SUPPORTING INFORMATION

Spectroscopic Properties of Benzene at the Air–Ice Interface: A Combined Experimental–Computational Approach

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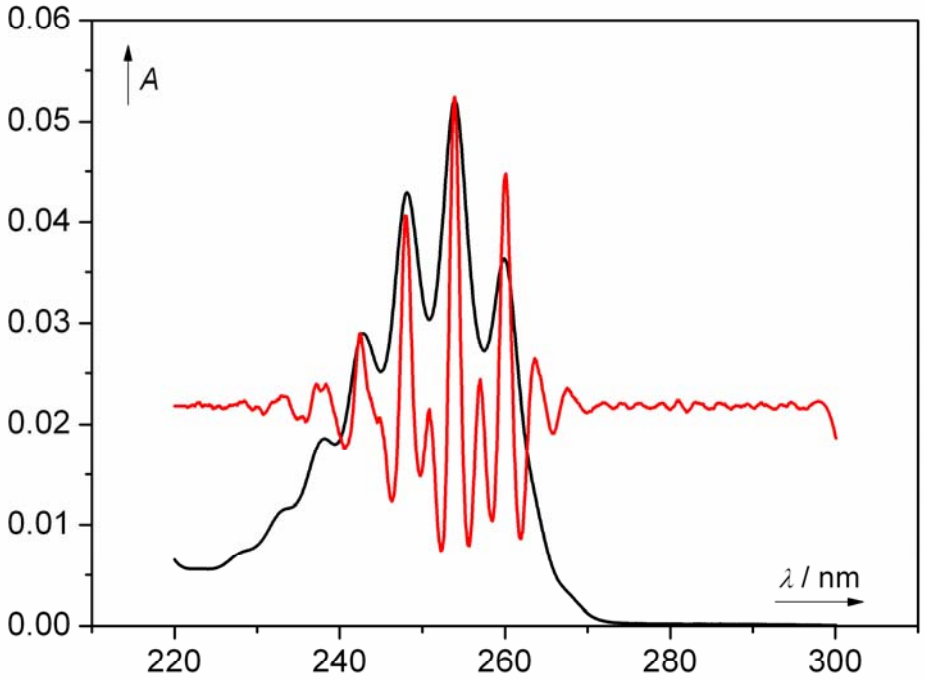

Figure S1. The absorption spectrum of benzene aq solution (black) with its 4th derivative (red).

Table S1. The literature survey of the experimentally found vibrations of the $S_0 \rightarrow S_1$ ($1^1A_{1g} \rightarrow 1^1B_{2u}$) transitions of benzene in various phases and environments. The values are given in the wavenumbers and wavelengths: [a] ref. 1, [b] ref. 2, [c] ref. 3, [d] ref. 4.

		benzene absorption maxima / cm^{-1}				
		vapor[a]	solid 20 K[b]	solid 279 K[c]	liquid 299 K[c]	free-jet (vapor)[d]
6_1^0	B_0^0 (hot)	37482	37200	37180	37180	
1_0^0	K_1 (0–0)	38089	37835	37800		
$6_0^1 1_0^0$	A_0^0	38609	38355	38300	38300	38611
1_0^1	K_2		38760	38760		
$6_0^1 1_0^1$	A_1^0	39532	39280	39200	39200	39533
1_0^2	K_3		39685	39680		
$6_0^1 1_0^2$	A_2^0	40455	40205	40130	40130	40458
1_0^3	K_4		40610	40630		
$6_0^1 1_0^3$	A_3^0	41378	41130		41030	41377
$6_0^1 1_0^4$	A_4^0					42297

		benzene absorption maxima / nm				
		vapor[a]	solid 20 K[b]	solid 5.45 °C[c]	liquid 299 K[c]	free-jet (vapor)[d]
6_1^0	B_0^0 (hot)	266.8	268.8	269.0	269.0	
1_0^0	K_1 (0–0)	262.5	264.3	264.6		
$6_0^1 1_0^0$	A_0^0	259.0	260.7	261.1	261.1	259.0
1_0^1	K_2		258.0	258.0		
$6_0^1 1_0^1$	A_1^0	253.0	254.6	255.1	255.1	253.0
1_0^2	K_3		252.0	252.0		
$6_0^1 1_0^2$	A_2^0	247.2	248.7	249.2	249.2	247.2
1_0^3	K_4		246.2	246.1		
$6_0^1 1_0^3$	A_3^0	241.7	243.1		243.7	241.7
$6_0^1 1_0^4$	A_4^0					236.4

