Electronic Supplementary Information (ESI) for New J. Chem. *Letter*

Self-Assembly Route from a Bis-aminal Derivative to a New Cyclam Based Macropentacycle

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1. ^{1}H NMR spectra of 2a (D_2O, 298K, 100 MHz)

2. X-ray structure of 3b : asymmetric unit.

3. Space Filling models for 3b and structure views with bromide atoms.

3a. View along axis a (b horizontal right, c vertical up).

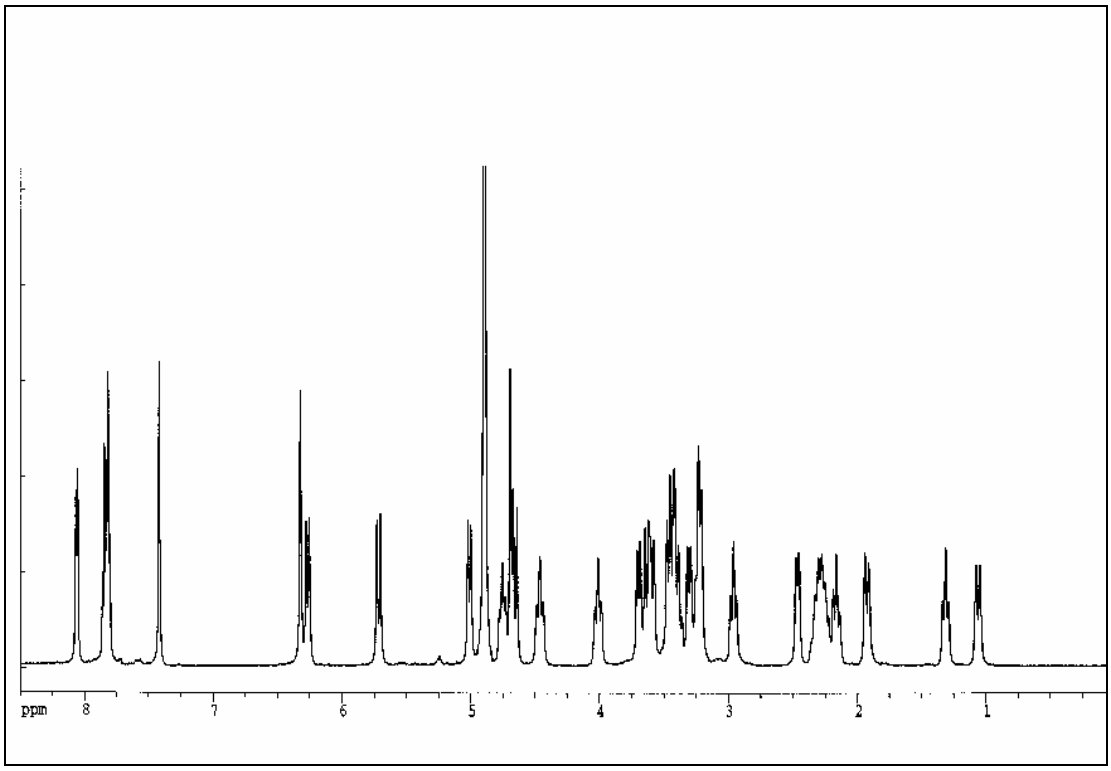
3b. View along axis b (c vertical up, a horizontal left).

3c. View along axis c (a horizontal right, b vertical up).

