Materials Physics and Mechanics 45 (2020) 60-78 Received: March 11, 2020

NATURAL ISOMERS OF FULLERENES FROM C_{30} TO C_{40}

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Abstract. We have systematized possible ways of forming the isomers of midi-fullerenes, namely C_{30}, C_{32}, C_{34} C_{36}, C_{38} and C_{40}. Similar to the isomers of midi-fullerenes from C_{20} to C_{28}, there are three the most natural mechanisms of their formation: 1) Embedding carbon dimers into initial fullerenes; 2) Fusion of carbon cupolas having the same symmetry; and 3) Fusion of fullerenes having compatible symmetry. The energies of the fullerenes calculated through the use of molecular mechanics are presented together with their graphs. It is found that in the majority of cases the minimum-energy fullerenes are those, having perfect and topological three-fold symmetries.

Keywords: atomic isomer, dimer embedding, energy, fullerene, fusion reaction, graph representation, growth, periodic system, self-organization, symmetry, topological symmetry

1. Introduction

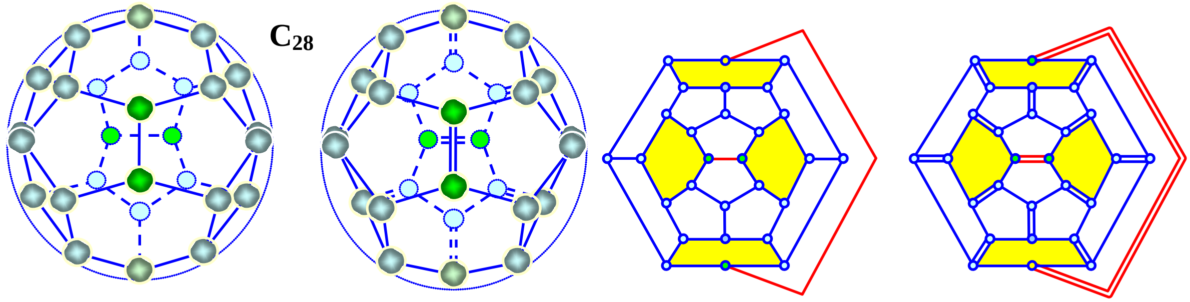
In Ref. [1] we have classified the most natural mechanisms of obtaining new fullerenes, namely: embedding a carbon dimer into an initial fullerene, fusion of the carbon cupolas having the same symmetry and fusion of the fullerenes having compatible symmetry. Once the classification of the fullerenes is embodied, the crucial point is the space isomerism of the fullerene molecules.

In this contribution we present the structure and energy of the fullerenes and their isomers in the range from C_{30} to C_{40} obtained through the use of these mechanisms. We will give the structure of the fullerenes of two extreme electronic configurations: with single bonds only and with single and double ones, the maximum number of possible double bonds being positioned symmetrically.

2. Isomers of fullerene C_{30}

a) Dimer embedding into a penta$_{12}$-hexa$_{4}$ eccaidecahedron (90º). The starting configuration is fullerene C_{28} (90^0) shown in Fig. 1. The polyhedron consists of twelve pentagons and four hexagons, has sixteen faces, and so is designated as an *eccaidecahedron*. It is a perfect fullerene having rotation-reflection symmetry [1]. The rotation axis goes through the centers of the bonds between the atoms marked in green.

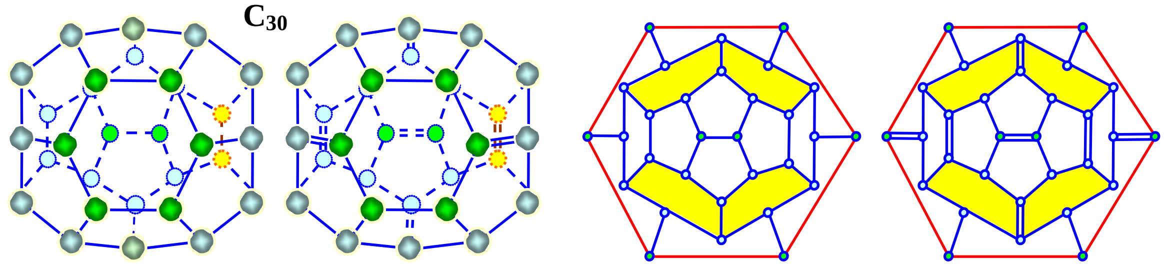
http://dx.doi.org/10.18720/MPM.4512020_7



E=924 E=1790

Fig. 1. Initial fullerene C_{28}: structure and graphs; energy in kJ/mol

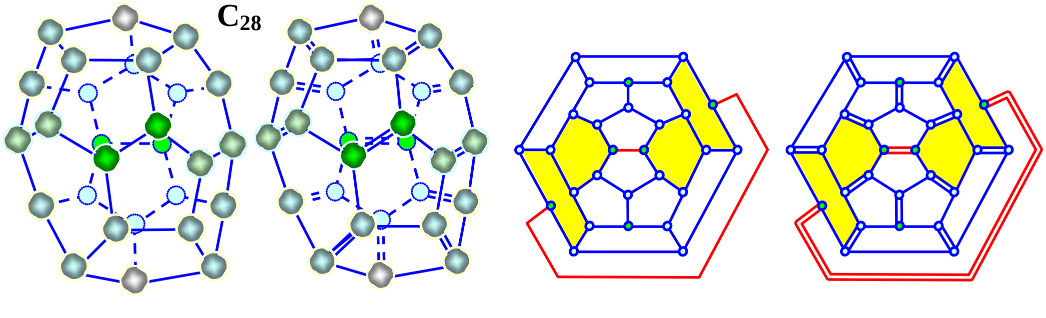
The new fullerene can be got in the following way: a carbon dimer, marked in yellow, is embedded into one of two hexagons at the equator of the initial fullerene that transform the C_{28} fullerene into fullerene C_{30} (Fig. 2). The polyhedron obtained contains twelve pentagons, five hexagons and has seventeen faces; therefore it can be named symmetric penta$_{12}$-hexa$_{5}$ *eptacaidecahedron* C_{30}.



E=832 E=847

Fig. 2. Fullerene C_{30} obtained by embedding a dimer into an initial fullerene C_{28} (90º): structure and graphs; energy in kJ/mol

b) Dimer embedding into a penta$_{12}$-hexa$_{4}$ eccaidecahedron (30º). The starting configuration is shown in Fig. 3. Here we have also a perfect fullerene having rotation-reflection symmetry. Contrary to the previous case, where the initial fullerene half is needed to be rotated through 90º to get a mirror image, here the rotation is done only through 30 ones. The fullerene also contains twelve pentagons and four hexagons. Another distinction: to get a new fullerene, here embedding is done at an angle of 60º to the axis going through the atoms marked in grey. It transforms the initial fullerene into fullerene C_{30} (Fig. 4). The fullerene obtained contains also twelve pentagons and five hexagons, has seventeen faces, and so is termed asymmetric penta$_{12}$-hexa$_{5}$ *eptacaidecahedron* C_{30}.



E=689 E=1872

Fig. 3. Initial fullerene C_{28}: structure and graphs; energy in kJ/mol

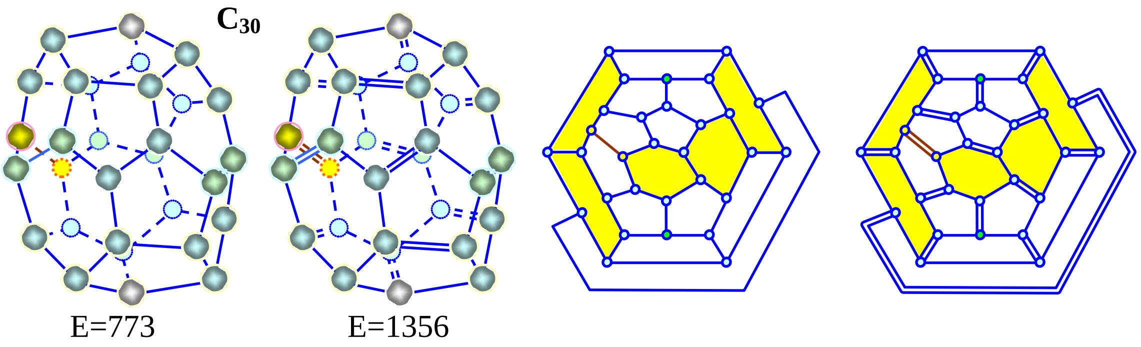


Fig. 4. Fullerene C_{30} obtained by embedding a dimer into an initial fullerene C_{28} (30°): structure and graphs; energy in kJ/mol

c) Dimer embedding into a tri$_2$-penta$_6$-hexa$_8$ eccaidecahedron. The initial atomic configuration of fullerene C_{28} is shown in Fig. 5. The polyhedron has two triangles, six pentagons, eight hexagons and has sixteen faces. Since it contains two extra dimers marked in yellow in comparison with the perfect tri$_2$-tetra$_3$-hexa$_9$ fullerene C_{24} [1], it is an imperfect fullerene having topological three-fold symmetry. A carbon dimer marked in yellow is incorporated into the hexagon at the equator of the initial C_{28} fullerene. The procedure restores the ordinary three-fold symmetry, because two fullerenes, C_{24} and C_{30}, refer to the column of the periodic system of basic fullerenes, which conserves three-fold symmetry; the mass difference between successive fullerenes being equal to $\Delta m = 6$. The new tri$_2$-penta$_9$-hexa$_6$ polyhedron, having seventeen faces, is referred to as an eptacaidecahedron C_{30}. It is a perfect fullerene having a three-fold symmetry axis (Fig. 6).

