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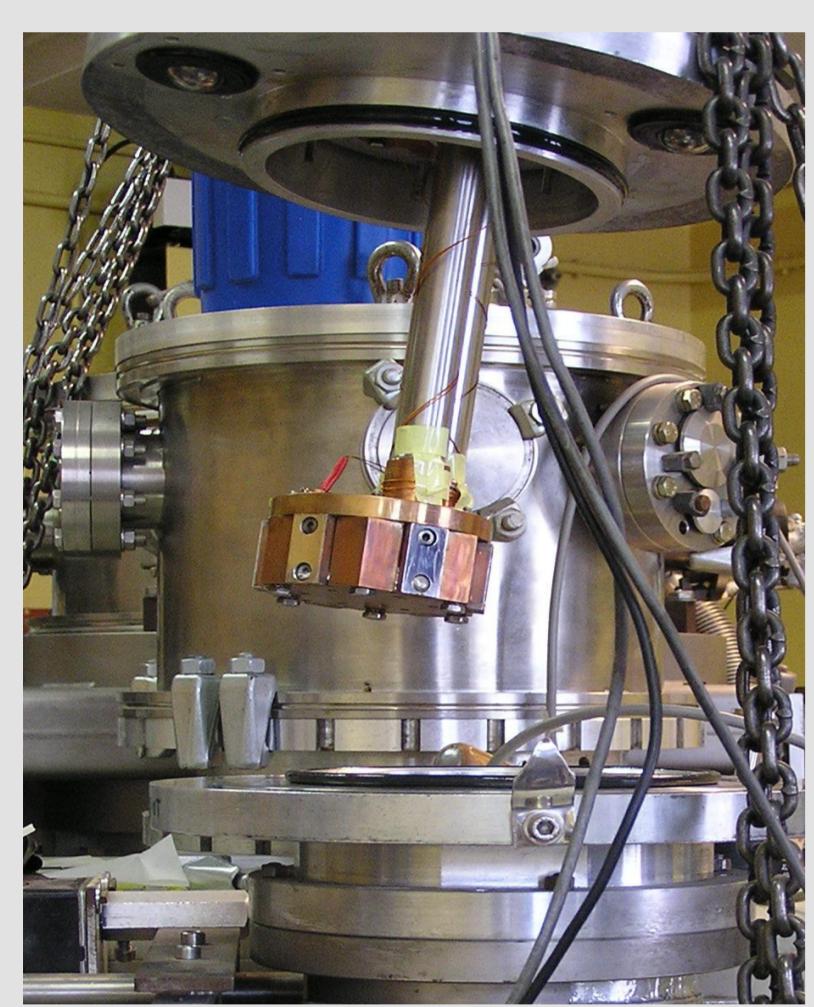
First infrared spectra of the acrylonitrile-water

hydrogen-bonded complexes isolated in solid neon

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The nitrile molecules have been detected in a variety of interstellar environments and these molecules are interest in astrochemistry. The experimental study of the complexation of acrylonitrile molecule (AN) with water has been undertaken from a vibrational point of view in solid neon at 3 K from 80 to 6000 cm⁻¹ using Fourier transform infrared spectroscopy. With the help of theoretical results we have identified several vibrational transitions for AN-H₂O and AN-(H₂O)₂ complexes. For the AN-H₂O complex, in which the two submolecules interacting through hydrogen bonding, the infrared spectral changes (frequencies as well as intensities) indicate that the water plays the role of the proton donor. We highlight the presence of three isomers for the AN-H₂O complex and two isomers for the AN-(H₂O)₂ complex. Theoretical calculations at the MP2/AVTZ level have been performed to obtain their equilibrium geometries and vibrational spectra at the harmonic level and comparison with experimental data allows us to give structures of these complexes.

