Caterina Fraschetti, Marco Pierini,* Claudio Villani, Francesco Gasparrini, Antonello Filippi, and Maurizio Speranza*

GAS-PHASE STRUCTURE AND RELATIVE STABILITY OF PROTON-BOUND HOMO- AND HETEROCHIRAL CLUSTERS OF TETRA-AMIDE MACROCYCLES WITH AMINES.

SUPPORTING INFORMATION

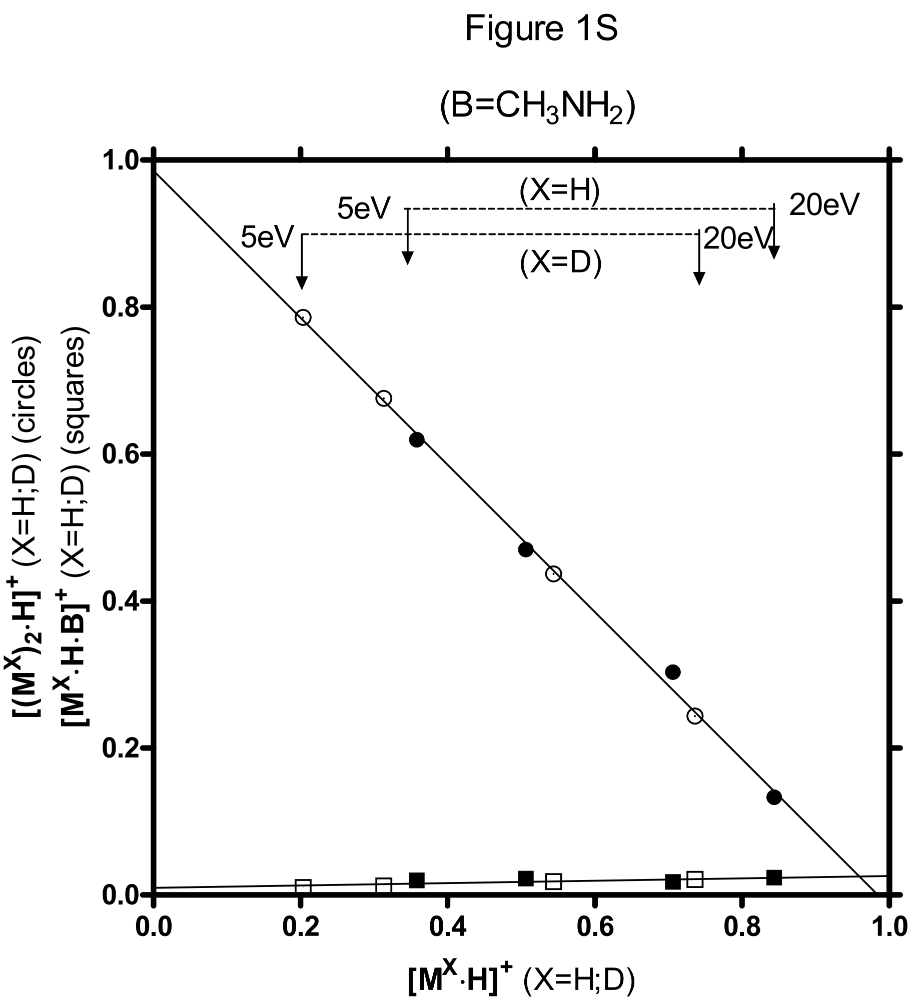

Figure 1S. Comparative plots of the relative abundances of the products from CID of the homochiral $[(M^{X})_2\bullet H\bullet B]^+$ (X=H;D) complexes from ESI of the ***(S)-M***$^{\mathbf{H}}$/***(R)-M***$^{\mathbf{D}}$/B=CH_3NH_2 mixture: *i*- open circles: $[((S)\text{-}M^{H})_2\bullet H]^+$ vs. $[(S)\text{-}M^{H}\bullet H]^+$; full circles: $[((R)\text{-}M^{D})_2\bullet H]^+$ vs. $[(R)\text{-}M^{D}\bullet H]^+$; open squares: $[((S)\text{-}M^{H}\bullet H\bullet B]^+$ vs. $[(S)\text{-}M^{H}\bullet H]^+$; full squares: $[(R)\text{-}M^{D}\bullet H\bullet B]^+$ vs. $[(R)\text{-}M^{D}\bullet H]^+$. The upper broken arrows denote the collision energy (E_{lab}) range for $[((S)\text{-}M^{H})_2\bullet H\bullet B]^+$ and the lower ones that for $[((R)\text{-}M^{D})_2\bullet H\bullet B]^+$ (see Table 1).

