Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Disentangling the molecular polarizability and first hyperpolarizability of methanol-air interfaces

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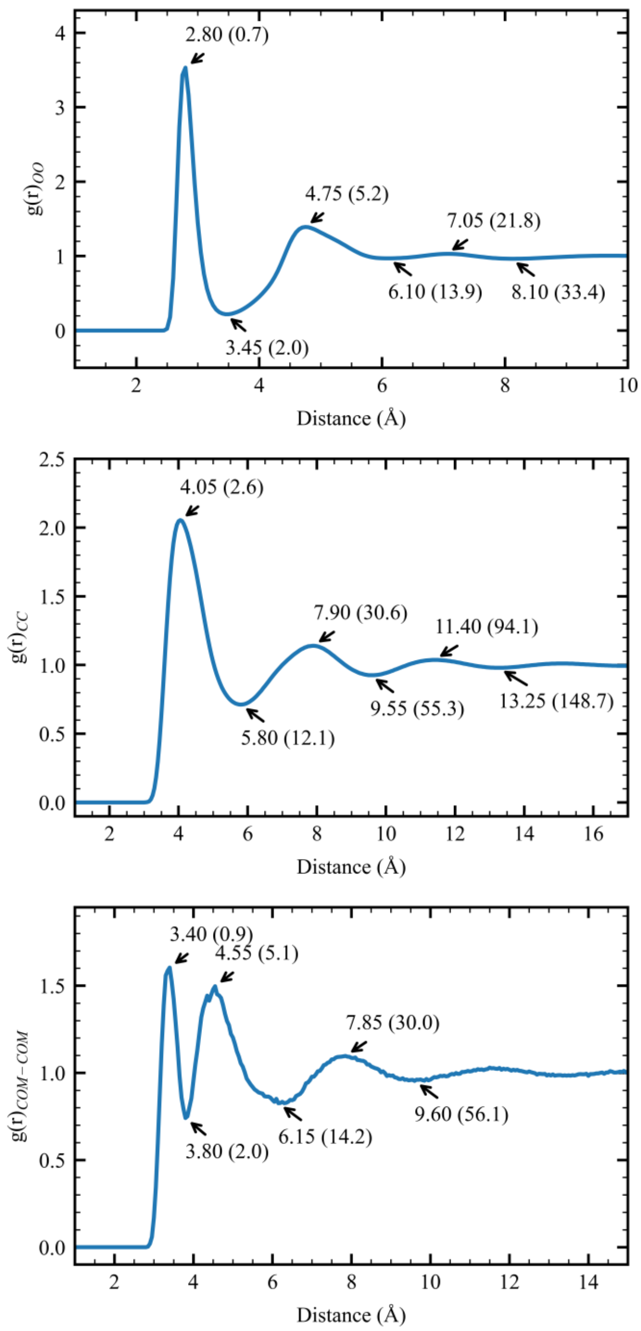

Figure S1. Radial distribution functions of Oxygen [$g(r)_{OO}$], Carbon [$g(r)_{CC}$], and center-of-mass [$g(r)_{COM\text{-}COM}$] for bulk MD simulations at T = 260 K. For each maximum/minimum, the first value corresponds to the distance in g(r) (in Å) while the quantity in parentheses is the number of molecules as obtained by integration up to the corresponding point.

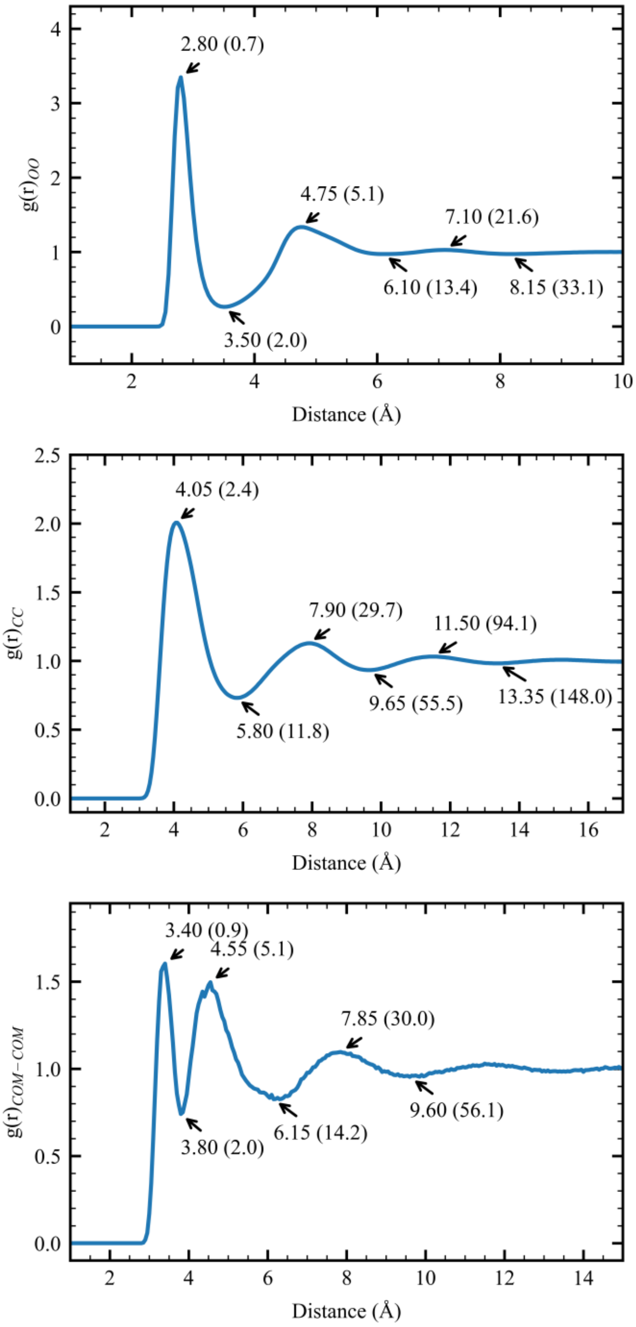

Figure S2. Radial distribution functions of Oxygen [$g(r)_{OO}$], Carbon [$g(r)_{CC}$], and center-of-mass [$g(r)_{COM\text{-}COM}$] for bulk MD simulations at T = 280 K. For each maximum/minimum, the first value corresponds to the distance in g(r) (in Å) while the quantity in parentheses is the number of molecules as obtained by integration up to the corresponding point.

