Supplementary Information

Azidoacetylene - interpretation of gas phase infrared spectra based on high-level vibrational configuration interaction calculations

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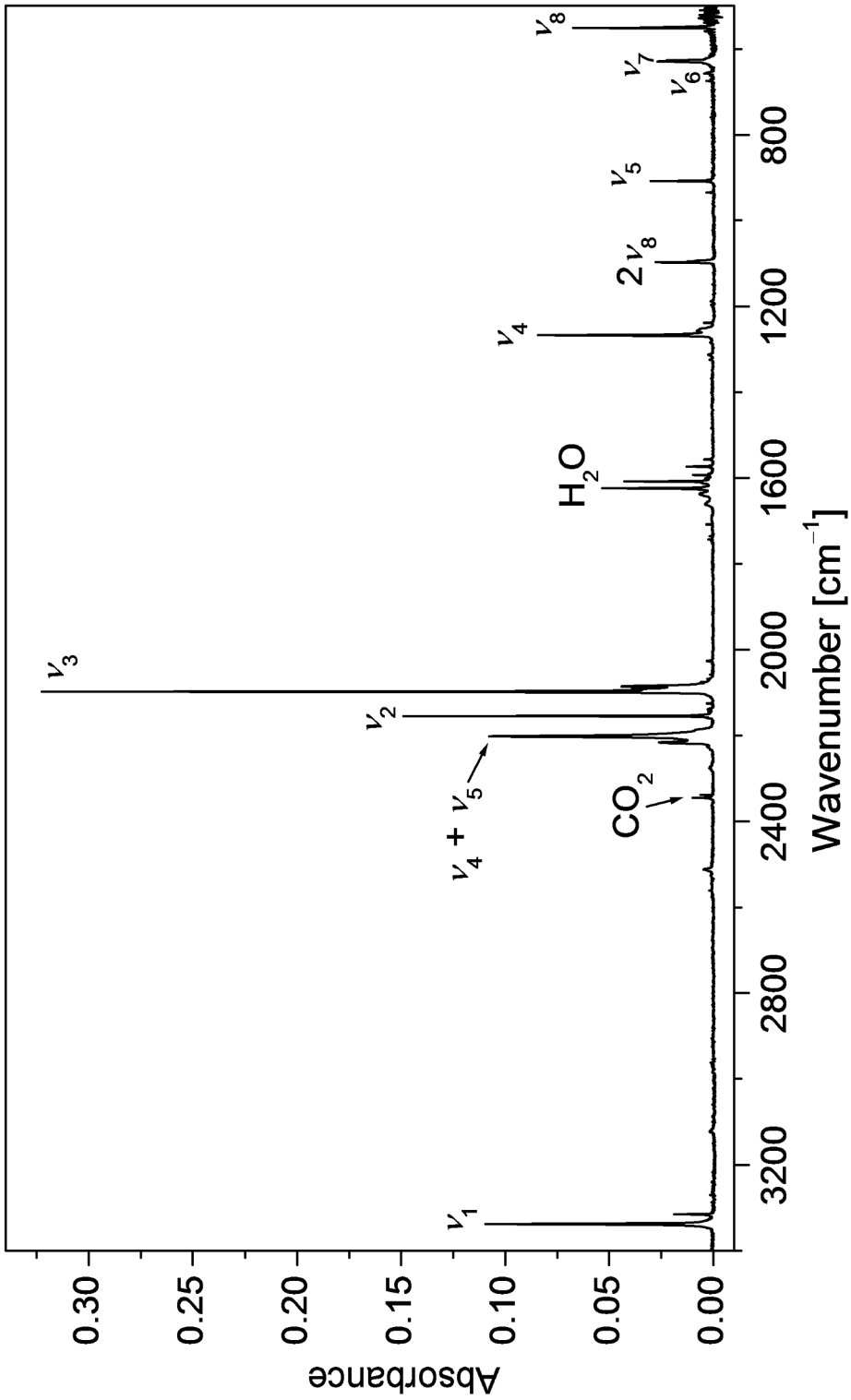
- **Table S1: CCSD(T)-F12a/cc-pVTZ-F12 geometry of azidoacetylene.**

C	-0.0851248138	0.0000000000	-1.1520521261
N	-0.7572864967	0.0000000000	0.0311230351
N	-0.0376583311	0.0000000000	1.0541530508
N	0.4617463870	0.0000000000	2.0664497723
C	0.4025896430	0.0000000000	-2.2554187260
H	0.8495752156	0.0000000000	-3.2189989220

- **Table S2: Scaled (0.969) and unscaled harmonic B3LYP/cc-pVTZ frequencies of azidoacetylene.** Deviations (Δ) refer to the scaled values relative to our gas phase data.

	DFT	DFT(scaled)	Δ
ν_1	3479.1	3371.2	30.2
ν_2	2273.7	2203.2	54.3
ν_3	2230.0	2160.9	68.9
ν_4	1349.9	1308.0	51,0
ν_5	918.3	889.8	21.2
ν_6	673.1	652.2	15.8
ν_7	666.8	646.1	12.1
ν_8	574.8	557.0	5.0
ν_9	532.5	515.9	3.9
ν_{10}	441.6	427.9	13.9
ν_{11}	413.6	400.7	20.7
ν_{12}	160.8	155.8	-

- **Figure S1: Matrix IR spectrum of azidoacetylene.**



- **Figure S2: Section of the IR spectrum of azidoacetylene measured at -20°C in $CHCl_3$ solution.**