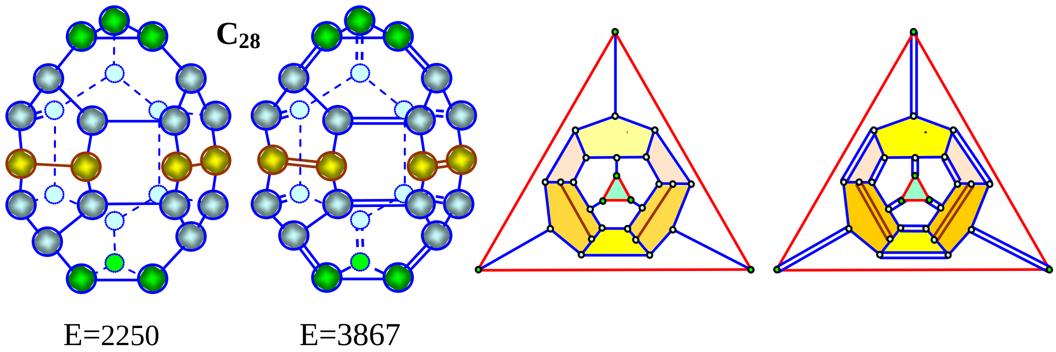


Fig. 5. Initial fullerene C_{28}: structure and graphs; energy in kJ/mol

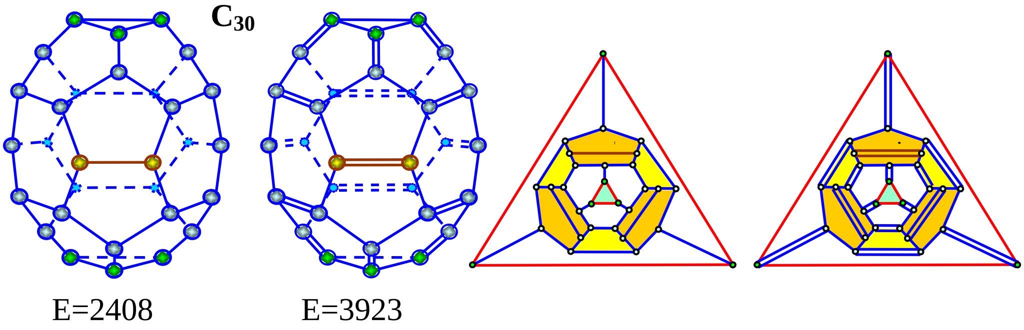


Fig. 6. Fullerene C_{30} obtained by embedding a dimer into a tri$_2$-penta$_6$-hexa$_8$ fullerene C_{28}: structure and graphs; energy in kJ/mol

d) Fusion of plane cluster C_{10} with cupola C_{20}. Here both initial configurations have five-fold symmetry [2]. The fullerene obtained consists of five squares, two pentagons and ten hexagons. Although it also contains seventeen faces, it is better to name this perfect isomer, having five-fold symmetry, a truncated five angular bipyramid (Fig. 7)

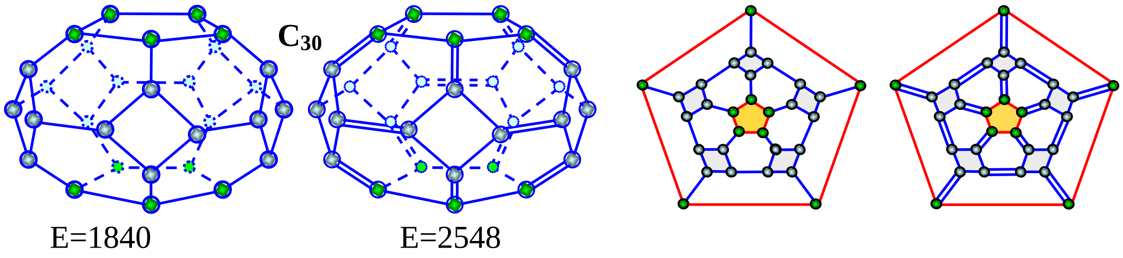


Fig. 7. Joining plane cluster C_{10} with cupola C_{20}; structure and graphs; energy in kJ/mol

e) Fusion of two cupolas C_{15} having five-fold symmetry. Here both cupolas have five-fold symmetry [2]. The fullerene produced has twelve pentagons and five hexagons, and contains also seventeen faces (Fig. 8). This penta$_{12}$-hexa$_5$ isomer of eptacaidecahedrons, is also perfect one having five-fold symmetry.

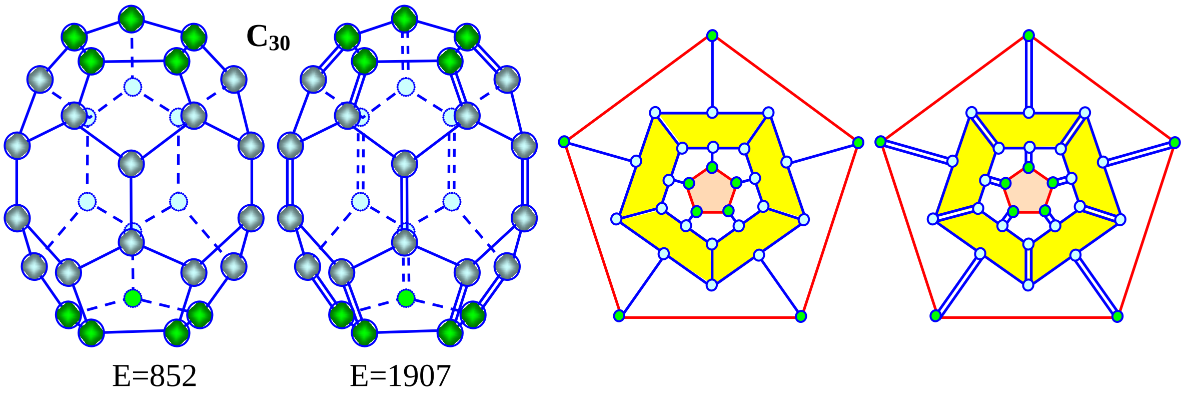


Fig. 8. Joining two cupolas C_{15}; structure and graphs; energy in kJ/mol

f) Fusion of regular pentagonal prism C_{10} and dodecahedron C_{20}. The reaction is possible since the both configurations have five-fold symmetry and therefore they are compatible with each other. However, the fullerene C_{30} formed [3], as a whole, is identical to the fullerene constructed by means of the fusion of two cupolas C_{15} having five-fold symmetry (Fig. 8). Therefore we have only another way of obtaining this isomer.

3. Isomers of fullerene C_{32}

a) Dimer embedding into penta$_{12}$-hexa$_5$ eptacaidecahedron C_{30} The initial fullerene is shown above in Fig. 2. Embedding a dimer into the hexagon at the equator transforms fullerene C_{30} into fullerene C_{32}. The fullerene succeeded contains twelve pentagons, six hexagons, eighteen faces, and therefore can be named penta$_{12}$-hexa$_6$ *octocaidecahedron* C_{32}. It is presented in Fig. 9 together with the graphs illustrating its symmetry.

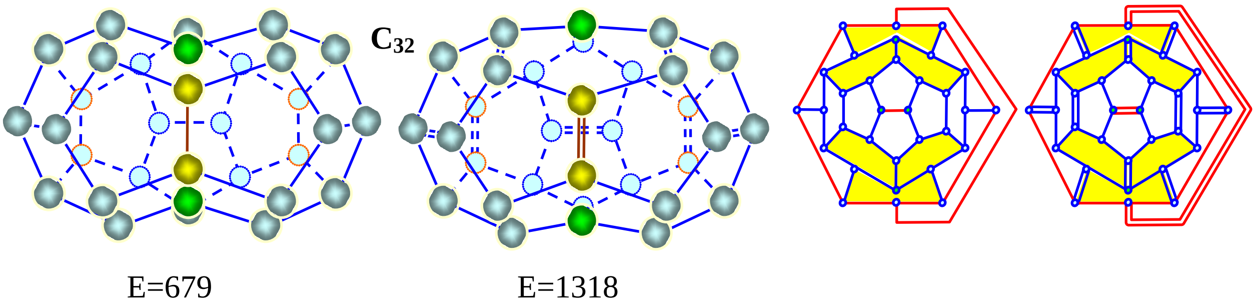


Fig. 9. Fullerene C_{32} obtained by embedding a dimer into penta$_{12}$-hexa$_6$ fullerene C_{30}: structure and graphs; energy in kJ/mol

b) Dimer embedding into asymmetric penta$_{12}$-hexa$_5$ eptacaidecahedron C_{30}. The starting fullerene is shown earlier in Fig. 4. As before, embedding a dimer into the hexagon at the equator transforms fullerene C_{30} into fullerene C_{32}, which also contains twelve pentagons and six hexagons. This penta$_{12}$-hexa$_6$ octocaidecahedron C_{32} is presented in Fig. 10 together with the corresponding graphs.

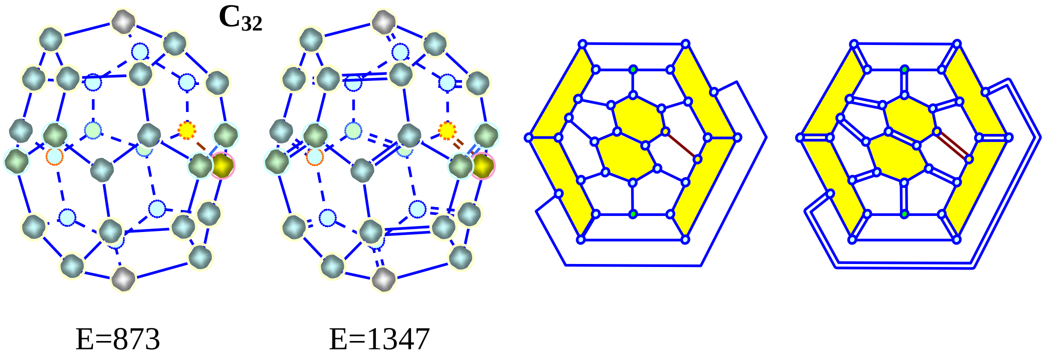


Fig. 10. Fullerene C_{32} obtained by embedding a dimer into asymmetric penta$_{12}$-hexa$_6$ fullerene C_{30}: structure and graphs; energy in kJ/mol

c) Dimer embedding into a tri$_2$-penta$_9$-hexa$_6$ eptacaidecahedron. Here a carbon dimer marked in yellow is incorporated into one of three hexagons at the equator of the initial perfect fullerene C_{30} (Fig. 6) at an angle of 60° to the three-fold axis of symmetry as shown in Fig. 11. The new polyhedron, tri$_2$-penta$_9$-hexa$_7$ octocaidecahedron C_{32}, having an extra dimer, possesses topological three-fold symmetry that follows from its structure and graphs (Fig. 11).

