Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Chiral discrimination between tyrosine and β-cyclodextrin revealed by cryogenic ion trap infrared spectroscopy

Keisuke Hirata,[1,2,3] Yuta Mori,[1,2] Shun-ichi Ishiuchi*,[1,3,5] Masaaki Fujii*[1,2,3] and Anne Zehnacker*[3,4]

[1]*Laboratory for Chemistry and Life Science, Institute of Innovative Research, Tokyo Institute of Technology, 4259, Nagatsuta-cho, Midori-ku, Yokohama, 226-8503, Japan.*

[2]*School of Life Science and Technology, Tokyo Institute of Technology. 4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa, 226-8503, Japan.*

[3]*Tokyo Tech World Research Hub Initiative (WRHI), Institute of Innovation Research, Tokyo Institute of Technology, 4259, Nagatsuta-cho, Midori-ku, Yokohama, Japan.*

[4] *Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405, Orsay, France.*

[5] *Department of Chemistry, School of Science, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8550, Japan.*

Supplementary Information

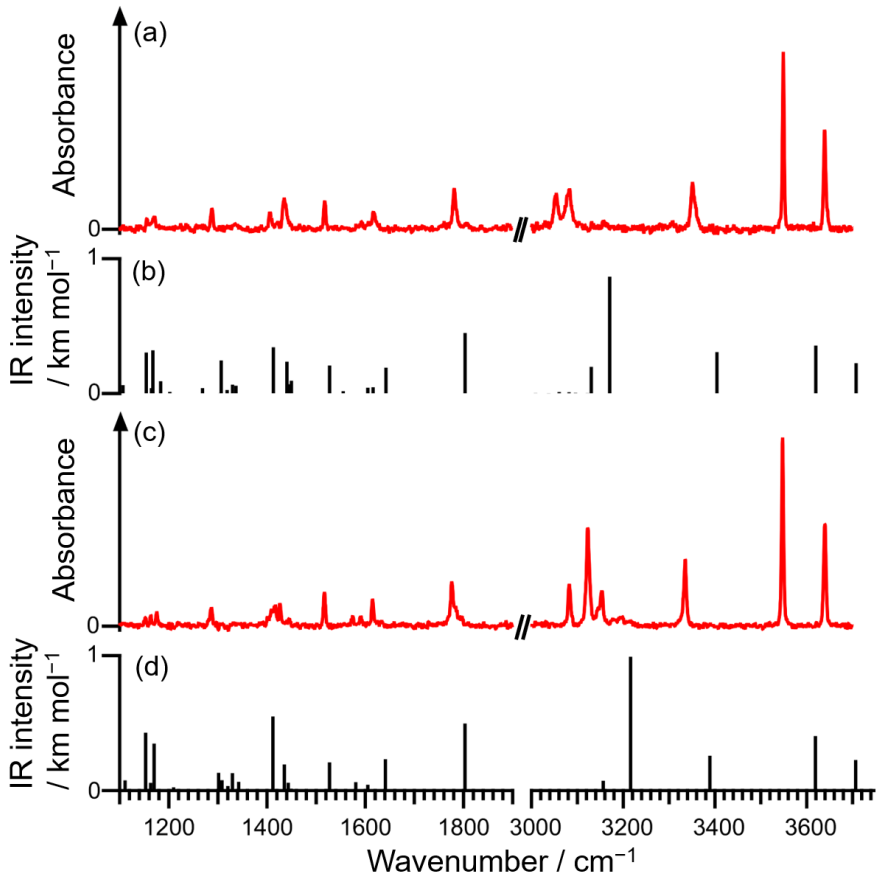

Figure S1 IR-UV ion dip spectra of L-TyrH$^+$ at (a) 35082 (Conf. A) and (c) 35112 cm^{-1} (Conf. B) and calculated IR spectra of (b) Conf. A and (d) B (cam-B3LYP/6-31G(d,p) Scaling factor = 0.961). The nomenclature of the conformers follows that of reference 1. See reference 2 for the experimental scheme.

