Electronic Supplementary Information

New Journal of Chemistry

New Insights into Metal Ion-Crown Ether Complexes Revealed by SEIRA Spectroscopy

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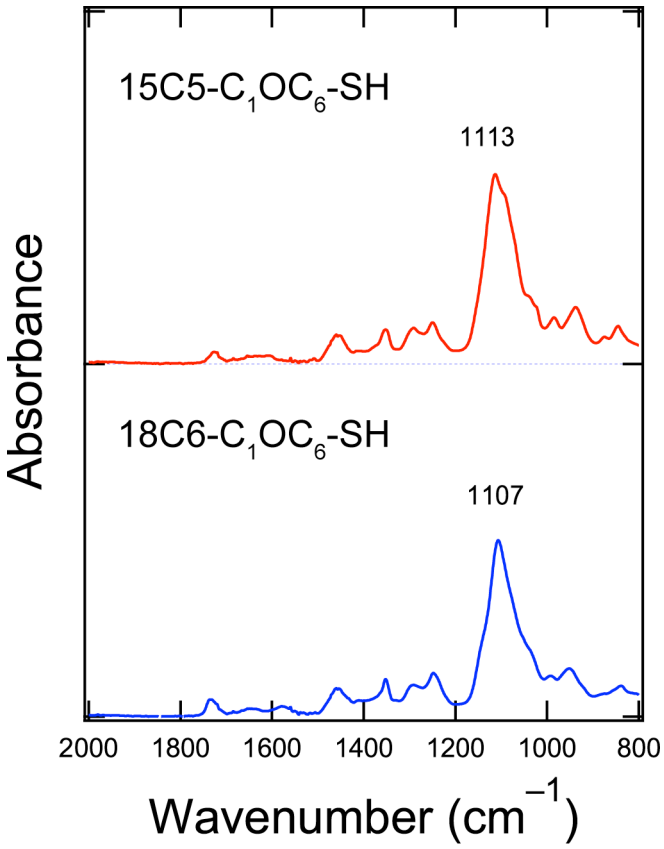

Figure 1S. The IR absorption spectra of the thiol derivatives used in this study. These IR spectra are measured by an ATR (attenuated total reflection) configuration.

