Electronic Supplementary Material (ESI) for Analytical Methods
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# Electronic Supplementary Information

# for

# Alkali Metal Ions Transfer across Water/1, 2-DCE Interface

# Facilitated by a Series of Crown Ethers

## Computational details

Density functional calculations were carried out with Becke's three-parameters hybrid exchange functional and Lee-Yang-Parr correlation functional approach B3LYP.[1-4] The basis sets for C, O, H, Li and Na atoms of investigated molecules were 6-311+G(d, p), which included the polarization function in all the atoms and diffuse function in C, O, Li and Na atoms.[5,6] The polarizable continuum model (PCM) was used in our system and DiChloroEthane with dielectric constant ($\varepsilon = 10.125$) was chosen as the solvent.[1] All the above quantum chemical calculations, including geometry optimizations, were carried out by using Gaussian 09 package.[7]

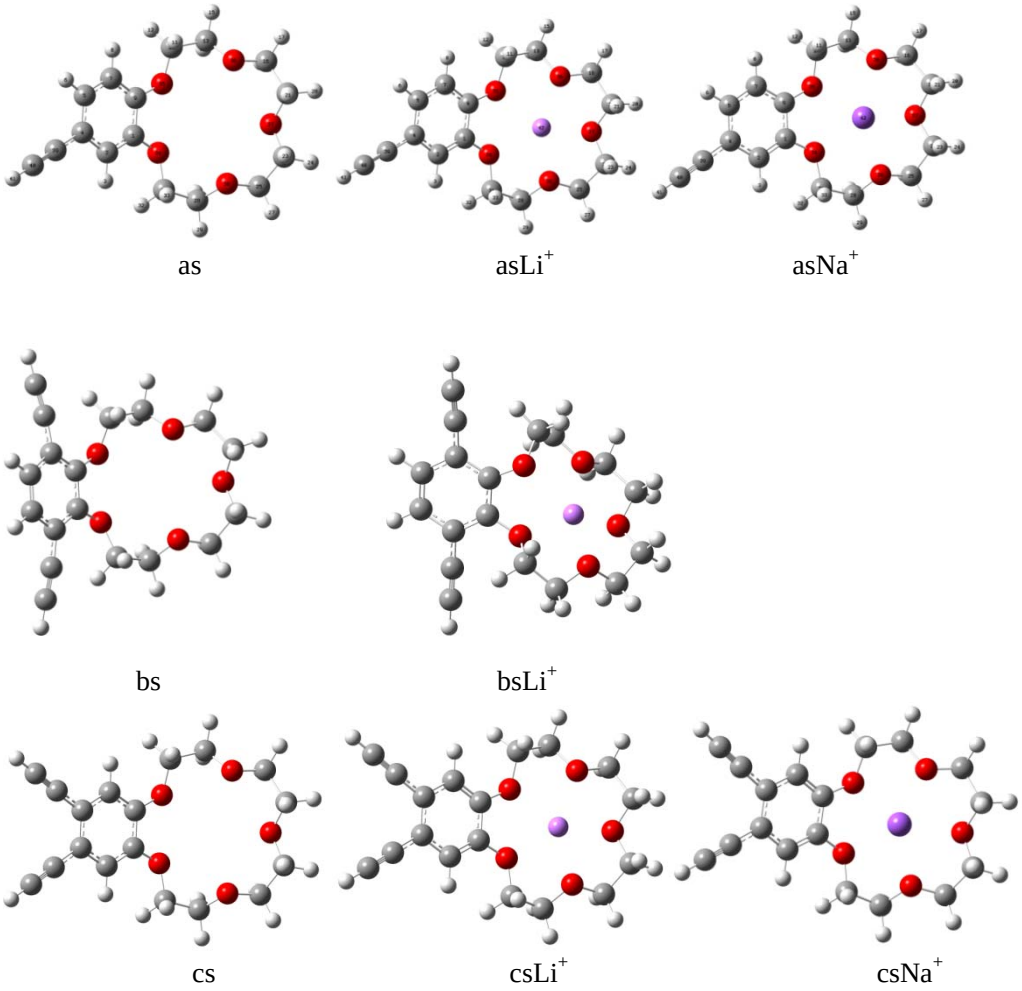


Figure 1 Optimized geometries of a, b and c as well as interacting with $Li^+$ and $Na^+$ with the PCM model calculated at the B3LYP/6-311+G(d, p) level.

