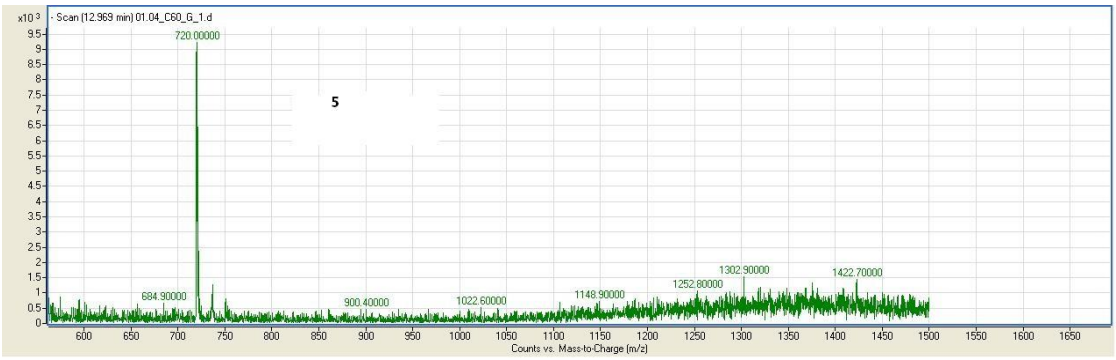

Fig. 5. Mass spectrum of the fifth peak.

For this reason, the following study was decided to do in favour of computer simulations, choosing the most probable isomers of C_{60} fullerene for investigation.

2. Structures of isomers

Selection of C_{60} isomers was limited by the number of paired pentagons, because it was supposed that they cause local strains decreasing formation probability of such structures and their stability. So we have confined structures with four contact pentagons. The simulation was performed with Avogadro visualization package. The resulting structures were optimized in Gaussian 09 W by the RHF method with a basis 3-21 G.

a) Three pairs of two adjacent pentagons on an equator at angle 45^0 (Fig. 6). The axis z passes through the centers of two hexagons, each of which being surrounded with three pentagons and three hexagons.

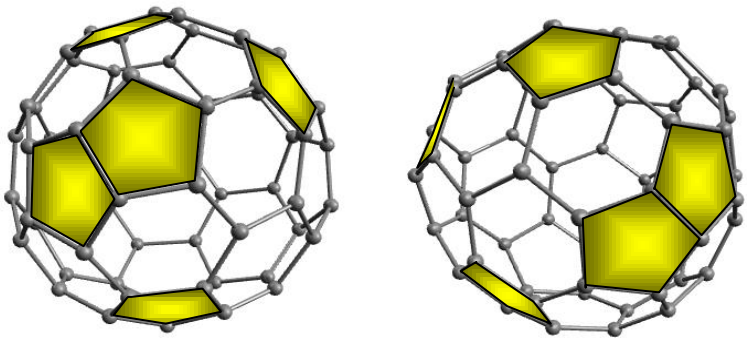

Fig. 6. Three pairs of pentagons on an equator at angle 45^0 (C_{60m3}).

The bond lengths range from 1.342 Å to 1.482 Å (Fig. 7), unlike buckminsterfullerene, whose bond lengths range from 1.373 Å to 1.449 Å.

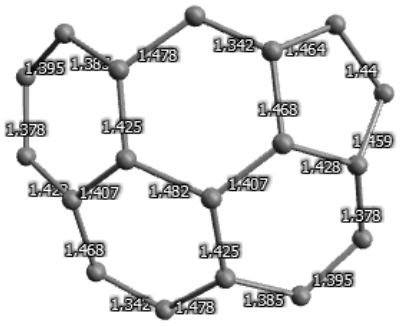

Fig. 7. Part of the structure with the largest value of a bond length.

Here the axis z passes through the central bond of each of two pyracylene units. Contrary to the previous case, one of the unit pentagons has an adjacent pentagon which is shown on the right side of the unit (Fig. 10, on the top).

The bond lengths range from 1.33 Å to 1.481 Å (Fig. 11).

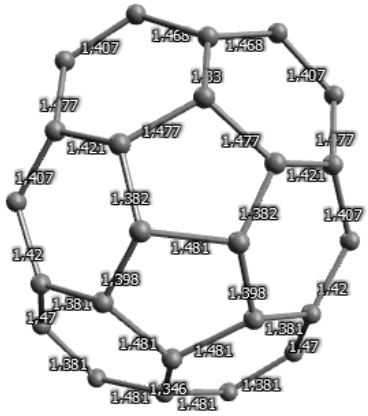

Fig. 11. Part of the structure with the largest value of a bond length.

d) Two chains of four adjacent pentagons normal to each other (Fig. 12). Here the bond lengths range from 1.331 Å to 1.511 Å (Fig. 13).

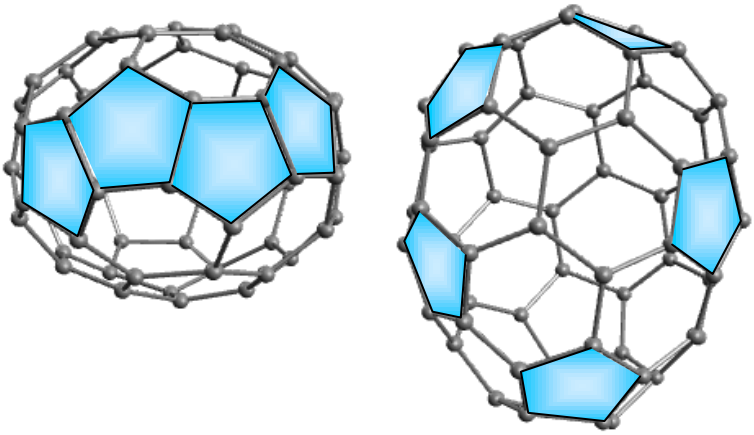

Fig. 12. Two chains of four adjacent pentagons **(**C_{60m6}).

