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

Supplementary Information for

Structural features of monohydrated 2-(4-fluoro-phenyl)-ethylamine: A combined spectroscopic and computational study

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Table S1. Vibrational transition frequencies (cm^{-1}) and intensities (arb. units) as obtained from the measured ionization-loss stimulated Raman and calculated scaled harmonic Raman spectra.

	Measured		Calculated			Measured		Calculated	
	Freq.	Int.	Freq.	Int.		Freq.	Int.	Freq.	Int.
ν_1	3719.8	0.6	3717.1	0.6	ν_{27}	1212.8	0.5	1208.1	0.3
ν_2	3401.6	0.4	3413.2	0.4	ν_{28}			1195.6	0.1
ν_3	3355.6	0.4	3354.7	0.6	ν_{29}	1165.4	0.3	1152.6	0.1
ν_4	3328.6	0.6	3331.2	0.8	ν_{30}	1141.3	0.2	1139.2	0.1
ν_5	3083.4	0.9	3080.1	0.9	ν_{31}	1109.2	0.2	1097.2	0.0
ν_6			3078.8	0.9	ν_{32}	1080.0	0.2	1081.3	0.2
ν_7	3028.4	0.2	3043.7	0.4	ν_{33}	1030.3	0.3	1036.3	0.1
ν_8	3017.4	0.2	3041.1	0.4	ν_{34}			1010.1	0.0
ν_9	2972.5	0.5	2984.1	0.3	ν_{35}			993.9	0.0
ν_{10}	2963.9	0.6	2946.0	1.2	ν_{36}			951.2	0.0
ν_{11}	2939.2	0.5	2918.7	0.8	ν_{37}	901.9	0.1	919.9	0.1
ν_{12}	2868.0	0.4	2867.3	0.7	ν_{38}	893.9	0.4	908.0	0.2
ν_{13}	1639.7	0.1	1640.6	0.3	ν_{39}	869.8	0.2	872.4	0.1
ν_{14}	1618.8	0.1	1626.0	0.2	ν_{40}	840.6	0.3	841.0	0.4
ν_{15}	1606.8	0.1	1606.2	0.1	ν_{41}	822.3	0.4	832.1	1.1
ν_{16}	1584.8	0.2	1595.5	0.1	ν_{42}	816.5	0.2	826.4	0.0
ν_{17}	1556.6	0.1	1522.5	0.0	ν_{43}			735.3	0.0
ν_{18}	1474.2	0.2	1475.1	0.2	ν_{44}			715.2	0.1
ν_{19}	1453.0	0.2	1456.7	0.2	ν_{45}			703.9	0.1
ν_{20}	1436.9	0.1	1424.9	0.0	ν_{46}	612.1	0.2	632.2	0.4
ν_{21}			1382.3	0.0	ν_{47}	561.0	0.3	555.8	0.0
ν_{22}	1348.6	0.3	1343.4	0.3	ν_{48}	490.1	0.3	499.3	0.1
ν_{23}			1309.1	0.2	ν_{49}	468.0	0.3	472.4	0.1
ν_{24}			1298.5	0.0	ν_{50}	414.9	0.1	430.0	0.1
ν_{25}			1288.7	0.0	ν_{51}			416.9	0.0
ν_{26}	1234.7	0.3	1249.9	0.6	ν_{52}			414.9	0.2