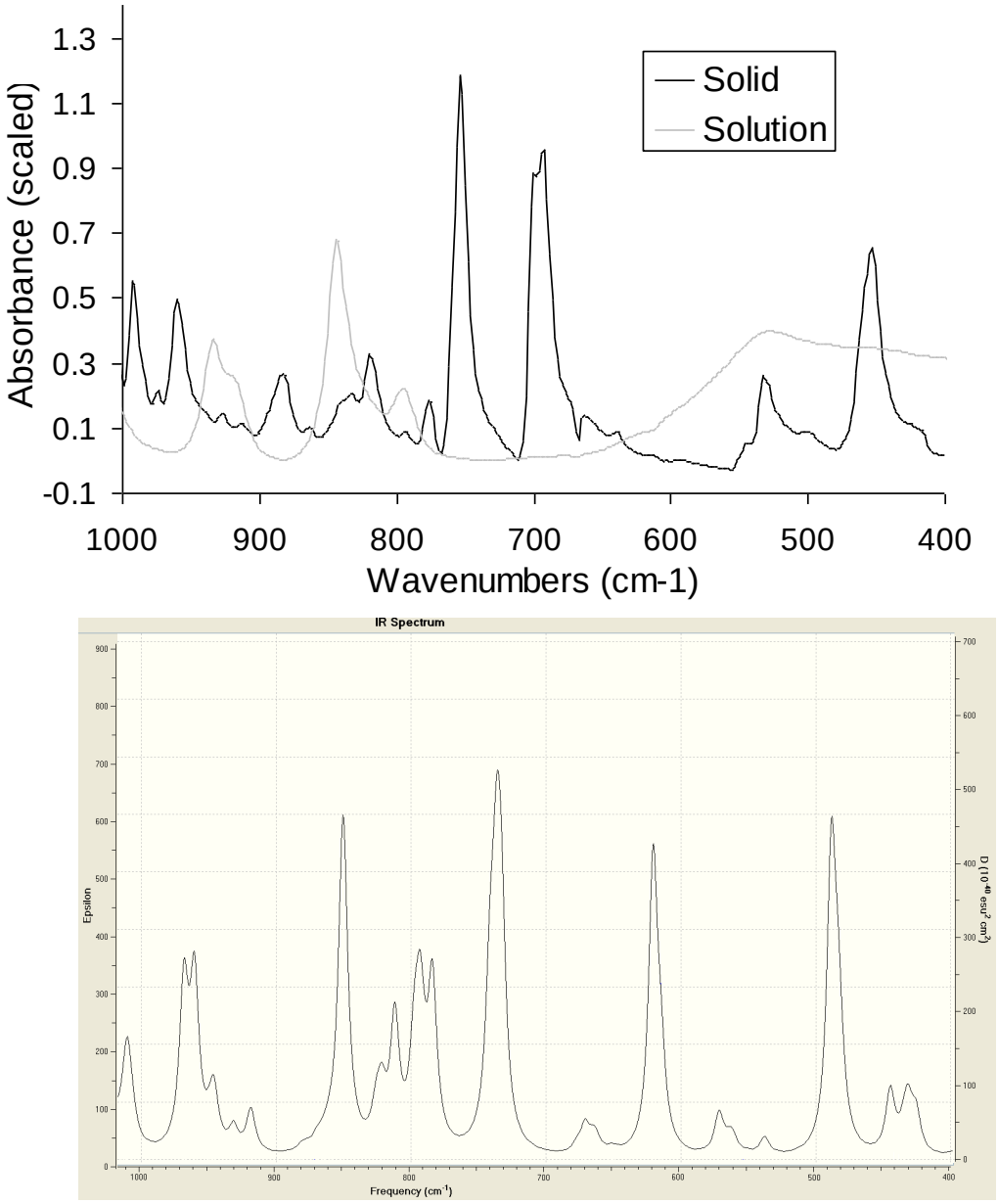

Figure S2. Infrared spectrum from experiment (solid and in diethyl ether) and calculated IR spectrum from Density Functional Theory using the B3LYP functional and 3-21G basis set.