Scientific paper

Polybenzene Revisited

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Abstract

Polybenzene was described by O'Keeffe *et al.*, as an embedding of a 6.8^2 net in the infinite periodic minimal *D*-surface, with a single type of carbon atoms and was predicted to have a substantially lower energy per atom in comparison to C_{60}, the reference structure in Nanoscience. They also described a 6.8^2 net embedded in the periodic minimal *P*-surface. We give here a rational structure construction for three benzene-based units (a third one described here for the first time in literature) and the corresponding networks. Their stability, relative to C_{60} but also to diamonds (the classical diamond D_6 and the pentagon-based diamond D_5), was calculated at the Hartree-Fock level of theory. The results confirmed the previous stability evaluation and support these structures for laboratory preparation. A Graph-theoretical description, in terms of Omega polynomial, of the three infinite networks is also presented.

Keywords: Polybenzene, periodic network, Hartree-Fock, omega polynomial

1. Introduction

O'Keeffe *et al.*[1] have published about twenty years ago a letter dealing with two 3D networks of benzene: the first one (Figure 1), called 6.8^2 *D* (also polybenzene), is described to belong to the space group *Pn3m* and has the topology of the diamond. The second structure (Figure 2) was called 6.8^2 *P* and belongs to the space group *Im3m*, corresponding to the *P*-type-surface. In fact these are embeddings of the hexagon-patch in the two surfaces of negative curvature, *D* and *P*, respectively. These are triple periodic minimal surfaces (as in the soap foame) that can embed networks of covalently bonded sp^2 atoms, called *periodic schwarzite*,[2–5] in the honor of H. A. Schwarz,[6,7] who first investigated, in the early nineteen century, the differential geometry of such surfaces. Various repeating units of schwarzites can be designed by applying the map operations (see below). If two such repeating units, of tetrahedral symmetry, join together to form an "intercalate-dimer", they can be used to build an sp^2 diamond lattice embeddable in the D-surface. The P-type surface is directed to the Cartesian coordinates in the Euclidean space. More about these periodic surfaces the reader can find in refs.[8,9]

The two proposed structures show stability comparable, or even higher, to that of C_{60} fullerene, the reference structure in nanoscience. The structure 6.8^2 *D* was predicted to be insulator while 6.8^2 *P* metallic. Of interest in Chemistry is their spongy-structure (see refs.,[3,10] the large ordered hollows could host alkali metal ions, as in natural zeolites.[11]
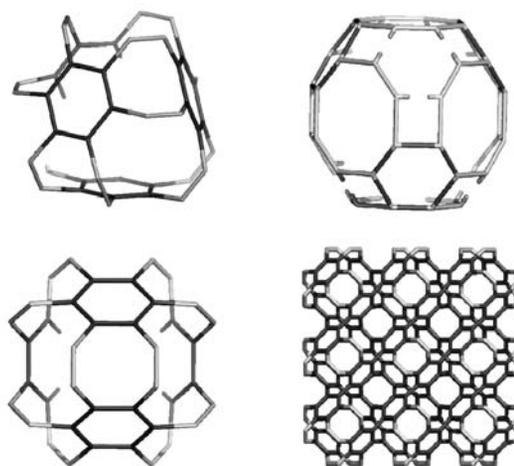
Figure 1. Benzene ring embedded in the *D*-surface; top row: BTA_48 = 6.8^2 *D* (left), designed by spanning of the parent $Le(P_4(T))$, T = Tetrahedron (right); bottom row: the face-centered BTA_48 unit (left) and the corresponding diamondoid BDia_*fcc*-network (in a (*k,k,k*)-domain, *k* = 3, right).
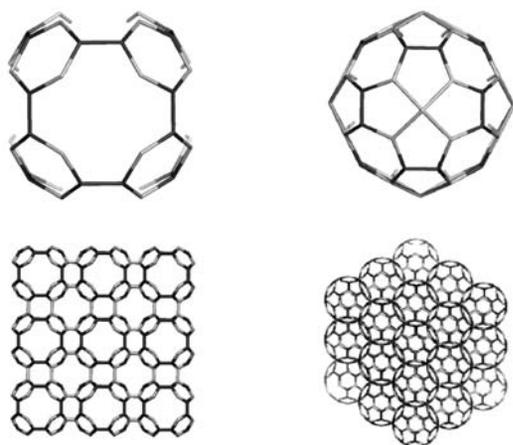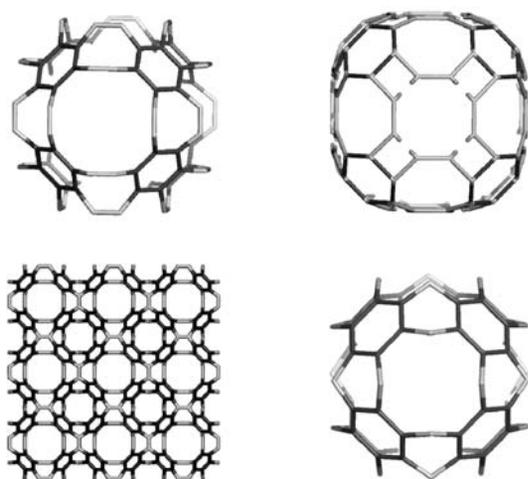
Figure 2. Benzene ring embedded in the *P*-type-surface: BCZ_48 = 6.8^2 *P* (top row, left corner), designed by spanning of the parent $S_2(Oct)$, Oct=Octahedron (top row, right corner) and the corresponding networks in a cubic (*k,k,k*)-domain, *k* = 3 (bottom row).