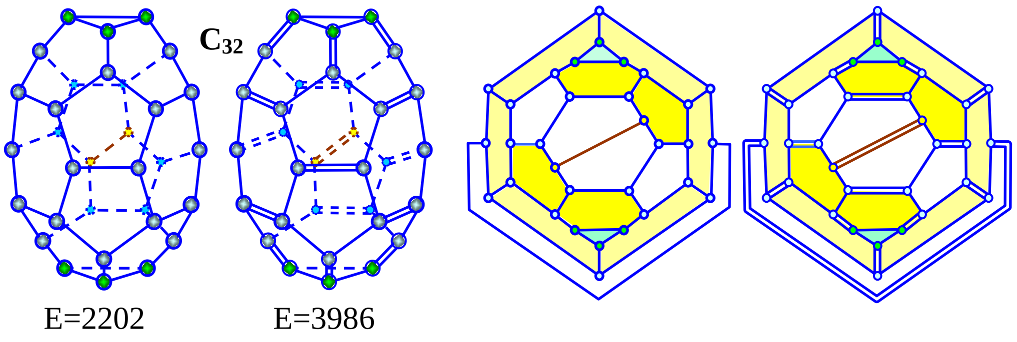


Fig. 11. Fullerene C_{32} obtained by embedding a dimer into tri$_2$- penta$_9$-hexa$_6$ fullerene C_{30}: structure and graphs; energy in kJ/mol

d) Fusion of two cupolas C_{16} having three-fold symmetry. This reaction was earlier studied in Ref. [4]. The final atomic configuration is presented in Fig. 12. It consists of twelve pentagons and six hexagons and forms a perfect penta$_{12}$-hexa$_{6}$ octocaidecahedron, which is an isomer of the fullerene shown in Fig. 10.

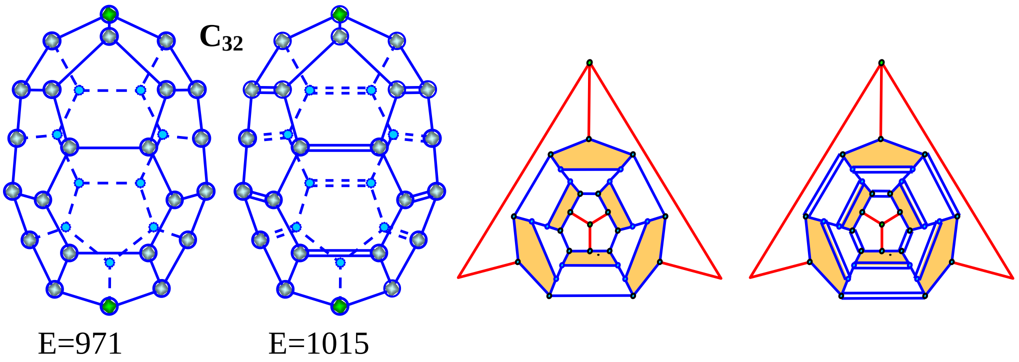


Fig. 12. Joining two half fullerenes C_{16} of three-fold symmetry; structure and graphs; energy in kJ/mol

e) Fusion of two cupolas C_{16} having four-fold symmetry. There are two ways of joining: mirror symmetry and rotation-reflection one [5]. In the first case (Fig. 13, above) the lower cupola is a mirror copy of the upper one. The fullerene got consists of six squares and twelve hexagons, has eighteen faces and therefore, as before, can be named a tetra$_{6}$-hexa$_{12}$ octocaidecahedron. In the second case (Fig. 13, below) the lower cupola is a rotary reflection of the upper one. The fullerene obtained contains two squares, eight pentagons and eight hexagons; it is a tetra$_{2}$-(penta-hexa)$_{8}$ octocaidecahedron.

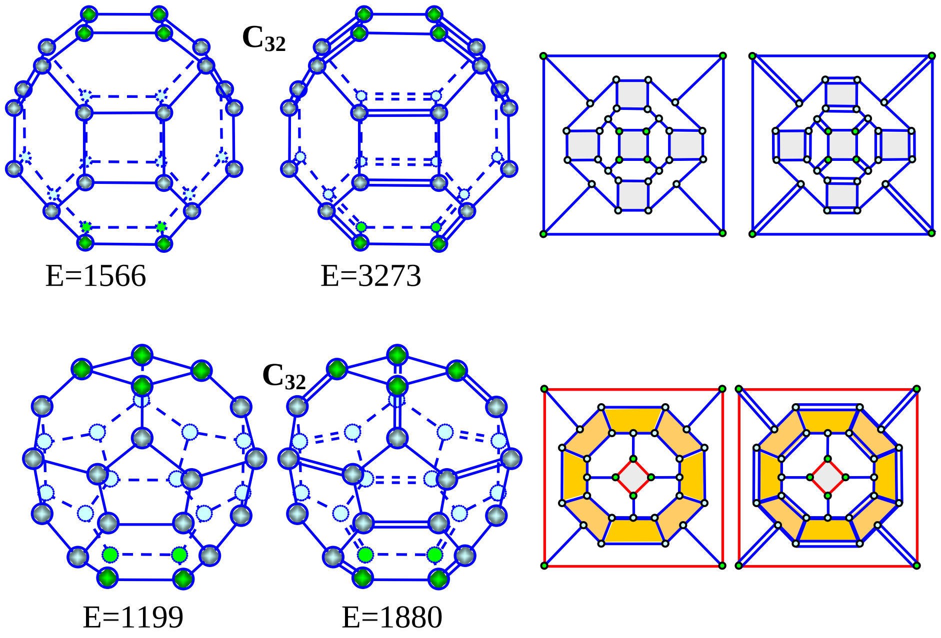


Fig. 13. Joining two half fullerenes C_{16} of four-fold symmetry: the mirror symmetry fusion (above) and the rotation-reflection symmetry (below); structure and graphs; energy in kJ/mol

f) Fusion of two mini-fullerenes C_{16}. There is only one way of joining: rotation-reflection symmetry. However, contrary to the previous cases, we have a narrow nanotube capped with two fragments of the C_{16} fullerene (Fig. 14).

It is worth noting that at first extremely narrow nanotubes were considered only as a new type of nanotubes being of academic interest [3,6]. Recently it has been discovered that small diameter single-walled carbon nanotubes were mimics of ion channels found in natural systems [7]. These properties make them a promising material for developing membrane separation technologies [8].

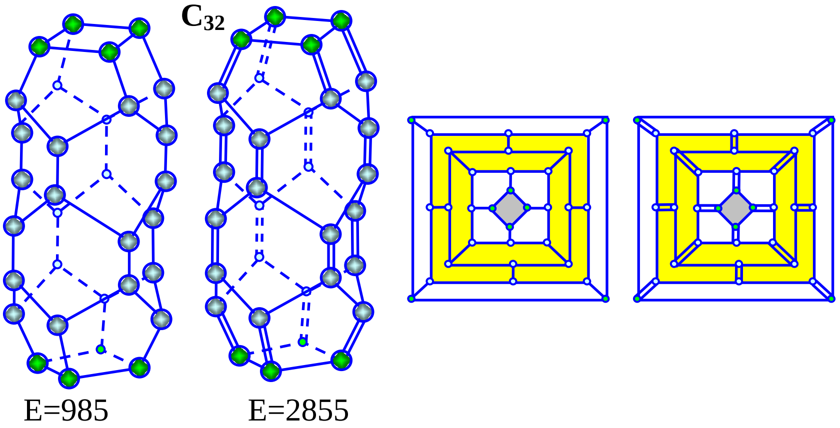


Fig. 14. Joining two mini-fullerenes C_{16} of four-fold symmetry: the rotation-reflection symmetry; structure and graphs; energy in kJ/mol

4. Isomers of fullerene C_{34}

***a) Dimer embedding into penta$_{12}$-hexa$_6$ octocaidecahedron C_{32}** (having three-fold symmetry).* The initial fullerene is shown above in Fig. 12. Embedding a dimer into one of the hexagon at the equator parallel to the three-fold axis transforms fullerene C_{32} into fullerene C_{34}. The fullerene formed contains fourteen pentagons, five hexagons, has nineteen faces and therefore can be named penta$_{12}$-hexa$_7$ *enneacaidecahedron* C_{34}. It is presented in Fig. 15 together with the graphs illustrating its symmetry.