Figure 2S

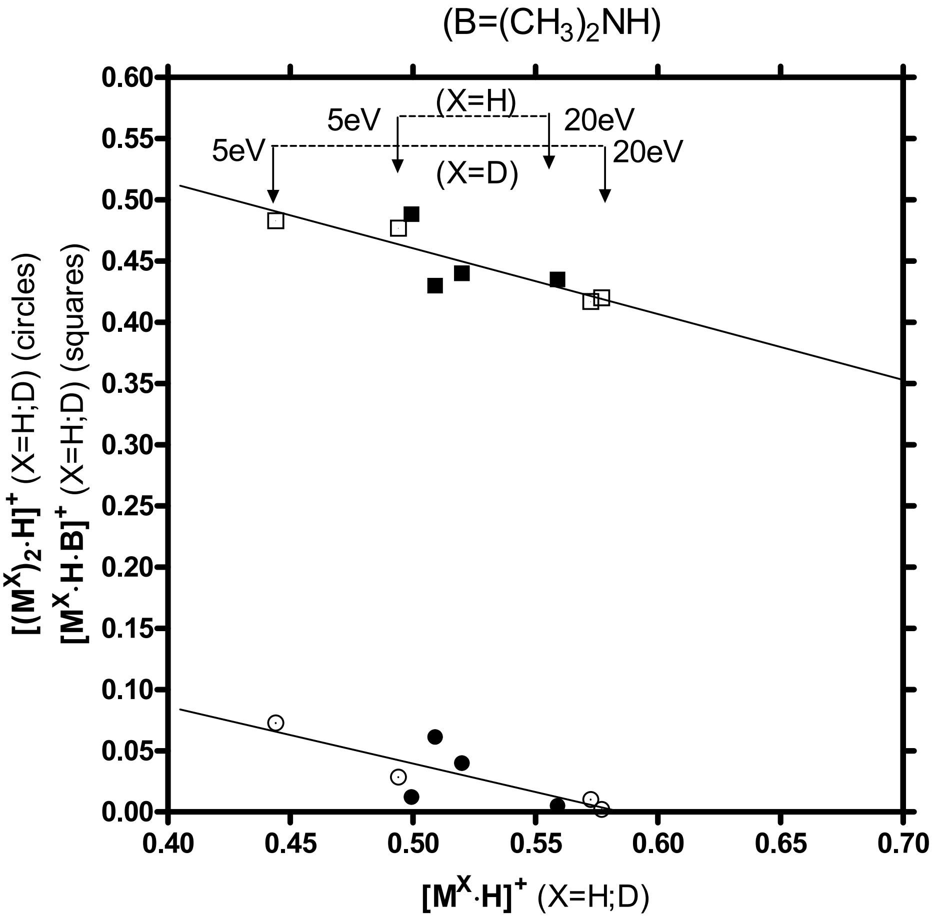

Figure 2S. Comparative plots of the relative abundances of the products from CID of the homochiral [(M^{X})$_2$•H•B]$^+$ (X=H;D) complexes from ESI of the ***(S)-M***$^{\mathbf{H}}$/***(R)-M***$^{\mathbf{D}}$/B=(CH_3)$_2$NH mixture: *i-* open circles: [(***(S)-M***$^{\mathbf{H}}$)$_2$•H]$^+$ vs. [***(S)-M***$^{\mathbf{H}}$•H]$^+$; full circles: [(***(R)-M***$^{\mathbf{D}}$)$_2$•H]$^+$ vs. [***(R)-M***$^{\mathbf{D}}$•H]$^+$; open squares: [(***(S)-M***$^{\mathbf{H}}$•H•B]$^+$ vs. [***(S)-M***$^{\mathbf{H}}$•H]$^+$; full squares: [***(R)-M***$^{\mathbf{D}}$•H•B]$^+$ vs. [***(R)-M***$^{\mathbf{D}}$•H]$^+$.. The upper broken arrows denote the collision energy (E_{lab}) range for [(***(S)-M***$^{\mathbf{H}}$)$_2$•H•B]$^+$ and the lower ones that for [(***(R)-M***$^{\mathbf{D}}$)$_2$•H•B]$^+$ (see Table 2).

