

High Selectivity Boolean Olfaction Using Hollow-Core Wavelength-Scalable Bragg Fibers

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Simulations

We present detailed simulation results of the fiber array based optoelectronic nose system. 180 fibers are created in the 600-4000 cm^{-1} wavenumber range using simple Gaussian peaks as shown in Figure S1. We took into account gradually widening fiber transmission bands and the PES/As₂Se₃ waveguide absorption that affects the fiber transmission bands. Three groups of 60 equally spaced (spectrally) fibers are simulated between 600-1200 cm^{-1} (fibers 1-60) 1200-1800 cm^{-1} (fibers 61-120) and 1800-4000 cm^{-1} (121-180). For the simulations where 25 fibers are used we selected fibers 11, 17, 23, 30, 36, 42, 45, 48, 51, 55, 61, 67, 73, 80, 86, 93, 97, 100, 106, 114, 148, 150, 155, 161, 166; for the 50 fiber simulations we used additional 25 fibers 8, 14, 20, 26, 33, 39, 44, 47, 50, 53, 58, 64, 70, 77, 83, 90, 95, 99, 103, 110, 140, 149, 152, 158, 164. For the 90 fiber simulations we used the odd numbered fibers from the whole set.

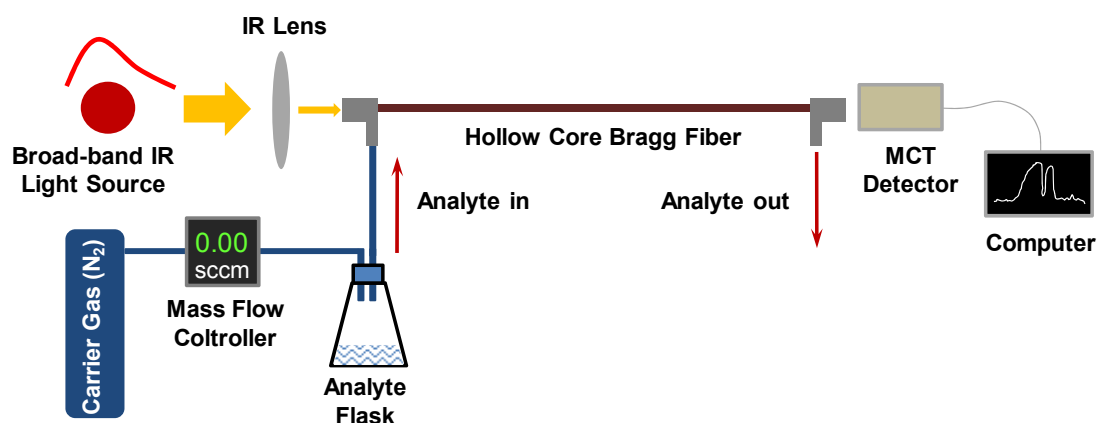


Figure S1. Schematic representation of experimental set up. The analyte vapors were delivered to the fibers using nitrogen as carrier gas. The gas flow rate was controlled with a mass flow controller and adjusted to 1000 sccm.

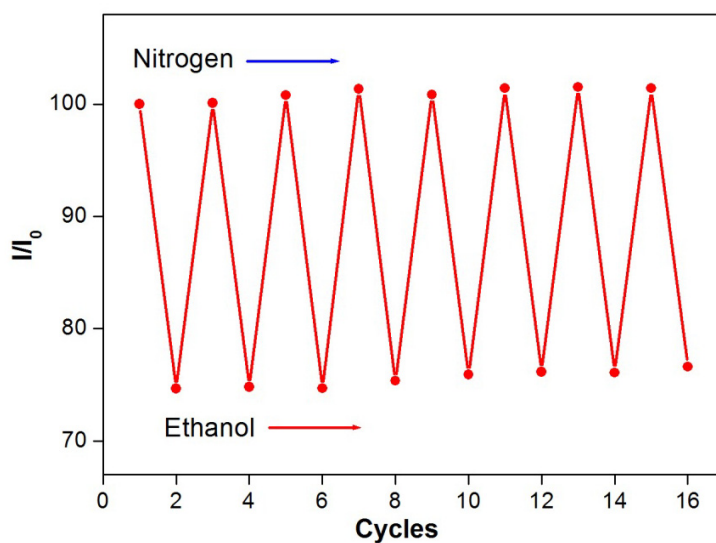


Figure S2. Repeatability of the fiber nose experimental set up is tested with ethanol and a fiber which has a transmission maximum around 1030 cm⁻¹. Transmission signal of the fiber was quickly recovered after flushing with nitrogen.

