

Conformational effects in molecular tectons containing protonated benzimidazole cations.

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Supplementary material

Table S1 : Details of Hydrogen bonds

Fig. S1. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for
[**1b**H₂][MnCl₄]

Fig. S2. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the cation
in [**3b**H₂]Cl₂·0.5 CH₃CN

Fig. S3. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the cation
in [**3b**H₂][MnCl₄]H₂O

Fig. S4. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the
complex in [Cu(**4b**)₂](PF₆)·CH₃CN

Fig. S5. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the cation
in [**5a**H₃]Cl₃·2MeOH

Fig. S6. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the cation
in [**5b**H₃]Br₃·4 H₂O.

Table S1. Data for hydrogen bonds

Donor, D	Hydrogen, H	Acceptor, A	D-H (Å)	H...A (Å)	D...A (Å)	Angle D-H...A (°)	Equivalent position for A
[1bH₂][MnCl₄]							
N1	H1	Cl1	0.96(4)	2.34(5)	3.269(4)	163(4)	1/2+ x , 1/2-y , -z
[3bH₂]Cl₂ 0.5 CH₃CN							
N2a	H02a	Cl1	1.06	1.93	2.978(5)	168	x , y , z
N4a	H04a	Cl2	1.00	2.09	3.020(5)	154	x , y , z
N2b	H02b	Cl3	0.91	2.16	3.020(5)	156	x , y , z
N4b	H04b	Cl4	0.86	2.15	2.978(6)	162	1-x , 1-y , 1-z
[3bH₂][MnCl₄]H₂O							
N1	H01	O1w	0.89(3)	1.79(3)	2.677(3)	171(3)	x , y , z
N3	H03	Cl1	0.85(3)	2.37(3)	3.172(2)	156(2)	x , y-1 , z
O1w	H1w	Cl3	0.86(2)	2.42(3)	3.199(3)	151(3)	x , y-1 , z
O1w	H2w	Cl3	0.85(3)	2.43(3)	3.156(3)	143(2)	x , y , z
[5aH₃]Cl₃.2MeOH							
N1	H01	O1a	0.92(10)	1.77(10)	2.681(10)	172(9)	x , y , z
N2	H02	Cl1	0.99(9)	2.10(9)	3.062(8)	165(7)	-x , y-3/2 , 1-z
N3	H03	Cl2	0.85(9)	2.20(9)	3.034(8)	166(9)	-x , 1/2+y , 1-z
N4	H04	Cl3	0.93(9)	2.22(9)	3.144(8)	171(9)	x , y , z
N5	H05	Cl3	1.12(9)	2.09(9)	3.163(8)	159(7)	x , y , z
N6	H06	Cl1	0.99(10)	2.19(10)	3.075(8)	149(7)	1-x , y-3/2 , 1-z
O1a	H1a	Cl2	1.01(9)	2.12(9)	3.085(7)	160(8)	1-x , 1/2+y , 1-z
O1b	H1b	Cl3	1.18(8)	1.97(8)	3.127(8)	166(7)	1-x , 1/2+y , 1-z
[5bH₃]Br₃.4 H₂O							
O1w	H11w	Br	0.89(3)	2.53(3)	3.419(3)	175(2)	2/3-y , 1/3+x-y , 1/3+z
O1w	H12w	Br	0.90(3)	2.46(2)	3.340(2)	166(2)	1-x , 1-y , 1-z
N1	H01	O1w	0.98	1.79	2.732(5)	161	1-x+y , 1-x , z