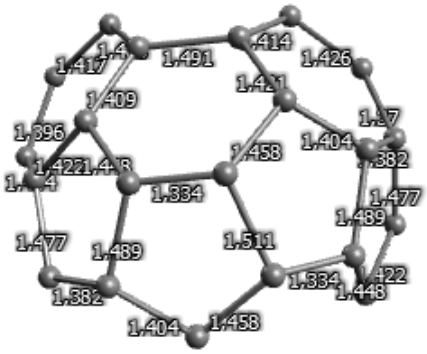

Fig. 13. Part of the structure with the largest value of a bond length.

e) Four triple adjacent pentagons (Fig. 14). Here the bond lengths range from 1.359 Å to 1.502 Å (Fig. 15).

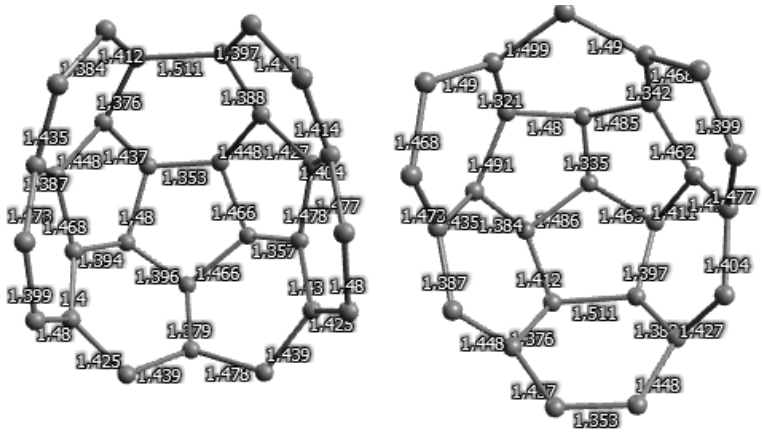

Fig. 17. Bond lengths related to two types of location pentagons.

3. Energies of formation and bond lengths

We have calculated formation energies of isomers. They are given below.

Table 1. Number of adjacent pentagons and formation energies.

Name	2 adjacent pentagons	3 adjacent pentagons	4 adjacent pentagons	Gibbs free energy, kJ/mol
Buckminster fullerene C_{60}	0	0	0	2573
C_{70}	0	0	0	2975
C_{60m3}	3	0	0	3039
C_{60m1}	4	0	0	3129
C_{60m2}	4	0	0	3134
C_{60m6}	0	0	2	3436
C_{60m5}	0	4	0	3636
C_{60m4}	0	4	0	3975

A comparison between the energies of isomers and their structures shows that the less is a surface the less is energy. The least surface has a sphere and so the least energy has a buckminsterfullerene. The adjacent pentagons induce declination from a sphere what leads to an energy increase.

We have also compared formation energies of isomers with their bond length (see below).

Table 2. Bond lengths and formation energies.

Name	Bond lengths, Å	Difference, Å	Gibbs free energy, kJ/mol
Buckminster fullerene C_{60}	1.373 (5-6) ÷ 1.449 (6-6)	0.076	2573
C_{60m3}	1.342 (6-6) ÷ 1.482 (6-6)	0.140	3039
C_{60m1}	1.345 (6-6) ÷ 1.502 (5-5)	0.157	3129
C_{60m2}	1.330 (6-6) ÷ 1.481 (5-6)	0.151	3134
C_{60m6}	1.331 (5-6) ÷ 1.512 (5-5)	0.181	3436
C_{60m5}	1.359 (6-6) ÷ 1.502 (5-6)	0.143	3636
C_{60m4}	1.331 (5-6) ÷ 1.512 (5-5)	0.181	3975

For the first three isomers, which shape is close to a sphere (C_{60m3}) and to an ellipsoid (C_{60m1} and C_{60m2}), it seems that there is a correlation, but for the isomers with a large declination from these shapes a correlation is absent.

Now discuss a possible form of the stable isomer synthesised in 2008. It has the retention time equal to 11.833 min which is close to that of C_{70}, 11.957 min respectively, so we suppose that their formation energies are also close. On the basis of the calculations done, one can concede that the form of this isomer is (C_{60m3}). The energy difference is only 64 kJ/mol.

4. Conclusion

In this paper we analyzed chromatograms and mass spectra of buckminsterfullerene and its isomers. We have calculated possible structures and formation energies of those isomers. A comparison between the energies of isomers and their structures shows that the less is a surface the less is energy. The least surface has a sphere and so the least energy has a buckminsterfullerene. The adjacent pentagons induce declination from a sphere what leads to an energy increase.

We have also compared formation energies of isomers with their bond length. For the isomers, which shape is close either to a sphere or to an ellipsoid, it seems that there is a correlation, but for the isomers with a large declination from these shapes a correlation is absent. We suppose that the most stable isomer which stability is comparable with that of C_{70} has the form close to a sphere. It has the symmetry axis of third order that passes through the centers of two hexagons, each of which being surrounded with three pentagons and three hexagons.

References

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[2] S.Y. Xie, S.L. Deng, R.B. Huang, L.J. Yu, L.S. Zheng // *Chemical Physics Letters* **343** (2001) 458.