This journal is © The Royal Society of Chemistry 2005

Table SF1: Intermolecular contacts in 3

Number	Atom1	Atom2	Symm.op.1	Symm.op.2	Length	Length-VdW
1	N9	O16	x,y,z	x,y,z 2.568		-0.502
2	N19	O26	x,y,z	x,y,z 2.579	-0.491	
3	O1W	O26	x,y,z	-x,-y,-z 2.802	-0.238	
4	O26	O1W	x,y,z -x,-y,-z	2.802		-0.238
5	O1W	O16	x,y,z	-x,-y,1-z 2.654	-0.386	
6	O16	O1W	x,y,z	-x,-y,1-z 2.654	-0.386	
7	O2W	O26	x,y,z	1-x,-y,-z 2.721		-0.319
8	O26	O2W	x,y,z	1-x,-y,-z 2.721		-0.319
9	O2W	O16	x,y,z	1-x,-y,1-z	2.752	-0.288
10	O16	O2W	x,y,z	1-x,-y,1-z	2.752	-0.288
11	N9	O16	1-x,-y,-z	1-x,-y,-z 2.568	-0.502	
12	N19	O26	1-x,-y,-z	1-x,-y,-z	2.579	-0.491
13	N9	O16	1-x,-y,1-z	1-x,-y,1-z	2.568	-0.502
14	N19	O26	1-x,-y,1-z	1-x,-y,1-z	2.579	-0.491
15	N9	O16	-x,-y,-z	-x,-y,-z	2.568	-0.502
16	N19	O26	-x,-y,-z	-x,-y,-z	2.579	-0.491
17	N9	O16	-x,-y,1-z	-x,-y,1-z	2.568	-0.502
18	N19	O26	-x,-y,1-z	-x,-y,1-z	2.579	-0.491
19	H1WB	O26	x,y,z	-x,-y,-z	1.974	-0.746
20	H1WB	C26	x,y,z	-x,-y,-z 2.620		-0.280
21	O26	H1WB	x,y,z	-x,-y,-z 1.974		-0.746
22	C26	H1WB	x,y,z	-x,-y,-z 2.620		-0.280
23	H1WA	O16	x,y,z	-x,-y,1-z	1.816	-0.904
24	H1WA	C16	x,y,z	-x,-y,1-z	2.769	-0.131
25	C6	C15	x,y,z -x,-y,1-z	3.353	-0.047	
26	C7	C15	x,y,z	-x,-y,1-z	3.340	-0.060
27	H7AC	C16	x,y,z	-x,-y,1-z	2.866	-0.034
28	C15	C6	x,y,z	-x,-y,1-z	3.353	-0.047
29	C15	C7	x,y,z	-x,-y,1-z	3.340	-0.060
30	O16	H1WA	x,y,z	-x,-y,1-z	1.816	-0.904
31	C16	H1WA	x,y,z	-x,-y,1-z	2.769	-0.131
32	C16	H7AC	x,y,z	-x,-y,1-z	2.866	-0.034
33	H2WA	O26	x,y,z	1-x,-y,-z	1.883	-0.837
34	H2WA	C26	x,y,z	1-x,-y,-z	2.715	-0.185
35	C2	C25	x,y,z	1-x,-y,-z	3.381	-0.019
36	C25	C2	x,y,z	1-x,-y,-z	3.381	-0.019
37	O26	H2WA	x,y,z	1-x,-y,-z	1.883	-0.837
38	C26	H2WA	x,y,z 1-x,-y,-z	2.715	-0.185	
39	H2WB	O16	x,y,z	1-x,-y,1-z	1.914	-0.806
40	H2WB	C16	x,y,z	1-x,-y,1-z	2.887	-0.013
41	H7AA	C10	x,y,z	1-x,-y,1-z	2.839	-0.061
42	C10	H7AA	x,y,z	1-x,-y,1-z	2.839	-0.061
43	O16	H2WB	x,y,z	1-x,-y,1-z	1.914	-0.806
44	C16	H2WB	x,y,z 1-x,-y,1-z	2.887	-0.013	
45	C25	H15A	1-x,-y,-z	1-x,-y,1-z	2.774	-0.126
46	H25A	C15	1-x,-y,-z	1-x,-y,1-z	2.727	-0.173
47	H25A	H15A	1-x,-y,-z	1-x,-y,1-z	2.184	-0.216
48	H2WA	H1WB	1-x,-y,-z	-x,-y,-z	2.334	-0.066
49	H2WB	H1WA	1-x,-y,-z	-x,-y,-z	2.246	-0.154
50	H2WA	H1WB	1-x,-y,1-z	-x,-y,1-z	2.334	-0.066
51	H2WB	H1WA	1-x,-y,1-z	-x,-y,1-z	2.246	-0.154
52	C25	H15A	-x,-y,-z	-x,-y,1-z	2.774	-0.126
53	H25A	C15	-x,-y,-z	-x,-y,1-z	2.727	-0.173
54	H25A	H15A	-x,-y,-z	-x,-y,1-z	2.184	-0.216