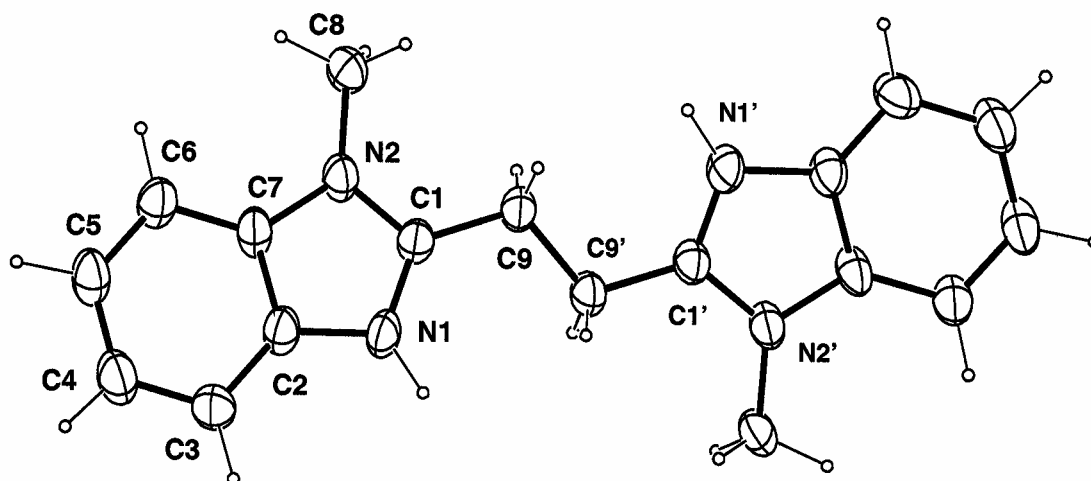


Fig. S1. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for $[1bH_2][MnCl_4]$

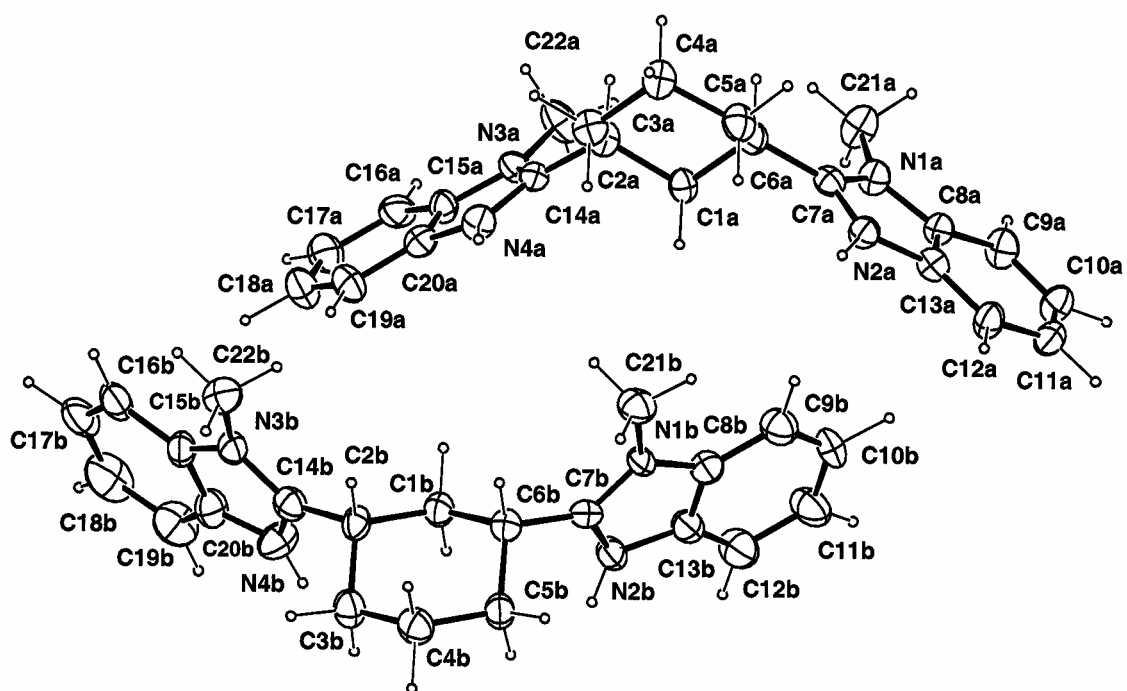


Fig. S2. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the cation in $[3bH_2]Cl_2 \cdot 0.5 CH_3CN$