These structures were expected to be synthesized as 3D carbon solids; however, in our best knowledge, no such a synthesis was reported so far. Our intention was to wake up the interest of scientists to the molecular realization of such nice ideas in Carbon Nanoscience, as much as the graphenes were gained a second Nobel prize, after C_{60}, and the direct synthesis of fullerenes is now a reality.[12,13]

2. Design of Networks

The design of units of the considered structures was made by using some operations on maps,[14–17] applied on the Platonic solids: the sequence of polygonal-4 and leap-frog operations, denoted $Le(P_4(M))$, M = T (tetrahedron)

Figure 3. Benzene ring embedded in the *P*-type-surface: BCA_96 (top row, left), designed by spanning the parent $Le(P_4(C))$, C = Cube (top row, right corner), the corresponding network BCA_96&BCZ_72 in a cubic (*k,k,k*)-domain, *k* = 3 (bottom row, left) and the co-net unit BCZ_72 (bottom row, right).

and C (cube) was used to build up the structures BTA_48 (Figure 1) and BCA_96 (Figure 3) while BCZ_48 (Figure 2) was designed by spanning the cage obtained by $S_2(Oct)$, Oct = Octahedron. In the above name of structures B represents the "benzene-patch" of tessellation, T or C indicate the Platonic solid on which the map operations acted, A/Z come from "armchair" and "zig-zag" nanotube ending, respectively, while the last number denotes the number of carbon atoms in structures.
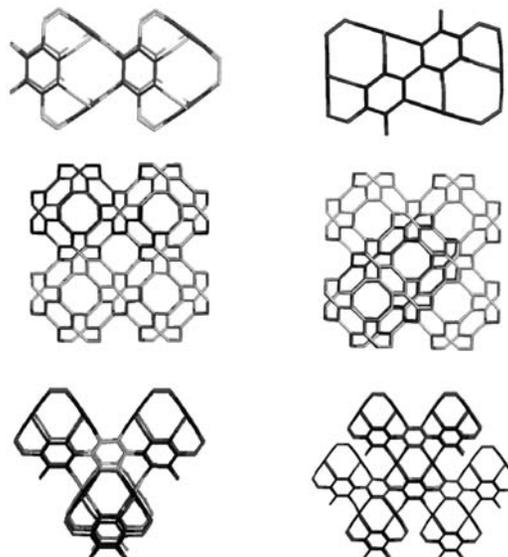
Figure 4. Top row: BTA_48 as an R(8)-dia-dimer (left) and R(12)-dendritic dimer (right). Middle row: superposition of R(8)-dimer (left) and R(12)-dimer (right) on the 222_288-domain of the *fcc*-network of BTA_48 unit (in black). Bottom row: dendrimers Den$_5$_192 and Den$_{17}$_624. In the name of dendrimers, the subscript number indicates the repeating units composing the structure while the last number counts the C-atoms.

