In a series of 1,4-dialkylcyclohexanes we studied the vibrational spectra of compounds with greatly differing conformational volumes of the radicals [1, 2], as well as compounds with the same hydrocarbon radicals [3]. In the vibrational spectra of all the cis-1-methyl-4-alkylcyclohexanes studied, there is a comparatively intense IR band at Raman line in the region of 600-650 cm⁻¹. In the spectra of the trans-isomers these bands and lines either are absent entirely, or are very weak. This agrees with the fact that in the latter hydrocarbons, both radicals are in a diequatorial position, since their diaxial arrangement is too energetically unprofitable.

In the spectra of the symmetrical 1,4-dialkylcyclohexanes studied [3], similar patterns were observed. Only in the IR spectra of stereoisomeric bis-(1-ethylpropyl)- and bis-(1-propylbutyl)-cyclohexanes is a deviation detected: for the stereoisomers that are recognized as trans-forms according to the Raman spectra, weak IR bands in the interval characteristic of the cis-forms were also observed. In view of this, an investigation of the spectra of stereoisomers of 1-methyl-4-(1-ethylpropyl)-cyclohexane (I), synthesized for the first time, the ethylpropyl radical which most likely occupies an equatorial position, was of special interest. The peculiarities of the spectra of these cis- and trans-isomers could be used to consider the nature of the deviation from the general principle observed in [3].

We also studied the vibrational spectra of two more pairs of newly synthesized stereoisomeric dialkylcyclohexanes: 1-n-propyl-4-isopropyl-(II) and 1-n-butyl-4-tert-butylcyclohexanes (III).

### EXPERIMENTAL SECTION

The conditions of obtaining the spectra were the same as in [4, 5].

The IR absorption spectra in the region of 450-3100 cm⁻¹ are cited in Figs. 1 and 2, while the frequencies and intensities of the Raman spectra are given in the text.

All the hydrocarbons studied, just like those described in our previous communication [2], were synthesized by hydrogenation of the corresponding dialkybenzenes, while the mixture of stereoisomers obtained was separated either by precise fractional distillation or by the new thiourea method [6, 7], permitting the separation of stereoisomers even if they both form adducts with thiourea. The constants are given for each hydrocarbon; the boiling points under vacuum are experimental, while the values calculated from the experimental data with the aid of the Dreisbach
cis-1-Methyl-4-(1-ethylpropyl)-cyclohexane. Produced from p-(1-ethylpropyl)-toluene [9] by hydrogenation on Pt-charcoal (20% Pt) in a flow-type system with a volume velocity 0.2 h⁻¹ in a stream of hydrogen at atmospheric pressure and 150°. The mixture of stereoisomers obtained, after freeing from the remains of the aromatic hydrocarbon by chromatography on silica gel, was separated by continuous multi-day round-the-clock distillation on a column with an efficiency of 100 theoretical plates. The distillation was conducted under a vacuum of 7-10 mm with a reflux ratio 200-250; the distillate was collected in portions of 3-4 g; a total of 42 fractions were collected. The fractions were analyzed on a capillary chromatograph, and those possessing a degree of purity no lower than 99.0% were combined. Properties [9]: bp 96.45° (17.5 mm); 214.1° (760 mm); nD 1.4540; d4 0.8276; degree of purity ~99.8%.

Raman spectrum* (Au, cm⁻¹): 184(7), 202(1), 216(5), 245(3), 262(1), 282(3), 307(10, br), 335(2), 354(2), 371(5, d), 377(4), 404(1), 426(2), 444(6), 461(5), 479(3), 491(1), 504(2), 547(3, br), 572(4, br), 599(3), 630(13), 648(9), 670(2), 706(3), 728(1), 747(2), 764(43), 778(20), 809(8), 825(3), 838(12), 854(10), 875(1), 907(12, br), 925(4), 945(6), 963(5), 1008(7), 1028(12), 1039(20, br), 1058(30), 1088(15, d, br), 1103(12, d, b), 1119(10, d), 1128(7, d), 1151(17, br), 1171(14), 1192(17), 1207(11), 1232(9), 1247(3, d), 1263(28, br), 1288(6, d), 1302(4, d), 1318(13), 1344(15), 1363(10), 1437(60), 1447(30, d, b), 1465(50, b), 2848(230, b), 2873(210, b), 2903(230, b), 2931(280, b), 2960(180, b).

cis-1-n-Propyl-4-isopropylcyclohexane. Produced by the hydrogenation of 1-n-propyl-4-isopropylbenzene [9] under the same conditions as those used for the production of the isomers of (I) (see above).

trans-1-Methyl-4-(1-ethylpropyl)-cyclohexane. Produced together with the cis-isomer and separated from it by fractional distillation on a column (see above). Properties [9]: bp 95.55° (17.5 mm); 213.0° (760 mm); nD 1.4478; d4 0.8133; degree of purity 99.8%.

Raman spectrum (Au, cm⁻¹): 186(1), 202(1), 216(0), 230(1), 246(2), 269(4, d), 286(7, d), 300(10, d), 381(3, d), 392(0), 425(1), 443(11), 466(9), 477(10), 486(1), 498(2), 513(5), 547(2), 592(1), 629(2), 653(0), 742(29), 747(6), 766(19), 777(20, br), 801(1), 823(2), 836(2), 860(6), 886(5), 901(4), 911(10), 942(5), 957(3), 994(9, b), 1005(8, b), 1019(3, d, b), 1038(25), 1066(26), 1074(15), 1099(6), 1153(22), 1172(26), 1222(3), 1236(5), 1250(26), 1261(4), 1287(3), 1304(12), 1316(3), 1346(24), 1359(15), 1378(2), 1442(33, br), 1455(60), 2843(200, b), 2871(230, br, b), 2910(200, d, b), 2926(280, br, b), 2955(160, d, b).

 cis-1-n-Propyl-4-isopropylcyclohexane. Produced by the hydrogenation of 1-n-propyl-4-isopropylbenzene [9] under the same conditions as those used for the production of the isomers of (I) (see above).

*Notations of the Raman lines: br – broad; v, br – very broad; d – diffuse; s – sharp; b – the line is situated against a background of substantial intensity.