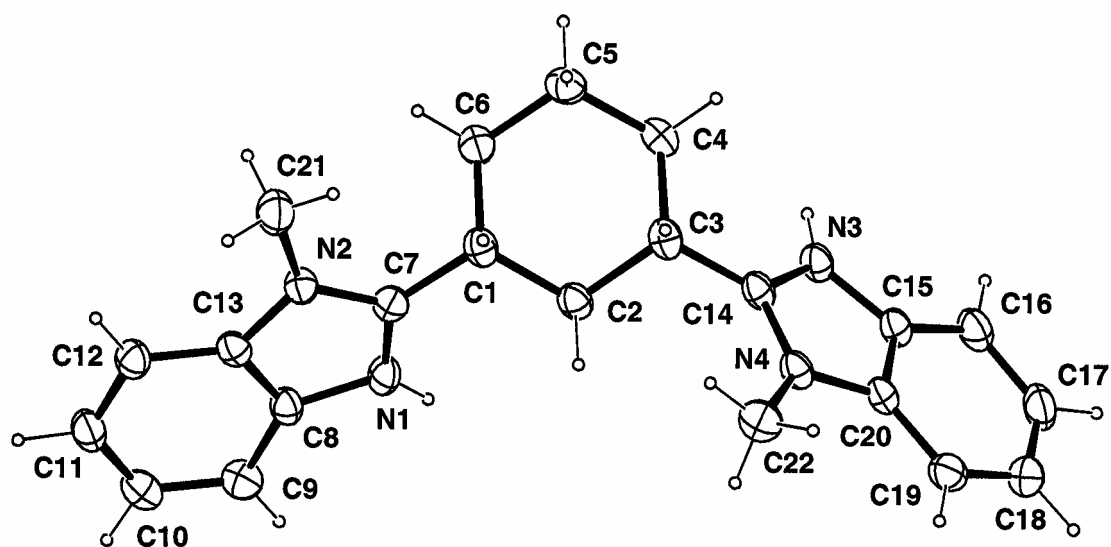


Fig. S3. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the cation in $[3bH_2][MnCl_4] \cdot H_2O$