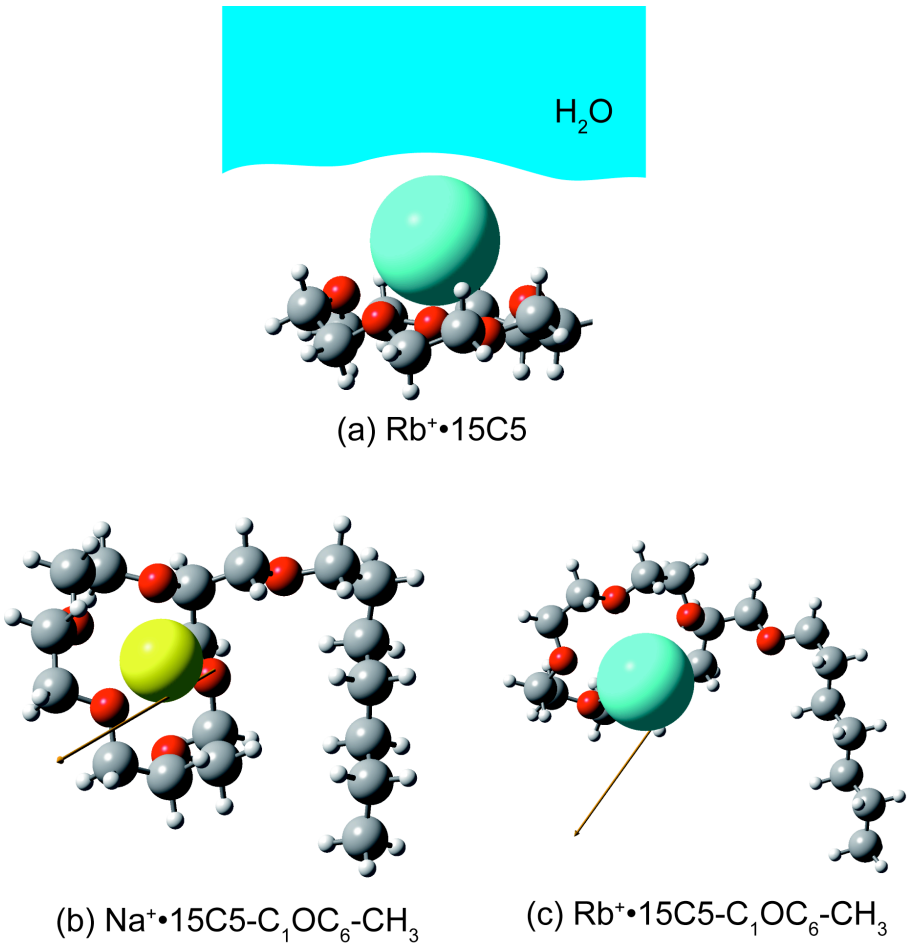

Figure 2S. (a) Proposed orientation of the Rb^+•15C5 component at the interface. (b, c) Dipole derivative of the most intense C–O stretching band for Na^+•15C5-C_1OC_6-CH_3 and Rb^+•15C5-C_1OC_6-CH_3.

