

Electronic Supplementary Information (ESI)

**Proton conduction in hydronium solvate ionic liquids affected by  
ligand shape**

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Table S1. Ionic conductivities and viscosities of  $[\text{H}_3\text{O}^+\cdot\text{Dh18C6}]\text{Tf}_2\text{N}$  at various temperatures.

| Temperature (°C) | Conductivity ( $\text{mS cm}^{-1}$ ) | Viscosity ( $\text{mPa s}$ ) |
|------------------|--------------------------------------|------------------------------|
| 50               | 0.15                                 | 677                          |
| 55               | 0.23                                 | 440                          |
| 60               | 0.32                                 | 300                          |
| 65               | 0.44                                 | 212                          |
| 70               | 0.58                                 | 155                          |
| 75               | 0.75                                 | 117                          |
| 80               | 0.95                                 | 90.0                         |
| 85               | 1.2                                  | 70.8                         |
| 90               | 1.4                                  | 56.7                         |

Table S2. Ionic conductivities and viscosities of  $[\text{H}_3\text{O}^+\cdot\text{B18C6}]\text{Tf}_2\text{N}$  at various temperatures.

| Temperature (°C) | Conductivity ( $\text{mS cm}^{-1}$ ) | Viscosity ( $\text{mPa s}$ ) |
|------------------|--------------------------------------|------------------------------|
| 60               | 0.37                                 | 263                          |
| 65               | 0.50                                 | 190                          |
| 70               | 0.65                                 | 140                          |
| 75               | 0.85                                 | 107                          |
| 80               | 1.1                                  | 83.1                         |
| 85               | 1.3                                  | 65.7                         |

Table S3. Ionic conductivities and viscosities of  $[\text{H}_3\text{O}^+\cdot\text{G5}]\text{Tf}_2\text{N}$  at various temperatures.

| Temperature (°C) | Conductivity ( $\text{mS cm}^{-1}$ ) | Viscosity ( $\text{mPa s}$ ) |
|------------------|--------------------------------------|------------------------------|
| 5                | 0.83                                 | 143                          |
| 15               | 1.4                                  | 81.0                         |
| 25               | 2.2                                  | 50.2                         |
| 35               | 3.3                                  | 33.5                         |
| 45               | 4.6                                  | 23.4                         |

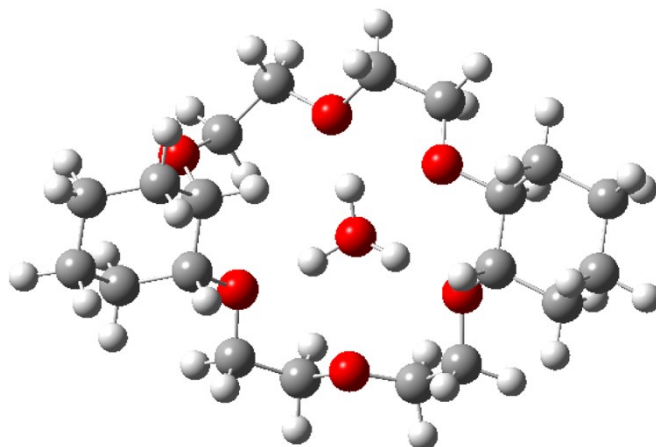


Fig. S1 Graphical representation of the equilibrium geometry of the most stable conformers of Dh18C6 complexes with  $\text{H}_3\text{O}^+$  (B3LYP/6-311+G\*\* level): oxygens in red, carbons in gray, and hydrogens in white.

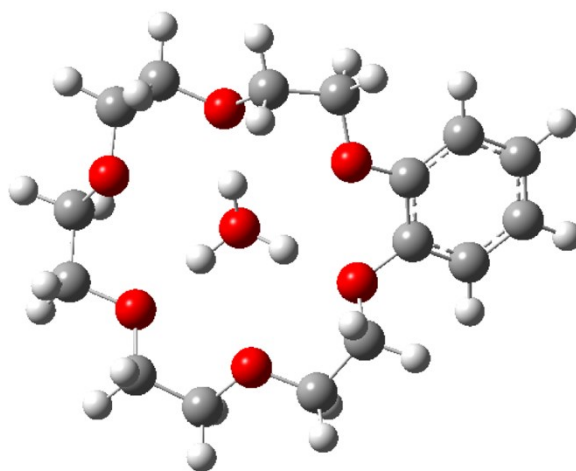


Fig. S2 Graphical representation of the equilibrium geometry of the most stable conformers of B18C6 complexes with  $\text{H}_3\text{O}^+$  (B3LYP/6-311+G\*\* level): oxygens in red, carbons in gray, and hydrogens in white.