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Table 1 Selected Bond Distances (Å) of Optimized Geometries of a, b and c as well as interacting with Li+ and Na+ with the PCM model calculated at the B3LYP/6-311+G(d, p) level.

| Species | $R_{34-35}$ | $R_{35-36}$ | $R_{36-37}$ | $R_{37-38}$ | $R_{38-34}$ | $R_{34-36}$ | $R_{34-37}$ | $R_{35-37}$ | $R_{35-38}$ |
|---|---|---|---|---|---|---|---|---|---|
| as | 2.601 | 2.838 | 2.902 | 2.899 | 2.836 | 4.490 | 4.435 | 4.432 | 4.485 |
| bs | 2.549 | 2.960 | 2.892 | 2.892 | 2.960 | 4.384 | 4.944 | 4.943 | 4.384 |
| cs | 2.590 | 2.825 | 2.899 | 2.899 | 2.825 | 4.477 | 4.415 | 4.414 | 4.476 |
| asLi+ | 2.556 | 2.656 | 2.650 | 2.644 | 2.656 | 4.218 | 4.285 | 4.287 | 4.223 |
| asNa+ | 2.578 | 2.754 | 2.773 | 2.774 | 2.749 | 4.380 | 4.290 | 4.293 | 4.387 |
| bsLi+ | 2.677 | 2.682 | 2.645 | 2.654 | 2.864 | 4.302 | 4.704 | 3.862 | 3.613 |
| csLi+ | 2.545 | 2.642 | 2.660 | 2.659 | 2.642 | 4.211 | 4.280 | 4.277 | 4.201 |
| csNa+ | 2.629 | 2.750 | 2.790 | 2.790 | 2.750 | 4.357 | 4.470 | 4.469 | 4.356 |

Table 2 Bond distances (Å) of Optimized Geometries of 15-5 (a, b and c) and Its Metal Cation ($Li^+$ and $Na^+$) Complexes

| Species | $R_{34-42}$ | $R_{35-42}$ | $R_{36-42}$ | $R_{37-42}$ | $R_{38-42}$ |
|---|---|---|---|---|---|
| asLi+ | 2.370 | 2.380 | 2.174 | 2.105 | 2.163 |
| asNa+ | 2.379 | 2.382 | 2.374 | 2.356 | 2.390 |
| bsLi+ | 2.782 | 2.083 | 2.045 | 2.061 | 2.022 |
| csLi+ | 2.298 | 2.296 | 2.194 | 2.184 | 2.184 |
| csNa+ | 2.352 | 2.352 | 2.352 | 2.341 | 2.351 |

Table3 Mulliken Charges (C)of Selected Atoms in the Optimized Geometries of 15-5 (a, b and c) and Its Metal Cation ($Li^+$ and $Na^+$) Complexes

| Species | C1 | C2 | C4 | C5 | C7 | C9 | O34 | O35 | O36 | O37 | O38 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| as | -0.0517 | 0.169 | 0.352 | -0.848 | 0.216 | -0.0234 | -0.136 | -0.127 | -0.183 | -0.201 | -0.183 |
| bs | -1.205 | 0.683 | -0.0677 | -0.0676 | 0.683 | -1.205 | -0.106 | -0.106 | -0.178 | -0.184 | -0.178 |
| cs | -0.155 | 0.273 | -0.230 | -0.230 | 0.273 | -0.155 | -0.125 | -0.125 | -0.184 | -0.184 | -0.201 |
| asLi+ | -0.0797 | 0.146 | 0.374 | -0.853 | 0.338 | -0.0769 | -0.130 | -0.118 | -0.178 | -0.169 | -0.177 |
| asNa+ | -0.0644 | -0.0302 | 0.251 | -1.165 | 0.655 | 0.103 | -0.194 | -0.183 | -0.248 | -0.249 | -0.245 |
| bsLi+ | -0.326 | 0.478 | -0.378 | -0.265 | 0.421 | -0.420 | -0.0736 | -0.0864 | -0.148 | -0.203 | -0.146 |
| csLi+ | -0.209 | 0.306 | -0.182 | -0.178 | 0.304 | -0.176 | -0.105 | -0.118 | -0.176 | -0.169 | -0.154 |
| csNa+ | -0.197 | 0.309 | -0.165 | -0.156 | 0.311 | -0.0884 | -0.153 | -0.194 | -0.261 | -0.239 | -0.188 |

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