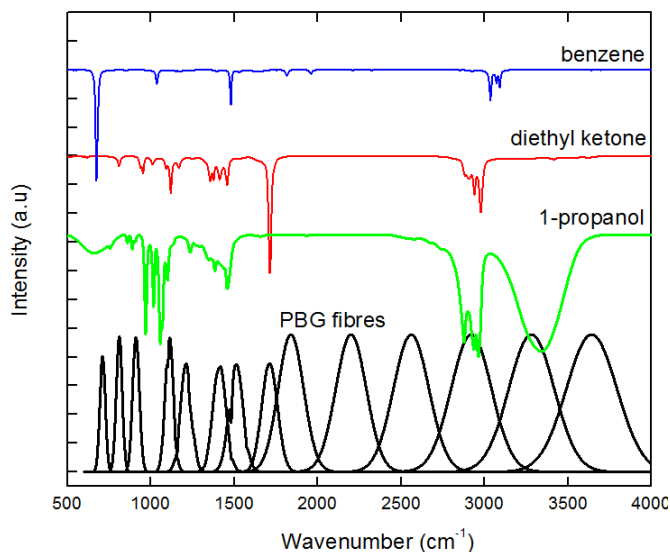


Figure S3. Typical transmission bands for PBG fibers and absorption spectra of chemicals used in the simulations.

Transmission bands for a selected number of fibers are generated in the 600-4000 cm^{-1} wavenumber range. The FTIR absorption spectra of a commercial chemicals library is imported. The intensity ratio for each chemical/fiber pair is obtained from $\frac{\int P_i A_i(\lambda) T_j(\lambda) d\lambda}{\int T_j(\lambda) d\lambda}$ where P_i is the partial atmospheric pressure and $A_i(\lambda)$ is the infrared absorption of the i^{th} gaseous analyte, and $T_j(\lambda)$ is the transmission of the j^{th} fiber. A visual representation is obtained from binary chemical codes obtained by selecting a threshold value for the quenching ratios.

Table S1. The calculated normalization factors.

Analyte	Fiber	Difference
Methanol	1	4
IPA	1	5.1
Acetone	2	15.1
IPA	5	3.9
Acetone	6	10.1
IPA	6	2.8

Table S2. The complete list of the successfully distinguished chemicals, their binary representation and corresponding decimal code.

No.	Chemical name	Binary code	Decimal code
1	Methyl Formate	0001 1111 1110 1110 0000 11111	4185119
2	Ethyl Formate	0000 0000 1111 0000 0011 00000	122976
3	Buthyl Formate	0000 0000 1110 0000 0011 11100	114812
4	Methyl Propyl Ketone	0000 0000 0110 1110 0011 11100	56444
5	N-Amyl Alcohol	0000 1111 1000 1111 0000 11111	2039327
6	Cumene	1100 0111 0000 1111 1000 11100	26091292
7	Tert-amyl Alcohol	0001 1011 1111 1110 0000 11111	3669023
8	Acetylacetone	0101 1110 0111 1111 1111 00000	12386272
9	Ethylene Glycol Monomethyl Ether	0011 1111 1111 1110 0000 11111	8387615
10	Benzylacetate	1100 0111 0011 1110 0011 00000	26115168
11	N,N-Dimethylacetamide	0000 0100 0010 1111 1111 00000	548832
12	Furfural	0101 1111 1111 1111 1111 00000	12582880
13	Furfuryl Alcohol	1111 1111 1111 1111 0000 11111	33553951
14	1-Hexanol	0000 0111 1000 0110 0000 11111	986143
15	Isopropyl Methyl Ketone	0000 0001 1110 1110 0011 11100	253052
16	2-Methoxyethyl Acetate	0000 0111 1111 1110 0011 11100	1047676
17	Nitroethane	0000 0000 0000 1111 1100 00000	8064
18	Styrene	1101 1100 0000 0010 0000 00100	28836868
19	Tert-buthyl Methyl Ether	0010 0011 1111 1110 0000 11100	4717596
20	Nitromethane	0000 0001 1000 1111 1100 00000	204672
21	L(-)-Ethyl Lactate	0000 0111 1111 1110 0011 11111	1047679
22	N,N-Dimethylformamide	0000 0011 1000 1111 0111 11000	466680
23	Carbon Tetrachloride	0110 0000 0000 0000 0000 00000	12582912
24	Tetrahydrofuran	0001 1111 1000 0000 0000 11100	4128796
25	4-Hydroxy-4-Methyl-2-Pentanone	0001 1000 1111 1111 0011 11111	3276415
26	Diethyl Ketone	0000 1001 1100 1110 0011 11100	1285244
27	Diethyl Ether	0010 0111 1111 1111 0000 11100	5242396
28	Ethyl Propionate	0000 0111 1111 1111 0011 11100	1048188
29	4-Methyl-2-Pentanol	1011 1111 1111 1111 0000 11111	25165343
30	Cyclohexanol	0000 1111 1001 1110 0000 11111	2047007
31	Propyl Acetate	0000 0111 0011 1110 0011 11100	949372
32	Mesityl Oxide	0000 1000 0111 1111 1111 11100	1114108
33	3-Methylcyclohexanol	0000 1111 1101 1110 0000 11111	2079775
34	4-Methylcyclohexanol	0000 1111 1000 1110 0000 11111	2038815
35	1,1,1-Trichloroethane	1101 0111 1100 1110 0000 11100	28285980
36	1,4-Dioxane	0001 0111 1111 1110 0000 11100	3144732
37	Benzene	1000 0000 0000 0000 0000 00000	16777216
38	Ethyl Acetate	0000 0111 0011 1100 0011 00000	948320
39	Trichloroethylene	0111 1000 0000 0000 0000 00000	15728640
40	Tetrachloroethylene	0101 0000 0000 0000 0000 00000	10485760
41	Cyclohexanone	0000 0000 0000 0000 0011 11100	124
42	3-Heptanone	0000 0111 1100 1110 0011 11100	1023100
43	Carbon Disulfide	0000 0000 0000 0011 1100 00000	1920
44	Isoxazole	0111 1111 1110 1111 1100 00110	16768902
45	Acrylonitrile	1000 1111 1000 0110 0000 00100	18811908