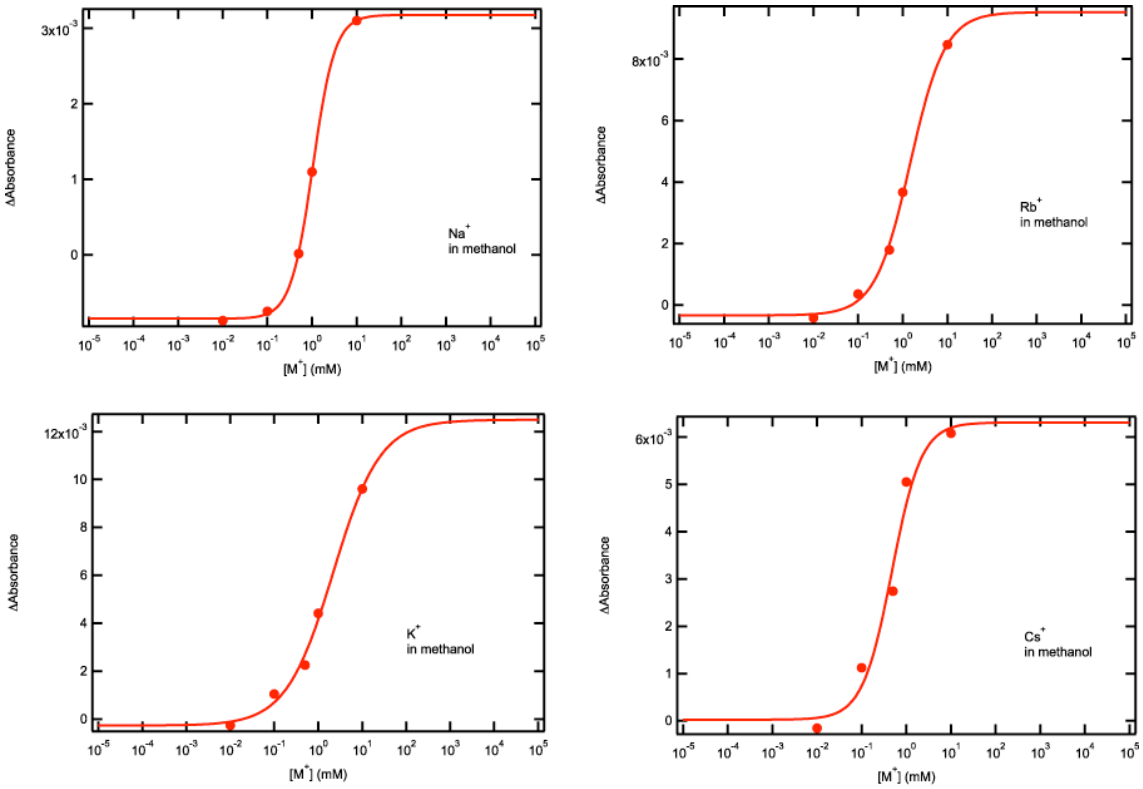

Figure 3S. The peak-to-peak amplitude at ~1100 cm^{-1} in the IR difference spectra of the M^+•18C6-C_1OC_6 (M = Li, Na, K, Rb, and Cs) complexes (Fig. 10) as a function of the concentration of the M^+ ions in methanol (closed circles). The data are reproduced by Hill equations (solid curves).

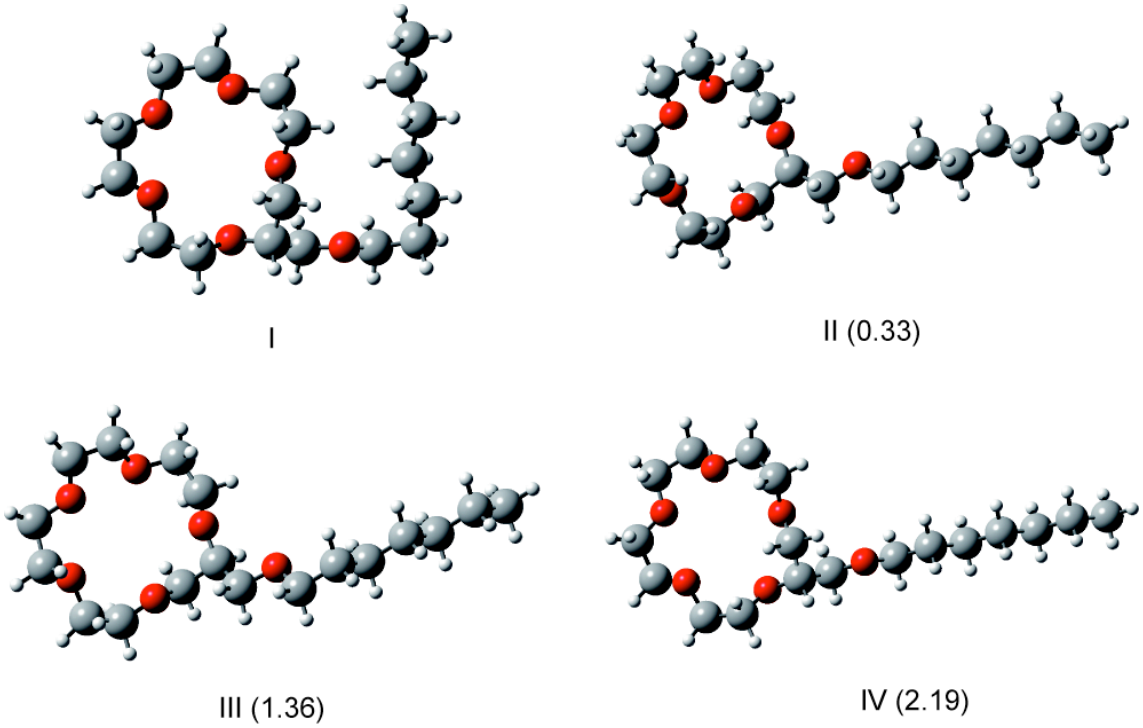

Figure 4S. Stable structures of bare 18C6-C_1OC_6-CH_3 calculated at the M05-2X/6-31+G(d) level of theory. The most stable conformer (conformer I) is the same as that shown in Fig. 6. The numbers in the parentheses show the total energy relative to that of the most stable one in kJ/mol.