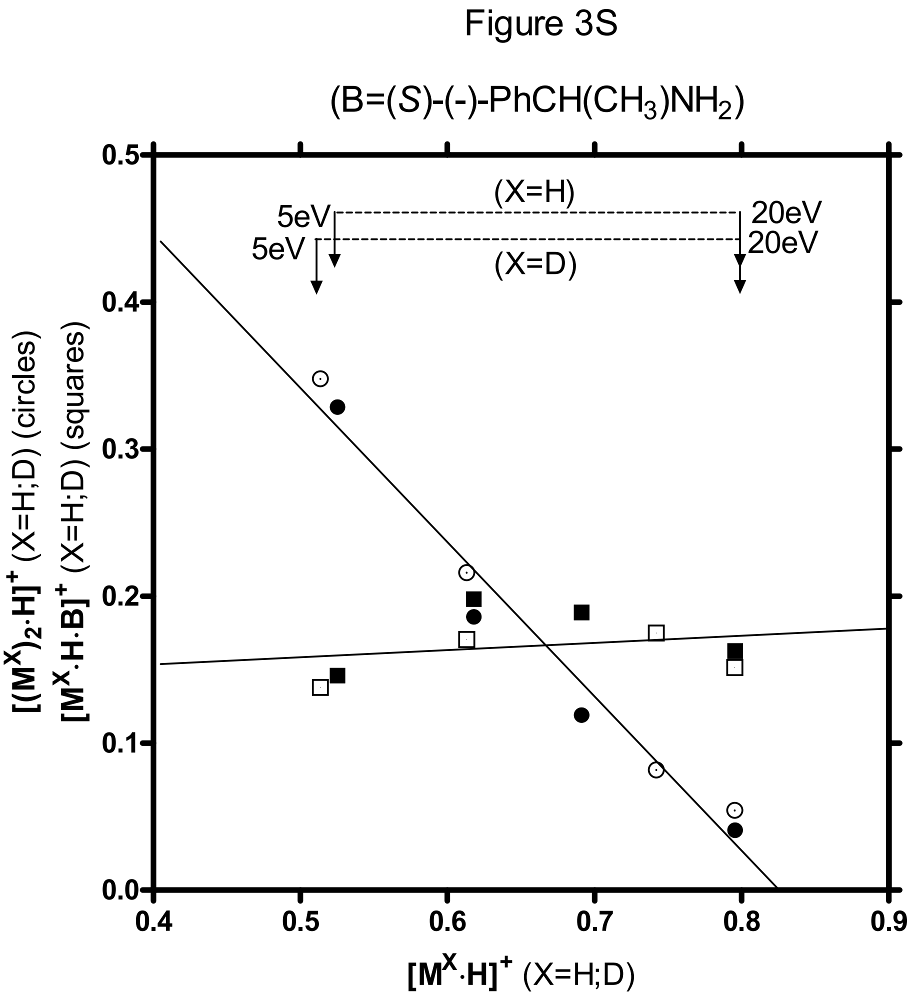

Figure 3S. Comparative plots of the relative abundances of the products from CID of the homochiral $[(M^{X})_2{\bullet}H{\bullet}B]^+$ (X=H;D) complexes from ESI of the ***(S)-M***$^{\mathbf{H}}$/***(R)-M***$^{\mathbf{D}}$/B=(*S*)-(-)-1-phenylethylamine mixture: *i*- open circles: $[((S)\text{-}M^{H})_2{\bullet}H]^+$ vs. $[(S)\text{-}M^{H}{\bullet}H]^+$; full circles: $[((R)\text{-}M^{D})_2{\bullet}H]^+$ vs. $[(R)\text{-}M^{D}{\bullet}H]^+$; open squares: $[((S)\text{-}M^{H}{\bullet}H{\bullet}B]^+$ vs. $[(S)\text{-}M^{H}{\bullet}H]^+$; full squares: $[(R)\text{-}M^{D}{\bullet}H{\bullet}B]^+$ vs. $[(R)\text{-}M^{D}{\bullet}H]^+$.. The upper broken arrows denote the collision energy (E_{lab}) range for $[((S)\text{-}M^{H})_2{\bullet}H{\bullet}B]^+$ and the lower ones that for $[((R)\text{-}M^{D})_2{\bullet}H{\bullet}B]^+$ (see Table 3).