

Influence of the Dushinsky effect on the vibronic spectra of 9,9,9',9'-tetramethyl-2,2'-bifluorene

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Fig.1 Equilibrium geometries of the S_0 state of 9,9,9',9'-tetramethyl-2,2'-bifluorene

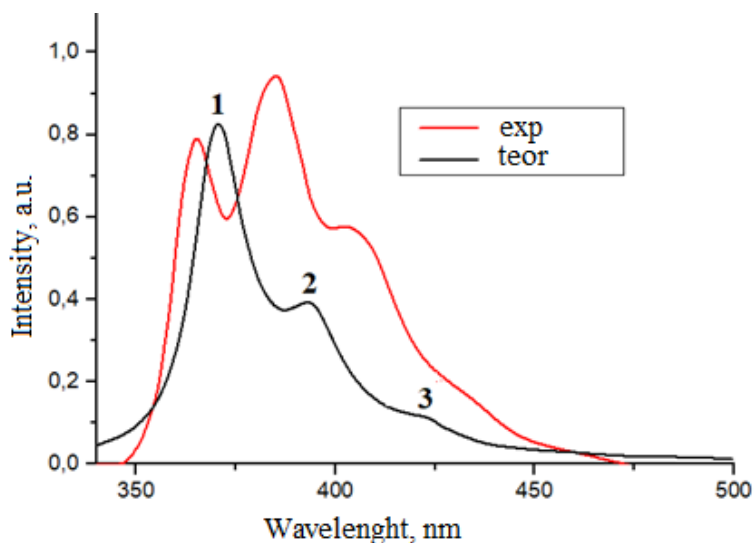


Fig.2 Vibronic fluorescence spectra of 9,9,9',9'-tetramethyl-2,2'-bifluorene

Table1. Spectral characteristics of 9,9,9',9'-tetramethyl-2,2'-bifluorene

Transit ion	Band	λ_{exp} [13], nm	λ_{teor} , nm	ω , cm^{-1}	FC (without Duschinsky effect)	ω , cm^{-1}	FC (with the Duschinsky effect[2])		
$S_1 \rightarrow S_0$	1	365	371	19	$2.7 \cdot 10^{-4}$	22	$1.4 \cdot 10^{-6}$		
				30	$3.5 \cdot 10^{-4}$	33	$2.2 \cdot 10^{-5}$		
				82	$3 \cdot 10^{-5}$	89	$3.2 \cdot 10^{-6}$		
				135	$1.9 \cdot 10^{-5}$	124	$3.1 \cdot 10^{-7}$		
				158	$3.7 \cdot 10^{-5}$	133	$1.6 \cdot 10^{-6}$		
					155	$9.1 \cdot 10^{-7}$			
	2	385	394	1692	$6.4 \cdot 10^{-5}$	1656	$9.5 \cdot 10^{-7}$		
				19×30	$3.4 \cdot 10^{-4}$	22×33	$1.0 \cdot 10^{-5}$		
				19×82	$3.0 \cdot 10^{-5}$	22×89	$1.5 \cdot 10^{-6}$		
				19×135	$1.9 \cdot 10^{-5}$	33×22	$1.1 \cdot 10^{-5}$		
				19×158	$3.7 \cdot 10^{-5}$	33×89	$2.4 \cdot 10^{-5}$		
				19×1692	$6.2 \cdot 10^{-5}$	33×124	$2.3 \cdot 10^{-6}$		
				30×19	$3.5 \cdot 10^{-4}$	33×133	$1.2 \cdot 10^{-5}$		
				30×135	$2.5 \cdot 10^{-5}$	33×155	$7.1 \cdot 10^{-6}$		
						33×1656	$7.2 \cdot 10^{-6}$		
					133×33	$1.2 \cdot 10^{-5}$			
					133×89	$1.8 \cdot 10^{-6}$			
					155×33	$7.1 \cdot 10^{-6}$			
3				404	424	135×19	$1.9 \cdot 10^{-5}$	359×33	$1.4 \cdot 10^{-6}$
						135×30	$3.5 \cdot 10^{-5}$	564×33	$1.4 \cdot 10^{-6}$
						158×19	$3.6 \cdot 10^{-5}$	571×33	$2.3 \cdot 10^{-6}$
	1378×30	$1.6 \cdot 10^{-5}$	731×33			$2.3 \cdot 10^{-6}$			
	1692×19	$6.2 \cdot 10^{-5}$	731×89			$4.7 \cdot 10^{-7}$			
	1692×30	$8.1 \cdot 10^{-5}$	1656×22			$4.6 \cdot 10^{-7}$			
			1656×33			$7.0 \cdot 10^{-6}$			
			1656×89			$1.0 \cdot 10^{-6}$			
		1656×133	$5.5 \cdot 10^{-7}$						

[1] Jo J. et al. Synthesis and Characterization of Monodisperse Oligofluorenes // Chem. Eur. J. – 2004. – V. 10. – P. 2681-2688.