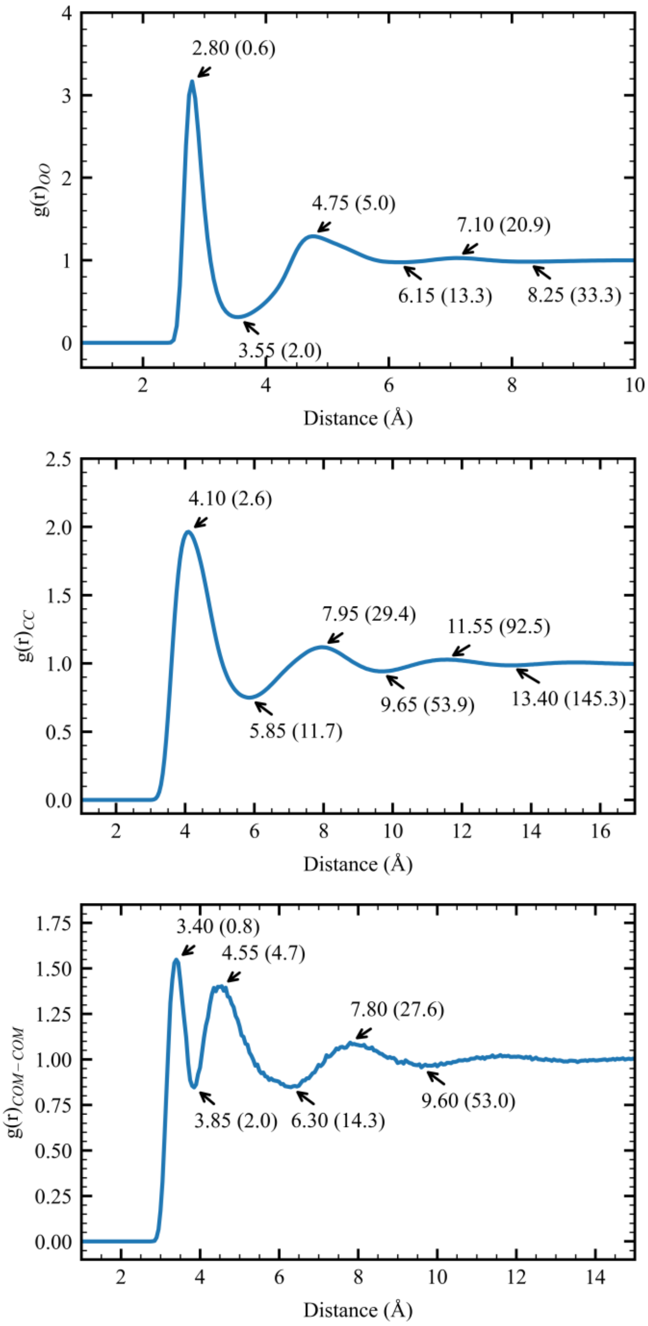

Figure S3. Radial distribution functions of Oxygen [$g(r)_{OO}$], Carbon [$g(r)_{CC}$], and center-of-mass [$g(r)_{COM\text{-}COM}$] for bulk MD simulations at T = 300 K. For each maximum/minimum, the first value corresponds to the distance in g(r) (in Å) while the quantity in parentheses is the number of molecules as obtained by integration up to the corresponding point.

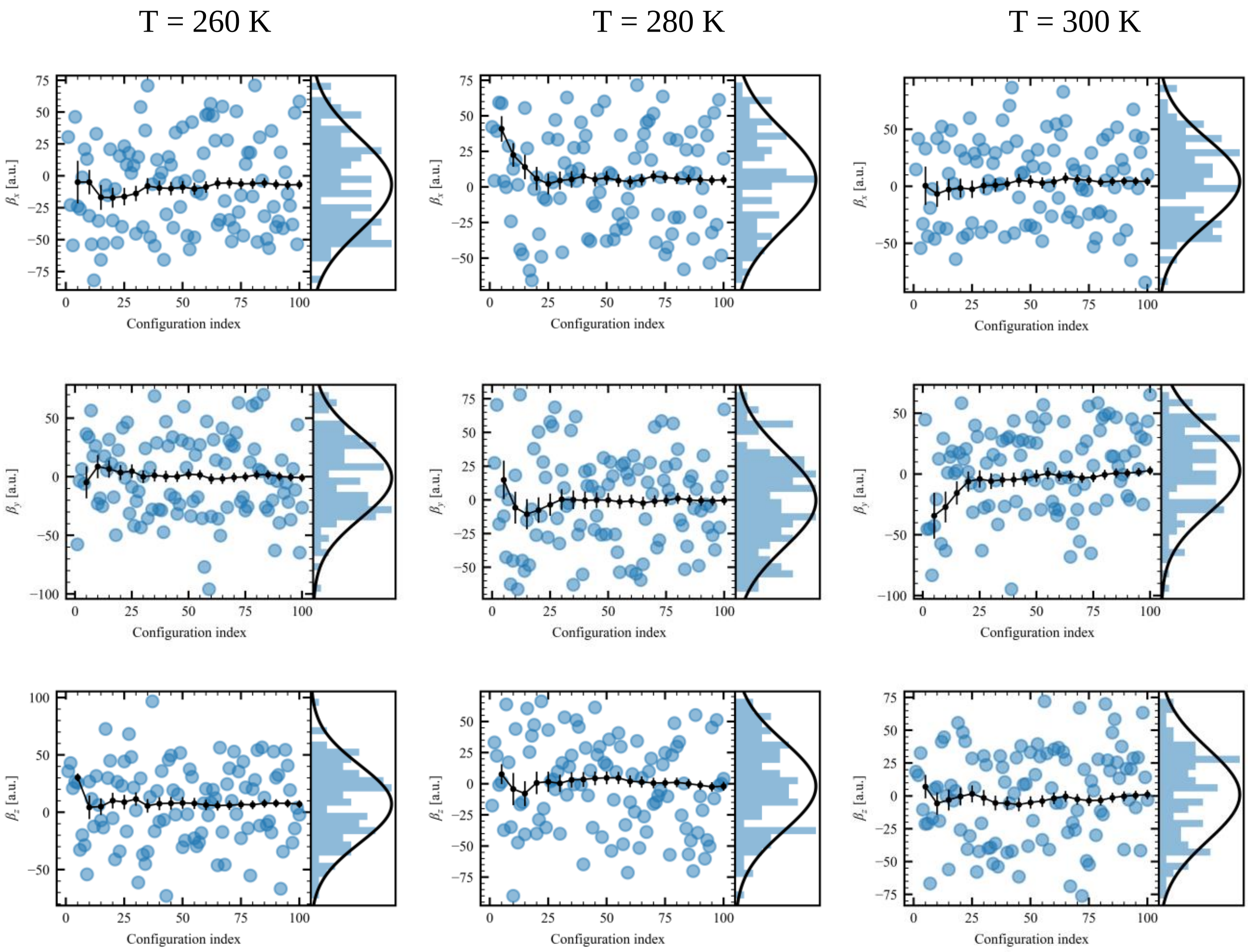

Figure S4. Convergence of the vectorial β components as obtained in bulk for N = 1 including an embedding with R=20Å. They oscillate around zero (the expectation value for an infinite number of snapshots), leading to either small negative or positive cumulative average values.