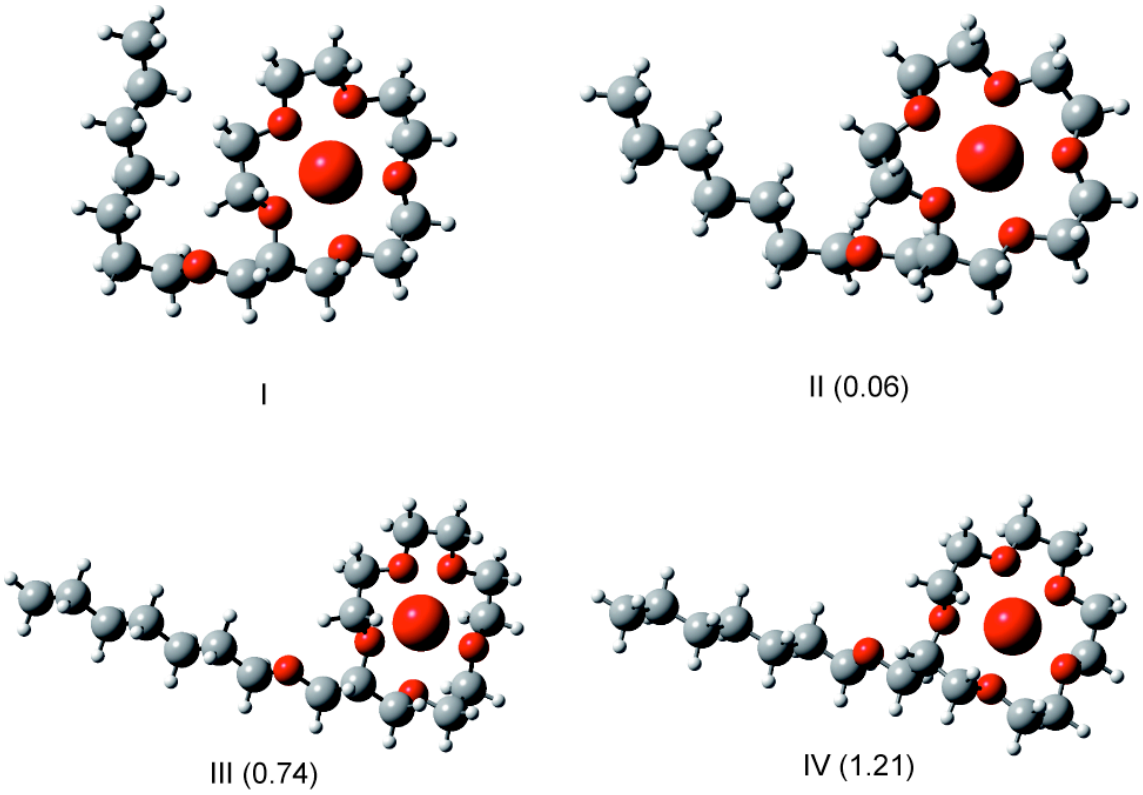

Figure 5S. Stable structures of the Li^+•18C6-C_1OC_6-CH_3 complexes calculated at the M05-2X/6-31+G(d) level of theory. The most stable conformer (conformer I) is the same as that shown in Fig. 6. The numbers in the parentheses show the total energy relative to that of the most stable one in kJ/mol.