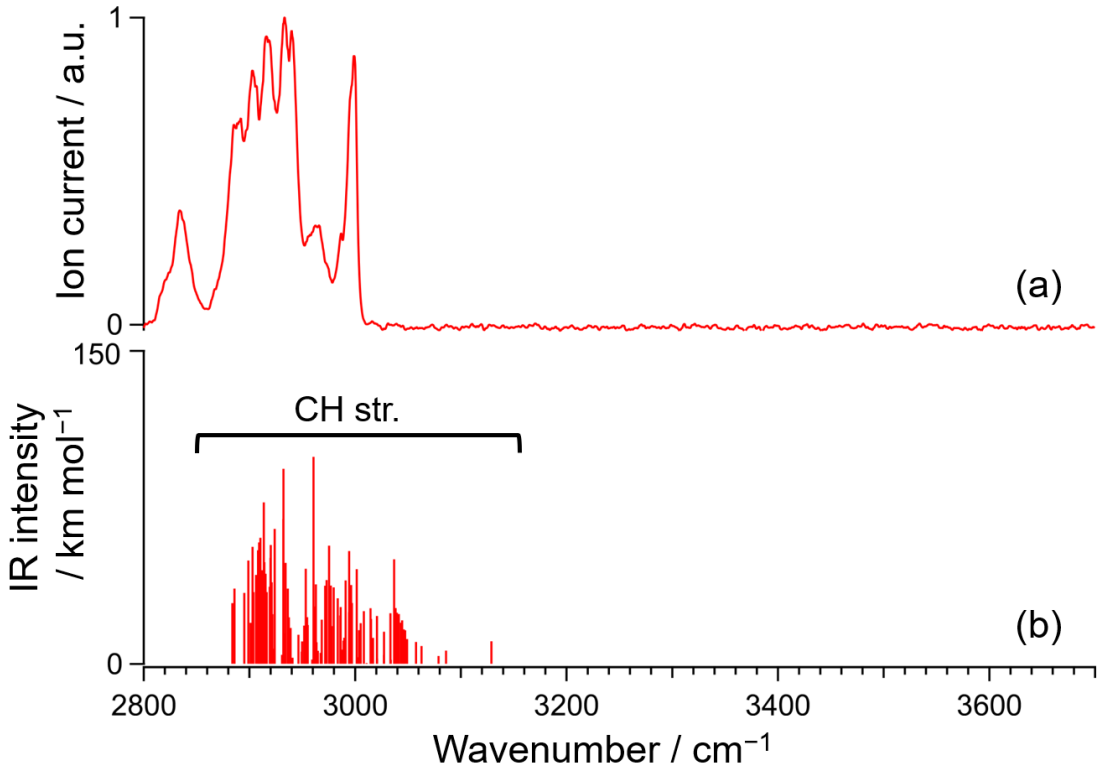

Figure S2 (a) IRPD spectrum of H_2-tagged β-MCDH$^+$ and calculated IR spectrum (cam-B3LYP/6-31G(d,p) Scaling factor = 0.961). Please note that the OH stretch is out of the experimental range.

