Supplementary Information

Enantioselective Raman spectroscopy (esR) for distinguishing between the enantiomers of 2-butanol

Claudia C. Rullich[1] and Johannes Kiefer[1,2]*

[1]University of Bremen, Technische Thermodynamik, Badgasteiner Str. 1, 28359 Bremen, Germany.

[2]University of Bremen, MAPEX Center for Materials and Processes, 28359 Bremen, Germany.

Corresponding author. Phone: +49 421 218 64777. Email: jkiefer@uni-bremen.de

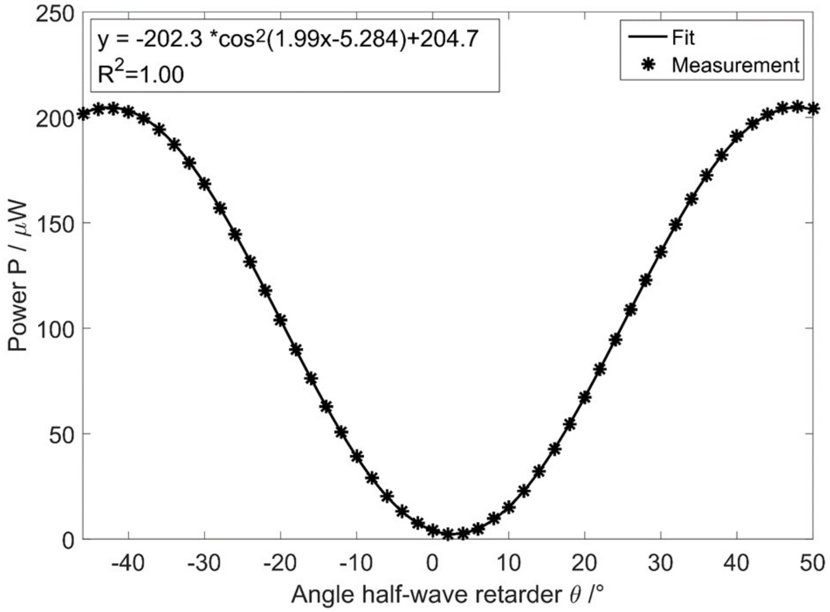

Figure S1. Calibration of orientation of half-wave Fresnel rhombus with a polarimeter set-up by fitting the measured values according to malus's law. The angular orientation at the intensity minimum (measured as power) is taken as 0.0° for the plane of incidence.

Table S1. Peak assignment of observed Raman peak positions and of observed ATR-IR peak positions of 2-Butanol in cm^{-1}(sh = shoulder, str. = stretching, def. = deformation, sciss. = scissoring, rock. = rocking, wagg. = wagging, tors. = torsion, s = symmetric, as = asymmetric).

Raman wavenumber /cm^{-1}	**IR wavenumber /cm^{-1}**	**Assignment**	**Reference**
407		skeletal	[1]
425 (sh)		skeletal	[1]
456		CCO def., CCC def.	[2]
518		CCO def., CCC def.	[2]
777	776	CH_2 rock.	[2]
794 (sh)	794 (sh)	CC str.	[2]
821	821	$(C)_2C$-O s str.	[3]
840 (sh)		CH_2 rock., CH_3 rock.	[2]
908	911	CC str., CH_3 rock.	[2]
971 (sh)	968	-	
984	991	CC s str., CH_3 rock., CO s str.	[2]
1023	1031	CCO s str., CH_2 tors.	[2, 4]
1045 (sh)		CC str.	[2]
1097	1109	CCO as str., CH_3 rock.	[3]
1114 (sh)	1120 (sh)	CCO as str., CH_2 rock.	[3]
1145	1148	CH_2 rock.	[2]
1166	1155 (sh)	CH_2 rock.	[2]
1244	1254	CH_2 wagg., COH def.	[2]
1282		CH_2 wagg., COH def.	[2]
	1300	CH_2 wagg., COH def.	[2]
	1326	CH sciss.	[3]
1338		CH sciss..	[3]
1359		CH sciss.	[3]
	1375	CH_3 s def.	[2]
1396		CH_2 sciss.	[2]

