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Electronic Supplementary Information to:

C_β-H stretching vibration as a new probe for conformation of n-propanol in gaseous and liquid States

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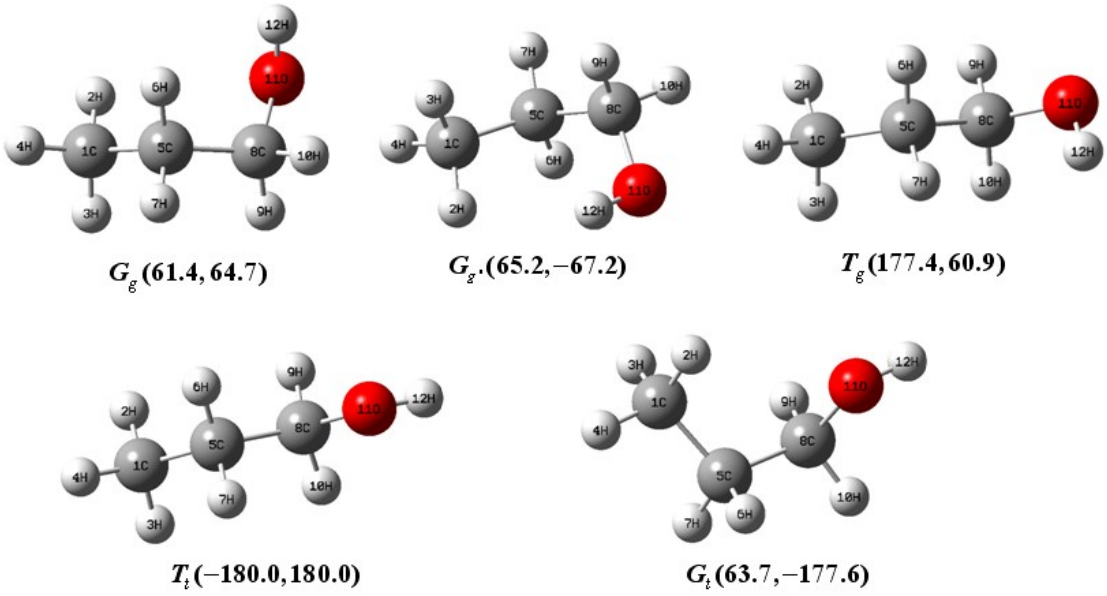

Figure S1. Geometry structures and labeling of atoms of n-propanol in the five conformers. The plane in n-propanol refers to C1-C5-C8-O11.

Table S1. The calculated vibrational frequencies (cm^{-1}) and Raman activities and depolarization ratio (ρ) as well as potential energy distribution (PED) analysis for five conformers of $CD_3CH_2CD_2OH$ in the C-H bending (1400-1500 cm^{-1}) and C-H stretching (2800-3100cm^{-1}) and OH stretching (3600-3700cm^{-1}) regions.

	G_g			T_g			G_g'			G_t			T_t		
Mode Description	υ_{cal} [a]	Activity (ρ)	PED(%) [b]	υ_{cal} [a]	Activity (ρ)	PED(%) [b]	υ_{cal} [a]	Activity (ρ)	PED(%) [b]	υ_{cal} [a]	Activity (ρ)	PED(%) [b]	υ_{cal} [a]	Activity (ρ)	PED(%) [b]
β-CH_2 bending	1442.9	7.7	95δ($C5H_2$)	1456.6	7.5	95δ($C5H_2$)	1437.8	7.7	95δ($C5H_2$)	1439.4	7.8	95δ($C5H_2$)	1459.9	7.7	95δ($C5H_2$)
β-CH_2-SS	2918.4	135.2 (0.08)	76υ(C5H7)+ 23υ(C5H6)	2923.1	118.8 (0.10)	88υ(C5H7)+12υ(C5H6)	2936.1	142.4 (0.08)	72υ(C5H7)+28υ(C5H6)	2939.9	134.7 (0.07)	63υ(C5H7)+36υ(C5H6)	2949.9	129.9 (0.06)	50υ(C5H7)+ 50υ(C5H6)
β-CH_2-AS	2951.6	85.3 (0.59)	76υ(C5H6)-24υ(C5H7)	2972.3	80.1 (0.49)	87υ(C5H6)-12υ(C5H7)	2974.1	77.8 (0.66)	71υ(C5H6)-28υ(C5H7)	2973.1	75.3 (0.7)	63υ(C5H6)-37υ(C5H7)	2983.4	72.3 (0.75)	50υ(C5H6) - 50υ(C5H7)
OH stretching	3661.2	74.8 (0.21)	100υ(OH)	3663.1	75.9 (0.21)	100υ(OH)	3674.8	57.5 (0.18)	100υ(OH)	3681.3	112.6 (0.25)	100υ(OH)	3678.7	125.6 (0.26)	100υ(OH)