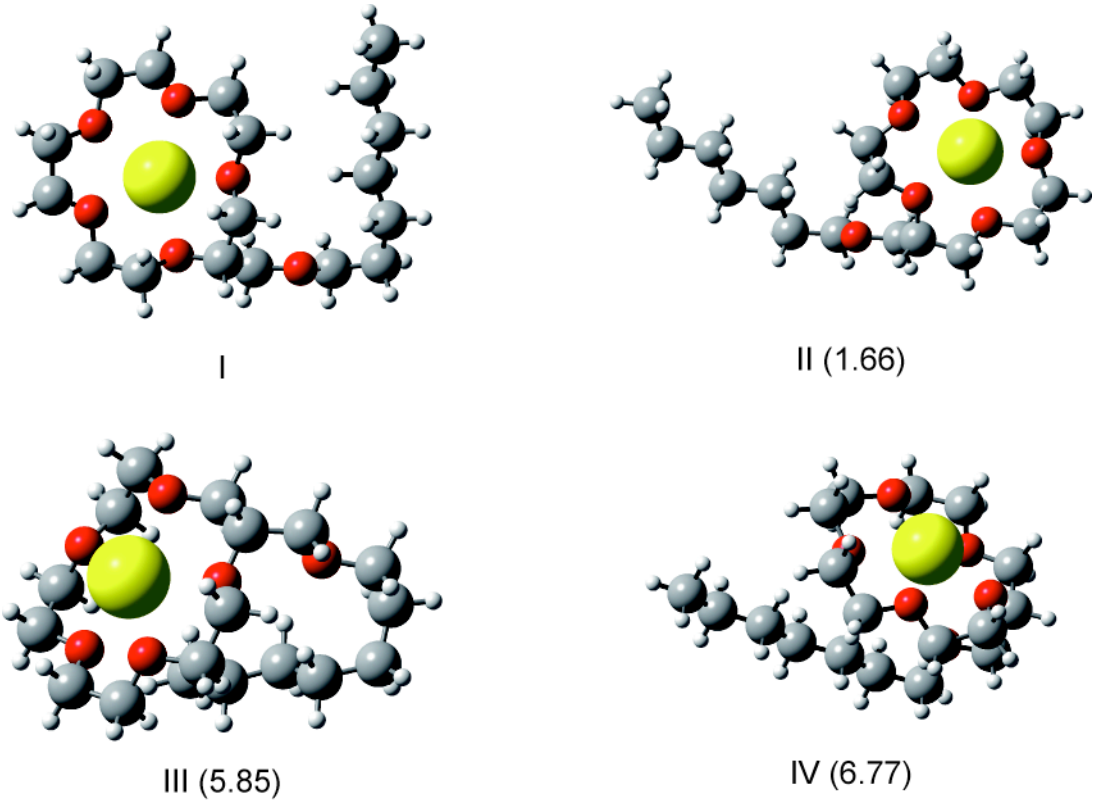

Figure 6S. Stable structures of the Na^{+}•18C6-C_1OC_6-CH_3 complexes calculated at the M05-2X/6-31+G(d) level of theory. The most stable conformer (conformer I) is the same as that shown in Fig. 6. The numbers in the parentheses show the total energy relative to that of the most stable one in kJ/mol.

