Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

A Helium Nanodroplet Setup for Mid and Far-Infrared Spectroscopy using Pulsed-Free Electron Lasers: Vibrational Spectra of Propargyl Alcohol.

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Table S1. Coordinates of the optimized geometries of gauche and trans-propargyl alcohol at MP2/6-311+G(3df,2p) level.

	gauche-PA			trans-PA		
Atom	x (Å)	y(Å)	z(Å)	x(Å)	y(Å)	z(Å)
C	1.92120	-0.21663	-0.01240	-1.94127	-0.20695	0.00000
C	0.76867	0.16507	-0.00497	-0.77694	0.13287	0.00007
H	2.93150	-0.54653	-0.03079	-2.95810	-0.51574	-0.00020
C	-0.63161	0.59001	0.03550	0.61353	0.57254	0.00011
O	-1.54097	-0.49073	-0.09835	1.45463	-0.57321	0.00020
H	-0.83943	1.25870	-0.79788	0.79143	1.19006	0.88521
H	-0.81288	1.14468	0.96031	0.79151	1.19006	-0.88497
H	-1.30104	-1.16173	0.54640	2.36620	-0.26947	-0.00268

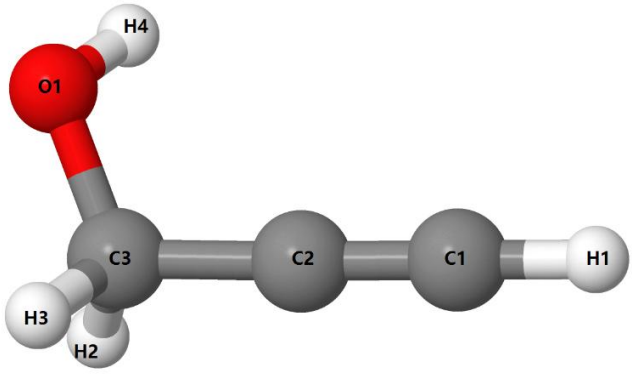

Figure S1. Optimized geometry of gauche-PA at MP2/6-311+G(3df,2p) level.

Table S2. Energies (E) in cm-1 and Integrated intensities in km.mol-1 for gauche and trans-PA for under harmonic and anharmonic approximations at MP2/6-311+G(3df,2p) level. An approximate description of corresponding normal modes is also given. Refer to Figure S1 for atom numberings.

gauche-PA					Trans-PA				
Mode (Quanta)	E (harm)	E (anharm)	I(harm)	I (anharm)	E (harm)	E (anharm)	I (harm)	I (anharm)	Approximate mode description
1(1)	3869.4	3682.4	44.3	38.7	3871.4	3690.5	42.1	37.3	O-H stretch
2(1)	3484.4	3356.9	57.0	51.2	3487.4	3359.9	55.0	49.4	acetylenic C-H stretch
3(1)	3147.4	3009.1	5.2	5.8	3092.9	2953.3	14.5	17.3	antisymmetric CH2 stretch
4(1)	3066.5	2905.9	28.3	29.6	3049.6	2908.3	34.1	35.3	symmetric CH2 stretch
5(1)	2133.2	2094.1	1.8	1.6	2146.3	2104.0	2.6	2.5	C≡C stretch
6(1)	1518.5	1477.4	1.9	1.6	1526.0	1480.3	1.1	1.1	CH2 Scissoring
7(1)	1423.0	1382.2	51.0	44.0	1454.0	1410.0	25.1	19.4	CH2 wagging coupled with C-OH bending
8(1)	1361.8	1320.6	2.8	4.0	1276.8	1247.6	0.0	0.0	O1C3H3 bending coupled with C3O1H4bending
9(1)	1227.5	1198.9	17.1	13.9	1247.1	1236.0	65.2	58.0	CH2 twist coupled with C3O1H4 bend for gauche-PA And CH2 wagging coupled with C3O1H4 bend for trans-PA
10(1)	1080.6	1044.1	106.5	97.7	1081.5	1044.3	112.4	118.5	C3O1 stretch
11(1)	1006.0	989.1	18.4	17.5	1042.1	1014.9	4.1	3.3	CH2 rock coupled with C3O1H4 bend
12(1)	923.3	912.5	23.8	24.8	922.5	912.6	9.7	8.9	C2C3 stretch coupled with C3O1H4 bend
13(1)	673.2	662.8	37.5	36.4	675.7	664.7	36.1	35.4	C2≡C1-H1 bend in the C-C-O plane
14(1)	647.8	637.0	45.8	44.4	645.3	635.9	44.7	44.0	C2≡C1-H1 bend perpendicular to C-C-O plane
15(1)	557.9	549.9	12.5	9.2	549.8	551.1	3.1	1.7	carbon chain bend parallel to C3-O1 bond, coupled with large amplitude COH motion
16(1)	326.9	298.9	67.5	25.2	308.1	308.6	0.2	7.1	carbon chain bend perpendicular to C3-O1 bond, coupled with large amplitude O-H and CH2 motions
17(1)	263.2	242.7	61.7	104.4	225.5	181.2	128.1	110.7	carbon chain bend perpendicular to C3-O1 bond, coupled with large amplitude O-H and CH2 motions
18(1)	190.5	189.7	7.9	16.9	202.6	199.8	8.7	8.0	carbon chain bend parallel to C3-O1 bond, coupled with large amplitude COH motion