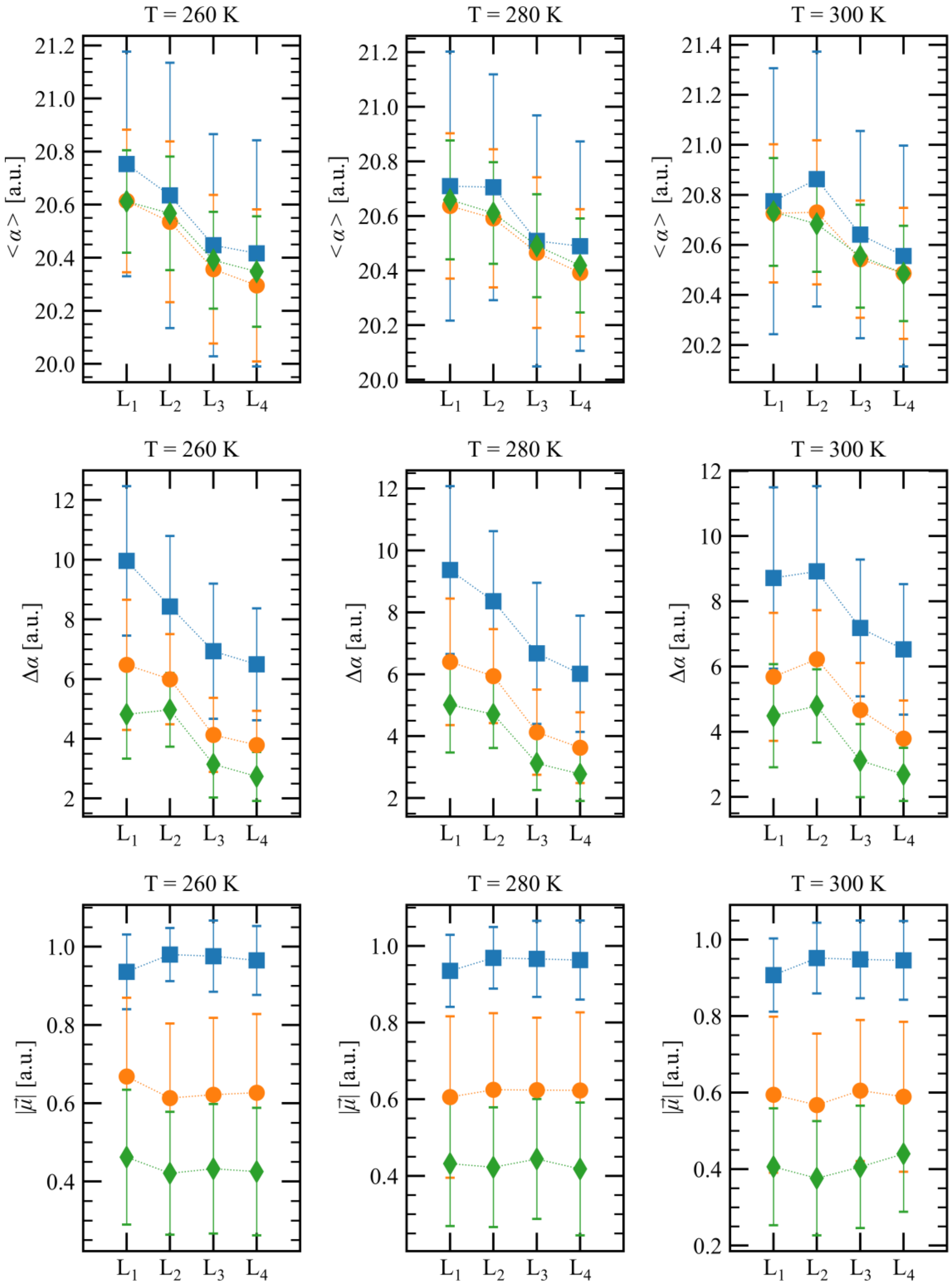

Figure S5. Comparison between the linear and nonlinear optical properties for different molecular layers, as calculated at λ=1064 nm for the α quantities. The average values are represented by symbols (blue squares for N = 1, orange circles for N = 3, and green diamonds for N = 6), whereas the standard deviations are given by error bars. All reported values are given per MeOH molecule.