[a] Scale factors of 0.973 for C-H bending and stretching regions and of 0.956 for O-H stretching region. [b] potential energy terms higher than 5% are included.

The following symbols stand for: ν - stretching; δ - CH_2 bending.

Table S2. The calculated vibrational frequencies (cm^{-1}) and Raman activities as well as potential energy distribution (PED) analysis for five conformers of $CH_3CH_2CH_2OH$ in the C-H bending (1400-1500 cm^{-1}) and C-H stretching (2800-3100cm^{-1}) and OH stretching (3600-3700cm^{-1}) regions.

	G_g			T_g			$G_{g'}$			G_t			T_t		
Mode	υ_{cal} [a]	Raman activity	PED(%) [b]	υ_{cal} [a]	Raman activity	PED(%) [b]	υ_{cal} [a]	Raman activity	PED(%) [b]	υ_{cal} [a]	Raman activity	PED(%)	υ_{cal} [a]	Raman activity	PED(%) [b]
β-CH_2 bending	1441.6	0.6	86δ ($C5H_2$)	1449.6	18.6	70δ ($C5H_2$)+ 18β_3($C1H_3$) +8δ ($C8H_2$)	1437.1	10.2	89δ ($C5H_2$)	1438.1	10.7	90δ ($C5H_2$)	1453.1	18.0	66δ ($C5H_2$)+26β_2($C1H_3$)
out-of-plane γ-CH_3 bending	1454.1	12.4	71β_2($C1H_3$)+17δ ($C8H_2$)	1460.8	7.2	89β_2($C1H_3$)	1470.3	2.2	52β_2($C1H_3$)-23β_3($C1H_3$) - 16δ ($C8H_2$)	1454.5	11.0	78β_2($C1H_3$)+6δ($C8H_2$)+ 6β_3($C1H_3$)	1461.3	7.5	91β_2($C1H_3$)
in-plane γ-CH_3 bending	1467.9	5.3	61β_3($C1H_3$)-22δ ($C8H_2$)	1462.7	0.3	52β_3($C1H_3$)-33δ($C8H_2$) -5δ ($C5H_2$)	1456.2	10.3	37β_2($C1H_3$)+28δ ($C8H_2$) +25β_3($C1H_3$)	1468.4	4.0	77β_3($C1H_3$)-7β_2($C1H_3$)	1466.6	0.3	52β_3($C1H_3$)-19δ ($C5H_2$) -19δ ($C8H_2$)
α-CH_2 bending	1466.7	0.6	61δ ($C8H_2$)-16β_2($C1H_3$)+ 14β_3($C1H_3$)	1475.4	3.2	57δ($C8H_2$)- 22δ($C5H_2$)+13β_3($C1H_3$)	1463.3	6.5	55δ ($C8H_2$) -34β_3($C1H_3$)	1476.8	4.8	88δ ($C8H_2$)	1482.6	4.5	74δ ($C8H_2$)-13δ ($C5H_2$) +5β_2($C1H_3$)
α-CH_2-SS	2907.2	69.1	69υ(C8H10)- 17υ(C5H6)- 10υ(C5H7)	2898.2	115.8	95υ(C8H10)	2897.3	126.5	95υ(C8H9)	2891.2	130.5	70υ(C8H9)+29υ(C8H10)	2889.2	127.1	50υ(C8H10)+49υ(C8H9)