The networks have been constructed either by identifying or joining the common faces in the corresponding repeating units. Face identification in case of the armchair-ended, tetrahedral unit BTA_48 is possible either by octagons (as in Figure 1, bottom row, detailed in Figure 4, top row, left) or by dodecagons (i.e., the opening faces of the repeating units – Figure 4, top row, right).

Identification by octagons R(8) in the BTA_48 units, disposed at the center of the six faces of the Cube, leads to a 6.8^2 net embedded as a cubic f_{cc}-net (Figure 1, bottom row), with the topology of D_6-diamond. The R(8)-dimer, leading to BTA_48_ f_{cc}-net, we call "dia-dimer". When dodecagons R(12) are identified, the resulting oligomeric structures are dendrimers (Figure 4, bottom row). The R(12)-dimer is named "dendritic dimer" (see Figure 4, middle row, right). Dendrimers, after the second generation, completely superimpose over the BTA_48_f_{cc}-net (see Figure 4, bottom row, right).

Atom orbit analysis performed on the armchair-zig-zag mixed net BCA_96&BCZ_72 had evidenced two

types of carbon atoms: one orbit includes only the atoms forming the benzene rings (6,6,8) while the second one consists of atoms belonging to octagons (6,8,8), (see Figure 3). Of course, in the case of the two networks described by O'Keeffe *et al.*[1], we also obtained a single orbit of carbon atoms (6,8,8).

3. Computational

The structures, as finite hydrogen-ended ones, were optimized at the Hartree-Fock HF (HF/6-31G**) level of theory. The calculations were performed in gas phase by Gaussian 09.[18] The single point energy minima obtained for the investigated structures are shown in Tables 1 to 3. Strain energy, according to POAV Haddon's theory[19,20] and HOMA index[21,22] were computed using the JSChem program.[23] Operations on maps were made by our CVNET program[24] while the network building, orbit analysis and Omega polynomial were calculated with the Nano Studio software package.[25]

4. Results and Discussion

Stability evaluation was performed on the finite hydrogen-ended repeating units BTA_48, and BCZ_48, corresponding to the O'Keeffe *et al.* networks and on BCA_96 and BCZ_72 units of our BCA_96&BCZ_72 network (Figure 3). As a reference, we considered C_{60}, the most used reference structure in Nanoscience. Table 1 lists the total energy per Carbon atom, E_{tot}/atom, HOMO-LUMO HL Gap, strain energy according to POAV Haddon's theory and HOMA index for the benzene patch R[6].

Among the considered structures, the most stable appears to be the armchair-ended unit BTA_48, with a tetrahedral embedding of benzene patch (Table 1, entry 1), followed by BCA_96 (Table 1, entry 3). The last structure makes a co-net with BCZ_72 (Table 1, entry 4) which is the least stable structure herein discussed. The BCZ_48 structure (Table 1, entry 2) shows the highest value of HOMA geometry based index of aromaticity, even the benzene patch is less planar in comparison to the same patch in BTA_48 and the structure is most strained among all ones in Table 1. This put a question mark on the HOMA index, as the C_C bond length is not the only parameter reflecting the pi-electron conjugation. Looking at the data in Table 1, the reference fullerene C_{60} appears the least stable among all the considered structures. For BTA_48, and BCZ_48 the simulated vibrational spectra are given in Appendix.

Comparison of BTA_48_222_f_{cc} with the classical diamond D_6–f_{cc} and the pentagon-based diamond D_5[26,27] (also known as the f_{cc}_C_{34} structure,[28] was made (Table 2) because of their face-centered cubic lattice, all of them belonging to the space group *Fd3m*. One can see that the stability (E_{tot}/C and HOMO-LUMO HL Gap) of polybenzene (Table 2, entry 1) immediately follows that of the diamond networks (Table 2, entries 2 and 3) and is over that of the reference C_{60} fullerene (Table 2, entry 4), as suggested by the results of O'Keeffe *et al.*[1]