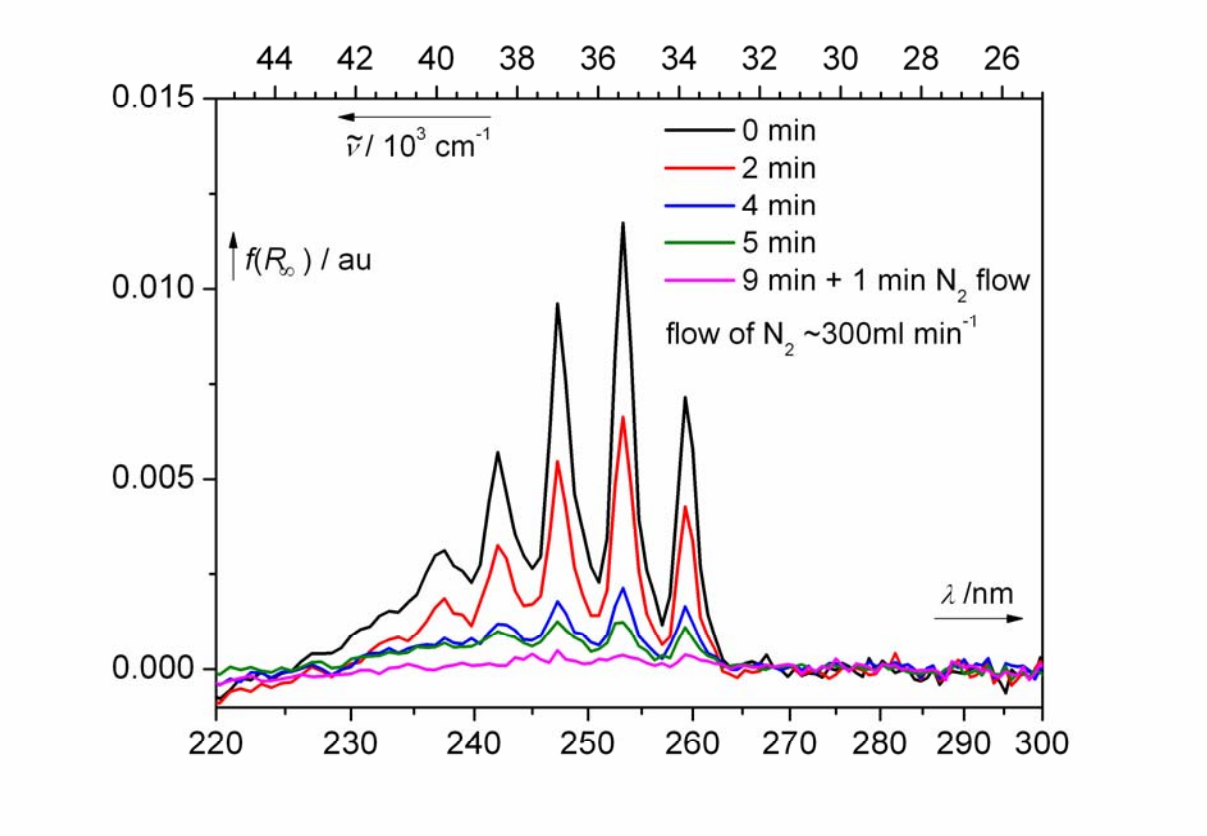

Figure S2. The UV-Vis absorbance spectra changes over a diffusion controlled sublimation of benzene from supersaturated (VD) ice grain surface at 253 K. The last trace represents a UV-Vis spectrum of a sample under N_2 gas flow reducing the benzene concentration below the detection capacity of the spectrometer. The spectra of the solid samples were recorded using a diffuse reflectance accessory.