[2] Duschinsky F. Meaning of the Electronic Spectrum of Polyatomic Molecules. The Frank-Condon Principle // Acta Physicochim. URSS 7 1937. P.551-566.

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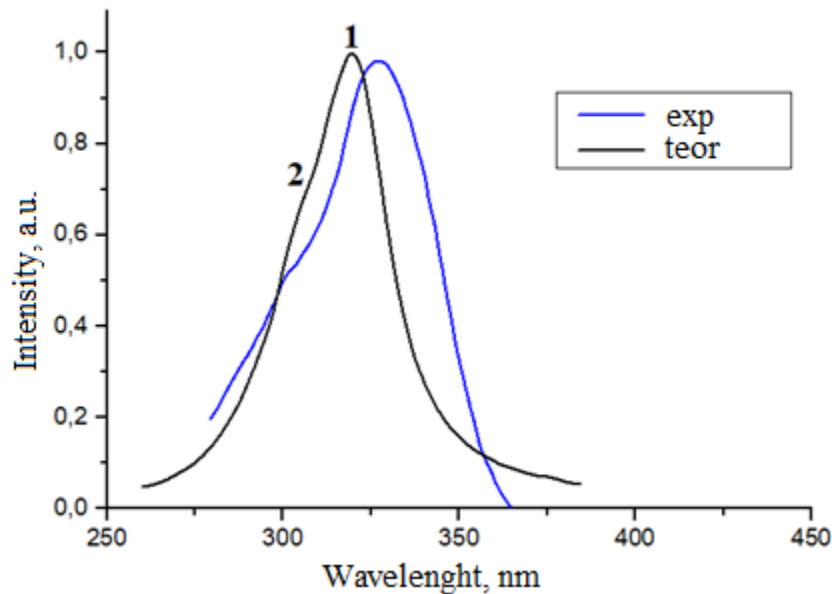


Fig.3 Vibronic absorption spectra of 9,9,9',9'-tetramethyl-2,2'-bifluorene

Table2. Spectral characteristics of 9,9,9',9'-tetramethyl-2,2'-bifluorene

Transition	Band	$\lambda_{exp}[1]$, nm	λ_{teor} , nm	ω , cm^{-1}	FC (without Duschinsky effect)	ω , cm^{-1}	FC (with the Duschinsky effect[2])
$S_0 \rightarrow S_1$	1	327	319	22	$2.4 \cdot 10^{-7}$	19	$7.8 \cdot 10^{-8}$
				33	$9.9 \cdot 10^{-7}$	30	$1.7 \cdot 10^{-7}$
				89	$1.3 \cdot 10^{-7}$	82	$2.0 \cdot 10^{-8}$
				120	$3.0 \cdot 10^{-8}$	126	$4.9 \cdot 10^{-9}$
				133	$2.0 \cdot 10^{-7}$	135	$3.3 \cdot 10^{-9}$
				153	$1.8 \cdot 10^{-8}$	158	$1.2 \cdot 10^{-8}$
				155	$5.4 \cdot 10^{-8}$	571	$1.2 \cdot 10^{-8}$
	2	301	303	1656	$6.1 \cdot 10^{-8}$	1692	$1.3 \cdot 10^{-8}$
				22×33	$1.0 \cdot 10^{-6}$	19×30	$5.4 \cdot 10^{-7}$
				22×133	$2.0 \cdot 10^{-7}$	19×82	$6.9 \cdot 10^{-8}$
				33×22	$1.0 \cdot 10^{-6}$	19×126	$1.6 \cdot 10^{-8}$
				33×89	$5.6 \cdot 10^{-7}$	19×135	$1.0 \cdot 10^{-8}$
				33×120	$1.2 \cdot 10^{-7}$	19×158	$4.5 \cdot 10^{-8}$
				33×133	$8.2 \cdot 10^{-7}$	30×19	$5.5 \cdot 10^{-7}$
33×1656	$2.5 \cdot 10^{-7}$	30×42	$4.9 \cdot 10^{-8}$				
			89×22	$1.4 \cdot 10^{-7}$	30×82	$1.5 \cdot 10^{-7}$	
			89×33	$5.6 \cdot 10^{-7}$	30×126	$3.5 \cdot 10^{-8}$	
			89×133	$1.1 \cdot 10^{-7}$	30×135	$2.4 \cdot 10^{-8}$	
			120×33	$1.2 \cdot 10^{-7}$	30×158	$8.3 \cdot 10^{-8}$	
					1692×19	$4.2 \cdot 10^{-8}$	
					1692×30	$8.9 \cdot 10^{-8}$	
					1692×82	$1.1 \cdot 10^{-8}$	

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Thanks for watching

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