The aqueous ROA spectra of 4(R)-hydroxyproline: theory and experiment: supplementary material.

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- Figure S2: The calculated Boltzman averaged Raman spectrum of the zwitterion 4(R)-hydroxyproline (in arbitrary units) and the experimental Raman spectrum of 4(R)-hydroxyproline (less than 100mg/ml) collected at pH=6, acquisition time: 5679s, power at sample 598mW.

- Figure S3: The calculated Boltzman averaged Raman spectrum of the cationic 4(R)-hydroxyproline (in arbitrary units) and the experimental Raman spectrum of 4(R)-hydroxyproline (100mg/ml) collected at pH=1, acquisition time: 3523s, power at sample 524mW.

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Table 1: Description of the wave numbers and amplitudes of the vibrations of the C*4, H4 O7 or H7 atoms in 4-(R)-hydroxyproline as compared to proline.

Zwitterionic form, conformer I				**Cationic form, conformer 1**				**Anionic form conformer A**			
	Amplitude of vibration for:				**Amplitude of vibration for:**				**Amplitude of vibrations for:**		
Wave numbers		**O7H7**	**C*4H4**	Wave numbers		**O7H7**	**C*4H4**	Wave numbers		**O7H7**	**C*4H4**
				1773		/	/				
1674		/	/								
1596		/	w	1599		w	w	1591		/	/
1485		w	w	1483		w	w	1491		w	w
1472		/	w	1470		w	w	1473		w	w
				1433		/	w	1440		m	m
1404		s, in phase	s	1419		s, in phase	s	1406		s	s
1383		/	w	1382		w	w	1385		w	w
1371		w	m	1371		w	s				
1347		w	s	1340		w	m	1339		w	m
1332		w	s	1331		w	m				
1325		s	m								
1319		m	s	1310		m	s	1308		m	m
								1304		m	s
1292		m	m	1296		/	i	1290		m	s
				1260		s	m	1258		w	m
1238		m	m					1235		m	m
1220		w, C*4O7 str	m, C*4O7 str	1227		w, C*4O7 str	m, C*4O7 str				
1194		s	s	1196		w, C*4O7 str	w, C*4O7 str	1195		m	m
1176		w	w	1176		w	m	1168		w	m
								1114		w	/
1087		s, C*4O7 stretch		1094		s, C*4O7 stretch, H4 //		1087		s, C*4O7 stretch	
1057		m	m	1067		w	m	1069		w, C*4O7 str	m, C*4O7 str
1055		w, C*4O7 stretch									
				1030		s	m	1029		w, C*4O7 str	m, H4 perp
1010		w, C*4O7 stretch		1019		w, C*4O7 stretch, H4 perp		975		/	i
951		m, O7 deform	/	958		m, O7 deform		959		C*4O7 stretch	
937		w	m	949		w	m				
919		w	m	909		i	m	905		/	s
879		C*4O7 torsion		870		i	i	873		i	i

853		w	w	851		w, i	i	856		s, O7 deformation	
822		w	/	819		w	w	830		w	i
772		i, O7 deform	w					768		w, C*4O7 def	w
747		w, C*4O7 deformation		740		w, C*4O7 deform		750		w	i
				730		w	w				
701		w	w								
				668		w	i	655		i	i
613		i	i	610		i	i				
				567		i	i	593		i, w	i
462		C*4O7 deform	/	440		i	w	466		i	i
412		C*4O7 deform	i	411		m	i	439		s, //	i
396		w	/	394		i	i	395		m, //	i
331		s, //	/	319		s, //	w	386		s, //	i
308		w, //	s/	284		i	i	298		w, //	i

Description of the amplitude of vibrations: strong=s, medium=m, weak=w, / = no vibration, i=indirect (when the movement of the atom is due to the vibration of other atoms), H7 // = desplacement of hydrogen H7 in a plane parallel to the pyrrolidine ring. If not specified the movement of H7 is in a plane almost perpendicular to the ring, H4 perp or H4 // = desplacement of H4 perpendicular or parallel to the C4*O7 bond.