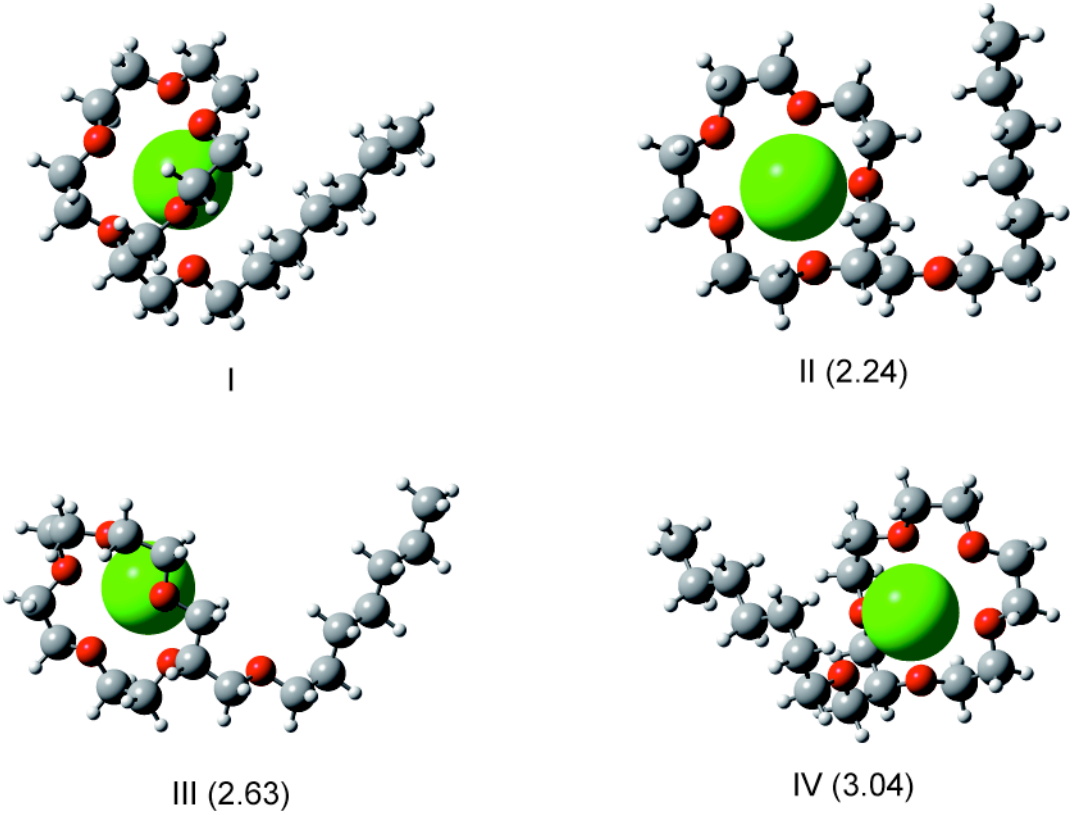

Figure 7S. Stable structures of the K^+•18C6-C_1OC_6-CH_3 complexes calculated at the M05-2X/6-31+G(d) level of theory. The most stable conformer (conformer I) is the same as that shown in Fig. 6. The numbers in the parentheses show the total energy relative to that of the most stable one in kJ/mol.