No.	Chemical name	Binary code	Decimal code
46	Dimethyl Phosphite	0110 1111 1111 1111 0000 11111	14679583
47	Dimethyl Sulfone	0101 1001 1111 1100 0000 00000	11794432
48	Ethanol	0001 0111 1001 1111 0000 11111	3096095
49	Dimethyl Sulphoxide	1000 1111 1000 0110 0000 00000	18811904
50	Acetaldehyde	0001 0011 1100 1110 0111 11100	2596092
51	Chloroacetamide	1110 0011 1111 1111 1111 11111	29884415
52	Methyl Acetate	0010 0111 1011 1111 0011 01100	5209708
53	1,3-Dioxolane	0001 1111 1111 0000 0000 11100	4186140
54	Acetone	0000 0000 0011 1110 0011 00000	31840
55	Ethylthiocyanate	0100 1011 0011 1110 0000 11100	9862172
56	Epichlorohydrin	1111 1000 1111 1110 0000 11100	32635932
57	2-Propyn-1-ol	1001 1111 0011 1110 0000 11111	20872223
58	Furan	1101 1111 0110 0011 0000 00000	29279744
59	Maleimide	1011 1001 1101 1101 1111 01111	24361967
60	Trimethyl Borate	0000 0110 0111 1111 1000 11100	851740
61	1-Propanol	1101 1111 1111 1111 0000 11111	29359647
62	Dimethyl Carbonate	0101 1000 0011 1110 0011 00000	11566176
63	Formamide	1100 0111 1111 1111 1111 11111	26214399
64	Thiophosgene	0110 0001 1100 0000 0000 00000	12812288
65	Formic Acid	1111 1011 1111 1111 1111 11111	33030143
66	Acetonitrile	0000 0111 0000 1111 1000 00100	925444
67	Methylhydrazine	0111 1111 1111 1111 1110 11111	16777183
68	Methanol	0000 0111 0000 0110 0000 11111	920607
69	1,2-Epoxybutane	0111 1000 0001 0111 0000 11100	15740444
70	Vinyl Acetate	1111 1111 1111 1111 1111 00000	33554400
71	Methyl Acrylate	0010 1111 0111 1110 0111 00000	6225120
72	Methacrylic Acid	0011 1100 0111 1111 1111 11111	7929855
73	Pyrrole	1100 0111 1000 0111 0000 00011	26152451
74	Tert-Butanol	0001 0000 0111 1110 0000 11111	2161695
75	Isobuthanol	0000 0111 0000 1111 0000 11111	925215
76	Morpholine	0111 0111 1111 1110 0000 11110	15727646
77	Pyrrolidine	0111 0011 1000 0000 0000 11110	15138846
78	Cyclopentene	1001 0110 0000 0010 0000 11100	19661852
79	Pyridine	1100 0110 0000 0111 1100 00100	25956228
80	Methyl Methacrylate	0010 1000 0111 1110 0011 00000	5307488
81	Ethyl Acrylate	0010 1111 1111 1110 1111 01100	6290924
82	Chlorobenzene	1100 0111 1000 0011 1100 00000	26150784
83	Hexafluorobenzene	0000 1110 0000 0011 1100 00000	1836928
84	Aniline	1100 0000 0111 1011 1110 00111	25229255
85	Dipropyl Ether	0000 0111 1100 1110 0000 11100	1023004
86	Cyclohexane	0000 0000 0000 0010 0000 11100	1052
87	ϵ -Caprolactone	0000 1111 1111 1110 0011 11100	2096252
88	Cyclohexene	1001 0000 0000 0110 0000 11100	18877468
89	Thiophenethanol	1010 0111 1111 1111 0000 11111	22019615
90	Bromoethane	0100 1000 0011 1110 0000 11100	9468956
91	Phosphoryl Chloride	0000 0000 0001 1000 0000 00000	12288
92	Trichlorosilane	0110 0111 1100 0000 0000 00000	13598720
93	Tripropylamine	0000 0111 1111 1110 0000 11100	1047580
94	α -Methylstyrene	1101 0100 0001 1111 1110 11100	27803612