Fig. SF1: Fourier difference map for [Mn.dapS_2.2H_2O] (3). DMF

This journal is © The Royal Society of Chemistry 2005

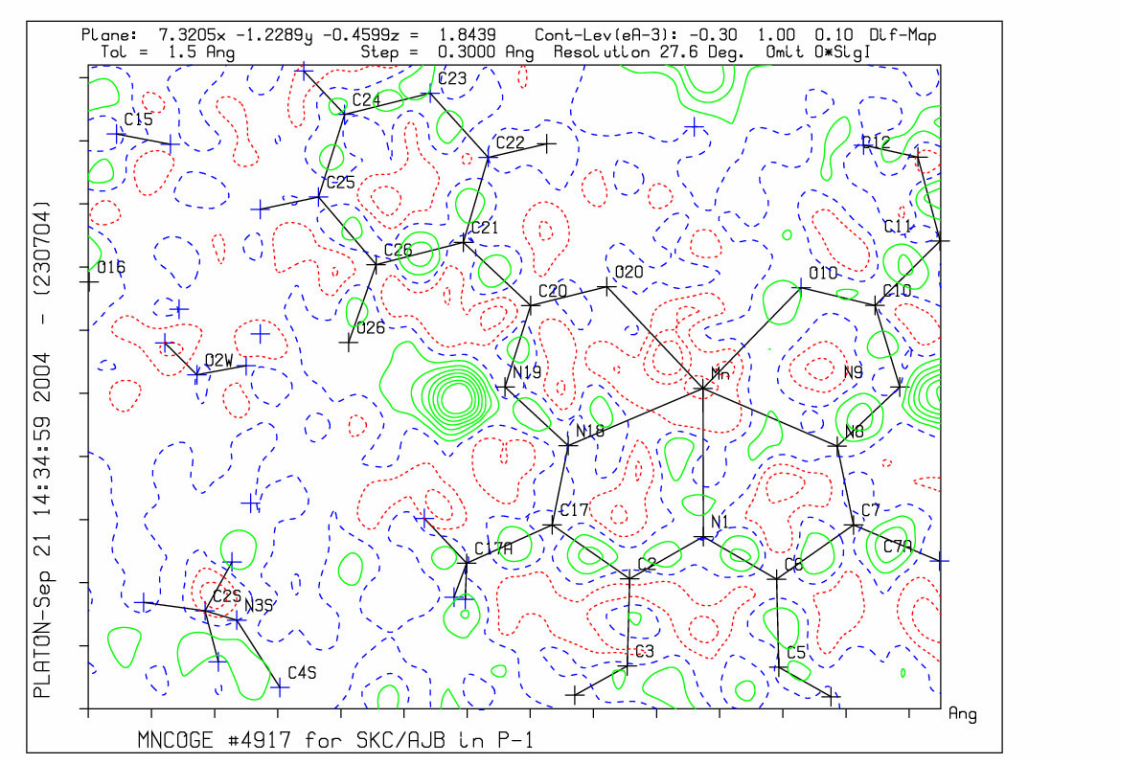
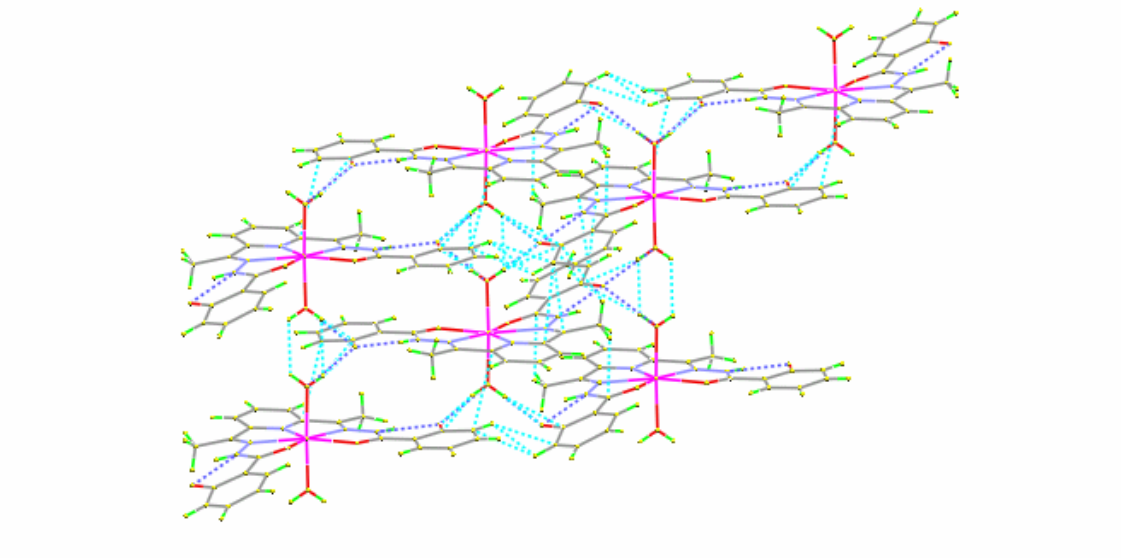