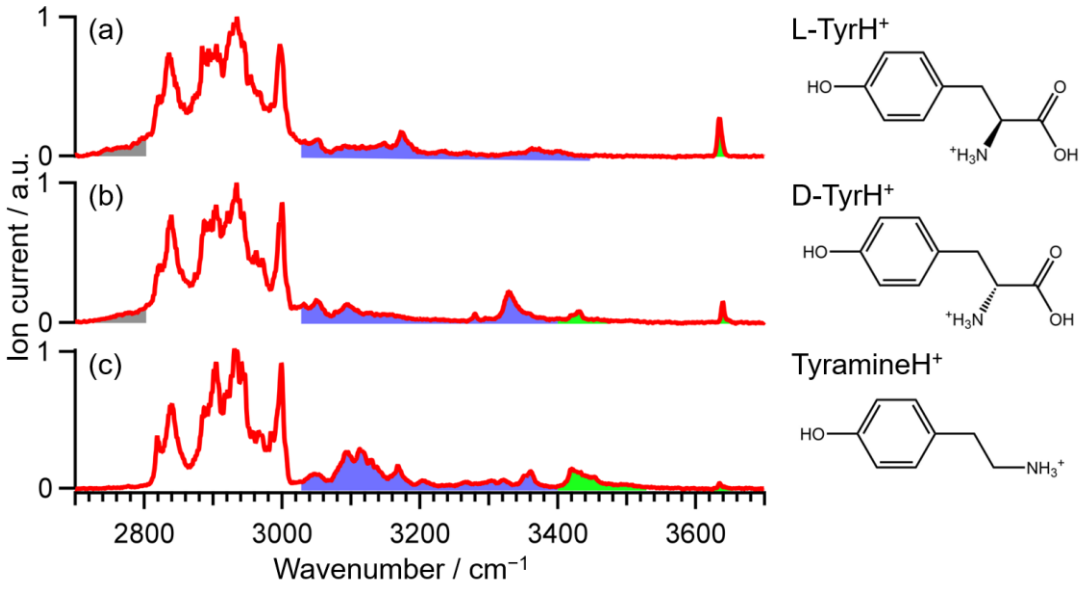

Figure S3 IRPD spectra of H_2-tagged (a) L-TyrH^+-β-MCD, (b) D-TyrH^+-β-MCD, and (c) tyramineH^+-β-MCD in the 3μm region. Green-, gray-, and blue-colored areas correspond to the bands assigned to $\nu(OH_{phenol})$, $\nu(OH_{acid})$, and ν(NH), respectively.

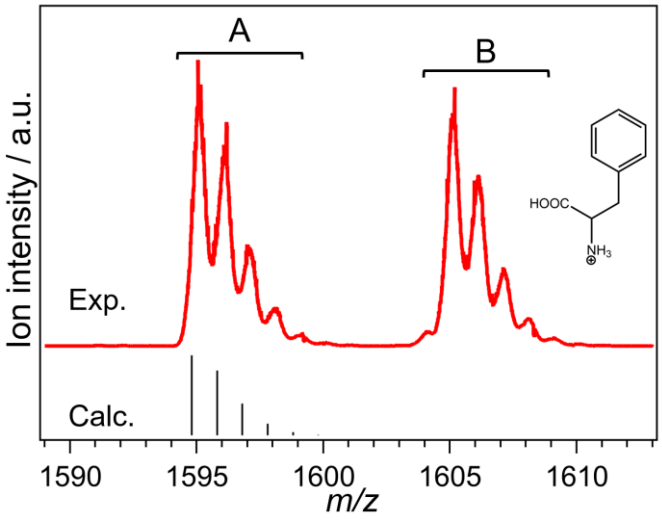

Figure S4 ESI mass spectrum of the solution containing β-MCD, D-phenylalanine (Phe), and isotope (^{13}C, ^{15}N) -labelled L-Phe with the calculated isotope pattern of D-PheH^+-β-MCD. Peak A (B) corresponds to the complex with D-PheH^+ (L-PheH^+). The concentrations of D- and L-Phe are equivalent.

Table S1 Summary of the assignment of the experimentally observed and calculated bands of L-TyrH^+ (Conf. A and B) in the fingerprint region.

	Conf. A		Conf. B	
	Exp.	Calc.*	Exp.	Calc.*
$\nu(OH_{phenol})$	3639	3708	3640	3707
$\nu(OH_{acid})$	3549	3620	3548	3619
$\nu(NH)$	3351	3404	3335	3389
$\nu(NH)_{asym}$	3082	3170	3123	3216
$\nu(NH)_{sym}$	3054	3130	3083	3156
$\nu(CO)$	1781	1803	1776	1803
$\beta(C_{arom}H)$ / $\nu(CC_{arom})$	1617, 1288	1642, 1307	1615,1287	1641, 1302
$\beta(CH)$	1518	1527	1517	1527
$\beta(NH)_{sym}$	1435	1440	1426	1435
$\beta(NH)_{sym}$ / $\nu(C–OH_{arom})$	1407	1412	1417	1412
$\beta(OH_{acid})$	1170	1168	1176	1170
$\beta(OH_{phenol})$	1156	1154	1164	1153

* cam-B3LYP/6-31G(d,p) Scaling factor = 0.961.

References

[1] J. A. Stearns, S. Mercier, C. Seaiby, M. Guidi, O. V. Boyarkin and T. R. Rizzo, *J. Am. Chem. Soc.*, 2007, **129**, 11814–11820.

[2] S. Ishiuchi, H. Wako, D. Kato and M. Fujii, *J. Mol. Spectrosc.*, 2017, **332**, 45-51.