No.	Chemical name	Binary code	Decimal code
95	2-Methylcyclohexanol	0000 1111 1000 0110 0000 11111	2034719
96	Chloroform	1100 0000 0010 0000 0000 00000	25182208
97	Toluene	1000 0000 0000 0011 0000 00100	16778756
98	Thiophen	1010 0001 0000 0100 0000 00000	21104640
99	cis-Cycloocatene	1100 0000 0000 0110 0000 11100	25168924
100	Piperidine	0110 0000 1000 0010 0000 11100	12649500

Table S3. The complete list of all possible mixes of the five chemicals sets, *i.e.*, DMF, ethanol, methanol, acetone and toluene. All 31 mixes were distinctly identified and their binary chemical codes and decimal codes are given. Mixings are denoted by sets of single chemical numbers.

No.	Chemical name	Binary code	Decimal code
1	Dimethylformamide	0000 0001 0000 1100 1110 00000	137,664
2	Ethanol	0000 1011 0000 1100 0000 11111	1,447,967
3	Methanol	0000 0000 0101 1100 0110 00000	47,296
4	Acetone	0000 0011 0000 0000 0000 11111	393,247
5	Toluene	0100 0000 0000 0000 0000 00000	8,388,608
6	{1, 2}	1000 1011 0001 1110 1110 11111	18,234,847
7	{1, 3}	0000 0001 0101 1110 1111 00000	179,680
8	{1, 4}	1000 0011 0001 1110 1110 11111	17,186,271
9	{1, 5}	0100 0001 0001 1111 1110 01100	8,536,012
10	{2, 3}	0000 1011 0111 1110 0110 11111	1,506,527
11	{2, 4}	0000 1011 0001 1110 0000 11111	1,457,183
12	{2, 5}	0100 1011 0000 1111 0000 11111	9,838,111
13	{3, 4}	0000 0011 0101 1110 0110 11111	441,567
14	{3, 5}	0100 0000 0101 1100 0110 00000	8,435,904
15	{4, 5}	0100 0011 0000 0011 0000 11111	8,783,391
16	{1, 2, 3}	1000 1011 0111 1111 1111 11111	18,284,543
17	{1, 2, 4}	1000 1011 1001 1111 1110 11111	18,300,895
18	{1, 2, 5}	1100 1011 0001 1111 1110 11111	26,623,967
19	{1,3,4}	1000 0011 0111 1111 1111 11111	17,235,967
20	{1,3,5}	0100 0001 0101 1111 1111 11100	8,568,828
21	{1,4,5}	1100 0011 0001 1111 1110 11111	25,575,391
22	{2,3,4}	0000 1011 0111 1111 0110 11111	1,507,039
23	{2,3,5}	0100 1011 0111 1111 0110 11111	9,895,647
24	{2,4,5}	0100 1011 0001 1111 0000 11111	9,846,303
25	{3,4,5}	0100 0011 0101 1111 0110 11111	8,830,687
26	{1,2,3,4}	1000 1011 1111 1111 1111 11111	18,350,079
27	{1,2,3,5}	1100 1011 0111 1111 1111 11111	26,673,151
28	{1,2,4,5}	1100 1011 1001 1111 1110 11111	26,689,503
29	{1,3,4,5}	1100 0011 0111 1111 1111 11111	25,624,575
30	{2,3,4,5}	0100 1011 0111 1111 0110 11111	9,895,647
31	{1,2,3,4,5}	1100 1011 1111 1111 1111 11111	26,738,687