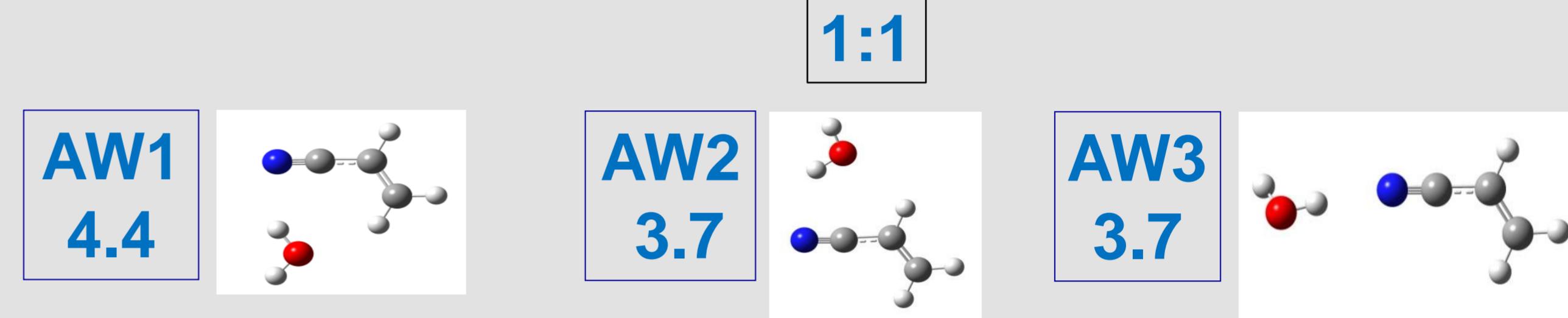


Advantages of our matrix isolation apparatus coupled with FTIR

Absorption spectra collected on the same sample from the Far IR (intermolecular region) to Near IR (combinations and overtones region) from 80 to 6000 cm⁻¹ with a Bruker 120 FTIR spectrometer (InSb or MCT or bolometer detectors).