Fig. SF2: View of the hydrogen bonding and other short contacts in [Mn.dapS_2.2H_2O] (3). DMF



Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2005

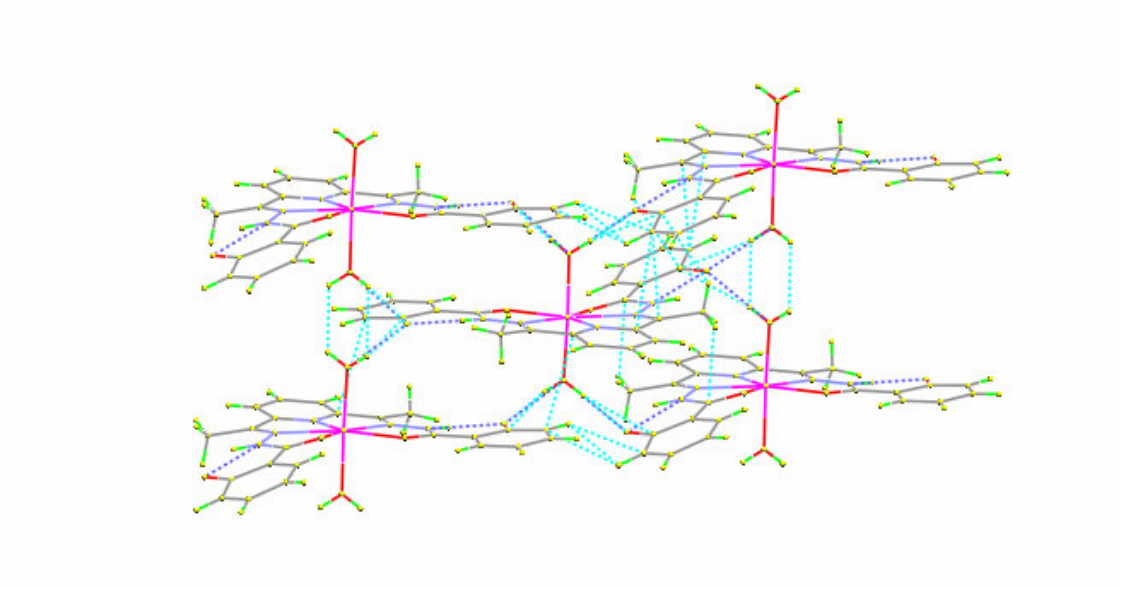
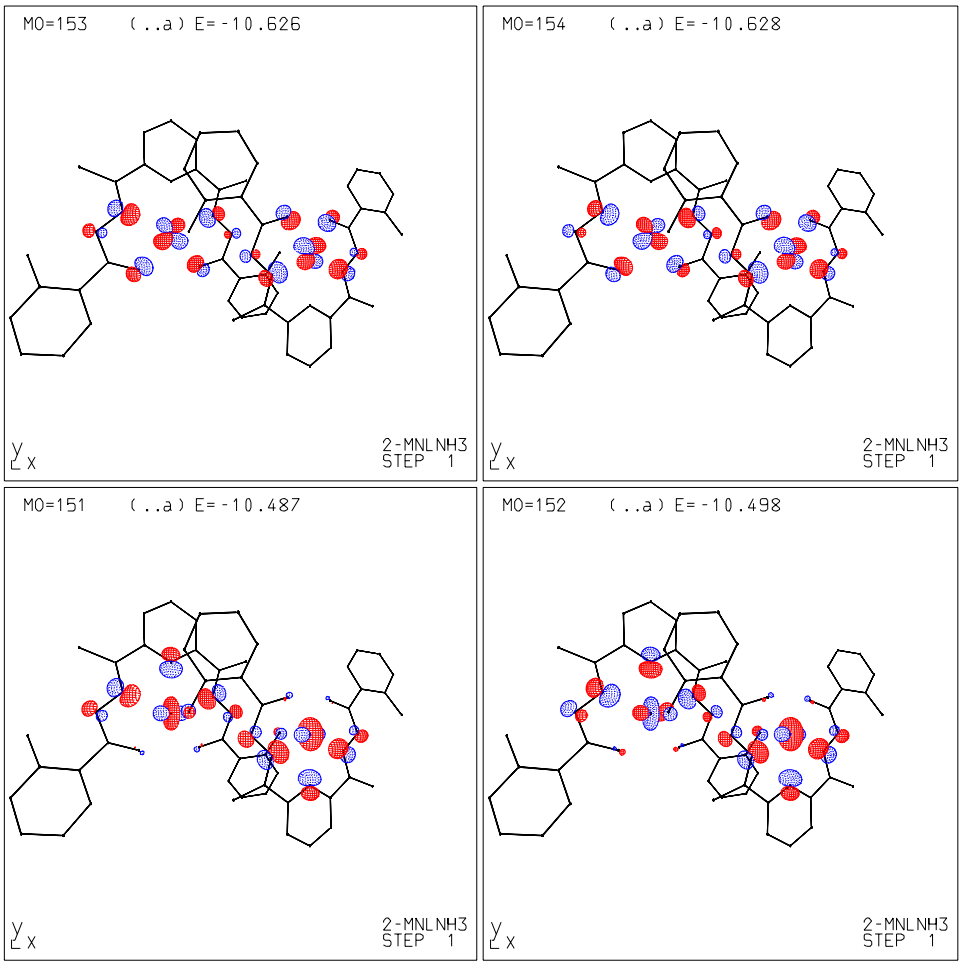
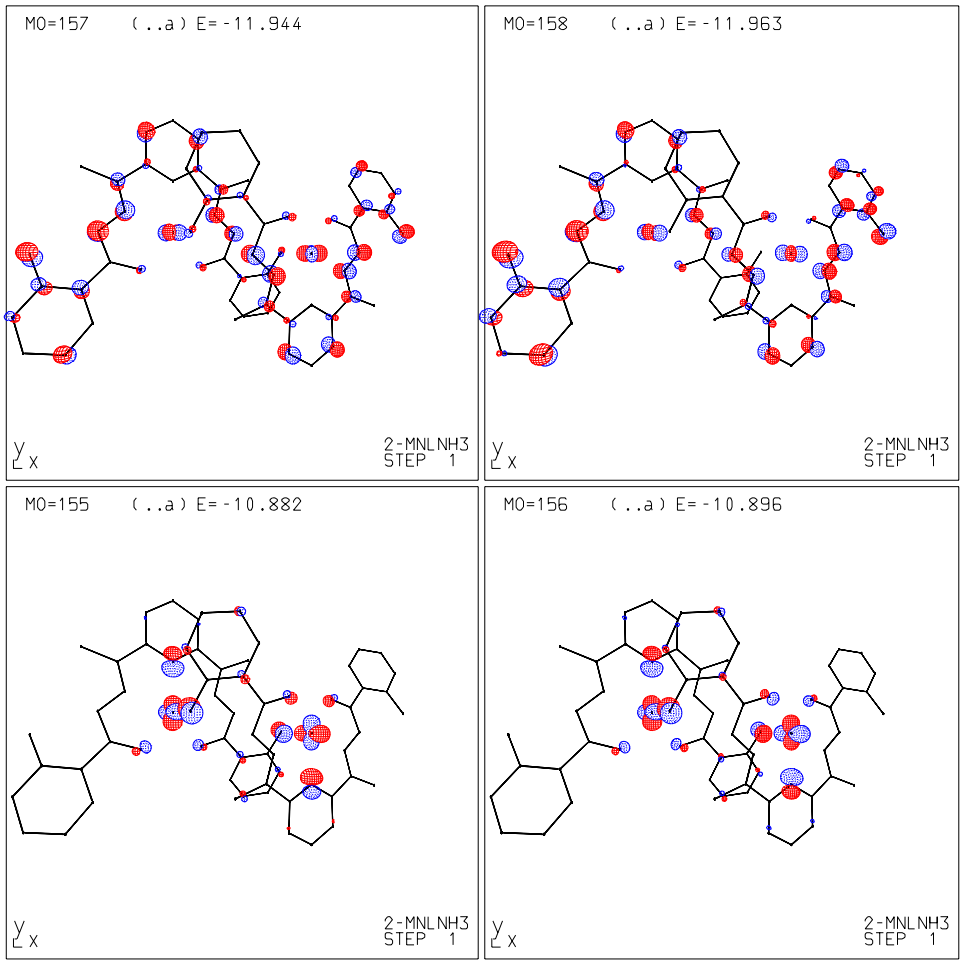