Table S2. The fluorescence emission maxima (λ_{exc} = 248 nm) of benzene aq solution and benzene in artificial snow prepared by a SF method (77 K).

experimental fluorescence emission maxima / nm	
benzene aq solution	benzene snow 77 K
268	269
271.3	273.2
275.2	276
279	280.2
283	284.1
286.4	288.1
291.1	292
294.6	296.3
299.6	300.5

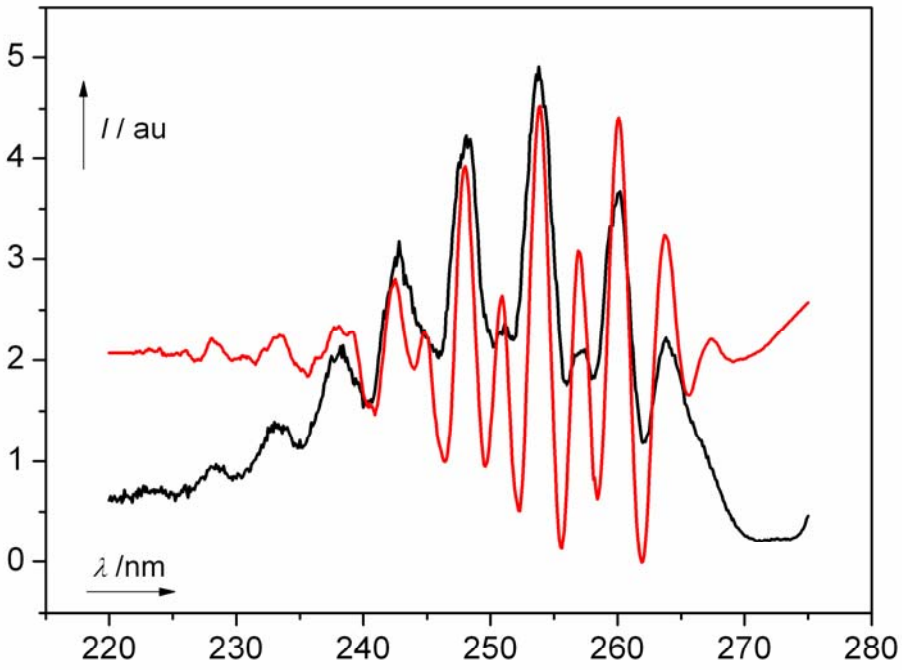

Figure S3. The excitation spectra of benzene in artificial snow at 77 K (SF; black) with its 4th derivative (red).