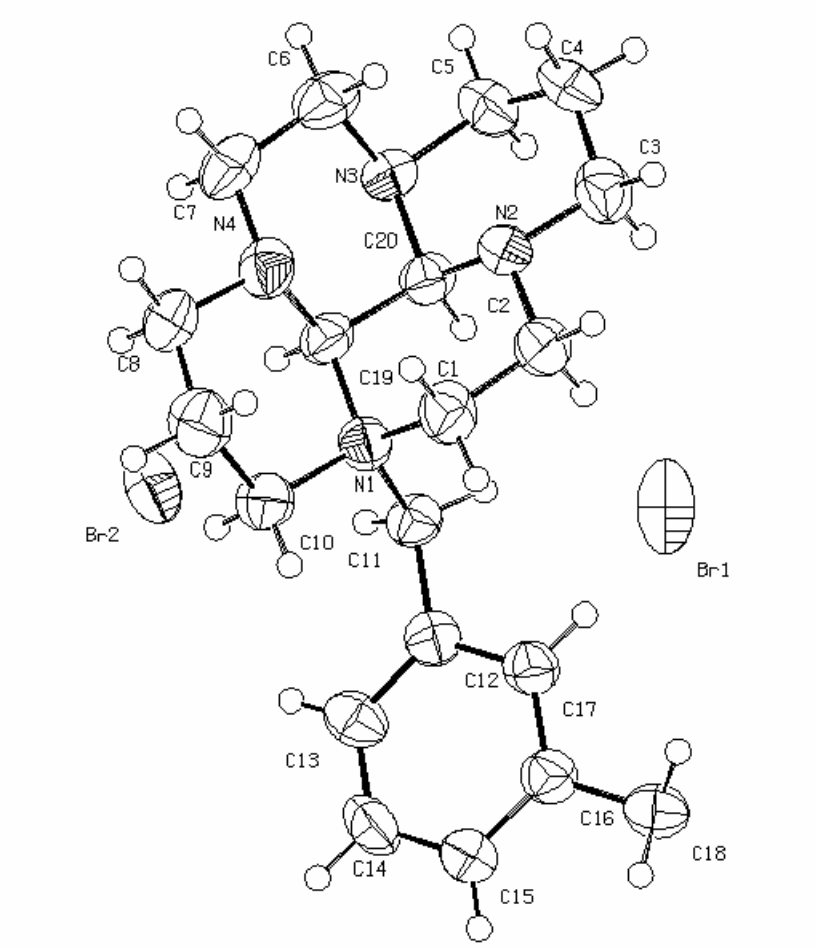
4. Molecular Packing showing the void occupied by disordered water molecules and bromide ions

ATTACHED FILES : Crystallographic data in CIF file and other electronic format

1. ^{1}H NMR spectra of 2a (D_2O, 298K, 100 MHz)



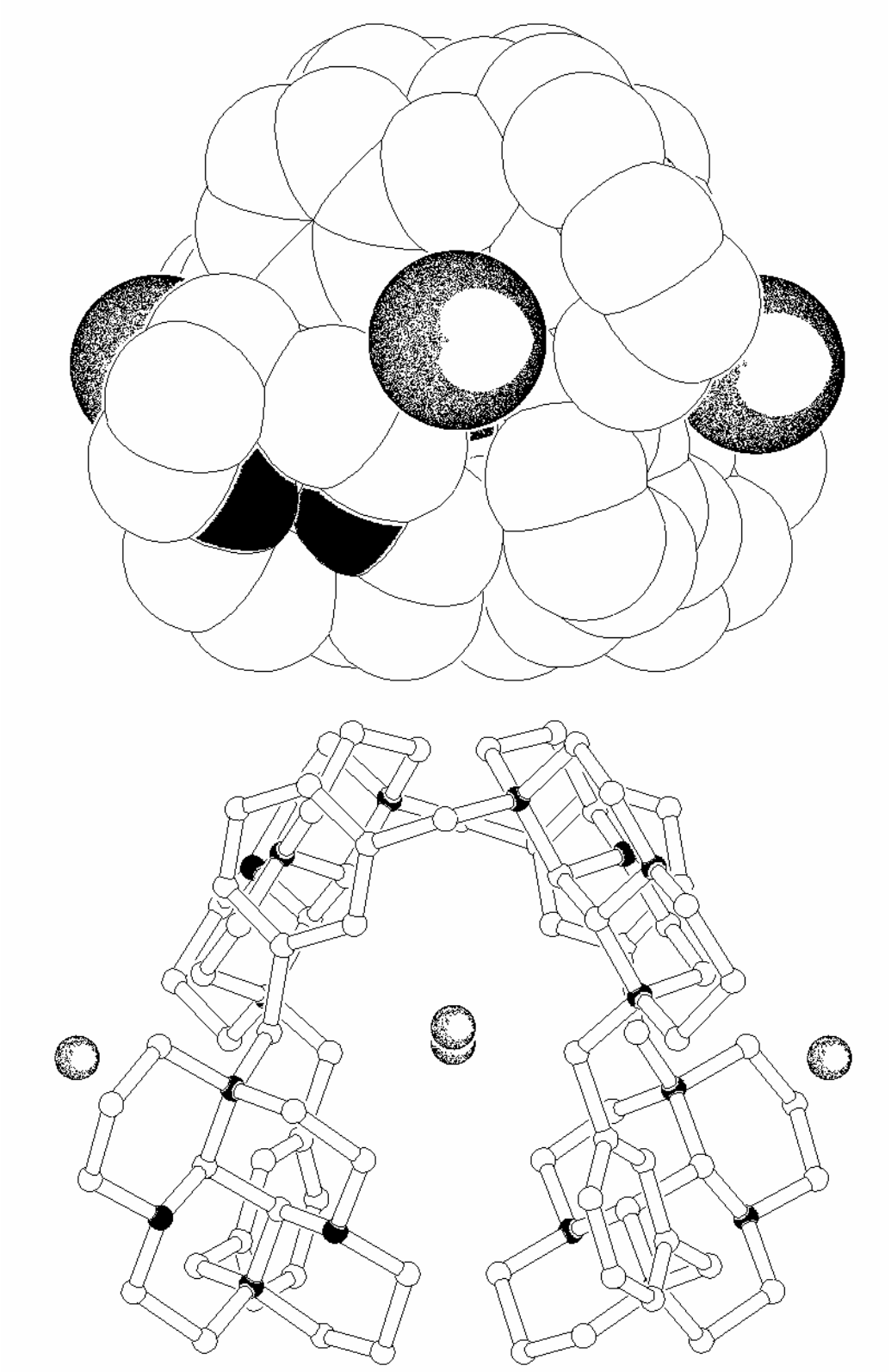
2. X-ray structure of 3b : asymmetric unit.