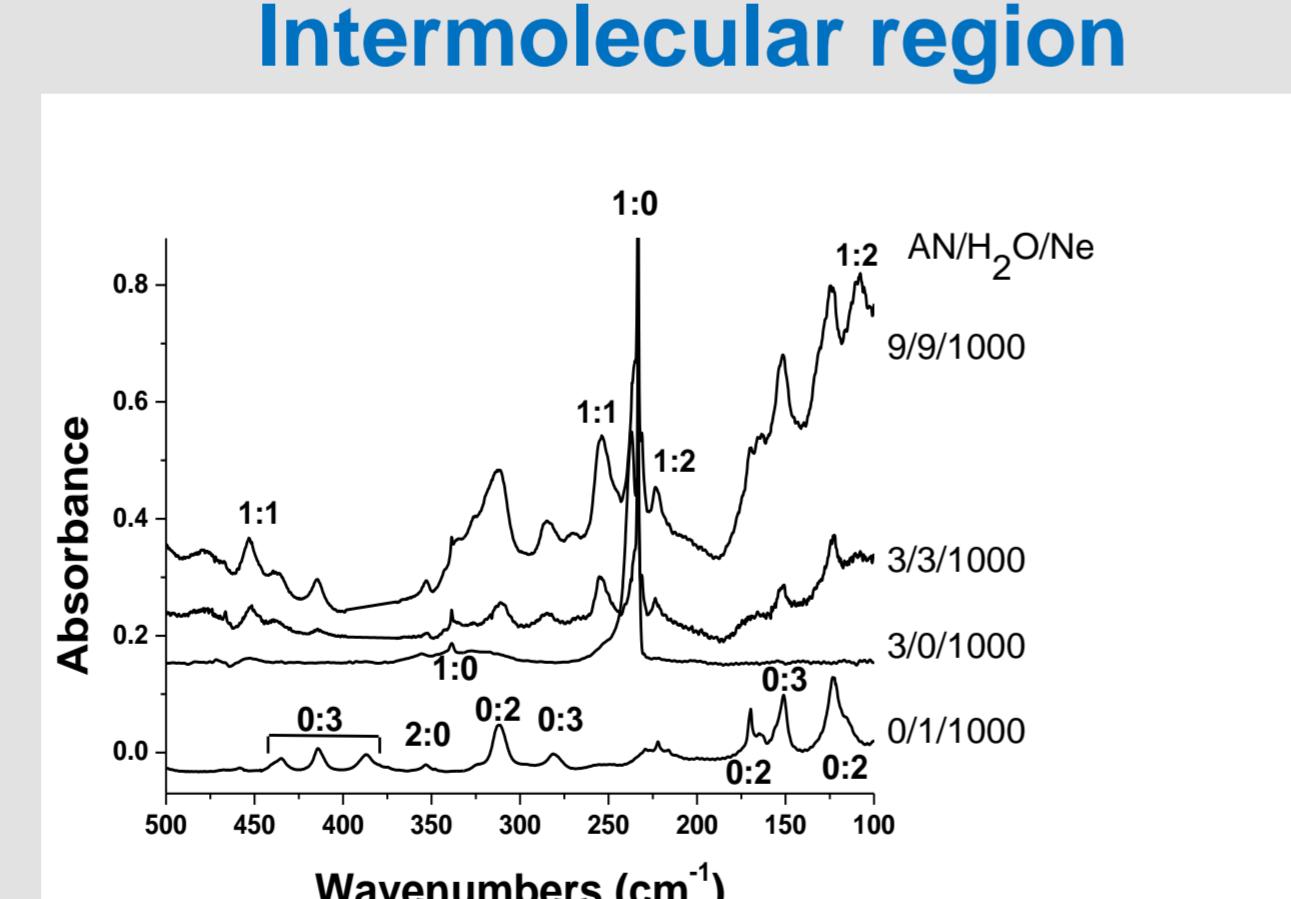