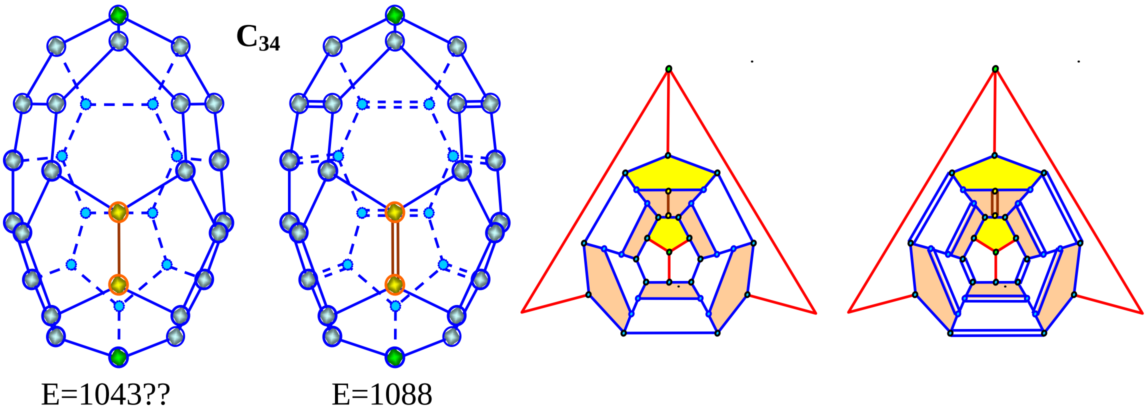


Fig. 15. Fullerene C_{34} obtained by embedding a dimer into penta$_{12}$-hexa$_6$ fullerene C_{32}: structure and graphs; energy in kJ/mol

***b) Dimer embedding into penta$_{12}$-hexa$_6$ octocaidecahedron C_{32}** (having disk shape).*
The initial fullerene is shown earlier in Fig. 9. Embedding a dimer into one of the hexagon on the top transforms fullerene C_{32} into fullerene C_{34}. The fullerene formed contains fourteen pentagons, seven hexagons, consists of nineteen faces, and therefore can be referred to as penta$_{12}$-hexa$_7$ enneacaidecahedron C_{34}. It is presented in Figure 16 together with the graphs showing its structure.

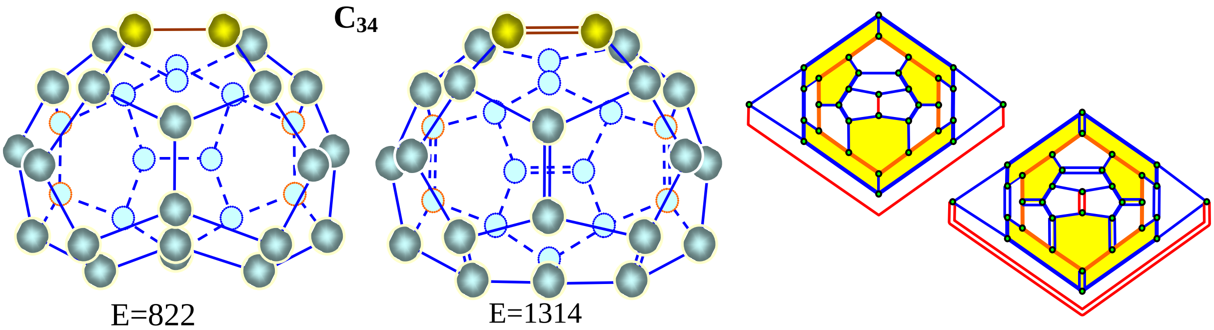


Fig. 16. Fullerene C_{34} obtained by embedding a dimer into penta$_{12}$-hexa$_6$ fullerene C_{32}: structure and graphs; energy in kJ/mol

c) Dimer embedding into tri$_2$-penta$_9$-hexa$_7$ octocaidecahedron C_{32}. From the standpoint of symmetry, the initial fullerene C_{32} has an extra dimer marked in brown, and therefore possesses topological three-fold symmetry (Fig. 11). A carbon dimer is incorporated into one of two hexagons at the equator of the initial fullerene at an angle of 60° to the three-fold axis of symmetry (Fig. 17). Now having two extra dimers, the new tri$_2$-penta$_9$-hexa$_8$ polyhedron having nineteen faces, enneacaidecahedron C_{34}, also conserves topological three-fold symmetry (Fig. 17).

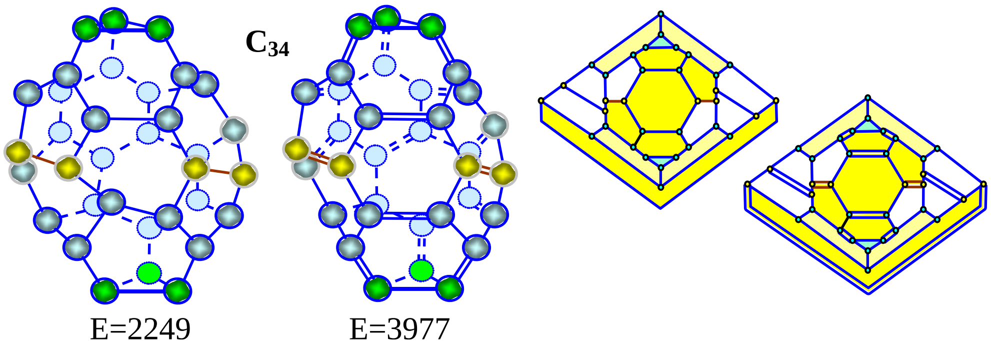
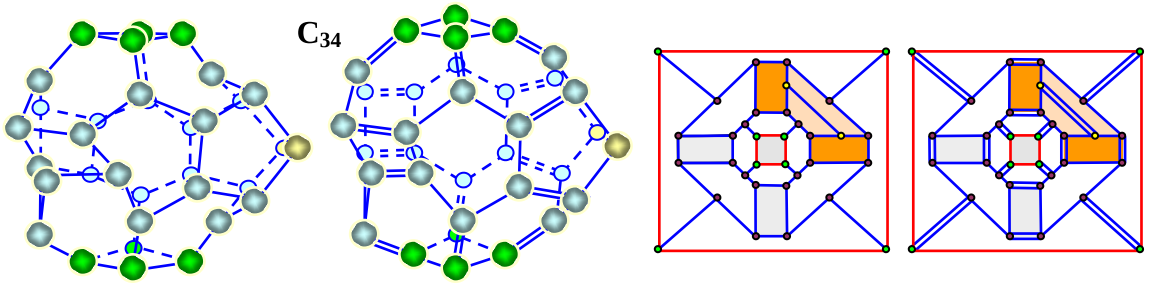


Fig. 17. Fullerene C_{34} obtained by embedding a dimer into penta$_{12}$-hexa$_6$ fullerene C_{32}: structure and graphs; energy in kJ/mol

d) Dimer embedding into tetra$_6$-hexa$_{12}$ octocaidecahedron C_{32}. The initial perfect fullerene is shown above in Fig. 13. Embedding a dimer into one of four hexagons at the equator transforms fullerene C_{32} into fullerene C_{34}. The process resembles that of reaction $C_{24}+C_2 \rightarrow C_{26}$ [1]. In both cases the fullerenes formed contain an extra interstitial; they are imperfect ones having topological three-fold and four-fold symmetry, respectively. The symmetry can be discovered by looking at the graphs. In our case the fullerene obtained contains four squares, four pentagons, eleven hexagons, has nineteen faces and therefore is referred to as (tetra-penta)$_4$-hexa$_{11}$ enneacaidecahedron C_{34}.

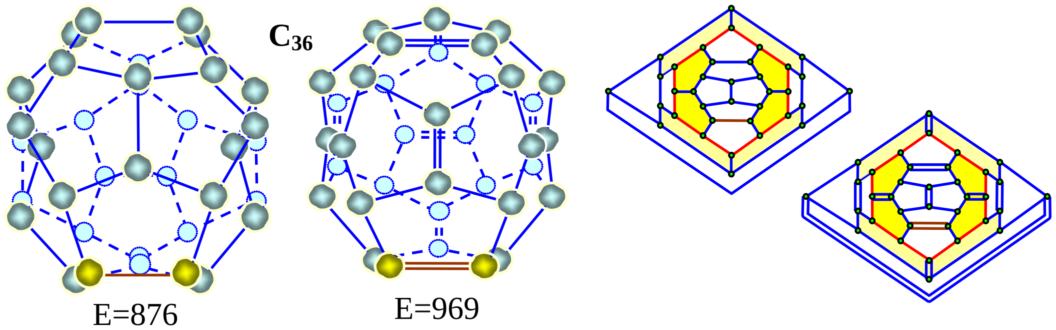


E=1637 E=3141

Fig. 18. Fullerene C_{34} obtained by embedding a dimer into tetra$_6$-hexa$_{12}$ fullerene C_{32}: structure and graphs; energy in kJ/mol

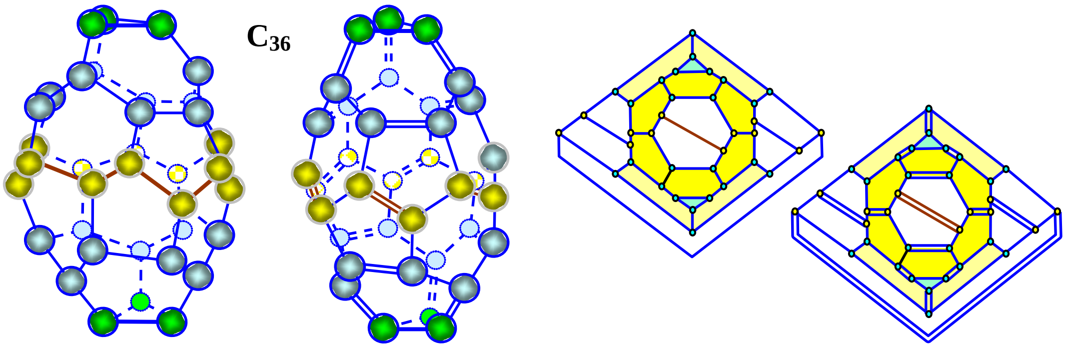
5. Isomers of fullerene C_{36}

a) Dimer embedding into penta$_{12}$-hexa$_7$ enneacaidecahedron C_{34}. Having two extra dimers, the initial polyhedron, penta$_{12}$-hexa$_7$ enneacaidecahedron C_{34}, possesses topological three-fold symmetry (Fig. 15). Adding one more dimer into the irregular (lower) part of the fullerene changes the symmetry. The fullerene becomes a perfect one having rotation-reflection four-fold symmetry (Fig. 18). It has twelve pentagons, eight hexagons and twenty faces. It is a penta$_{12}$-hexa$_8$ *eicosahedron* C_{36}.