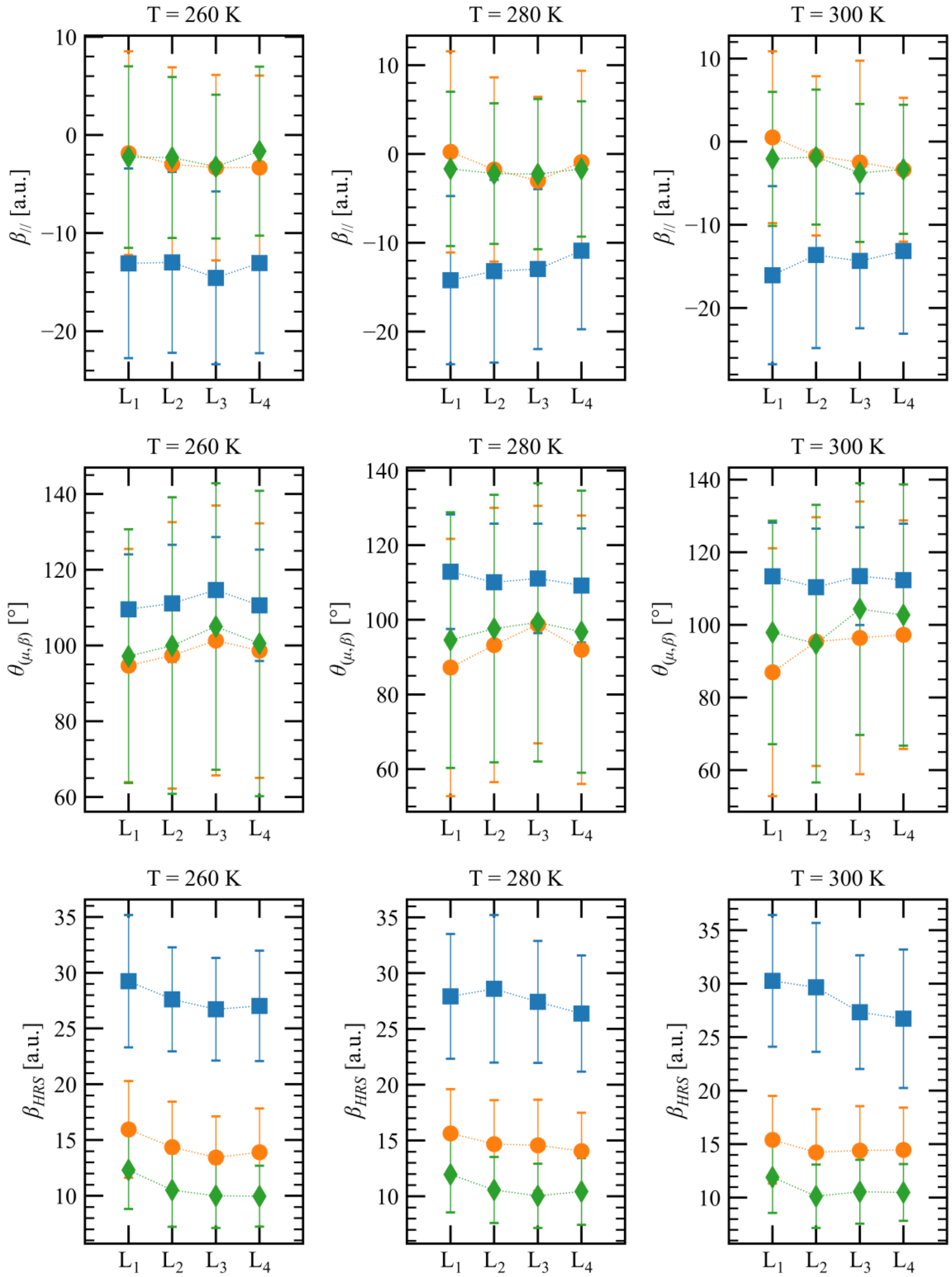

Figure S6. Comparison between the linear and nonlinear optical properties for different molecular layers, as calculated at λ=1064 nm for the β quantities. The average values are represented by symbols (blue squares for N = 1, orange circles for N = 3, and green diamonds for N = 6), whereas the standard deviations are given by error bars. All reported values are given per MeOH molecule.

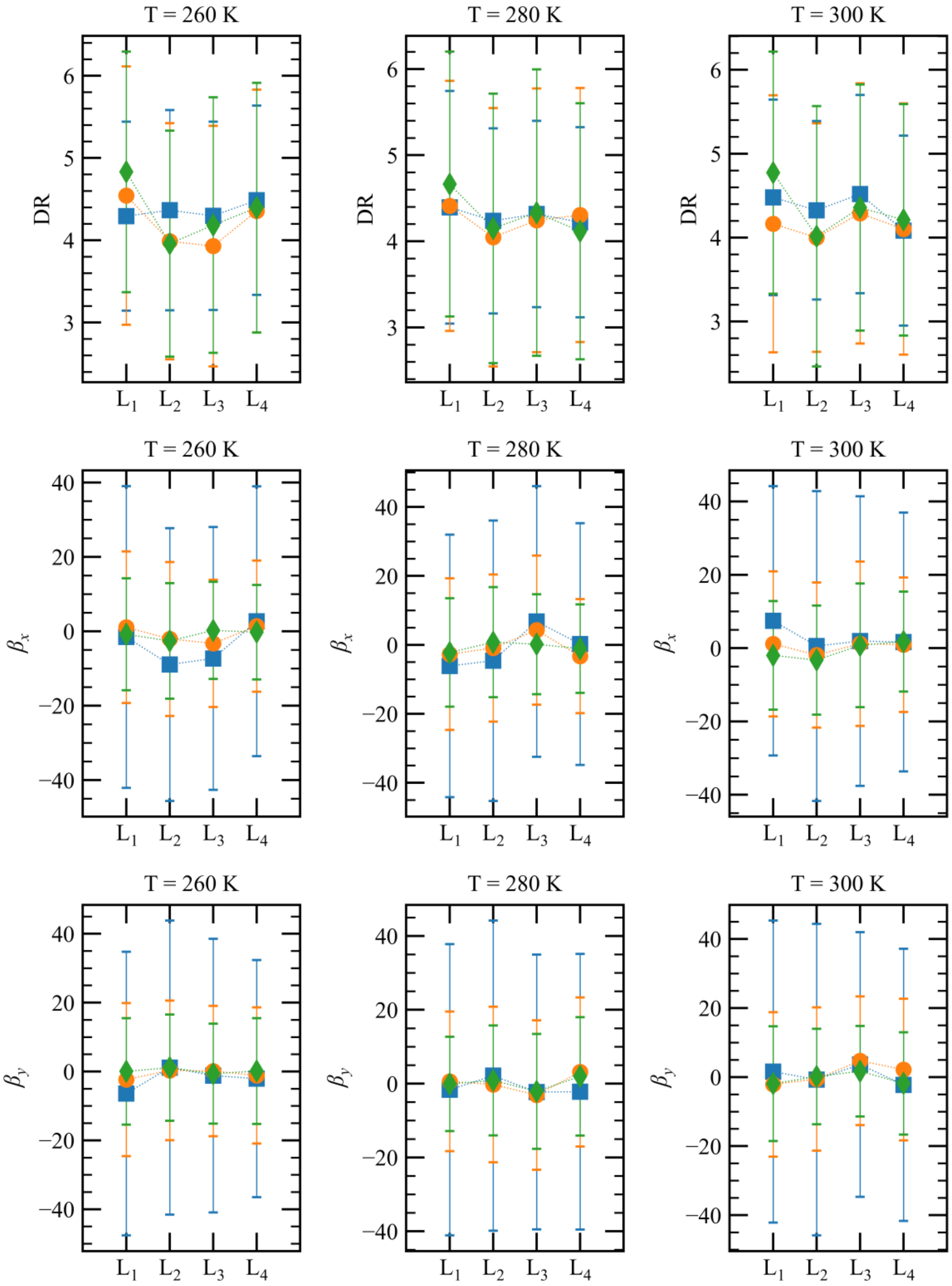

Figure S7. Comparison between the linear and nonlinear optical properties for different molecular layers, as calculated at λ=1064 nm for the β quantities. The average values are represented by symbols (blue squares for N = 1, orange circles for N = 3, and green diamonds for N = 6), whereas the standard deviations are given by error bars. All reported values are given per MeOH molecule.