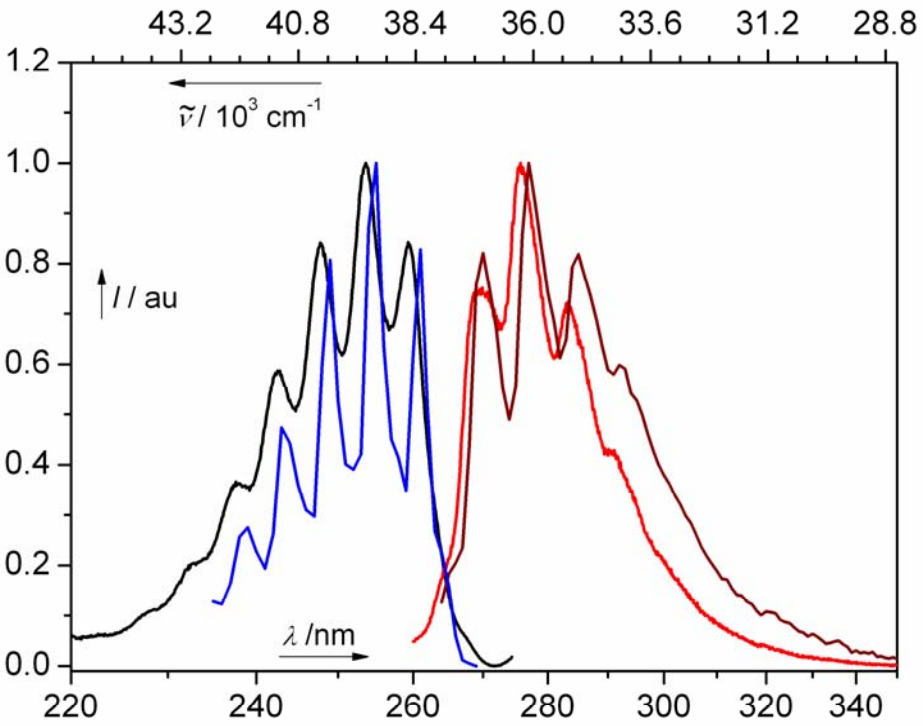

Figure S4. The fluorescence emission (λ_{exc} = 248 nm, red line) and excitation (λ_{em} = 283 nm, black line) spectra of aq benzene solution (c = 1.4 mM; 295 K), and the emission (λ_{exc} = 248 nm, brown line) and excitation (λ_{em} = 290 nm, blue line) spectra of benzene in artificial snow prepared by a SF method (253 K).