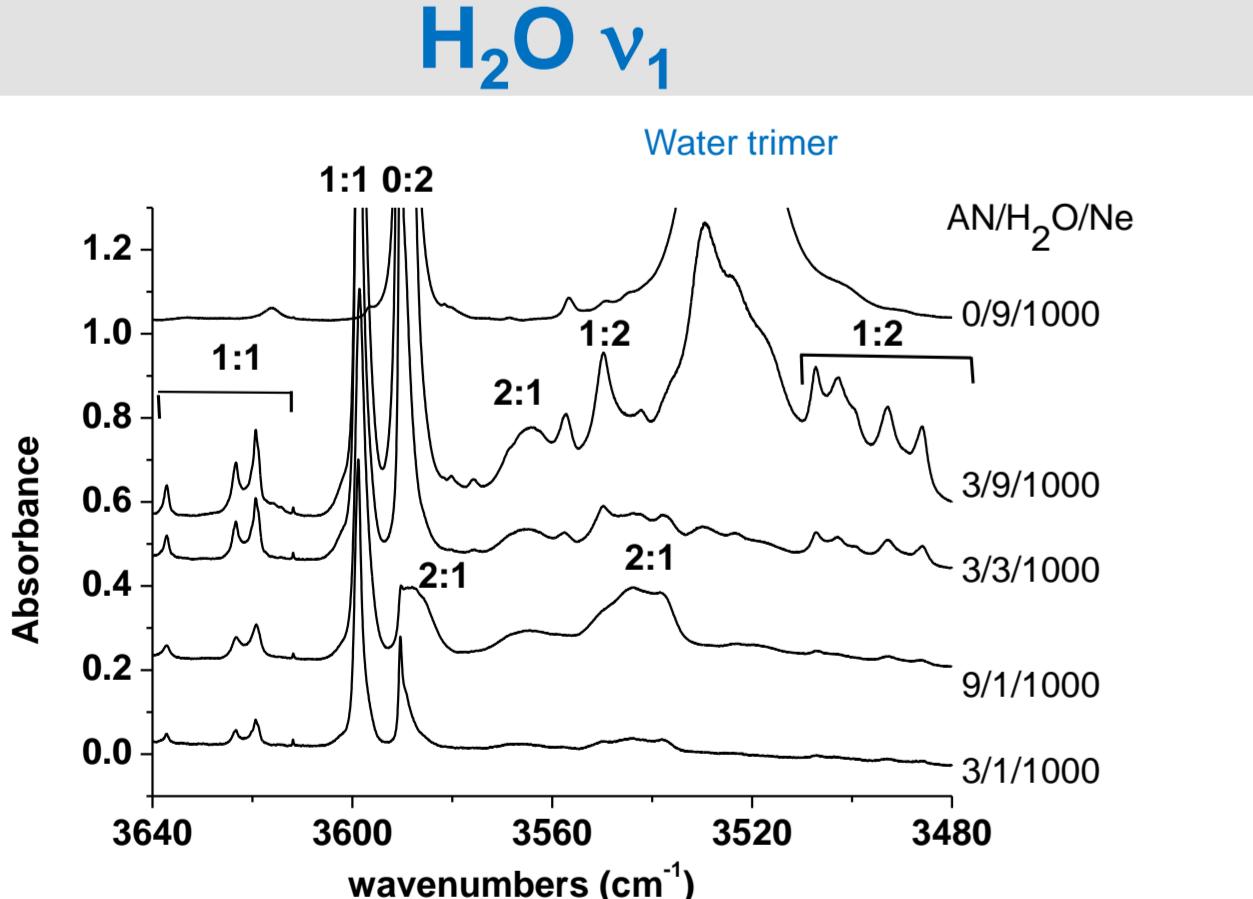
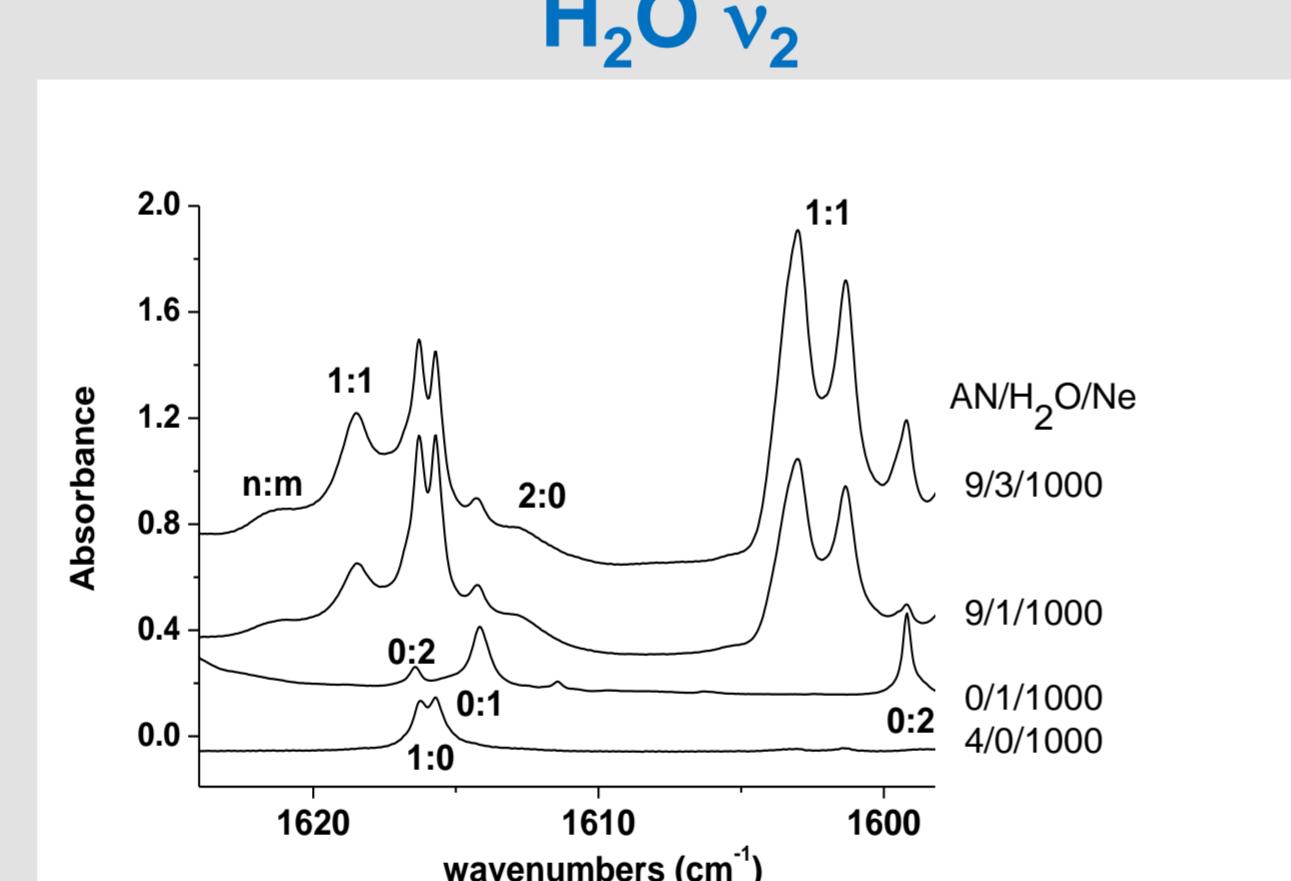