Table S1. Linear and nonlinear optical properties in bulk obtained at T = 300 K as a function of the size of the spherical embedding (of radius R). The quantum region comprises only one MeOH molecule. [a] Up to R = 20 Å polarizable atomic sites with extra shell of point charges from R = 20 Å to R = 30 Å. All results are in atomic units, except $\theta_{(\mu,\beta)}$ (°) and DR (dimensionless).

Property	R = 15 Å	R = 20 Å	R = 30 Å[a]	R = 30 Å
$\langle\alpha\rangle$	20.44 ± 0.44	20.37 ± 0.43	20.37 ± 0.43	20.30 ± 0.43
$\Delta\alpha$	6.10 ± 1.81	6.08 ± 1.80	6.08 ± 1.80	6.04 ± 1.79
$\|\vec{\mu}\|$	0.95 ± 0.10	0.95 ± 0.10	0.95 ± 0.10	0.95 ± 0.10
$\beta_{//}$	-14.80 ± 9.91	-14.54 ± 9.84	-14.53 ± 9.74	-14.42 ± 9.64
$\theta_{(\mu,\beta)}$	113.86 ± 15.04	113.57 ± 14.96	113.63 ± 14.85	113.60 ± 14.86
β_{HRS}	26.78 ± 5.50	26.59 ± 5.40	26.51 ± 5.35	26.34 ± 5.29
DR	4.43 ± 1.20	4.43 ± 1.19	4.42 ± 1.19	4.41 ± 1.19
β_x	4.17 ± 37.41	4.12 ± 36.97	4.18 ± 36.72	4.20 ± 36.46
β_y	3.01 ± 35.09	2.87 ± 34.97	2.79 ± 34.91	2.75 ± 34.70
β_z	1.48 ± 35.35	1.00 ± 35.04	0.80 ± 34.85	0.79 ± 34.57

Table S2. Linear and nonlinear optical properties in bulk obtained at T = 260 K and 280 K as a function of the size of the spherical embedding (of radius R). The quantum region comprises only one MeOH molecule. All results are in atomic units, except $\theta_{(\mu,\beta)}$ (°) and DR (dimensionless).

	T = 260K		T = 280K	
Property	R = 15Å	R = 20Å	R = 15Å	R = 20Å
$\langle\alpha\rangle$	20.46 ± 0.36	20.39 ± 0.36	20.44 ± 0.40	20.37 ± 0.39
$\Delta\alpha$	5.73 ± 1.91	5.69 ± 1.94	6.70 ± 1.90	6.67 ± 1.92
$\|\vec{\mu}\|$	0.98 ± 0.08	0.98 ± 0.08	0.95 ± 0.10	0.95 ± 0.10
$\beta_{//}$	-12.72 ± 9.39	-12.26 ± 9.26	-13.79 ± 9.75	-13.88 ± 9.61
$\theta_{(\mu,\beta)}$	110.52 ± 14.54	109.95 ± 14.49	112.95 ± 15.17	113.26 ± 14.98
β_{HRS}	26.95 ± 5.10	26.73 ± 5.05	26.38 ± 5.07	26.27 ± 4.94
DR	4.26 ± 1.05	4.25 ± 1.06	4.37 ± 1.15	4.38 ± 1.15
β_x	-7.38 ± 36.88	-6.86 ± 36.56	5.07 ± 34.33	5.06 ± 34.21
β_y	-0.86 ± 34.76	-0.86 ± 34.54	-0.39 ± 35.10	-0.33 ± 35.24
β_z	7.08 ± 34.40	7.15 ± 33.94	-1.93 ± 36.34	-1.98 ± 35.84

Table S3. Linear and nonlinear optical properties of MeOH molecules in **bulk** obtained at different temperatures as a function of the number of MeOH molecules in the quantum region. All results are in atomic units, except $\theta_{(\mu,\beta)}$ (°) and DR (dimensionless). μ, α, and β quantities are given per MeOH molecule.

Property	T = 260K	T = 280K	T = 300K
		N = 1	
$\langle\alpha\rangle$	20.39 ± 0.36	20.37 ± 0.39	20.37 ± 0.43
$\Delta\alpha$	5.69 ± 1.94	6.67 ± 1.92	6.08 ± 1.80
$\lvert\vec{\mu}\rvert$	0.98 ± 0.08	0.95 ± 0.10	0.95 ± 0.10
$\beta_{//}$	-12.26 ± 9.26	-13.88 ± 9.61	-14.53 ± 9.74
$\theta_{(\mu,\beta)}$	109.95 ± 14.49	113.26 ± 14.98	113.63 ± 14.85
β_{HRS}	26.73 ± 5.05	26.27 ± 4.94	26.59 ± 5.40
DR	4.25 ± 1.06	4.38 ± 1.15	4.43 ± 1.19
β_x	-6.86 ± 36.56	5.06 ± 34.21	4.12 ± 36.97
β_y	-0.86 ± 34.54	-0.33 ± 35.24	2.87 ± 34.97
β_z	7.15 ± 33.94	-1.98 ± 35.84	1.00 ± 35.04
		N = 3	
$\langle\alpha\rangle$	20.22 ± 0.24	20.26 ± 0.24	20.34 ± 0.21
$\Delta\alpha$	3.34 ± 1.04	3.70 ± 1.09	3.70 ± 1.13
$\lvert\vec{\mu}\rvert$	0.73 ± 0.19	0.73 ± 0.18	0.71 ± 0.16
$\beta_{//}$	-2.05 ± 8.43	-0.76 ± 8.85	0.73 ± 8.79
$\theta_{(\mu,\beta)}$	94.07 ± 30.48	90.77 ± 32.17	86.22 ± 32.00
β_{HRS}	13.30 ± 3.45	13.42 ± 3.73	13.55 ± 3.30
DR	4.13 ± 1.50	4.14 ± 1.55	3.92 ± 1.21
β_x	-1.53 ± 17.34	3.30 ± 18.97	0.21 ± 18.26
β_y	-0.46 ± 18.11	-0.13 ± 18.52	2.37 ± 17.51
β_z	0.80 ± 17.89	-3.60 ± 16.55	1.28 ± 17.17
		N = 6	
$\langle\alpha\rangle$	20.16 ± 0.18	20.23 ± 0.18	20.30 ± 0.20
$\Delta\alpha$	2.55 ± 0.77	2.56 ± 0.93	2.63 ± 0.93
$\lvert\vec{\mu}\rvert$	0.50 ± 0.15	0.48 ± 0.15	0.47 ± 0.17
$\beta_{//}$	-1.62 ± 7.43	-1.95 ± 6.29	-1.20 ± 7.08
$\theta_{(\mu,\beta)}$	96.47 ± 36.07	98.55 ± 30.46	95.04 ± 38.03
β_{HRS}	9.84 ± 2.92	9.48 ± 2.81	10.00 ± 2.83
DR	4.44 ± 1.46	4.01 ± 1.36	4.12 ± 1.44
β_x	0.53 ± 14.12	1.94 ± 13.45	1.04 ± 14.03
β_y	1.81 ± 13.40	1.07 ± 12.48	-0.22 ± 12.25
β_z	2.15 ± 13.97	-1.17 ± 12.79	2.35 ± 14.32