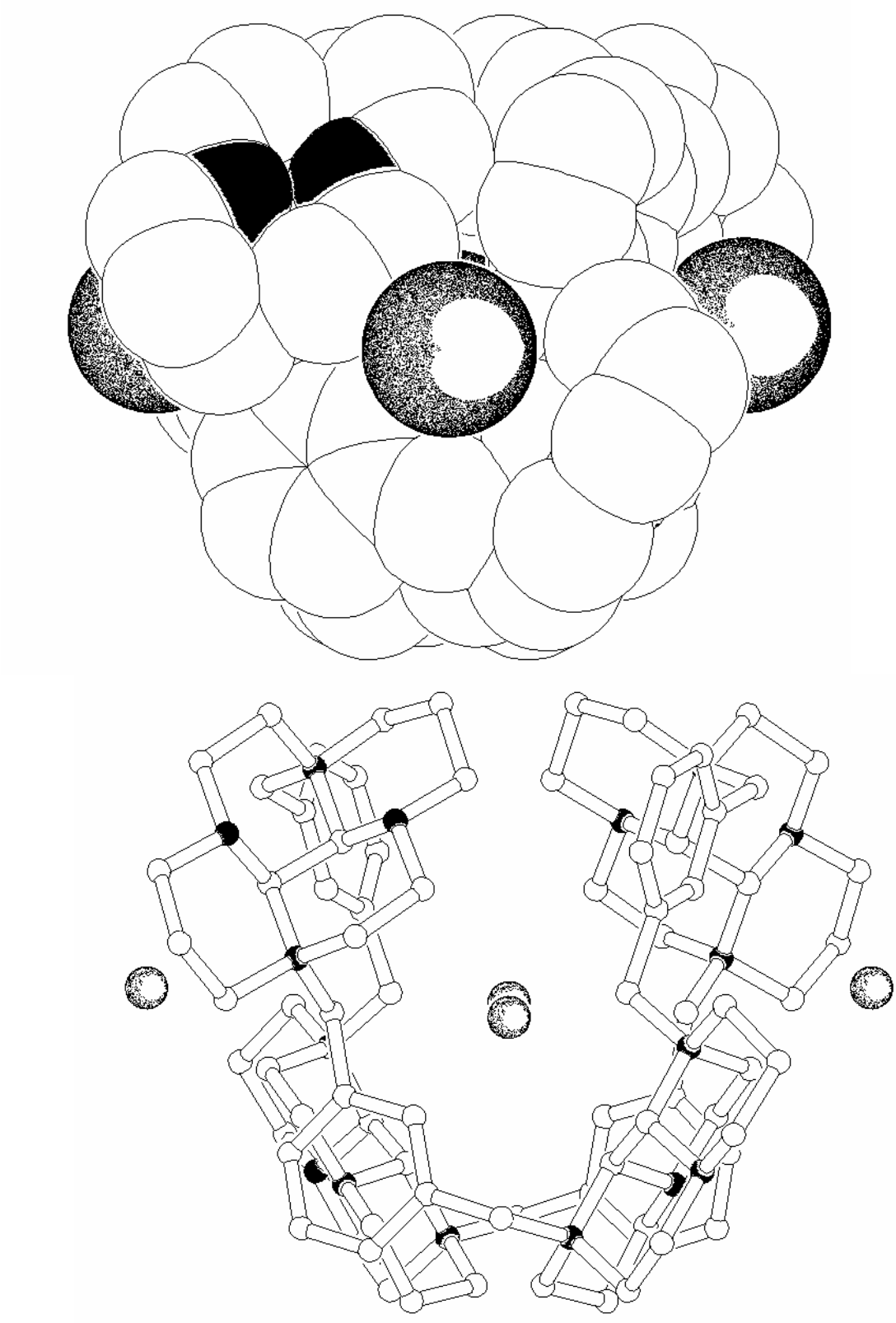
ORTEP drawing of asymmetric unit showing atom numbering viewed along ***b*** axis (***c*** points vertically up, ***a*** points horizontally left). Displacement ellipsoids are drawn at the 50% probability level. Br1 is on a centre –4 (occupation factor ¼). The expected 3 Br^- anions with statistical occupation factor 0.25 are not represented.