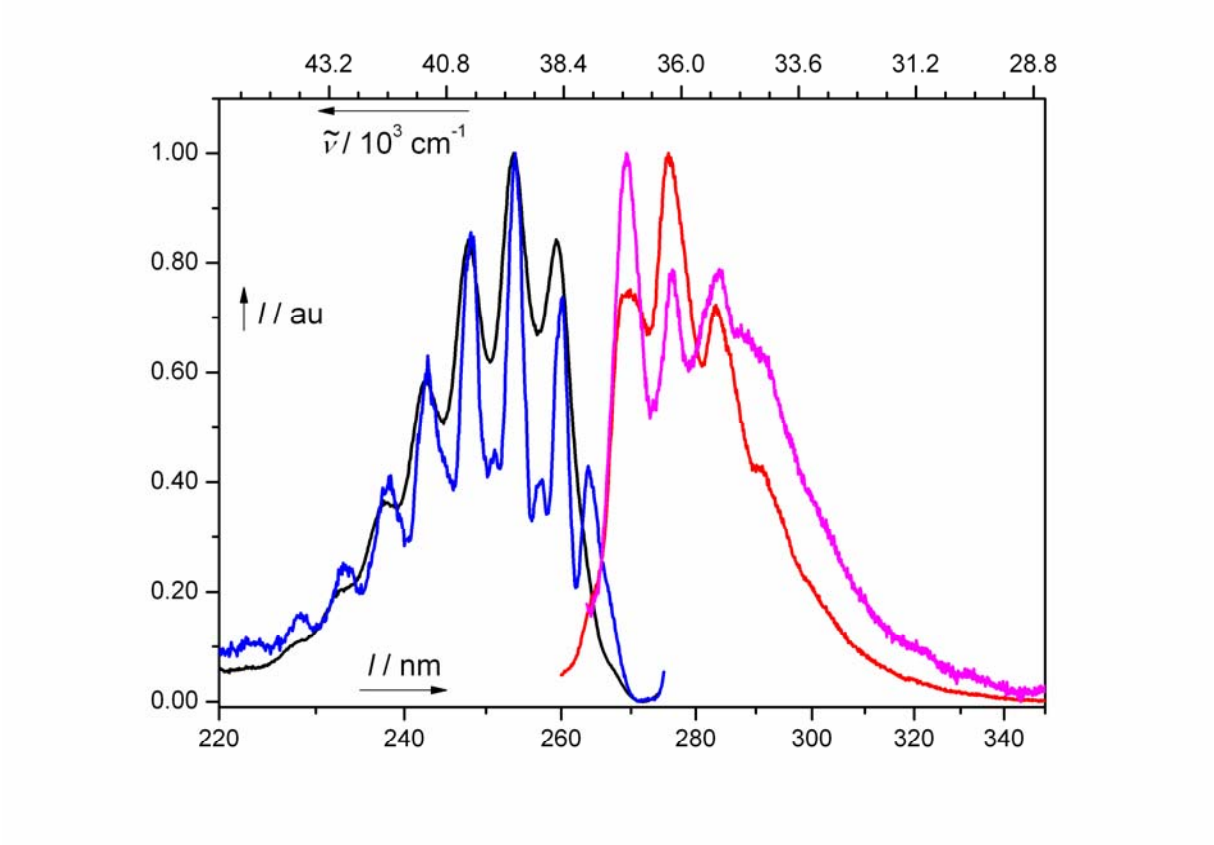

Figure S5. The fluorescence emission (λ_{exc} = 248 nm, red line) and excitation (λ_{em} = 283 nm, black line) spectra of aq benzene solution (c = 1.4 mM; 295 K), and the emission (λ_{exc} = 248 nm, magenta line) and excitation (λ_{em} = 290 nm, blue line) spectra of benzene in artificial snow samples (SF; 77 K).

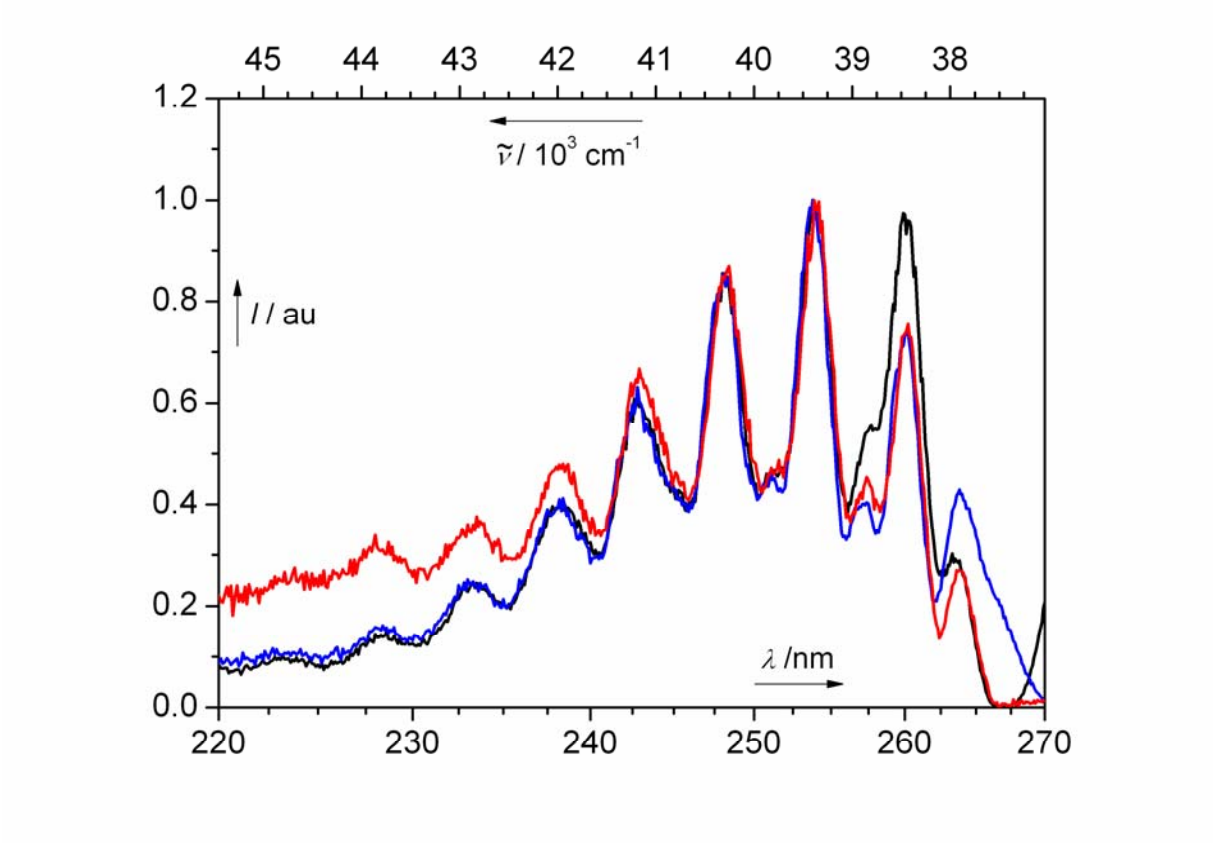

Figure S6. The fluorescence excitation spectra of benzene in artificial snow (SF, prepared from 1.4 mM solution) measured at 77 K: the emission wavelengths of 284 nm (black), 290 nm (blue) and 320 nm (red).