Table S4. Interfacial linear and nonlinear optical properties obtained at T = 300 K as a function of the radius in spherical embeddings. The quantum region comprises one MeOH molecule (N = 1). All results are in atomic units, except $\theta_{(\mu,\beta)}$ (°) and DR (dimensionless). These results were obtained for MeOH molecules belonging to the first molecular layer but differently from those identified as L_1.

Property	R = 15 Å	R = 20 Å	R = 30 Å
$\langle\alpha\rangle$	21.04 ± 0.50	20.90 ± 0.50	20.75 ± 0.50
$\Delta\alpha$	7.97 ± 2.42	8.11 ± 2.47	8.18 ± 2.52
$\lvert\vec{\mu}\rvert$	0.88 ± 0.09	0.88 ± 0.09	0.88 ± 0.10
$\beta_{//}$	-16.30 ± 11.06	-16.00 ± 11.15	-15.65 ± 11.14
$\theta_{(\mu,\beta)}$	112.67 ± 14.99	112.31 ± 15.15	112.00 ± 15.18
β_{HRS}	30.73 ± 5.63	30.70 ± 5.65	30.54 ± 5.56
DR	4.73 ± 1.22	4.69 ± 1.21	4.64 ± 1.21
β_x	5.47 ± 34.14	5.88 ± 33.41	5.84 ± 33.06
β_y	-2.41 ± 41.35	-2.58 ± 41.15	-2.47 ± 40.31
β_z	-32.97 ± 36.31	-32.62 ± 36.79	-32.48 ± 36.86

Table S5. Linear and nonlinear optical properties of MeOH molecules at **L2** obtained at different temperatures as a function of the number of MeOH molecules in the quantum region. All results are in atomic units, except $\theta_{(\mu,\beta)}$ (°) and DR (dimensionless). μ, α, and β quantities are given per MeOH molecule.

Property	T = 260K	T = 280K	T = 300K
N = 1			
$\langle\alpha\rangle$	20.63 ± 0.50	20.71 ± 0.41	20.86 ± 0.51
$\Delta\alpha$	8.43 ± 2.36	8.36 ± 2.26	8.92 ± 2.62
$\|\vec{\mu}\|$	0.98 ± 0.07	0.97 ± 0.08	0.95 ± 0.09
$\beta_{//}$	-12.99 ± 9.22	-13.20 ± 10.28	-13.62 ± 11.20
$\theta_{(\mu,\beta)}$	111.10 ± 15.48	110.05 ± 15.72	110.35 ± 16.14
β_{HRS}	27.61 ± 4.66	28.60 ± 6.61	29.65 ± 6.02
DR	4.36 ± 1.22	4.24 ± 1.07	4.32 ± 1.06
β_x	-8.95 ± 36.65	-4.60 ± 40.67	0.57 ± 42.25
β_y	1.12 ± 42.68	2.14 ± 42.01	-0.75 ± 45.10
β_z	-5.11 ± 27.39	-3.88 ± 31.73	-3.32 ± 29.87
N = 3			
$\langle\alpha\rangle$	20.54 ± 0.30	20.59 ± 0.25	20.73 ± 0.29
$\Delta\alpha$	5.99 ± 1.51	5.94 ± 1.52	6.22 ± 1.50
$\|\vec{\mu}\|$	0.61 ± 0.19	0.62 ± 0.20	0.57 ± 0.19
$\beta_{//}$	-2.99 ± 9.88	-1.75 ± 10.37	-1.71 ± 9.57
$\theta_{(\mu,\beta)}$	97.37 ± 35.16	93.24 ± 36.74	95.36 ± 34.26
β_{HRS}	14.37 ± 4.07	14.68 ± 3.93	14.23 ± 4.04
DR	3.99 ± 1.44	4.05 ± 1.50	4.00 ± 1.36
β_x	-2.07 ± 20.69	-0.91 ± 21.33	-1.89 ± 19.80
β_y	0.31 ± 20.27	-0.24 ± 21.05	-0.58 ± 20.73
β_z	0.47 ± 17.12	-0.95 ± 16.46	0.80 ± 16.67
N = 6			
$\langle\alpha\rangle$	20.57 ± 0.21	20.61 ± 0.19	20.68 ± 0.19
$\Delta\alpha$	4.97 ± 1.24	4.70 ± 1.09	4.79 ± 1.12
$\|\vec{\mu}\|$	0.42 ± 0.16	0.42 ± 0.16	0.38 ± 0.15
$\beta_{//}$	-2.30 ± 8.20	-2.21 ± 7.92	-1.85 ± 8.12
$\theta_{(\mu,\beta)}$	99.94 ± 39.16	97.63 ± 35.83	94.79 ± 38.23
β_{HRS}	10.51 ± 3.29	10.57 ± 2.96	10.13 ± 2.96
DR	3.96 ± 1.37	4.15 ± 1.56	4.01 ± 1.55
β_x	-2.61 ± 15.54	0.76 ± 15.96	-3.27 ± 14.87
β_y	1.11 ± 15.41	0.86 ± 14.88	0.15 ± 13.83
β_z	2.86 ± 10.97	1.14 ± 12.41	-0.42 ± 11.54

Table S6. Linear and nonlinear optical properties of MeOH molecules at **L3** obtained at different temperatures as a function of the number of MeOH molecules in the quantum region. All results are in atomic units, except $\theta_{(\mu,\beta)}$ (°) and DR (dimensionless). μ, α, and β quantities are given per MeOH molecule.

