Conformation of Alkali Metal Ion-Calix[4]arene Complexes Investigated by IR Spectroscopy in the Gas Phase

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Electronic Supplementary Information

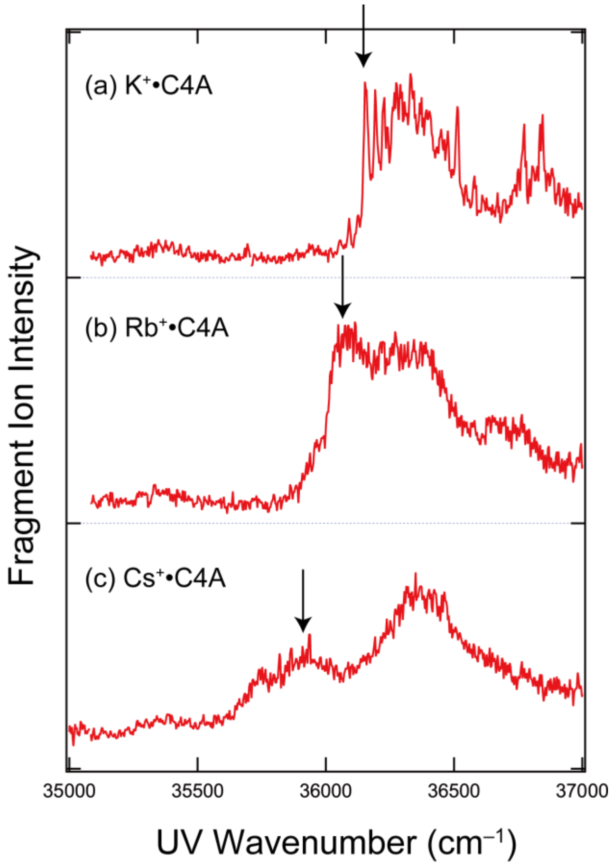
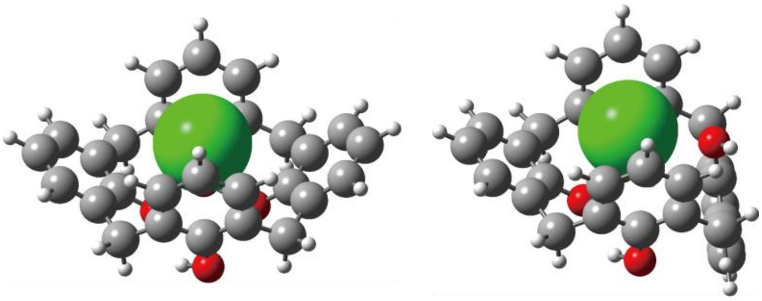
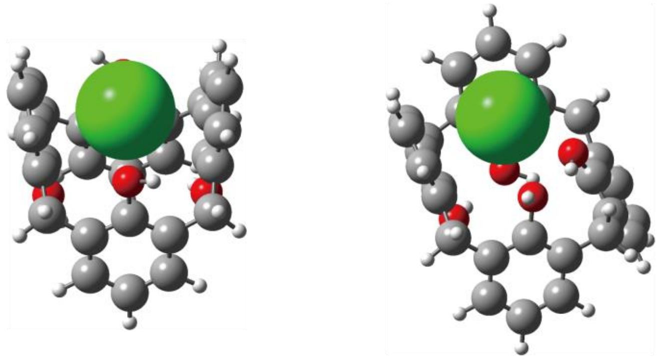


Figure S1. The UVPD spectra of the (a) K^+·C4A, (b) Rb^+·C4A, and (c) Cs^+·C4A complexes. These spectra are reproduced from our previous paper (*Phys. Chem. Chem. Phys.*, 2017, **19**, 12857). The IR-UV spectra in Figs. 1 and 3 are measured at 36156, 36080, and 35920 cm^{-1} for K^+·C4A, Rb^+·C4A, and Cs^+·C4A, respectively. The UV positions for the IR-UV measurement are shown with black arrows.



(a) cone

(b) partial cone



(c) 1,3-alternate

(d) 1,2-alternate

Figure S2. Stable structures of the K$^+$·C4A complexes. Geometry optimization is performed at the !B97X-D/6-311++G(d,p) level of theory

Table S1. Relative total energies (kJ/mol) of stable isomers for the $\mathrm{M}^+\cdot\mathrm{C4A}$ (M = K, Rb, and Cs) complexes calculated at the !B97X-D/6-311++G(d,p) level of theory. These values are corrected by the zero point energy.

M	cone	partial cone	1,3-alternate	1,2-alternate
K	0	15.9	34.2	63.5
Rb	0	20.7	48.1	59.1
Cs	0	26.1	57.6	62.2