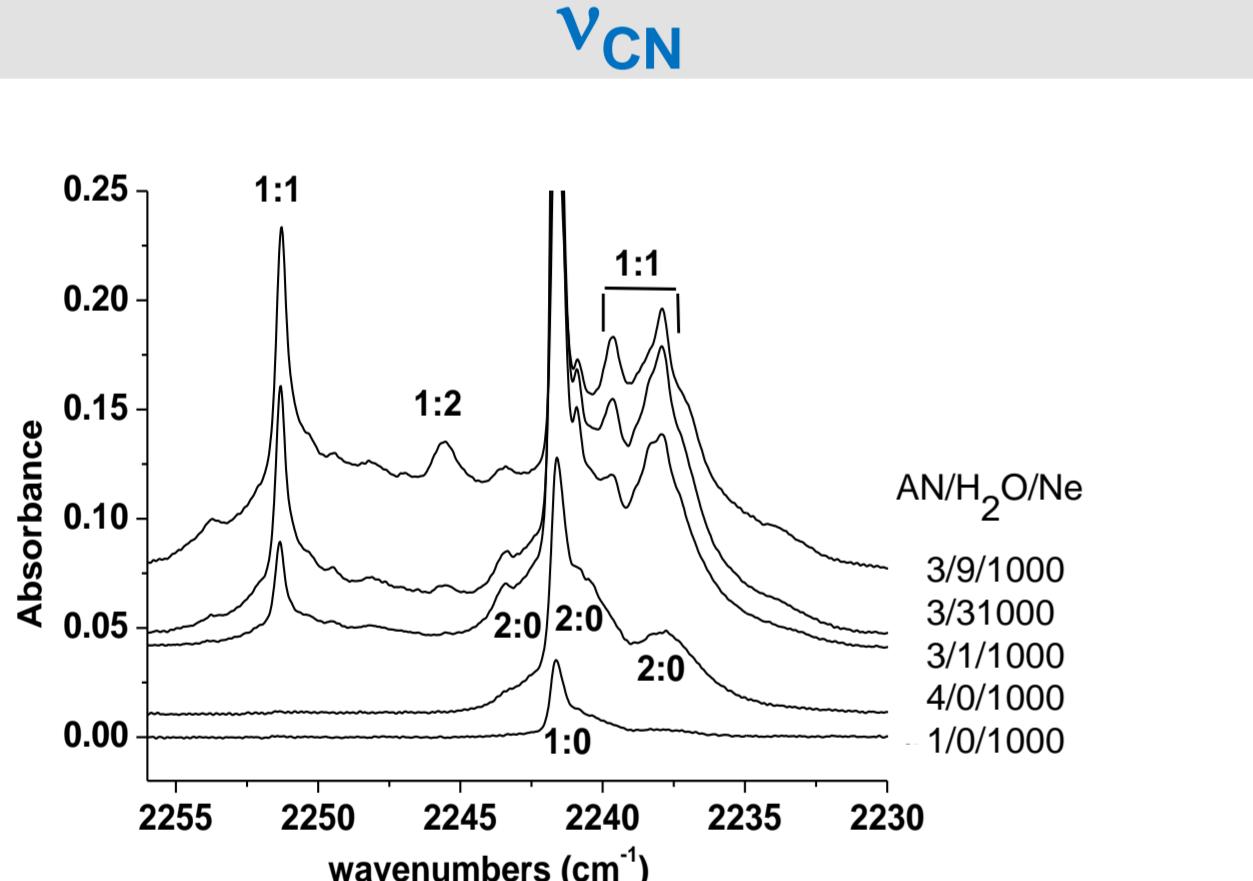