α-CH_2-AS	2988.5	57.6	86υ(C5C8) -5υ(C8H10)	2989.7	30.2	66υ(C8H9)+15υ(C1H3)- 14υ(C1H2)	2999.2	91.0	80υ(C8H10)+6υ(C1H2) - 5υ(C1H4)	2920.2	103.9	59υ(C8H10)-26υ(C8H9) -9υ(C5H6)-5υ(C5H7)	2914.9	105.3	48υ(C8H9)-47υ(C8H10)
γ-CH_3-SS	2943.4	121.1	47υ(C1H3)+ 25υ(C1H4)+ 13υ(C1H2)-11υ(C5H7)	2940.6	163.8	41υ(C1H3)+ 36υ(C1H2)+ 21υ(C1H4)	2935.8	40.7	35υ(C1H3)-21υ(C5H7)+ 21υ(C1H2)+16υ(C1H4)+ -6υ(C5H6)	2941.0	65.7	45υ(C1H3)+25υ(C1H4)- 15υ(C5H7)+11υ(C1H2)	2938.9	204.1	40υ(C1H2)+39υ(C1H3) +18υ(C1H4)
β-CH_2-SS	2920.1	222.5	62υ(C5H6)+22υ(C8H10) +9υ(C5H7)+ 5υ(C8H9)	2921.4	153.7	87υ(C5H7)+ 10υ(C5H6)	2934.2	254.8	49υ(C5H7)+22υ(C5H6)+ 13υ(C1H3)+13υ(C1H2)	2942.2	249.2	44υ(C5H7)+26υ(C5H6) +13υ(C1H3)+9υ(C8H10)	2948.8	80.9	48υ(C5H7)+48υ(C5H6)
β-CH_2-AS	2950.2	159.5	66υ(C5H7)- 14υ(C5H6)+ 8υ(C1H2)	2966.1	112.0	73υ(C5H6)-10υ(C8H9) - 6υ(C5H7)	2968.5	111.2	54υ(C5H6)-20υ(C5H7)- 14υ(C1H2)+9υ(C1H3)	2971.0	86.5	54υ(C5H6)-32υ(C5H7) -6υ(C5H7)-5υ(C1H4)	2976.2	99.5	29υ(C5H6)-29υ(C5H7) +19υ(C1H3)-19υ(C1H2)
out-of-plane γ-CH_3-AS	3001.4	66.8	48υ(C1H4) -42υ(C1H3)	3001.9	43.3	31υ(C1H2)- 30υ(C1H3)+18υ(C8H9)	3004.5	95.8	75υ(C1H4)-12υ(C1H3) - 5υ(C5H6)	3023.2	38.6	78υ(C1H2)-14υ(C1H4)	3001.1	5.38	31υ(C1H2)-30υ(C1H3) -19υ(C5H7)+19υ(C5H6)

in-plane γ-CH_3-AS	3018.3	41.4	74υ(C1H2)-18υ(C1H4) -5υ(C1H3)	3008.0	80.7	77υ(C1H4)-12υ(C1H2) +10 υ(C1H3)	2994.6	14.5	40υ(C1H2)-31υ(C1H3)+11υ(C5H6)-9υ(C8H10)+ -8υ(C5H7)	2998.9	63.2	54υ(C1H4)-36υ(C1H3) +8υ(C5H6)	3007.6	82.0	78υ(C1H4)-10υ(C1H3) -10υ(C1H2)
OH stretching	3724.1	73.3	100υ(O11H12)	3725.8	74.5	100υ(O11H12)	3737.5	56.1	100υ(OH)	3744.2	112.6	100υ(OH)	3741.5	125.6	100υ(O11H12)

[a] Scale factors of 0.973 for C-H bending and stretching regions and of 0.956 for O-H stretching region. [b] potential energy terms higher than 5% are included.

The following symbols stand for: ν - stretching; δ - CH_2 bending; β_1 - CH_3 umbrella bending; β_2 - CH_3 out-of-plane bending; β_3 - CH_3 in-plane bending; the plane denotes the atoms of C1-C5-C8-O11 in $CH_3CH_2CH_2OH$.