3. Space Filling models for 3b and structure views with bromide atoms.

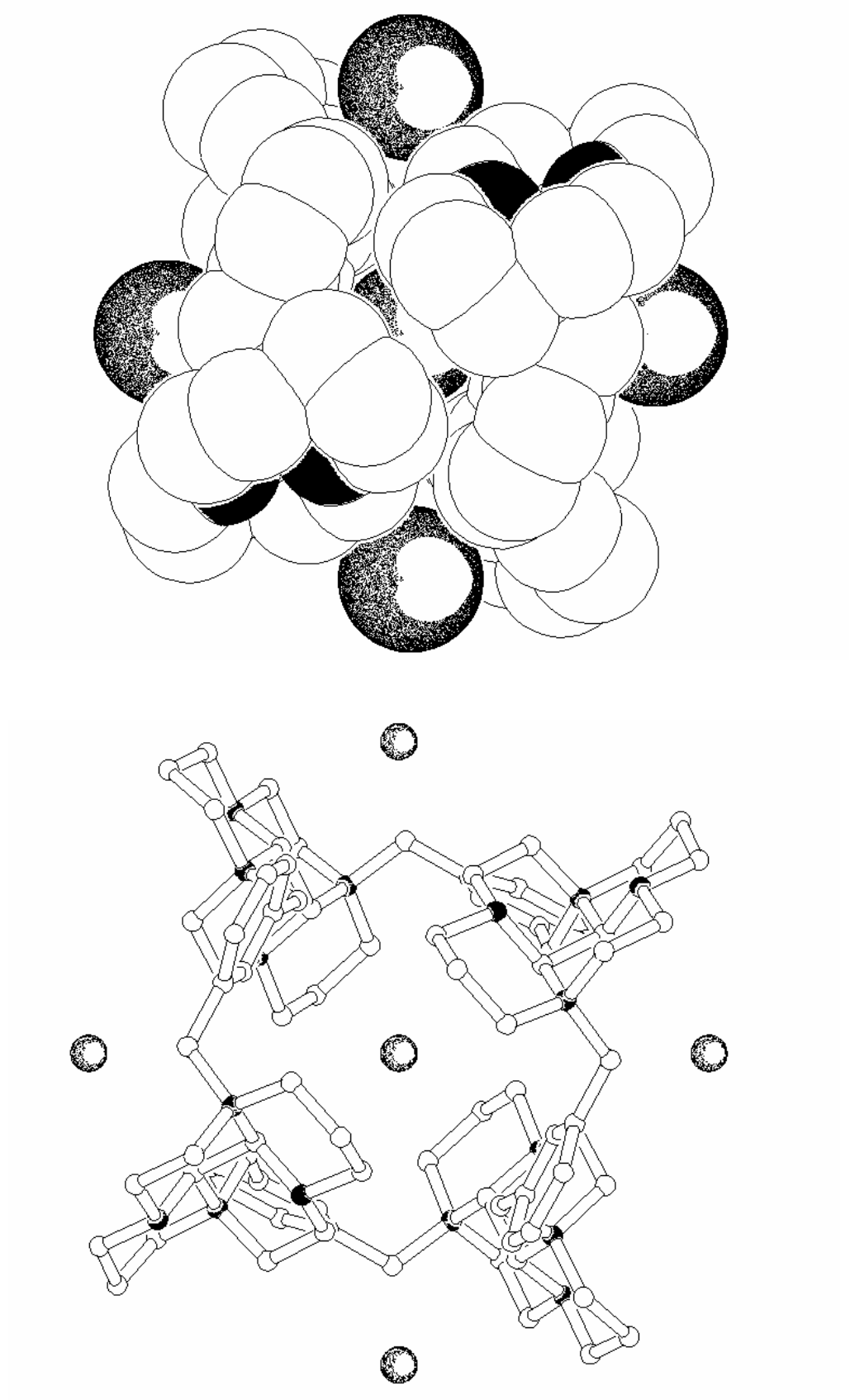
3a. View along axis a (b horizontal right, c vertical up).



