

Supporting information for

Induced VCD and conformational chirality in host-guest complexes of a chiral ammonium salt with crown ethers

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1. Additional figures

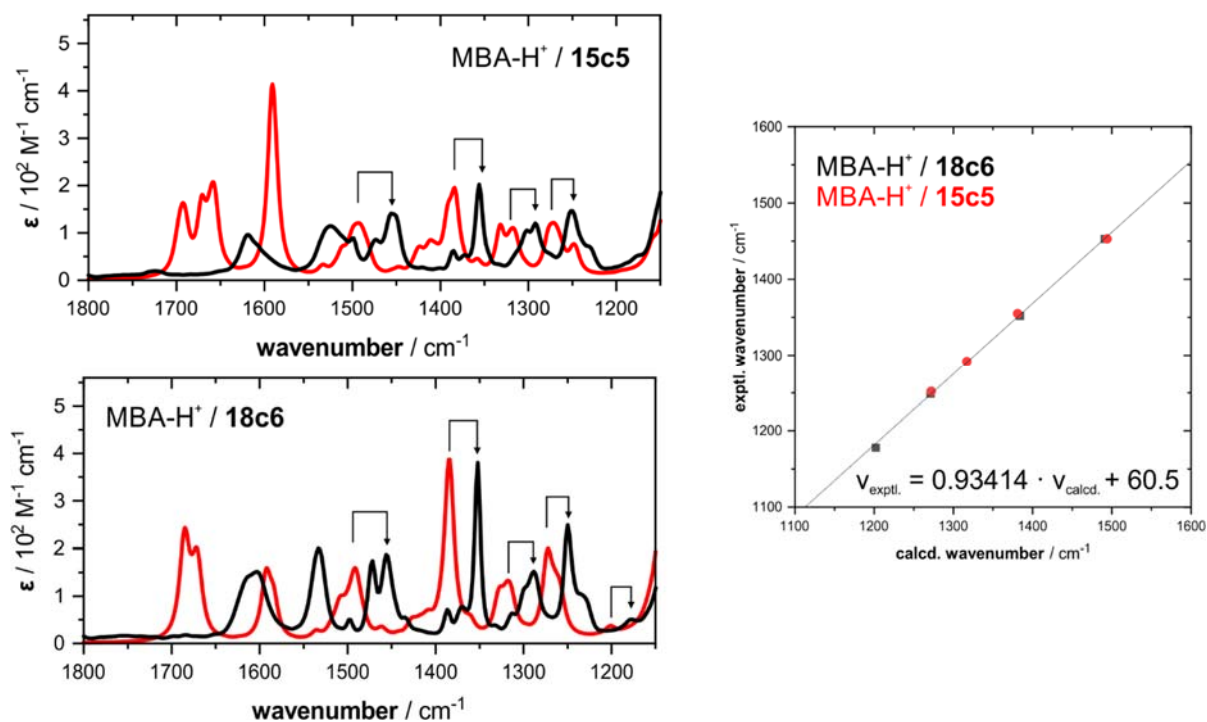


Figure S1. Determination of empirical scaling factor by assignment of unscaled band maxima to unambiguously assignable experimental bands.

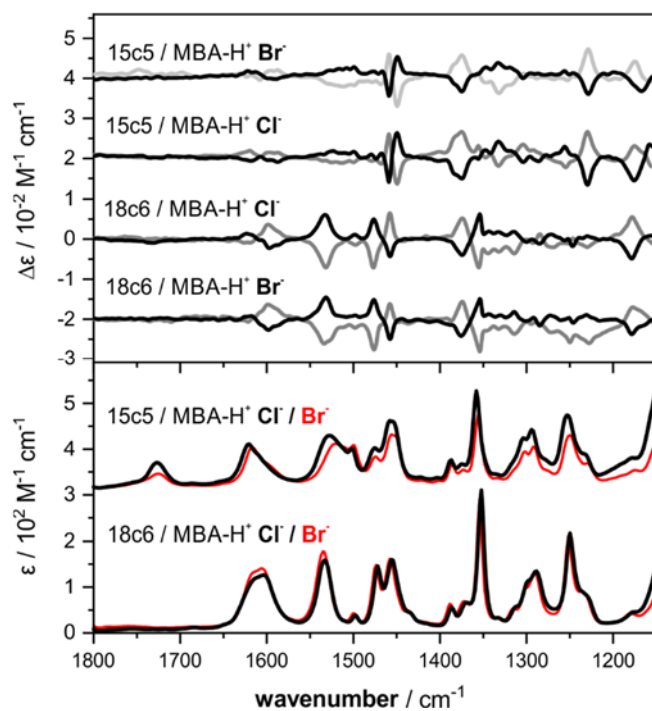


Figure S2. Comparison of the IR and VCD spectra of ammonium-halide salt host-guest complexes with MBA-H⁺ chloride and bromide.