E=876 E=969

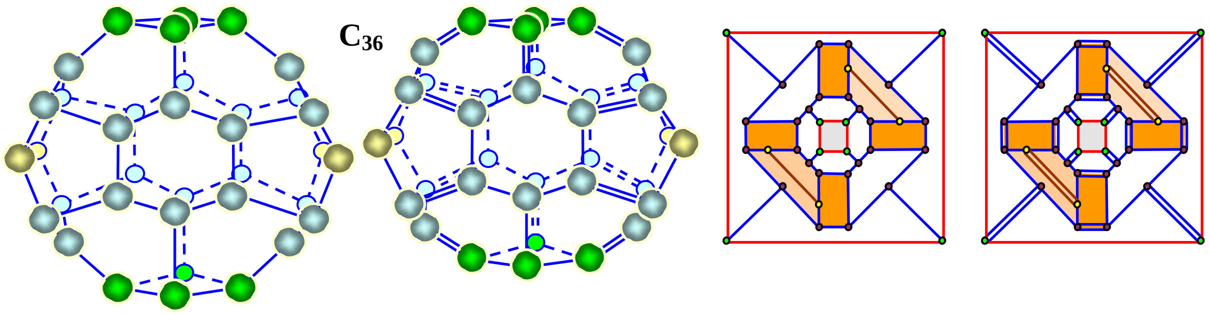
Fig. 19. Fullerene C_{36} obtained by embedding a dimer into penta$_{12}$-hexa$_7$ enneacaidecahedron C_{34}: structure and graphs; energy in kJ/mol



E=2400 E=3957

Fig. 20. Fullerene C_{36} obtained by embedding a dimer into tri$_2$-penta$_9$-hexa$_8$ enneacaidecahedron C_{34}: structure and graphs; energy in kJ/mol

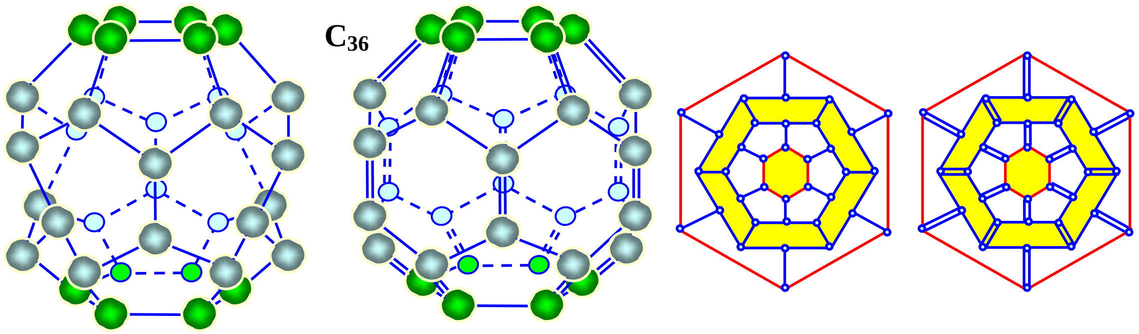
c) Dimer embedding into (tetra-penta)$_4$-hexa$_{11}$ enneacaidecahedron C$_{34}$. The dimer embedding transforms an imperfect fullerene, (tetra-penta)$_4$-hexa$_{11}$ enneacaidecahedron C_{34}, shown in Fig. 17, into a semi-perfect, tetra$_2$-penta$_8$-hexa$_{10}$ eicosahedron C_{36}, having two-fold symmetry (Fig. 20).



E=1096 E=1984

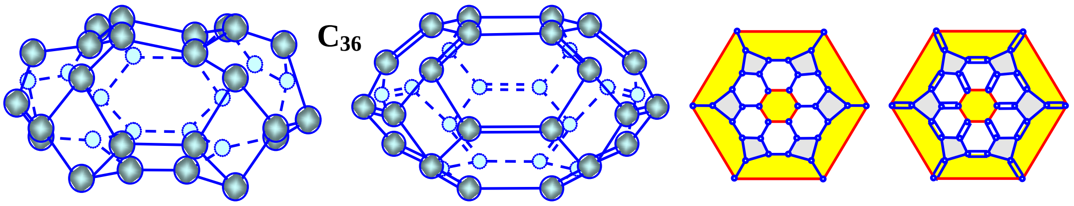
Fig. 21. Fullerene C_{36} obtained by embedding a dimer into (tetra-penta)$_4$-hexa$_{11}$ enneacaidecahedron C_{34}: structure and graphs; energy in kJ/mol

d) Fusion of two cupolas C$_{18}$. The final atomic configuration is presented in Fig. 22. It consists of twelve pentagons and eight hexagons. It is a perfect penta$_{12}$-hexa$_8$ eicosahedron having six-fold symmetry. It should be emphasized that the same structure can be obtained by fusion of prism C_{12} with barrel shape fullerene C_{24} [3].



E=1022 E=1884

Fig. 22. Joining two cupolas C_{18} of six-fold reflection symmetry: structure, graphs, energy



E=203 E=388

Fig. 23. Fullerene C_{34} obtained by embedding a dimer into penta$_{12}$-hexa$_6$ fullerene C_{32}: structure and graphs; energy in kJ/mol

e) Fusion of two graphene fragments C$_{12}$ and C$_{24}$. Although the process was considered in Ref. [2], the energy was calculated only for the configuration with single and double bonds. The final atomic configurations are presented in Fig. 23. They consist of six squares and eighteen hexagons and forms a tetra$_6$-hexa$_{14}$ eicosahedron. It is worth noting that a perfect shape is destroyed if the fullerene has only single bonds. In this case the hexagons take the conformations of a boat or a chair.

6. Isomers of fullerene C_{38}

a) Dimer embedding into penta$_{12}$-hexa$_8$ eicosahedron C_{36}. The initial perfect polyhedron is displayed in Fig. 19. It consists of twelve pentagons and eight hexagons and has rotation-reflection four-fold symmetry. We suppose that the dimer embedding takes place in the regions of the largest curvature attempting to do the fullerene surface looking like a sphere. The two cells of twelve atoms, each cell having four pentagons, the nearest three of which being adjacent, have the largest curvature. Therefore it is reasonable to assume that the dimer embedding occurs inside one of these cells in a manner shown in Fig. 24. As a consequence one obtains fullerene C_{38} which consist of one square, ten pentagons and ten hexagons (Fig. 25).

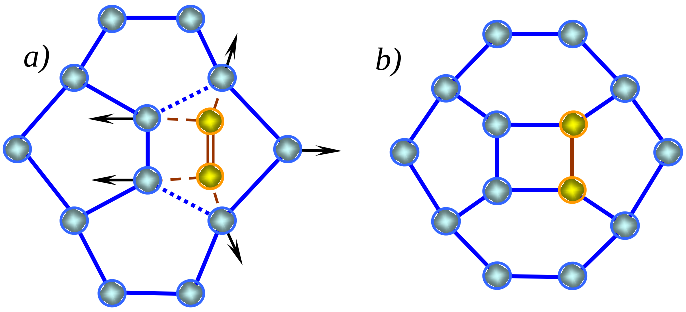


Fig. 24. Carbon dimer embedding into a pentagon (*a*) and forming a square (*b*)

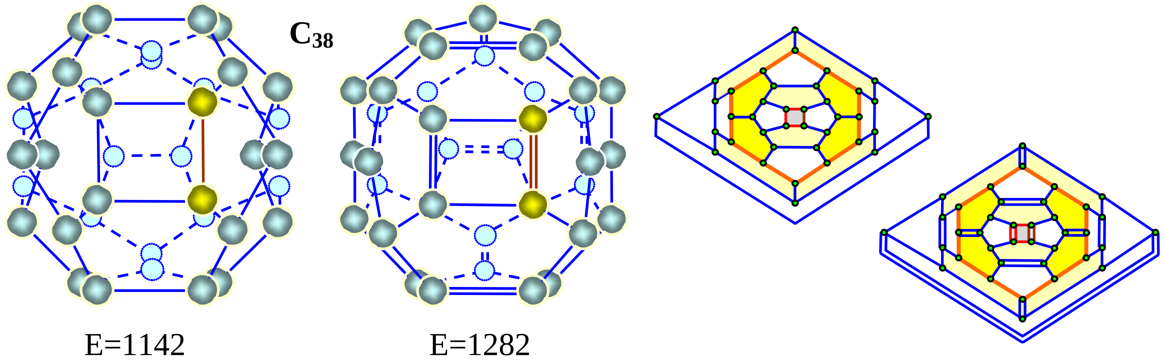


Fig. 25. Fullerene C_{38} obtained by embedding a dimer into penta$_{12}$-hexa$_8$ eicosahedron C_{36}: structure and graphs; energy in kJ/mol

b) Dimer embedding into tri$_2$-penta$_9$-hexa$_9$ eicosahedron C_{36}. The initial perfect polyhedron consists of two trigons, nine pentagons and nine hexagons. It is tri$_2$-penta$_9$-hexa$_9$ eicosahedral C_{36}, the structure being shown in Fig. 20. Similar to the previous case, we suppose that the dimer embedding takes place in the regions of the largest curvature, i.e. into one of the hexagons adjacent to an apex. The fullerene obtained has one trigon, one tetragon, ten pentagons and nine hexagons, the number of faces equals to twenty-one (Fig. 26).

