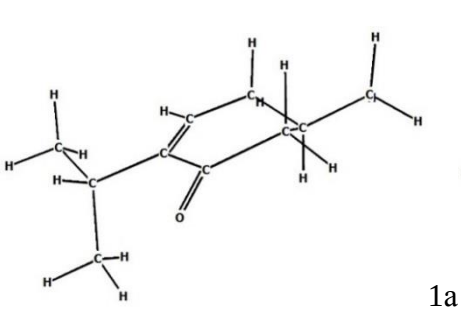
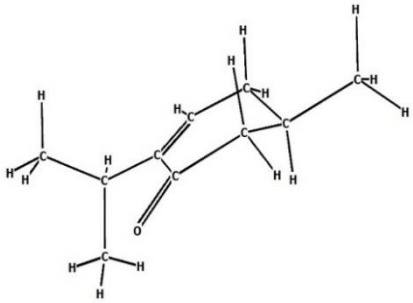
DEPENDENCE OF CONFORMAL STABILITY (R)-4-MENTENONE FROM TEMPERATURE

Belkina N. V.[1], Vakulin I. V.[1], Talipova G. R.[1], Latypova E. R.[1], Vakulina A. I.[2]
[1]Bashkir state University, Ufa, Russia
[2]Ural State University of Economics, Yekaterinburg, Russia

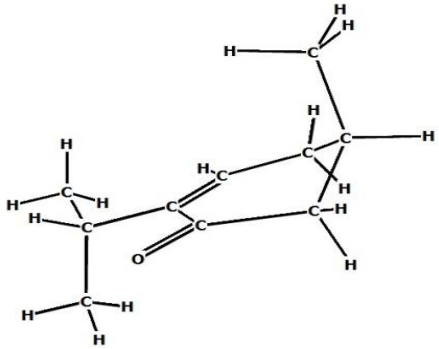
According to NMR spectroscopy in 13C spectra, the signals of conformers of (R)-4-menthenone are manifested when the temperature is lowered. Therefore, using the quantum-chemical approximation B3LYP / 6-311 ++ G (2d, p), the dependence of the population of conformers (R)-4-mentenone on temperature is considered.



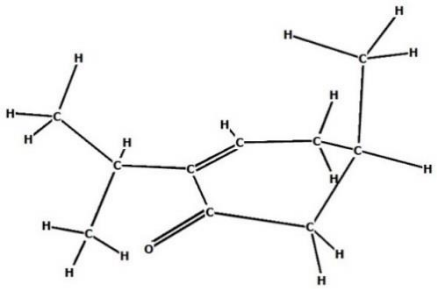
1a



1b



1c



1d

The relative stability of other conformers differs from 1a by not more than 7.97 kJ/mol according to B3LYP / 6-311 ++ G (2d, p). With increasing temperature, the difference in the population of these conformers decreases. First of all, the proportion of conformer 1c in which the methyl group occupies the axial position increases. The proportion of conformers 1b and 1d in which the angle of the isopropyl group is rotated by 180° varies little with increasing temperature (Table).

Table

conformer	**w, %**				
	243	**273**	**298**	**323**	**373**
1a	67.11	62.69	59.42	56.08	50.47
1b	24.98	26.13	26.65	26.98	26.99
1c	6.74	9.29	11.58	13.56	17.51
1d	1.18	1.90	2.54	3.37	5.03