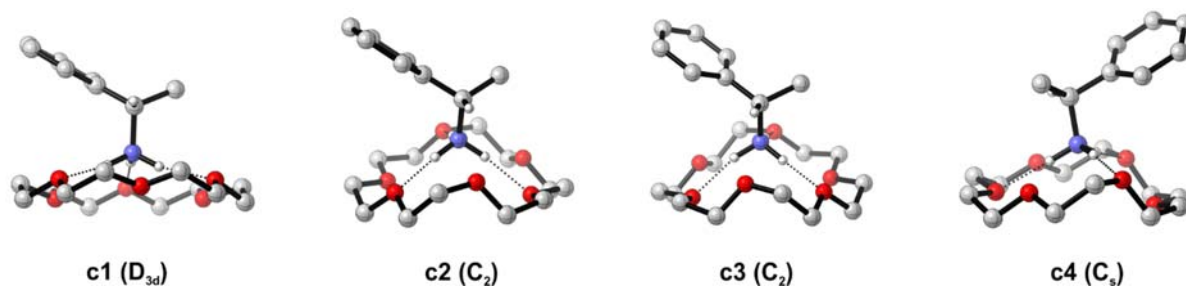


Figure S3. Side views of the four lowest energy conformers of $\text{MBA-H}^+/\text{18c6}$

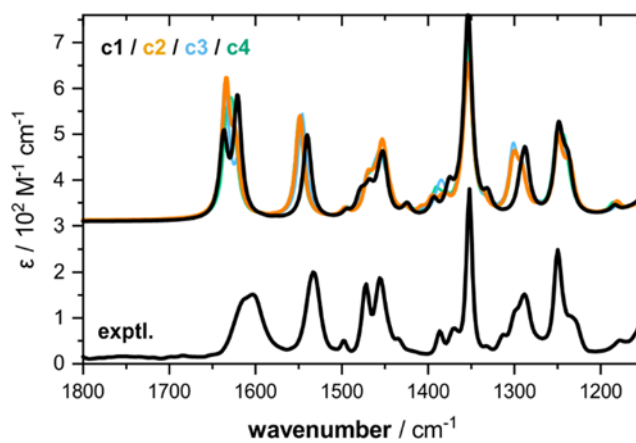


Figure S4. Comparison of the single-conformer IR spectra of $\text{MBA-H}^+/\text{18c6}$ -*c1* to *-c4*

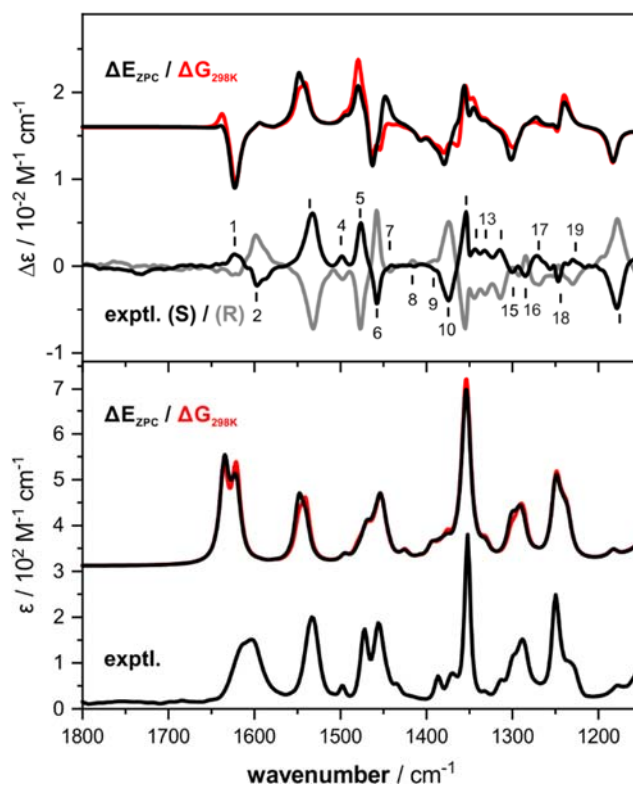


Figure S5. Comparison of the ΔE_{ZPC} and ΔG_{298K} -weighted spectra of **MBA- H^+ /18c6**