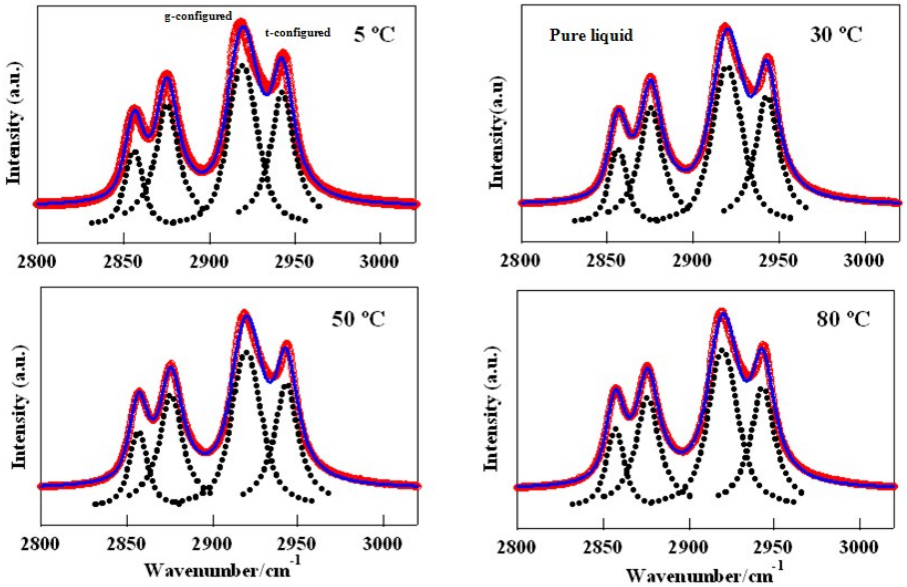

Figure S2. The temperature-dependent Raman spectra of liquid $CD_3CH_2CD_2OH$ in pure liquid state fitted with four Voigt profiles.

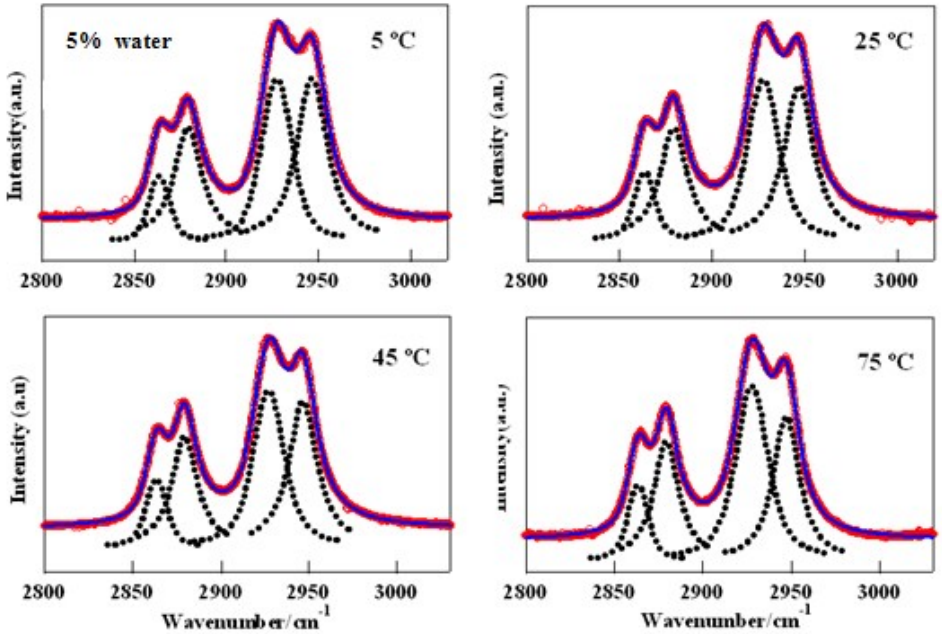

Figure S3. The temperature-dependent Raman spectra of liquid $CD_3CH_2CD_2OH$ in 5% water solution fitted with four Voigt profiles.