## **Electronic Structure and Conformational Conversion of**

## Calix[4] arene Complexes with Alkali Metal Ions

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## **Electronic Supplementary Information**



Figure S1. Structure of stable C4A conformers obtained in geometry optimization.



Figure S2. Structure of stable Na<sup>+</sup>•C4A conformers obtained in geometry optimization.





Figure S3. Structure of stable K<sup>+</sup>•C4A conformers obtained in geometry optimization.



Figure S3. Cont.



Figure S4. Structure of stable Rb<sup>+</sup>•C4A conformers obtained in geometry optimization.



RbC4A-IV





RbC4A-V



Figure S4. Cont.



Figure S5. Structure of stable Cs<sup>+</sup>•C4A conformers obtained in geometry optimization.





CsC4A-IV





CsC4A-V





CsC4A-VI

Figure S5. Cont.



C4A TS1 (cone-partial-cone)



C4A TS2 (partial-cone-1,3-alternate)



C4A TS3 (partial-cone-1,2-alternate)

Figure S6. Structure of transition-state conformers of C4A.



Na<sup>+</sup>•C4A TS1 (cone-partial-cone)



Na<sup>+</sup>•C4A TS2 (partial-cone-1,3-alternate)



Na<sup>+</sup>•C4A TS3 (partial-cone-1,2-alternate)



Na⁺•C4A TS4 (NaC4A-V–NaC4A-VII)

Figure S6. Structure of transition-state conformers of Na<sup>+</sup>•C4A.