Property	T = 260K	T = 280K	T = 300K
	N = 1		
$\langle\alpha\rangle$	20.45 ± 0.42	20.51 ± 0.46	20.64 ± 0.41
$\Delta\alpha$	6.93 ± 2.26	6.67 ± 2.28	7.18 ± 2.10
$\lvert\vec{\mu}\rvert$	0.98 ± 0.09	0.97 ± 0.10	0.95 ± 0.10
$\beta_{//}$	-14.56 ± 8.80	-12.96 ± 9.00	-14.35 ± 8.10
$\theta_{(\mu,\beta)}$	114.64 ± 13.99	111.08 ± 14.64	113.40 ± 13.47
β_{HRS}	26.72 ± 4.60	27.43 ± 5.47	27.34 ± 5.32
DR	4.30 ± 1.15	4.32 ± 1.08	4.52 ± 1.18
β_x	-7.30 ± 35.32	6.78 ± 39.26	1.91 ± 39.48
β_y	-1.19 ± 39.74	-2.27 ± 37.21	3.62 ± 38.33
β_z	-1.26 ± 30.19	-1.24 ± 33.11	-1.89 ± 32.48
	N = 3		
$\langle\alpha\rangle$	20.36 ± 0.28	20.47 ± 0.28	20.54 ± 0.23
$\Delta\alpha$	4.13 ± 1.24	4.13 ± 1.38	4.66 ± 1.44
$\lvert\vec{\mu}\rvert$	0.62 ± 0.20	0.62 ± 0.19	0.61 ± 0.18
$\beta_{//}$	-3.34 ± 9.45	-3.03 ± 9.47	-2.48 ± 12.21
$\theta_{(\mu,\beta)}$	101.31 ± 35.63	98.71 ± 31.81	96.38 ± 37.55
β_{HRS}	13.43 ± 3.68	14.57 ± 4.08	14.41 ± 4.14
DR	3.93 ± 1.46	4.24 ± 1.53	4.29 ± 1.55
β_x	-3.26 ± 17.10	4.27 ± 21.62	1.19 ± 22.42
β_y	0.12 ± 18.90	-3.09 ± 20.26	4.71 ± 18.65
β_z	2.23 ± 16.42	0.72 ± 17.45	1.11 ± 18.06
	N = 6		
$\langle\alpha\rangle$	20.39 ± 0.18	20.49 ± 0.19	20.55 ± 0.21
$\Delta\alpha$	3.15 ± 1.11	3.12 ± 0.86	3.11 ± 1.12
$\lvert\vec{\mu}\rvert$	0.43 ± 0.17	0.44 ± 0.16	0.41 ± 0.16
$\beta_{//}$	-3.23 ± 7.32	-2.26 ± 8.45	-3.75 ± 8.30
$\theta_{(\mu,\beta)}$	105.00 ± 37.82	99.30 ± 37.29	104.32 ± 34.67
β_{HRS}	10.00 ± 2.89	10.04 ± 2.88	10.55 ± 2.98
DR	4.18 ± 1.55	4.33 ± 1.66	4.36 ± 1.47
β_x	0.24 ± 13.03	0.18 ± 14.51	0.74 ± 16.87
β_y	-0.63 ± 14.51	-2.10 ± 15.56	1.68 ± 13.10
β_z	3.34 ± 13.10	1.05 ± 11.39	0.82 ± 13.92

Table S7. Linear and nonlinear optical properties of MeOH molecules at **L4** obtained at different temperatures as a function of the number of MeOH molecules in the quantum region. All results are in atomic units, except $\theta_{(\mu,\beta)}$ (°) and DR (dimensionless). μ, α, and β quantities are given per MeOH molecule.

Property	T = 260K	T = 280K	T = 300K
		N = 1	
$\langle\alpha\rangle$	20.42 ± 0.43	20.49 ± 0.38	20.56 ± 0.44
$\Delta\alpha$	6.49 ± 1.88	6.01 ± 1.88	6.52 ± 2.00
$\|\vec{\mu}\|$	0.96 ± 0.09	0.96 ± 0.10	0.95 ± 0.10
$\beta_{//}$	-13.05 ± 9.18	-10.89 ± 8.85	-13.16 ± 9.94
$\theta_{(\mu,\beta)}$	110.58 ± 14.72	109.18 ± 15.27	112.29 ± 15.56
β_{HRS}	27.02 ± 4.95	26.38 ± 5.21	26.72 ± 6.47
DR	4.49 ± 1.15	4.22 ± 1.10	4.08 ± 1.13
β_x	2.68 ± 36.26	0.22 ± 35.05	1.65 ± 35.31
β_y	-2.07 ± 34.40	-2.21 ± 37.32	-2.26 ± 39.38
β_z	-2.29 ± 39.02	1.51 ± 31.81	4.33 ± 30.92
		N = 3	
$\langle\alpha\rangle$	20.30 ± 0.29	20.39 ± 0.23	20.49 ± 0.26
$\Delta\alpha$	3.79 ± 1.15	3.63 ± 1.14	3.79 ± 1.17
$\|\vec{\mu}\|$	0.63 ± 0.20	0.62 ± 0.20	0.59 ± 0.20
$\beta_{//}$	-3.32 ± 9.38	-0.92 ± 10.29	-3.37 ± 8.64
$\theta_{(\mu,\beta)}$	98.62 ± 33.60	91.96 ± 35.96	97.27 ± 31.47
β_{HRS}	13.90 ± 3.93	14.06 ± 3.43	14.46 ± 3.95
DR	4.35 ± 1.48	4.30 ± 1.47	4.10 ± 1.50
β_x	1.37 ± 17.63	-3.27 ± 16.56	0.91 ± 18.34
β_y	-1.15 ± 19.77	3.15 ± 20.20	2.16 ± 20.49
β_z	2.29 ± 20.37	-1.02 ± 19.38	0.40 ± 19.78
		N = 6	
$\langle\alpha\rangle$	20.35 ± 0.21	20.42 ± 0.17	20.49 ± 0.19
$\Delta\alpha$	2.73 ± 0.82	2.78 ± 0.87	2.69 ± 0.81
$\|\vec{\mu}\|$	0.43 ± 0.16	0.42 ± 0.17	0.44 ± 0.15
$\beta_{//}$	-1.66 ± 8.61	-1.69 ± 7.62	-3.33 ± 7.76
$\theta_{(\mu,\beta)}$	100.52 ± 40.30	96.79 ± 37.78	102.69 ± 35.97
β_{HRS}	9.96 ± 2.73	10.43 ± 2.98	10.49 ± 2.65
DR	4.39 ± 1.52	4.12 ± 1.49	4.21 ± 1.38
β_x	-0.24 ± 12.69	-1.11 ± 12.83	1.78 ± 13.64
β_y	0.13 ± 15.36	1.96 ± 16.05	-1.83 ± 14.80
β_z	0.42 ± 13.71	-1.77 ± 12.88	0.67 ± 14.17