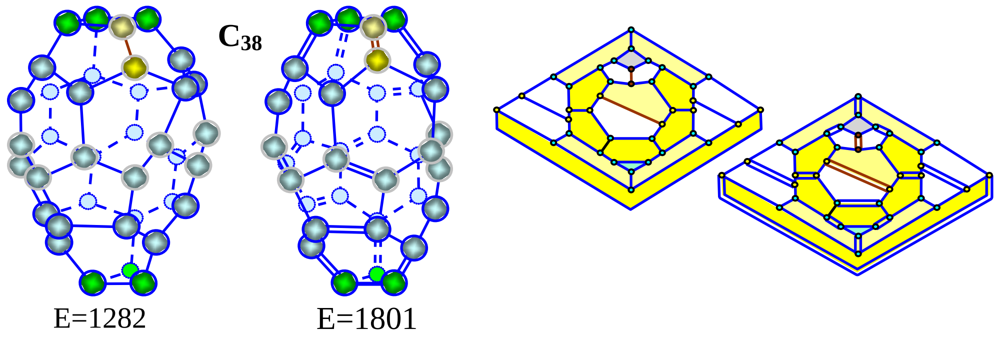


Fig. 26. Fullerene C_{38} obtained by embedding a dimer into fullerene C_{36} having three-fold symmetry: structure and graphs; energy in kJ/mol

c) Dimer embedding into tetra$_2$-penta$_8$-hexa$_{10}$ eicosahedron C_{36}. The starting fullerene is shown in Fig. 21. It is a semi-perfect tetra$_2$-penta$_8$-hexa$_{10}$ eicosahedron C_{36}, having two-fold symmetry. The dimer embedding into one of the equator hexagons increases the number of hexagons to eleven. The fullerene becomes imperfect but conserves topologic symmetry (Fig. 27).

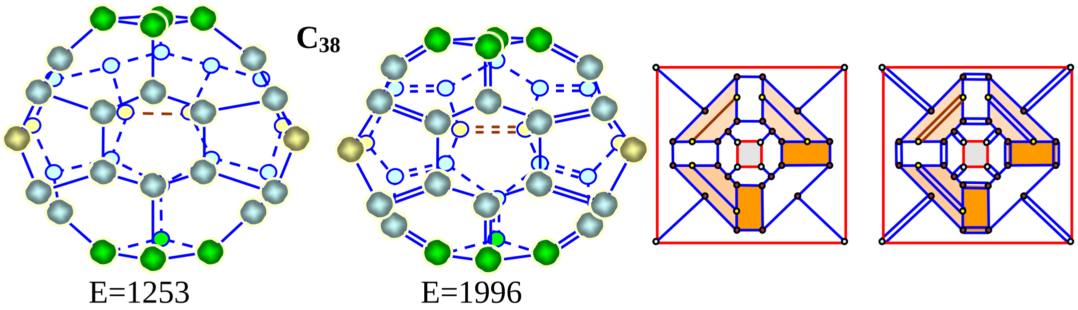


Fig. 27. Fullerene C_{38} obtained by embedding a dimer into fullerene C_{36} having two-fold symmetry: structure and graphs; energy in kJ/mol

d) Fusion of two cupolas: C_{16} and C_{22}. The process was considered in Ref. [9], but the energy was calculated only for the configuration with single and double bonds. The final atomic configurations of both only single bonds and single and double ones are shown in Fig. 28. They have twelve pentagons, nine hexagons, twenty-one faces and perfect three-fold symmetry.

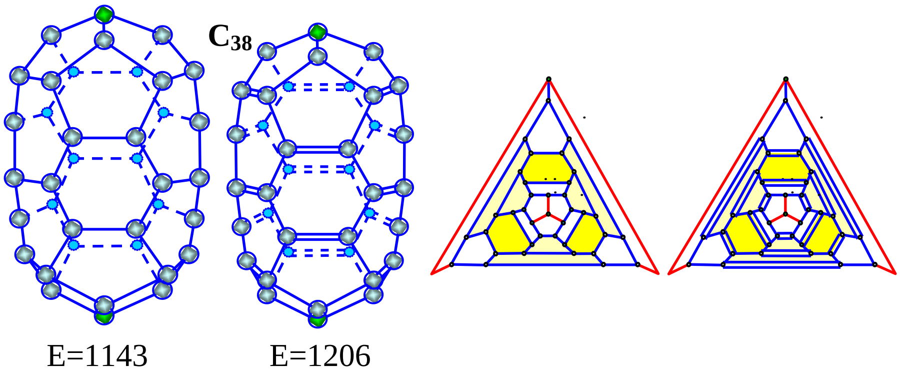


Fig. 28. Fullerene obtained by the fusion of two half-fullerenes C_{16} and C_{22}

7. Isomers of fullerene C_{40}

a) Dimer embedding into tetra-(penta-hexa)$_{10}$ polyhedron C_{38}. The initial polyhedron is composed of one square, ten pentagons and ten hexagons (Fig. 25). Similar to the creation of fullerene C_{38}, we suppose again that the dimer embedding takes place in the regions of the largest curvature, i.e. into the cell of twelve atoms formed by four pentagons, the nearest three of which being adjacent, in a manner shown in Fig. 24. As a consequence, we have fullerene C_{40} which consist of two tetragons, eight pentagons and twelve hexagons (Fig. 29). It has twenty-two faces and rotation-reflection four-fold symmetry.

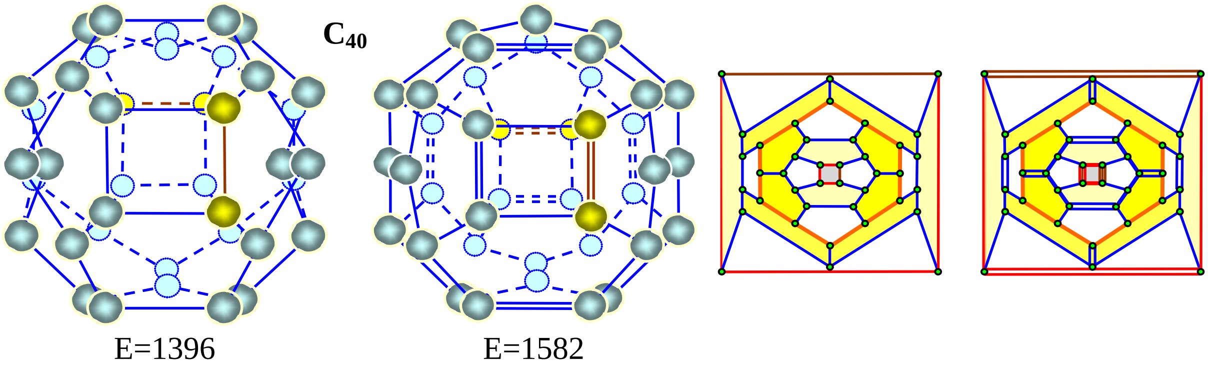


Fig. 29. Fullerene C_{40} obtained by embedding a dimer into tetra-(penta-hexa)$_{10}$ polyhedron C_{38}: structure and graphs; energy in kJ/mol

b) Dimer embedding into tri-tetra-penta$_{10}$-hexa$_9$ polyhedron C_{38}. The initial polyhedron consists of one trigon, one tetragon, ten pentagons and nine hexagons, the structure being shown in Fig. 26. The fullerene obtained has two tetragons, eleven pentagons and nine hexagons, the number of faces equals to twenty-one.

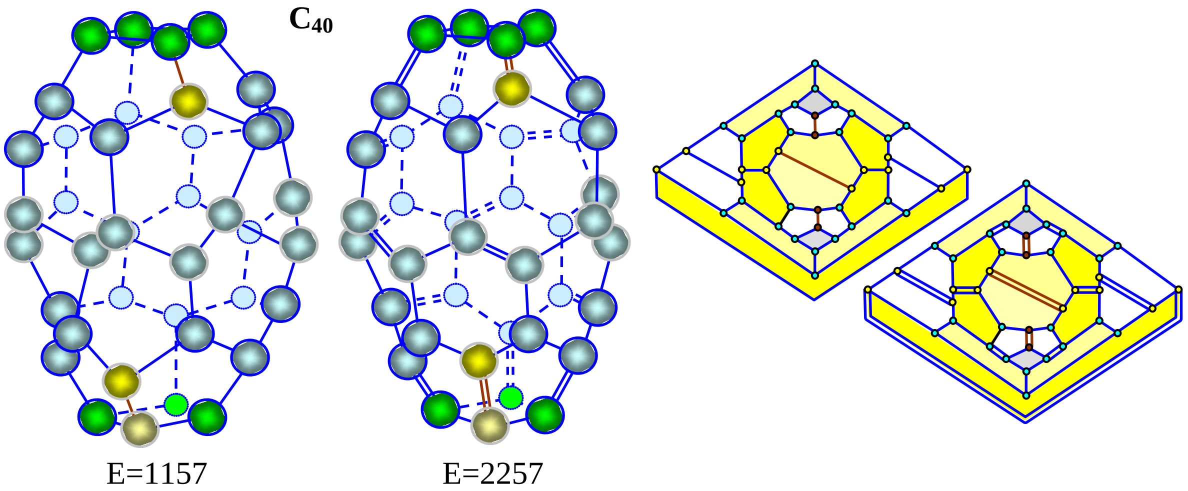


Fig. 30. Fullerene C_{40} obtained by embedding a dimer into asymmetric fullerene C_{38}: structure and graphs; energy in kJ/mol

c) Dimer embedding into tetra$_2$-penta$_8$-hexa$_{11}$ polyhedron C_{38}. . The starting fullerene is shown in Fig. 27. It is a semi-perfect tetra$_2$-penta$_8$-hexa$_{11}$ polyhedron C_{38}, having topologic four-fold symmetry. The dimer embedding into one of the equator hexagons increases the number of hexagons to twelve. The fullerene becomes perfect and obtains real four-fold symmetry (Fig. 31) as its ancestor, fullerene C_{32}, (Fig. 13, above).