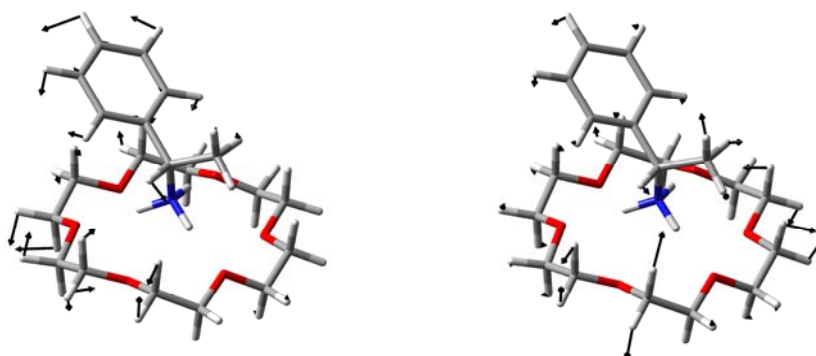


Figure S6. Mixed modes of **MBA- H^+ / 18c6-c1**. Left: Mode 130, 65% localized on ammonium; right: Mode 131, 35 % localized on ammonium.

2. Conformational analysis

Table S1. Energies and populations of the ten lowest energy conformers of **MBA-H⁺ / 18c6** (referenced to E(c1) = -1289.552963 hartree and G(c1) = -1289.613685 hartree)

conformer	ΔE_{ZPC} kcal mol ⁻¹	ΔG_{298K} kcal mol ⁻¹	pop(ΔE) %	pop(ΔG) %
MBA-H ⁺ / 18c6-c1	0.00	0.00	32.8	54.3
MBA-H ⁺ / 18c6-c2	0.10	0.64	27.8	18.5
MBA-H ⁺ / 18c6-c3	0.46	0.93	15.1	11.2
MBA-H ⁺ / 18c6-c4	0.56	1.49	12.8	4.4
MBA-H ⁺ / 18c6-c5	1.22	2.31	4.2	1.1
MBA-H ⁺ / 18c6-c6	1.51	1.46	2.5	4.6
MBA-H ⁺ / 18c6-c7	1.75	2.21	1.7	1.3
MBA-H ⁺ / 18c6-c8	1.94	2.01	1.2	1.8
MBA-H ⁺ / 18c6-c9	2.01	2.53	1.1	0.8
MBA-H ⁺ / 18c6-c10	2.29	1.94	0.7	2.0

Table S2. Energies and populations of the ten lowest energy conformers of **MBA-H⁺ / 15c5** (referenced to E(c1) = -1135.722499 hartree and G(c2) = -1135.779469 hartree)

conformer	ΔE_{ZPC} kcal mol ⁻¹	ΔG_{298K} kcal mol ⁻¹	pop(ΔE) %	pop(ΔG) %
MBA-H ⁺ / 15c5-c1	0.00	0.48	23.3	18.5
MBA-H ⁺ / 15c5-c2	0.13	0.00	18.8	41.2
MBA-H ⁺ / 15c5-c3	0.25	0.85	15.3	9.8
MBA-H ⁺ / 15c5-c4	0.27	1.28	14.7	4.7
MBA-H ⁺ / 15c5-c5	0.33	0.50	13.4	17.6
MBA-H ⁺ / 15c5-c6	0.47	1.20	10.6	5.4
MBA-H ⁺ / 15c5-c7	1.66	2.24	1.4	0.9
MBA-H ⁺ / 15c5-c8	2.01	2.89	0.8	0.3
MBA-H ⁺ / 15c5-c9	2.08	3.16	0.7	0.2
MBA-H ⁺ / 15c5-c10	2.12	2.33	0.7	0.8