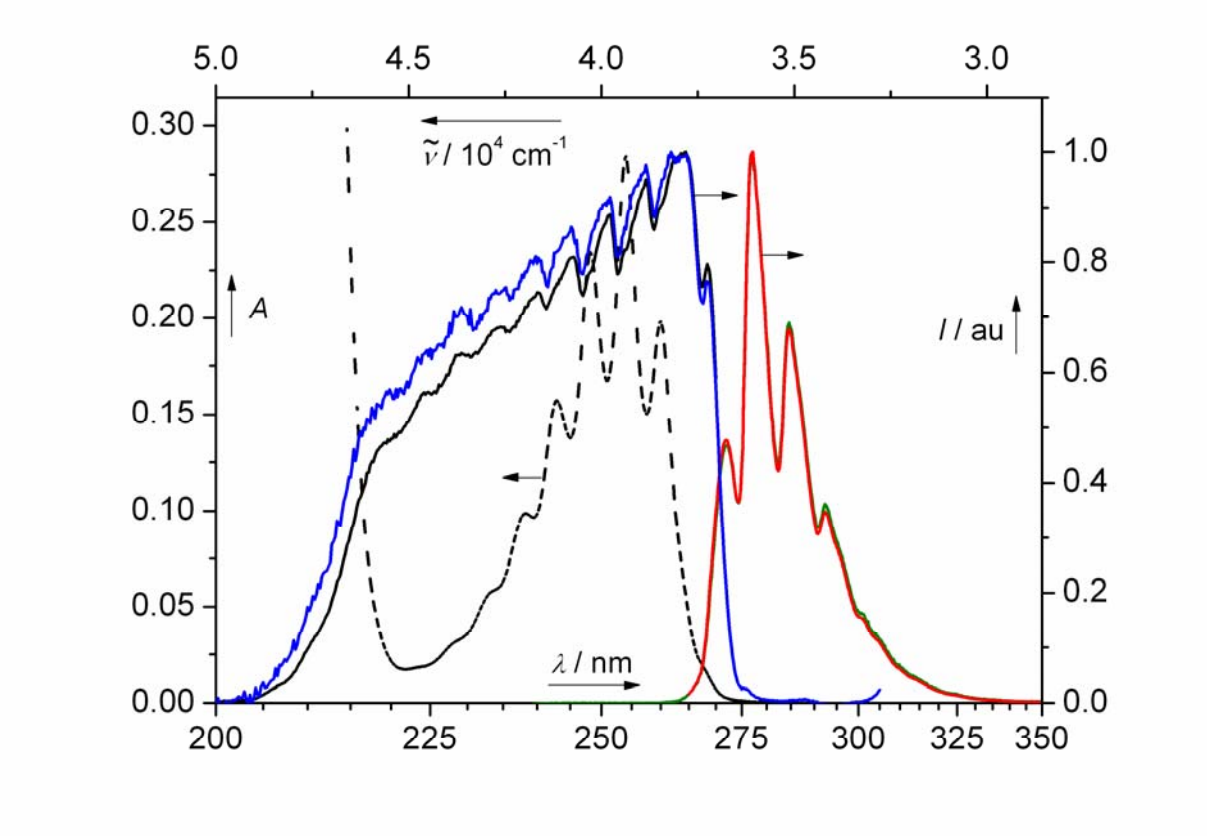

Figure S7. The fluorescence excitation (283 nm, black; 320 nm, blue) and emission (243 nm, red; 214 nm, green) spectra of benzene on artificial snow (VD) measured at 253 K. The absorption spectrum of melted sample is shown (black dashed line) for comparison. The total benzene concentration was 8.4 mM.

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