	1415	CH_2 sciss.	[2]
1433		CH_3 as sciss., CH_2 sciss.	[3]
	1458	CH_3 as sciss. CH_2 sciss.	[3]
2721		Combination	[2]
	2861 (sh)	Overtone	[2]
2876	2881	CH_2 s str	[2]
2887		CH_3 s str	[2]
	2929	CH_3 s str	[2]
2933	2934 (sh)	CH_3 s str	[2]
2967	2969	CH_2 as str. CH_3 as str.	[2]
3352	3344	OH str.	[2]

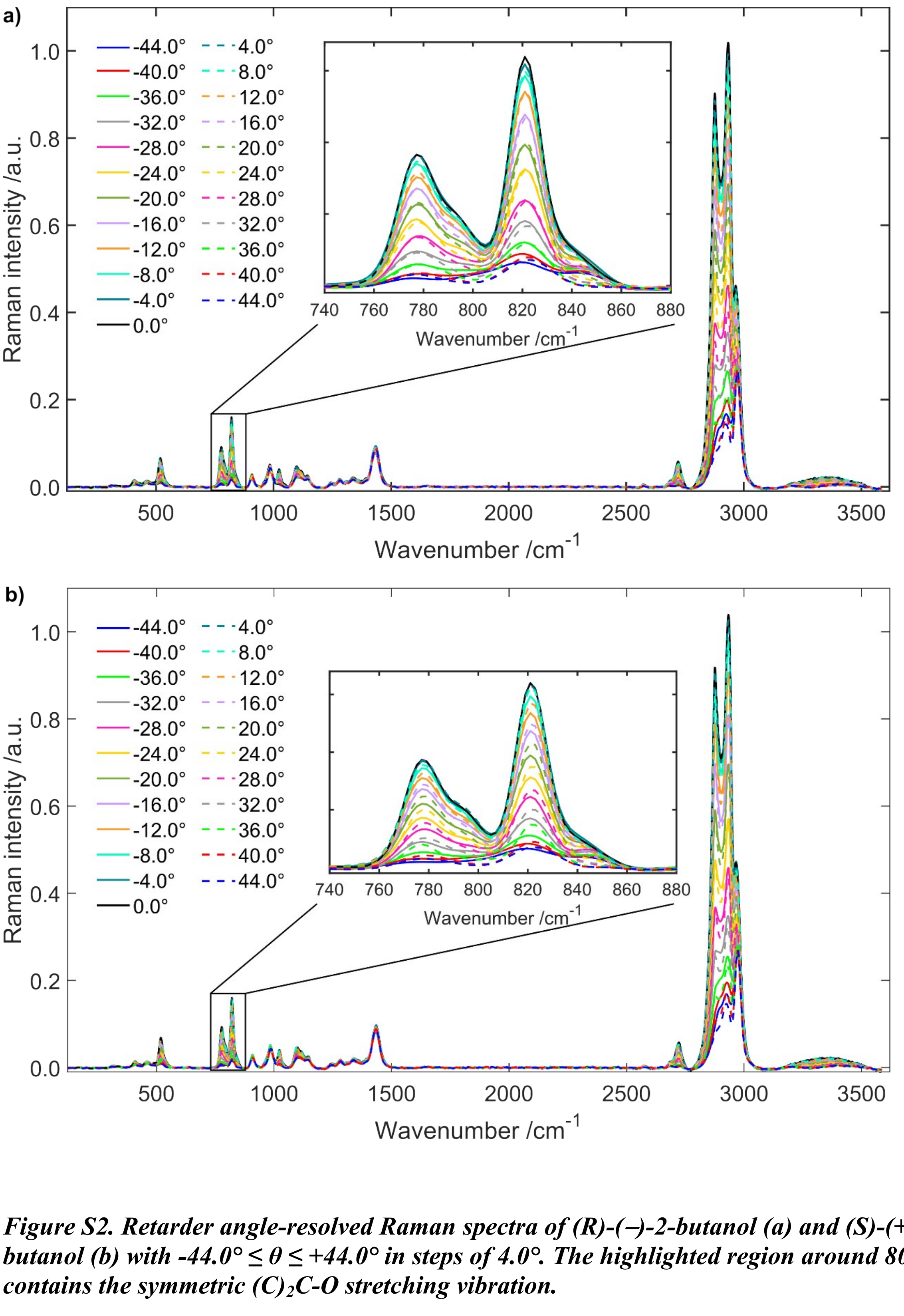

Figure S2. Retarder angle-resolved Raman spectra of (R)-(−)-2-butanol (a) and (S)-(+)-2-butanol (b) with -44.0° ≤ θ ≤ +44.0° in steps of 4.0°. The highlighted region around 800 cm^{-1} contains the symmetric (C)$_2$C-O stretching vibration.