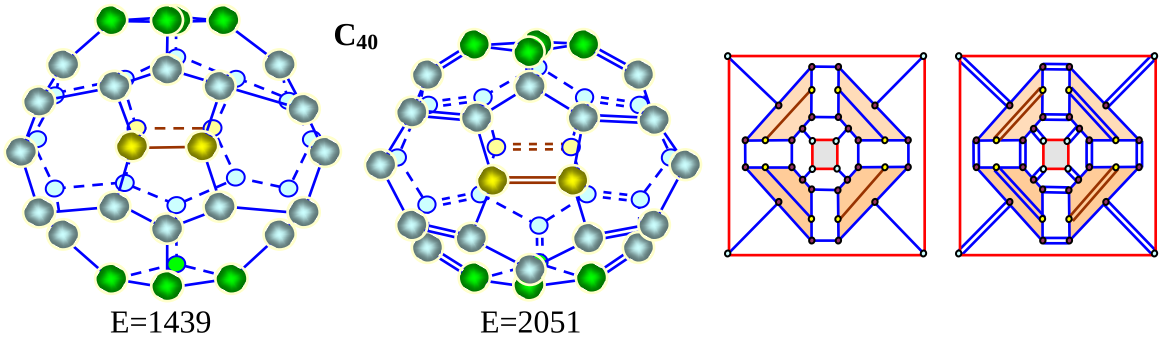


Fig. 31. Fullerene C_{40} obtained by embedding a dimer into fullerene C_{38} having topologic four-fold symmetry: structure and graphs; energy in kJ/mol

d) Dimer embedding into penta$_{12}$-hexa$_{9}$ polyhedron C_{38}. The initial fullerene, shown in Fig. 28, has twelve pentagons, nine hexagons, twenty-one faces and possesses perfect three-fold symmetry. Embedding a dimer begins the growth of this fullerene with conserving topological three-fold symmetry [9].

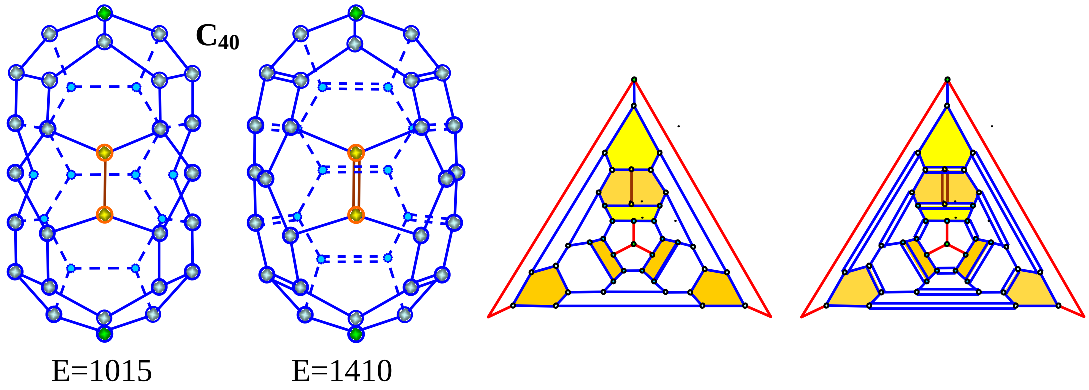


Fig. 32. Fullerene C_{40} obtained by embedding a dimer into fullerene C_{38} having perfect three-fold symmetry: structure and graphs; energy in kJ/mol

e) Fusion of two cupolas C_{20} having five-fold symmetry. The process was considered in Ref. [5], but the energy was not calculated. There are two ways of joining: mirror symmetry and rotation-reflection one. In the first case the lower cupola is a mirror copy of the upper one (Fig. 33). The fullerene got consists of five tetragons, two pentagons and fifteen hexagons, and has twenty-two faces.

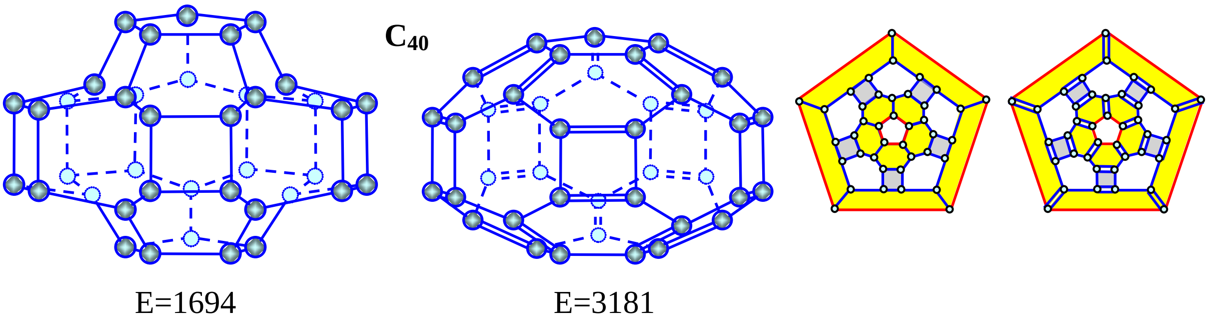


Fig. 33. Joining two cupolas C_{20} of five-fold symmetry: the mirror symmetry fusion, structure and graphs; energy in kJ/mol

In the second case the lower cupola is a rotary reflection of the upper one (Fig. 34). The fullerene obtained contains twelve pentagons and ten hexagons, the number of faces being the same.

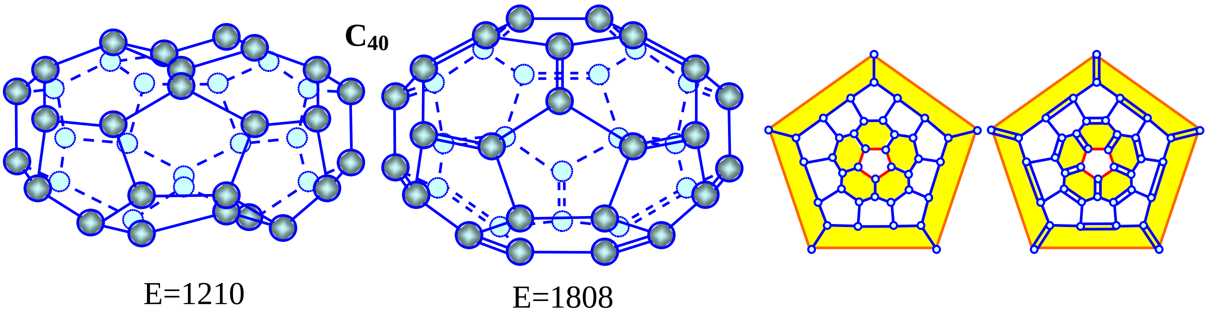


Fig. 34. Joining two cupolas C_{20} of five-fold symmetry: the rotation-reflection symmetry fusion, structure and graphs; energy in kJ/mol

f) Fusion of two asymmetric cupolas C_{20} having two-fold symmetry. There is only one way of joining: rotation-reflection symmetry. Although we have, as for the narrow nanotubes C_{32}, the structure which is typical for nanotubes (Fig. 35), the influence of double bonds leads to smoothing the nanotube surface.

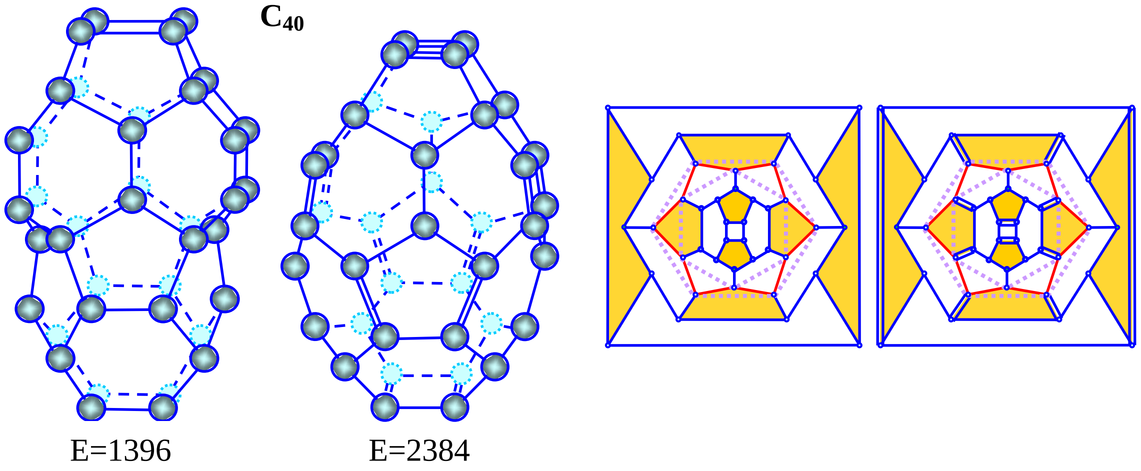


Fig. 35. Joining two cupolas C_{20} of two-fold symmetry: the rotation-reflection symmetry; structure and graphs; energy in kJ/mol

g) Fusion of two dodecahedron-fullerenes C_{20} having five-fold symmetry. As above, there is only one way of joining: rotation-reflection symmetry (Fig. 36). Here the influence of double bonds is stronger and the nanotube surface becomes perfect.