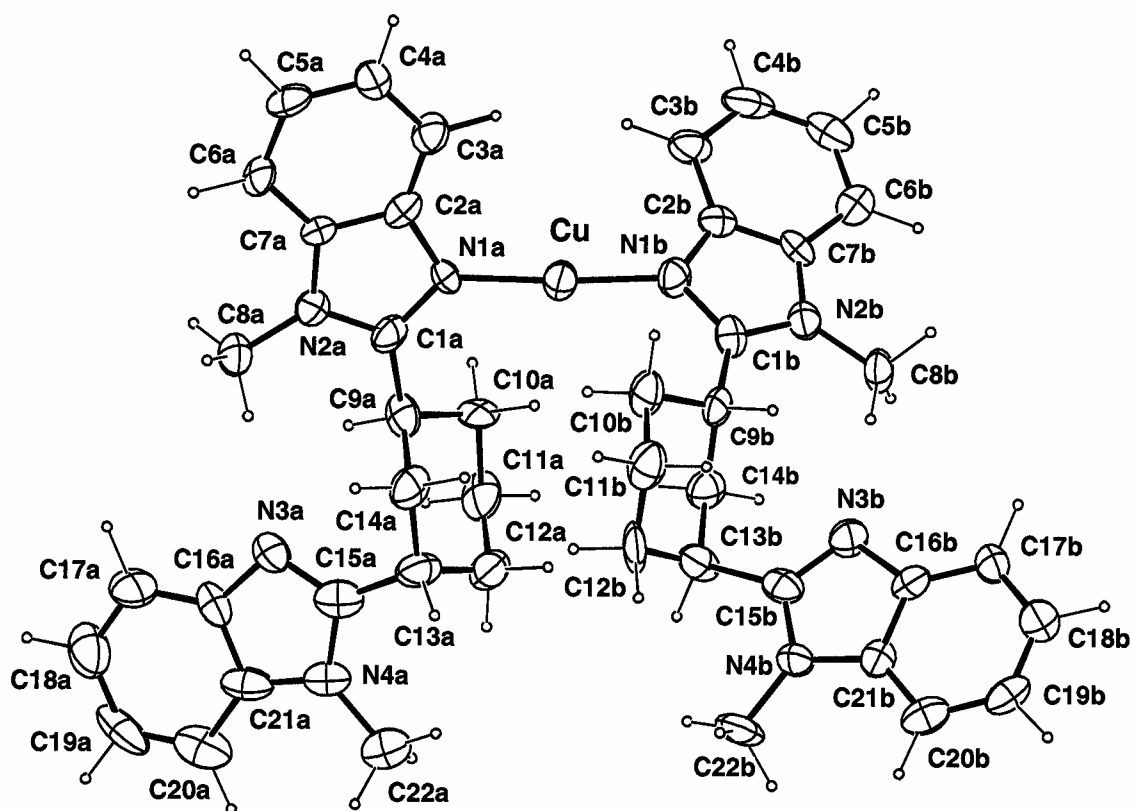


Fig. S4. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the complex in $[Cu(4b)_2](PF_6) \cdot CH_3CN$

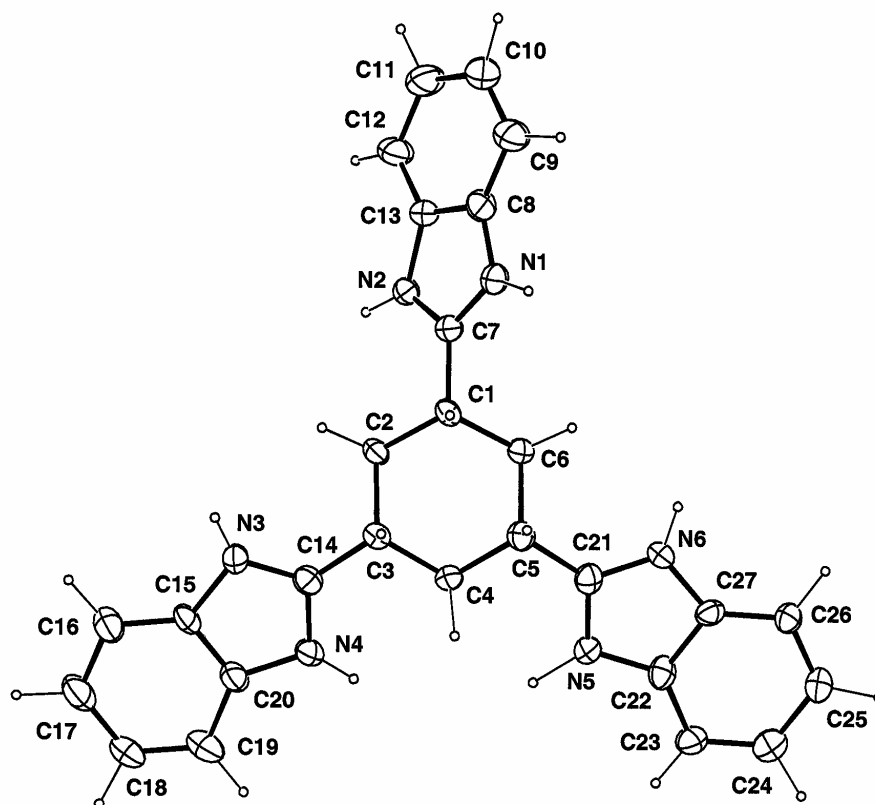


Fig. S5. Thermal ellipsoids (at 50% probability) and atomic numbering scheme for the cation in $[5aH_3]Cl_3 \cdot 2MeOH$