Table S8. β components corresponding to the non-vanishing $\chi^{(2)}$ ones associated with surface SHG measurements. The results were obtained for N = 1, 6, and 1(6) [See text for details of N = 1(6)]. All of them were obtained at T = 260 K and are in atomic units unless explicitly stated.

Property	N = 1	N = 6	N = 1(6)
		L_1	
β_{ZZZ}	-13.99 ± 20.34	-14.15 ± 9.10	-23.96 ± 74.08
β_{ZXX}	-2.33 ± 10.87	-1.55 ± 4.28	16.31 ± 88.26
β_{XZX}	-2.32 ± 10.93	-1.56 ± 4.29	-1.73 ± 19.96
		L_2	
β_{ZZZ}	-1.13 ± 15.76	2.47 ± 6.82	5.96 ± 54.32
β_{ZXX}	-0.34 ± 11.63	0.88 ± 4.46	8.86 ± 86.26
β_{XZX}	-0.34 ± 11.63	0.88 ± 4.46	1.82 ± 15.81
		L_3	
β_{ZZZ}	-0.34 ± 20.26	3.20 ± 8.87	-4.94 ± 74.29
β_{ZXX}	-1.69 ± 11.70	-0.75 ± 4.60	2.50 ± 94.53
β_{XZX}	-1.72 ± 11.74	-0.75 ± 4.61	0.84 ± 17.11
		L_4	
β_{ZZZ}	1.13 ± 27.07	1.47 ± 9.64	-2.92 ± 77.68
β_{ZXX}	-1.21 ± 11.33	-0.53 ± 4.46	11.23 ± 105.47
β_{XZX}	-1.21 ± 11.33	-0.53 ± 4.47	1.58 ± 17.86
		L_1	
$\chi^{(2)}_{ZZZ}$	-6.59 ± 9.58	-6.67 ± 4.29	-11.29 ± 34.89
$\chi^{(2)}_{ZXX}$	-1.10 ± 5.12	-0.73 ± 2.01	7.68 ± 41.57
$\chi^{(2)}_{XZX}$	-1.09 ± 5.15	-0.73 ± 2.02	-0.82 ± 9.40
		$L_1 - \chi^{(2)}$ values given in pm/V	
$\chi^{(2)}_{ZZZ}$	-12.82 ± 18.64	-12.97 ± 8.34	-21.96 ± 67.88
$\chi^{(2)}_{ZXX}$	-2.14 ± 9.96	-1.42 ± 3.92	14.94 ± 80.87
$\chi^{(2)}_{XZX}$	-2.13 ± 10.01	-1.43 ± 3.93	-1.59 ± 18.29

Table S9. β components corresponding to the non-vanishing $\chi^{(2)}$ ones associated with surface SHG measurements. The results were obtained for N = 1, 6, and 1(6) [See text for details of N = 1(6)]. All of them were obtained at T = 280 K and are in atomic units unless explicitly stated.

Property	N = 1	N = 6	N = 1(6)
		L_1	
β_{ZZZ}	-11.17 ± 19.85	-13.24 ± 8.86	-15.49 ± 83.61
β_{ZXX}	-0.69 ± 10.92	-1.42 ± 4.48	8.67 ± 120.15
β_{XZX}	-0.69 ± 10.96	-1.42 ± 4.49	0.80 ± 17.96
		L_2	
β_{ZZZ}	-0.24 ± 17.20	2.06 ± 7.73	2.26 ± 63.91
β_{ZXX}	-1.28 ± 12.93	-0.26 ± 5.07	17.19 ± 113.06
β_{XZX}	-1.30 ± 12.94	-0.25 ± 5.07	6.91 ± 18.34
		L_3	
β_{ZZZ}	-0.73 ± 20.25	0.97 ± 7.31	8.44 ± 70.12
β_{ZXX}	1.07 ± 12.75	0.10 ± 4.01	27.65 ± 86.10
β_{XZX}	1.03 ± 12.77	0.10 ± 4.01	6.67 ± 19.21
		L_4	
β_{ZZZ}	1.32 ± 23.12	0.17 ± 9.06	11.66 ± 76.02
β_{ZXX}	-0.53 ± 11.23	-1.26 ± 5.28	9.76 ± 101.93
β_{XZX}	-0.53 ± 11.27	-1.26 ± 5.28	2.38 ± 20.02
		L_1	
$\chi^{(2)}_{ZZZ}$	-4.87 ± 8.65	-5.77 ± 3.86	-6.75 ± 36.44
$\chi^{(2)}_{ZXX}$	-0.30 ± 4.76	-0.62 ± 1.95	3.78 ± 52.37
$\chi^{(2)}_{XZX}$	-0.30 ± 4.78	-0.62 ± 1.96	0.35 ± 7.83
		$L_1 - \chi^{(2)}$ values given in pm/V	
$\chi^{(2)}_{ZZZ}$	-9.48 ± 16.83	-11.23 ± 7.51	-13.13 ± 70.90
$\chi^{(2)}_{ZXX}$	-0.59 ± 9.26	-1.20 ± 3.80	7.35 ± 101.89
$\chi^{(2)}_{XZX}$	-0.59 ± 9.29	-1.21 ± 3.81	0.68 ± 15.23