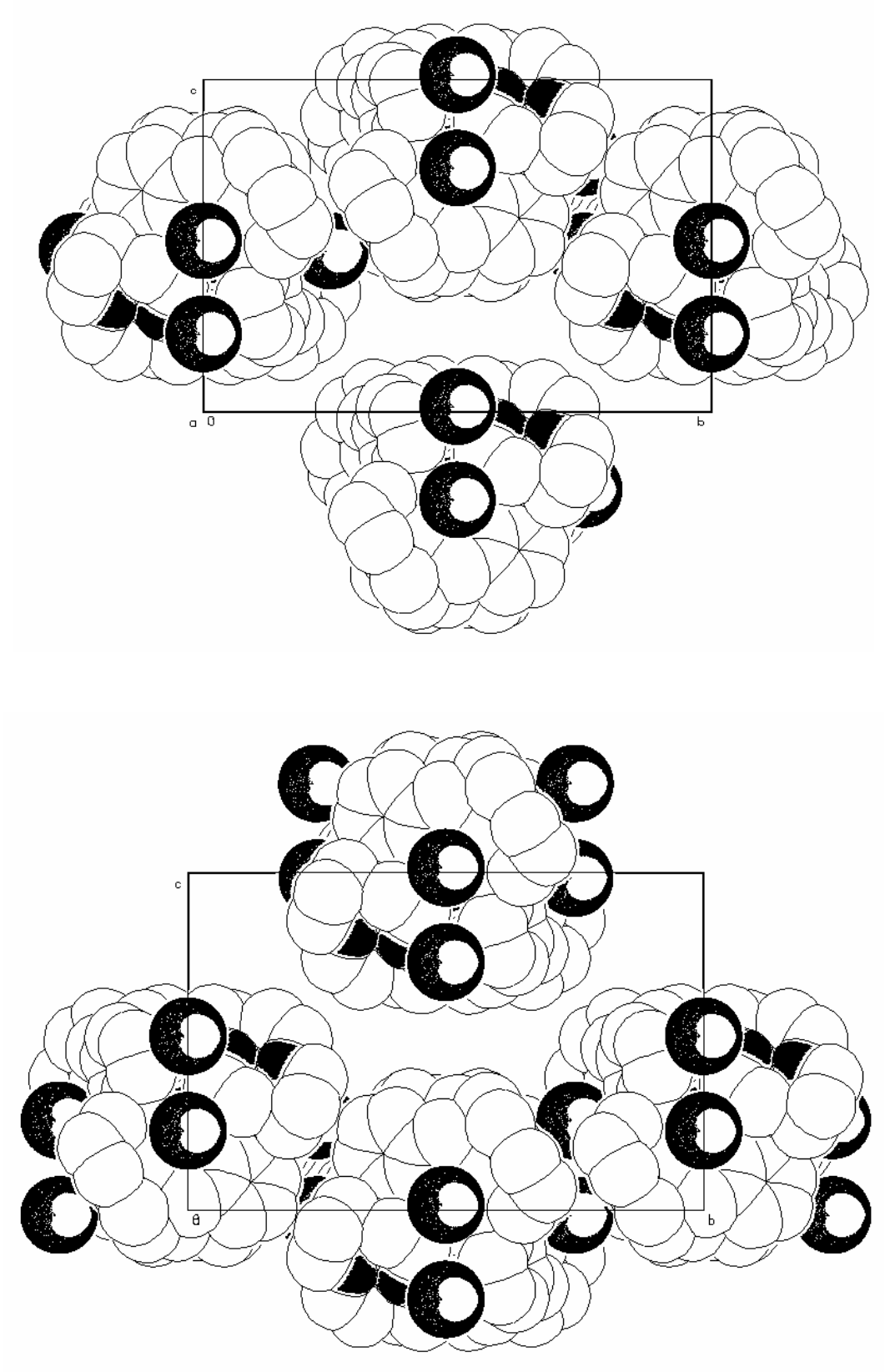
3b. View along axis b (c vertical up, a horizontal left).



