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

Chirality-dependent structuration of protonated or sodiated polyphenylalanines: IRMPD and ion mobility studies

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Supplementary Information

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Table S1. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for LLH^+.

Experiment	LL_{calc1}		LL_{calc2}	
	1088	bend CH	1111	bend CH
1150	1151	bend OH	1157	bend OH
	1395	bend CH	1386	bend CH
1390-1440	1434	Umbrella NH_3^+	1403	Umbrella NH_3^+
1524	1533	bend NH	1555	bend NH (+ scissoring NH_3^+)
1698	1703	stretch C=O	1706	stretch C=O
1772	1778	stretch C=O (Cter)	1764	stretch C=O (Cter)

Table S2. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for LDH^+.

Experiment	LD_{calc}	
	1081	stretch C-C
	1102	bend CH
	1113	bend CH
1155	1151	bend OH
1380-1420	1380	bend CH
	1409	Umbrella NH_3^+
1530	1552	bend NH (+ scissoring NH_3^+)
1697	1706	stretch C=O
1768	1786	stretch C=O (Cter)

Table S3. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for $LLNa^+$.

Experiment	$LLNa^+_{calc1}$		$LLNa^+_{calc2}$	
	1103	stretch C-N	1100	stretch C-N
1165	1158	bend OH	1152	bend OH
	1327	bend CH_2+CH	1333	bend CH_2
			1352	bend CH+CH_2
			1381	bend CH (aliphatic)
	1409	bend CH	1465	bend CH_2
			1501	bend CH (Phe)
1544	1546	bend NH	1537	bend NH
	1630	bend NH_2 (Nter)	1633	bend NH_2 (Nter)
1676	1666	stretch C=O	1655	stretch C=O
1754-1786	1740	stretch C=O (Cter)	1783	stretch C=O (Cter)

Table S4. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for $LDNa^+$.

Experiment	$LDNa^+_{calc}$	
	1088	stretch C-C
	1148	bend CH_2+CH
	1158	bend OH
1155	1213	bend CH_2
	1503	bend CH (Phe)
1380-1420	1508	bend NH
1530	1633	bend NH_2 (Nter)
1697	1653	stretch C=O
1768	1723	stretch C=O (Cter)

Table S5. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for $LLLLH^+$.

Experiment	$LLLL_{calc}$	
1141	1150	bend OH
	1253	bend CH
	1382	bend CH + stretch CC
1444	1474	Umbrella NH_3^+
1498-1520	1498	bend N(1)H
	1525	bend N(2)H
	1544	bend N(3)H
1650	1638	stretch C=O(3) scissoring NH_3^+
	1659	stretch C=O(3) scissoring NH_3^+
1700	1699	stretch C=O(1)
	1727	stretch C=O(2)
1772	1772	stretch C=O (Cter)

Table S6. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for $LDLDH^+$.

Experiment	$LDLD_{calc1}$		$LDLD_{calc2}$	
1241	1170	bend OH	1175	bend OH
	1492	Umbrella NH_3^+	1491	Umbrella NH_3^+
	1500	bend CH (+ bend N(2)H)	1502	bend CH
	1506	bend N(2)H	1509	bend N(2)H
	1543	bend N(3)H	1544	bend N(3)H
1545	1550	bend N(1)H	1560	bend N(1)H
	1641	stretch C=O(3) scissoring NH_3^+	1643	stretch C=O(3) scissoring NH_3^+
	1653	stretch C=O(3) scissoring NH_3^+	1660	stretch C=O(3) scissoring NH_3^+
	1685	stretch C=O(1)	1685	stretch C=O(1) scissoring NH_3^+
1700	1711	stretch C=O(2)	1715	stretch C=O(2)
	1745	stretch C=O (Cter)	1750	stretch C=O (Cter)

Table S7. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for $LLLLNa^+$.

Experiment	$LLLLNa^+_{calc}$	
	1147	bend OH
	1249	bend CH
	1369	bend CH
1500	1495	bend N(2)H
	1514	bend N(1)H
	1535	bend N(3)H
1680	1662	stretch C=O(1)
	1683	stretch C=O(3)
	1708	stretch C=O(2)
1750	1774	stretch C=O (Cter)

Table S8. Comparison between experimental and calculated vibrational frequencies (cm^{-1}) for $LDLDNa^+$.

Experiment	$LDLDNa^+_{calc}$	
	1129	bend CH
	1166	bend OH
	1245	bend CH + stretch CN
	1261	bend CH + stretch CN
1530	1526	bend N(2+3)H
	1528	bend N(2+3)H
	1535	bend N(1)H
1680-1700	1658	stretch C=O(1+2)
	1679	stretch C=O(1+2+3)
	1696	stretch C=O(1+2+3)
1760	1754	stretch C=O (Cter)