Figure SF3: MO for the dimer, (for clarity, the NH_3 groups and H atoms, are omitted).

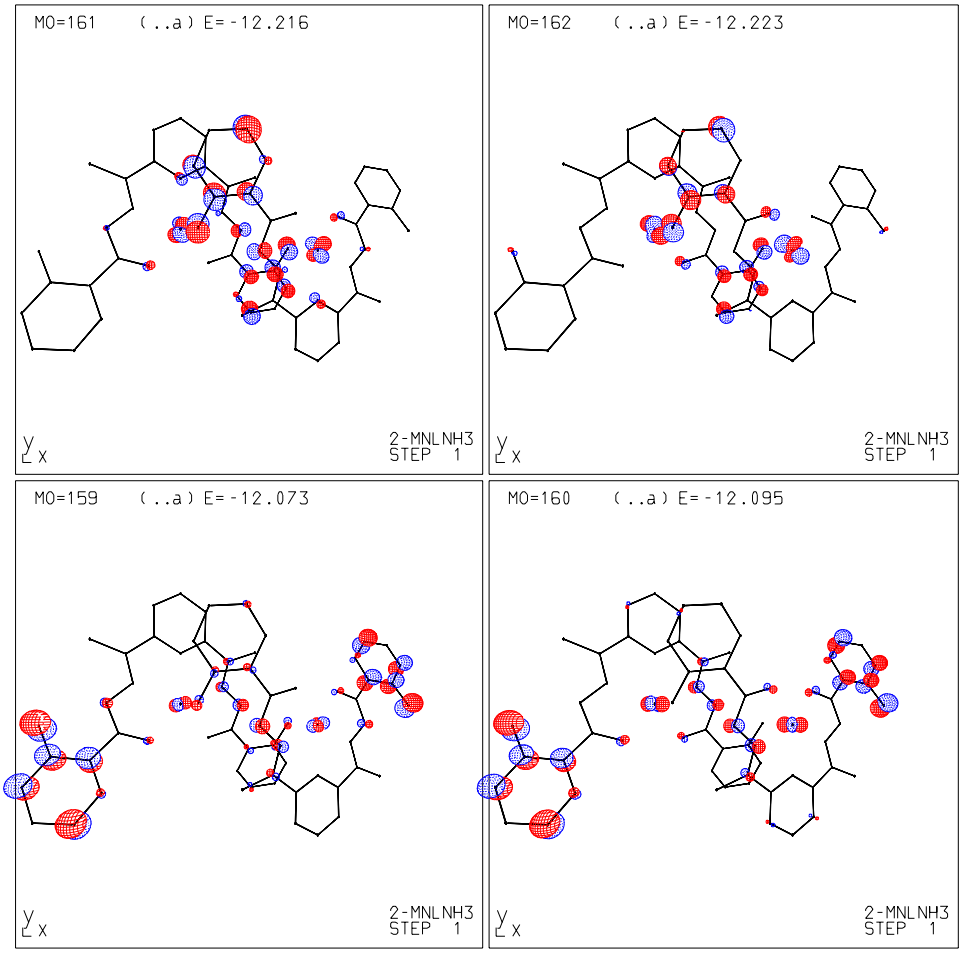
Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2005



Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2005



Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2005



Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2005