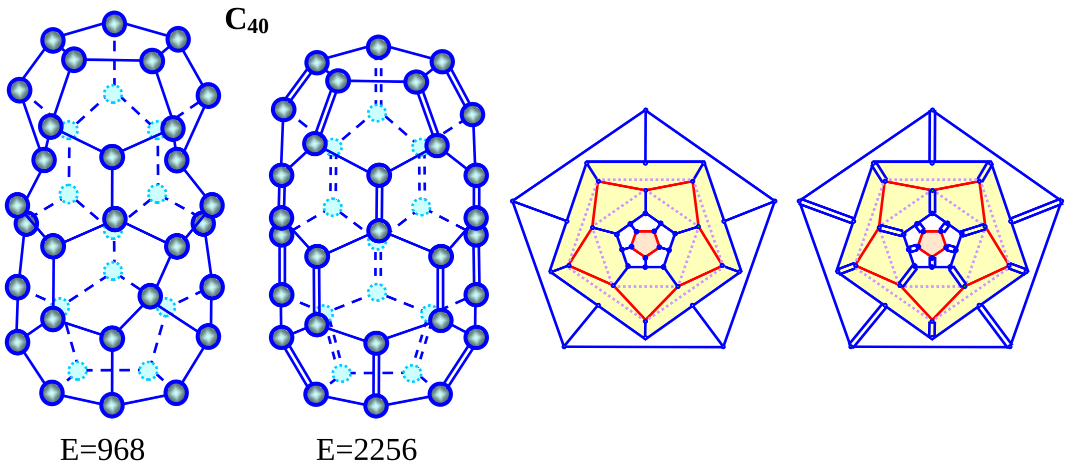


Fig. 36. Joining two mini-fullerenes C_{20} of five-fold symmetry: the rotation-reflection symmetry; structure and graphs; energy in kJ/mol

6. Conclusion and discussion

We have systematized possible ways of forming the isomers of midi-fullerenes, namely C_{30}, C_{32}, C_{34} C_{36}, C_{38} and C_{40}. Similar to the isomers of midi-fullerenes from C_{20} to C_{28}, there are three the most natural mechanisms of their formation:

1) Embedding carbon dimers into initial fullerenes;
2) Fusion of carbon cupolas having the same symmetry;
3) Fusion of fullerenes having compatible symmetry.

In Table 1 the calculated energies of fullerenes are presented, for different isomers the minimum energies being designated with bold figures.

Table 1. Energy of fullerenes in kJ/mol as a function of fullerene size and shape

	C_{30} (a, b, c, d, e)				**C_{32}** (a, b, c, d, e_u, e_d)				
E_{max}	847	1356	E_{max}	847	1356	E_{max}	847	1356	E_{max}
E_{min}	***832***	**773**	E_{min}	***832***	**773**	E_{min}	***832***	**773**	E_{min}
ΔE	15	583	ΔE	15	583	ΔE	15	583	ΔE

	C_{34} (a, b, c, d)				**C_{36}** (a, b, c, d, e)				
E_{max}	1088	1314	3977	3141	969	3957	1984	1884	3887
E_{min}	***1043***	**822**	2249	1637	**876**	2400	***1096***	***1022***	2034
ΔE	45??	492	1728	1504	93	1557	888	862	1853

	C_{38} (a, b, c, d)				**C_{40}** (a, b, c, d, e_u, e_d)					
E_{max}	1282	1801	1996	1206	1582	2257	2051	1410	3181	1808
E_{min}	**1142**	1282	***1253***	**1143**	1396	***1157***	1439	**1015**	1694	***1210***
ΔE	140	519	743	63	186	1100	612	395	1487	598

The isomers having the minimum energies are shown in Fig. 37 together with their graphs. From the figure it follows that in the majority of cases the minimum-energy fullerenes are those, having perfect and topological three-fold symmetries. Consider at first them. Their energy is seems easy to justify on the basis of the periodic system of basic perfect fullerenes [4].

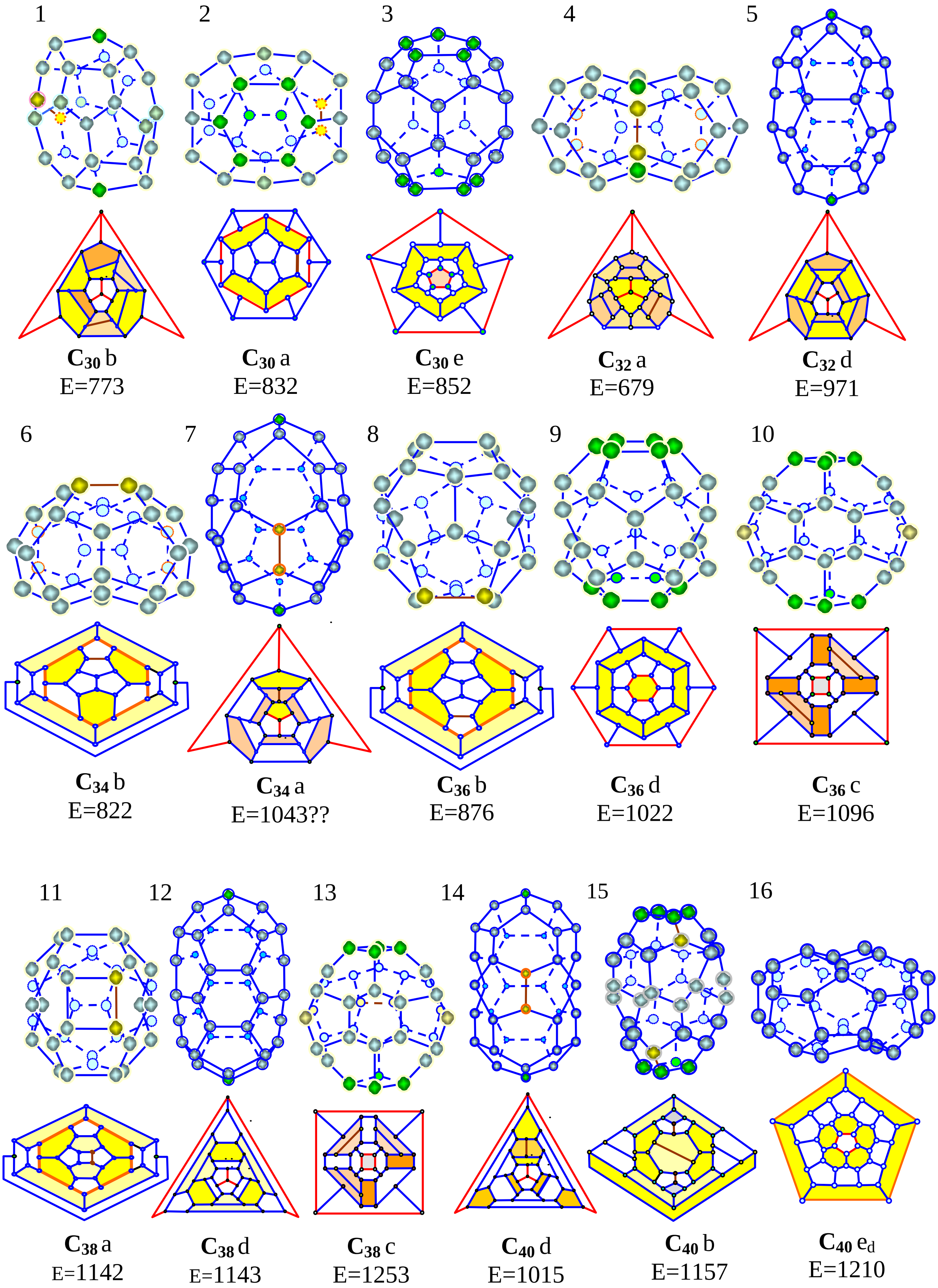


Fig. 37. Fullerene isomers of minimum energy, their graphs and energies in kJ/mol

In the range from 20 to 40 atoms the basic prefect fullerenes of three-fold symmetry having a minimum energy contain 20, 26, 32 and 38 atoms. The fullerenes of 20 and 26 atoms, C_{20} b E=1083 and C_{26} a E=801 were obtained earlier. Now we have three perfect fullerenes: (4) C_{32} a E=679, (5) C_{32} d E=971 and (12) C_{38} d E=1143. In addition to them there are three imperfect fullerenes having three-fold topological symmetry: (1) C_{30} b E=773, (7) C_{34} a E=1043 and (14) C_{40} d E=1015. Recall that we understand under the topological symmetry. In Ref. [9] by analogy with crystal physics, it was told that the imperfection is connected with the fact that the fullerenes have extra interstitial dimers or vacant dimers. That analogy was augmented in the following way. It is known that in real crystals a long-range order is impossible because dislocations violate translational symmetry. Nevertheless, the long-range order is observed experimentally, but this order is refer to as topological long-range order [10]. Following this example, we defined the imperfect fullerenes with extra interstitial dimers or vacant ones as having topological symmetry.

The perfect fullerenes of four-fold symmetry have 24, 32 and 40 atoms. The fullerene C_{24} c E=853 was obtained earlier; the perfect fullerenes C_{32} e_d E=1199 and C_{40} c E= 1439 have also not very large energy. However, the energy of the imperfect fullerenes, having four-fold topological symmetry: (10) C_{36} d E=1096 and (13) C_{38} c E=1253, is also small.

The perfect fullerenes of five-fold symmetry have 20, 30 and 40 atoms. Here we see the following picture: C_{20} b E=491 (obtained earlier), (3) C_{30} e E=852 and (16) C_{40} e_d E=1210. The perfect fullerenes of six-fold symmetry must consist of 24 and 36 atoms and here we have received before C_{24} a E=697 and now (9) C_{36} d E=1022. The rest fullerenes having the minimum energies include (2) $\mathbf{C_{30}}$ a E=832, (6) $\mathbf{C_{34}}$ b E=822, (8) $\mathbf{C_{36}}$ b E=876, (11) $\mathbf{C_{38}}$ a E =1142 and (15) $\mathbf{C_{40}}$ b E=1157. They refer to the two-fold symmetry.

It should be emphasized that all these fullerenes were produced through the use of quite different mechanisms of growth which knew nothing about the periodic system. Nevertheless, it is possible to classify them due to the periodic system of fullerenes. The question arises why the fullerenes formed the periodic system. We assume that the appearance of this system is connected with the self-organization of electronic and atomic degrees of freedom [11,12].

Acknowledgements. *No external funding was received for this study.*

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