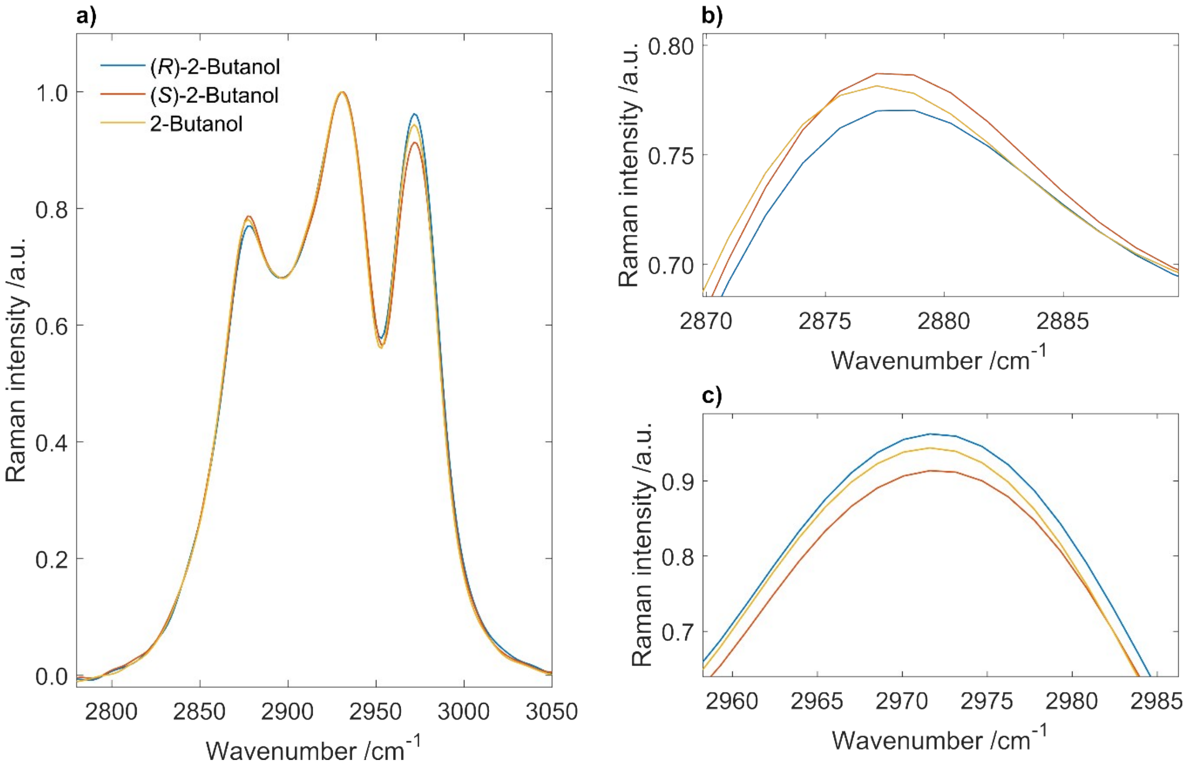

Figure S3. Enlarged Raman spectra of CH_2 and CH_3-stretching vibrations (a), symmetric CH_2 and CH_3 stretching vibrations (b), asymmetric CH_3 stretching vibration (c)): Spectra were recorded with vertically polarized incident laser light, of (R)-(-)-2-butanol, (S)-(+)-2-butanol, and 2-butanol with $\theta = +32.0°$. The full spectrum of each substance was normalized with respect to its strongest peak.

References

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