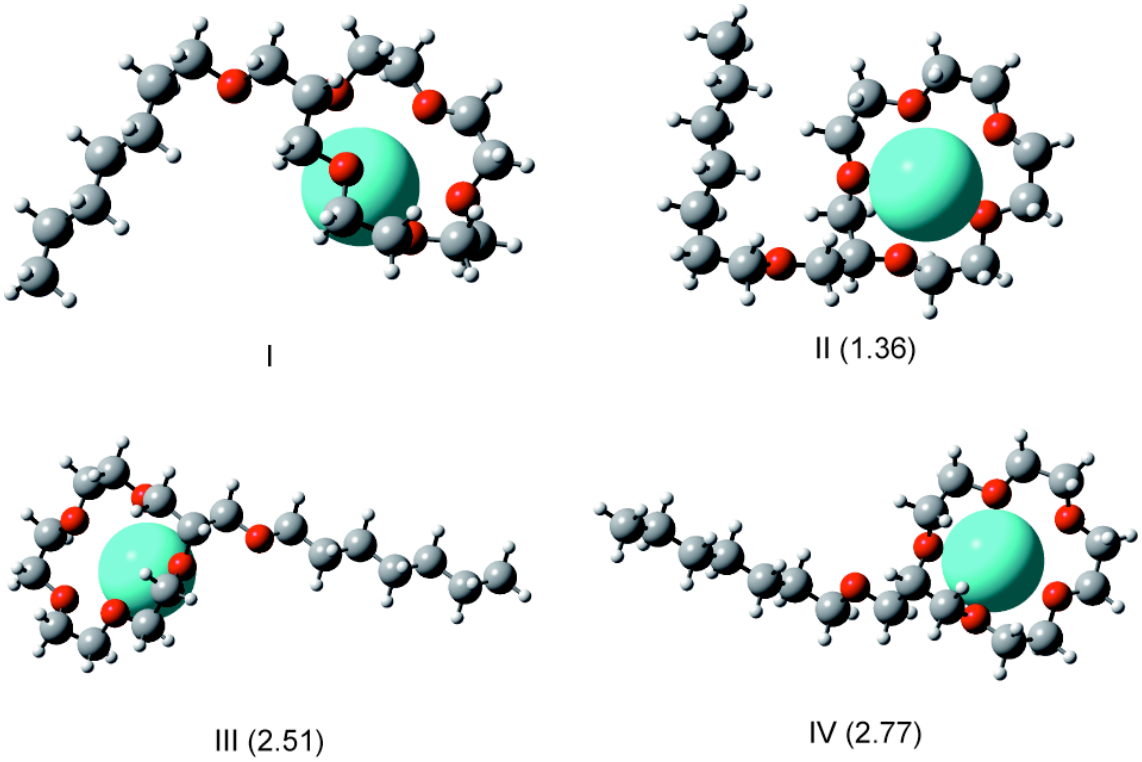

Figure 8S. Stable structures of the Rb^{+}•18C6-C_1OC_6-CH_3 complexes calculated at the M05-2X/6-31+G(d) level of theory. The most stable conformer (conformer I) is the same as that shown in Fig. 6. The numbers in the parentheses show the total energy relative to that of the most stable one in kJ/mol.

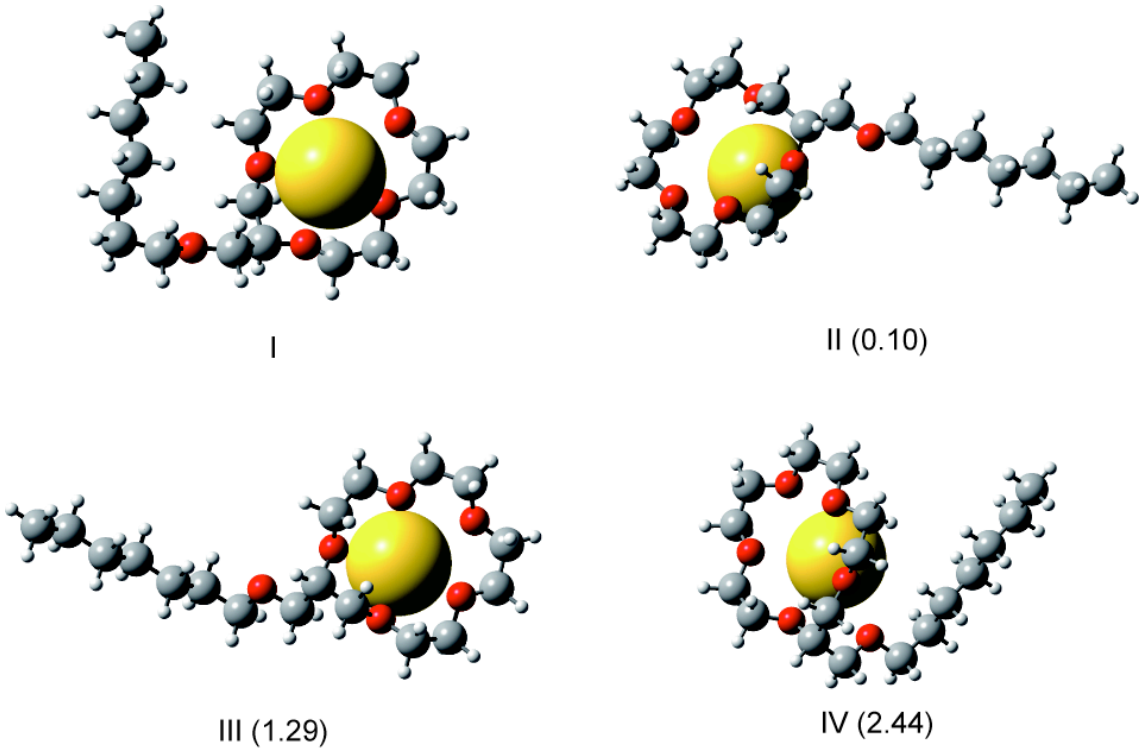

Figure 9S. Stable structures of the Cs^+•18C6-C_1OC_6-CH_3 complexes calculated at the M05-2X/6-31+G(d) level of theory. The most stable conformer (conformer I) is the same as that shown in Fig. 6. The numbers in the parentheses show the total energy relative to that of the most stable one in kJ/mol.