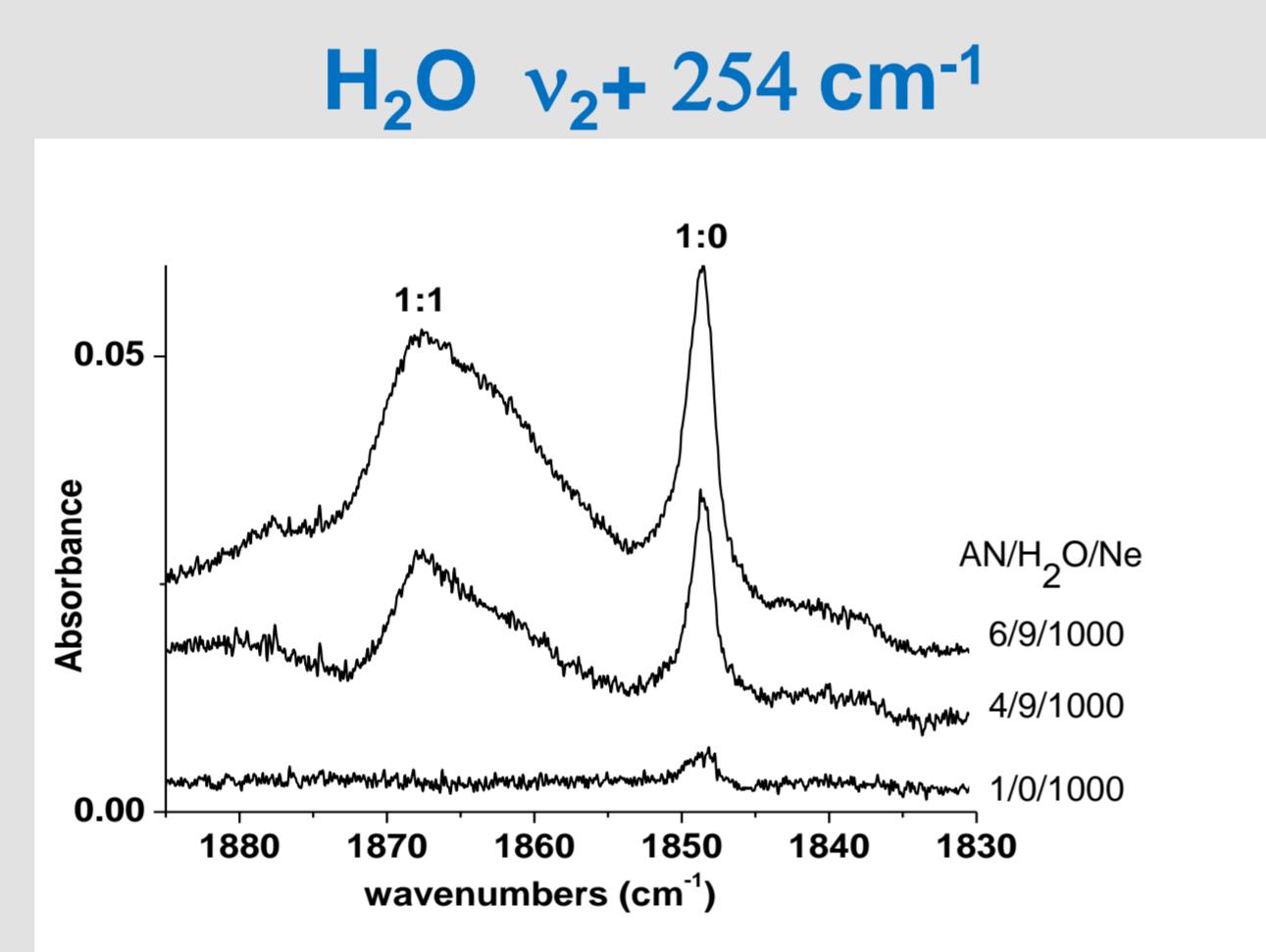
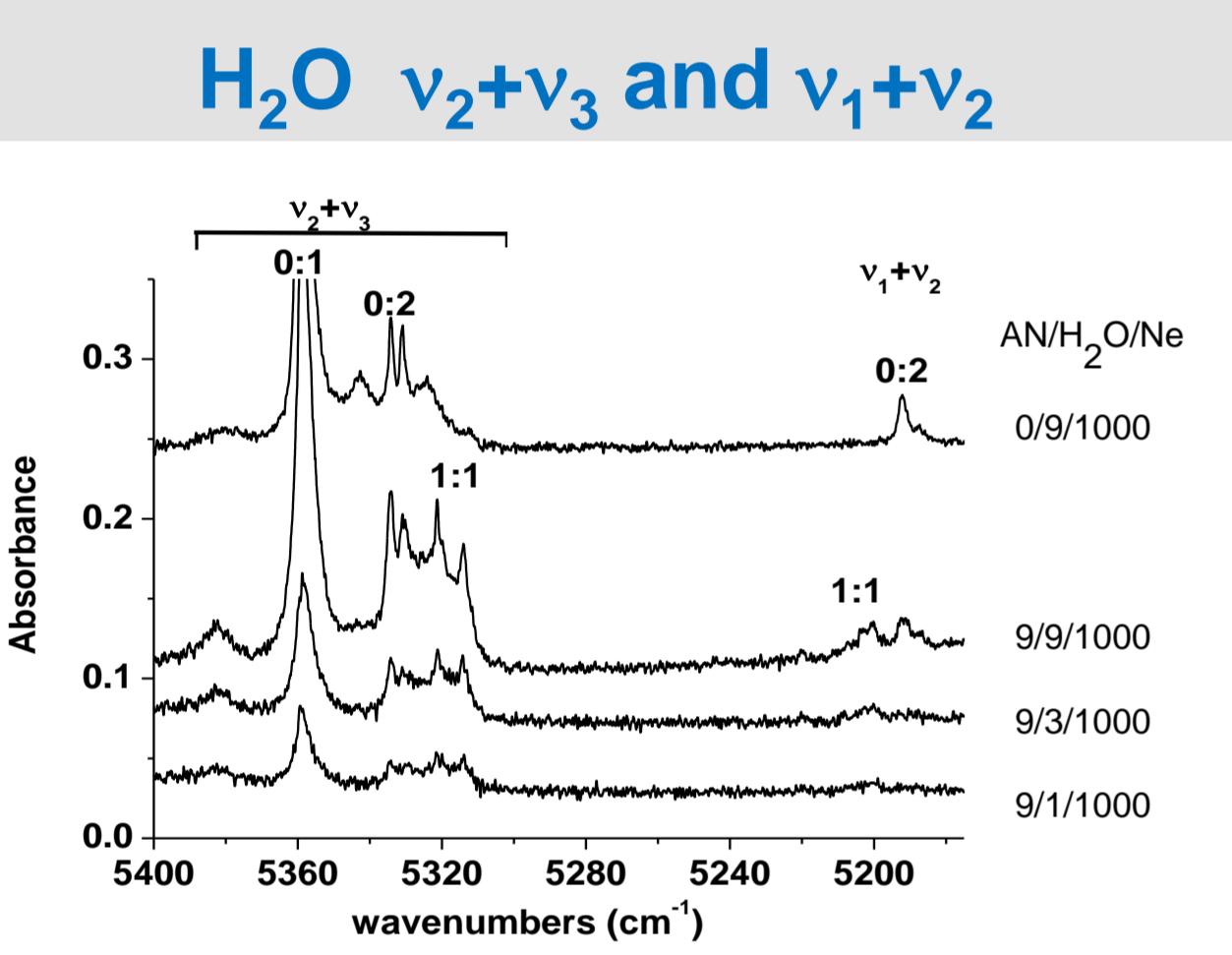
MP2/AVTZ calculations for energy, geometry and frequencies