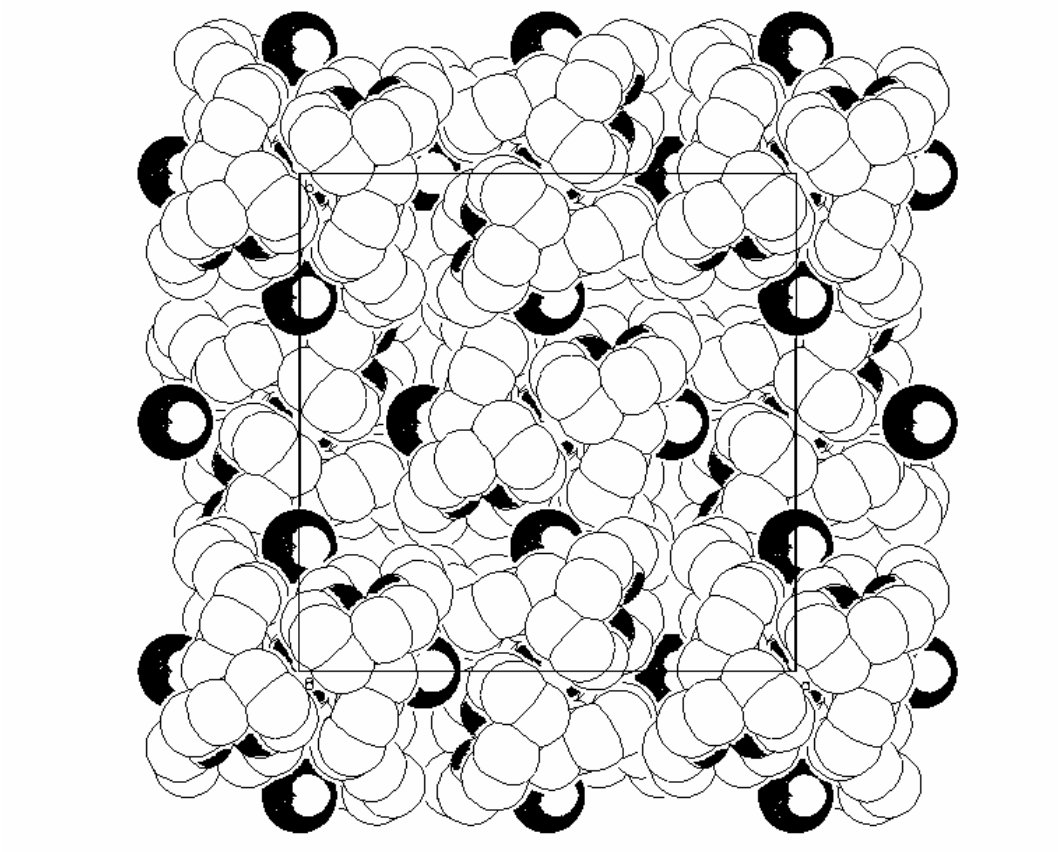
3c. View along axis c (a horizontal right, b vertical up).



4. Molecular Packing showing the void occupied by disordered water molecules and bromide ions



Up: x = 0 ; down: x = 0,5



R0 z = -0,5 ; 0,5