complexes structures with D₀(kcal/mol)



AW1 is the isomer observed in gas phase by millimeter spectroscopy¹

Infrared spectra in the acrylonitrile and water regions



Comparison with other nitrile-water complexes

	HCN	C ₆ H ₅ (CH ₂) ₂ CN	CH ₂ =CHCN	C ₆ H ₅ CN	CH ₃ CN
H ₂ O v ₁ red-shift	44	57	67	66	99
D ₀ (kcal/mol)	3.0	4.2	3.7	4.4	4.5
	Solid Ar	gas	Solid Ne	Solid Ar	Solid Ar
v _{CN} blue-shift	19	-	10	10	8
Ref	2,3	4	This work	5	6

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Comparison of frequencies (cm⁻¹) and shifts ($\Delta v = v_{\text{mono}} - v_{\text{complex}}$) for the 1:1 complex

	Calculated						Exp	Isomer
	AW1	ω	Δ	AW2	ω	Δ		
H₂O								
v ₃	3918	30		3925	23		3740	20
							3736	24
							3731	29
v ₁	3771	51		3791	31		3599	67
							3621	43
							3637	28
v ₂	1632	-8		1629	-5		1601	-6
							1603	-8
							1618	-23
								AW3
Acrylonitrile								
v ₄	2177	2		2176	3		2251	-10
							2240	2
							2238	4
v ₈	1111	-5		1108	-2		1095	-2
							1099	-6
v ₁₃	990	-17		975	-2		960	-6
							969	-15
v ₁₄	574	-16		561	-3		691	-6
v ₁₁	235	-9		226	0		231	2
Inter	367			303			453	
							291	
							262	
							302	
							254	
								AW1-2-3

Identification of three isomers for 1:1 complex: observation of three bands for the v₁ water mode separated by 12-25 cm⁻¹

Comparison of frequencies and shifts for the 1:2 complex

	Calculated				Exp	Isomer
	ADW1	ω	Δ	ADW2		
H₂O						
v ₁ PA	3679	135		3696	118	
					3507	154
					3550	111
v ₁ PD	3598	121		3609	110	
					3486	105
					3493	98
Acrylonitrile						
v ₄	2189	-10		2183	-4	
v ₁₂	1064	-29		1026	-21	
					998	-27
v ₁₄	581	-23		575	-17	
Inter	118			108		
				138		
				215		
				210		
				223		
						ADW1 or 2

PA: proton acceptor and PD: proton donor for H₂O dimer

Identification of two isomers for 1:2 complex: observation of two bands for the v₁ water mode