The stability of dendrimers (Table 3, entries 2 to 5) decreases monotonically with increasing the number of atoms (in bold, in Table 3), as suggested by the total energy per carbon atom and HOMO-LUMO gap. The strain of these dendrimers decreases with the increase in the number of their carbon atoms. This is reflected in the values of HOMA: the benzene patch seems to be few distorted from the ideal planar geometry (thus showing the unity value),

Table 1. Total energy E_{tot} per atom (kcal/mol) and HOMO-LUMO HL Gap, at Hartree-Fock HF level of theory, strain according to POAV theory and HOMA index in benzene-based structures vs C_{60} taken as the reference structure

	Structure	E_{tot}/ (au)	E_{tot}/atom (au)	HL Gap (eV)	Strain/C (kcal/mol)	HOMA R[6]
1	BTA_48	–1831.484	–38.156	11.285	0.083	0.951
2	BCZ_48	–1831.097	–38.148	8.134	3.395	0.989
3	BCA_96	–3662.991	–38.156	10.253	0.124	0.939
4	BCZ_72	–2740.025	–38.056	7.558	2.749	0.812
5	C_{60}	–2271.830	–37.864	7.418	8.256	0.493

Table 2. Total energy E_{tot} per atom (kcal/mol) and HOMO-LUMO HL Gap, at Hartree-Fock HF level of theory, in benzene-based structures and C_{60} taken as the reference structure

	Structure	No C atoms	E_{tot} (au)	E_{tot}/C (au)	HL Gap (eV)
1	BTA_48_222_f_{cc}	288	–10961.473	–38.061	10.343
2	D_6–f_{cc}	248	–9478.180	–38.218	12.898
3	D_5–f_{cc}	226	–8621.954	–38.150	13.333
4	C_{60}	60	–2271.830	–37.864	7.418

Table 3. Total energy E_{tot} and HOMO-LUMO HL Gap, at Hartree-Fock HF level of theory, Strain by POAV and HOMA index in BTA_48-based oligomeric structures and C_{60} taken as the reference structure

	Structure	No units	E_{tot} (au)	E_{tot}/Catom (au)	HL Gap (eV)	Strain/C (kcal/mol)	HOMA R[6]
1	BTA_48	1	–1831.484	–38.156	11.285	0.083	0.951
2	BTA_48(**84**)_dendr2	2	–3201.679	–38.115	10.895	0.061	0.975
3	BTA_48(**120**)_dendr3	3	–4571.874	–38.099	10.771	0.056	0.978
4	BTA_48(**156**)_dendr4	4	–5942.070	–38.090	10.684	0.054	0.978
5	BTA_48(**192**)_dendr5	5	–7312.265	–38.085	10.594	0.055	0.988
6	BTA_48(**88**)_R8_dia	2	–3355.431	–38.130	10.970	0.074	0.972
8	BCA_96(**184**)	2	–7013.828	–38.119	9.805	0.180	0.936
9	C_{60}	1	–2271.830	–37.864	7.418	8.256	0.493

with the maximum at the dendrimer with a complete first generation (Table 3, entry 5). The dia-dimer (Table 3, entry 6) appears more stable than the dendritic dimer (Table 3, entry 2), however, after the second generation (see Figure 4, bottom row, right), the dendritic structure completely superimposes over the BTA_48_f_{cc}-net, so that it is no matter which way the building process has followed. A similar stability shows the dimer BCA_96(184), Table 3, entry 8. (see also Figure 3). In comparison, the reference fullerene C_{60} (Table 3, entry 9) appears less stable and less aromatic.

5. Omega Polynomial in Polybenzenes

In a connected graph $G(V,E)$, with the vertex set $V(G)$ and edge set $E(G)$, two edges $e = uv$ and $f = xy$ of G are called *codistant e co f* if they obey the relation:[29]

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \quad (1)$$

which is reflexive, that is, *e co e* holds for any edge *e* of *G*, and symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive; if "*co*" is also transitive, thus it is an equivalence relation, then *G* is called a *co-graph* and the set of edges $C(e) := \{f \in E(G); f\ co\ e\}$ is called an *orthogonal cut oc* of *G*, $E(G)$ being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \varnothing, i \neq j$. Klavžar[30] has shown that relation *co* is a theta Djoković-Winkler relation.[31,32]

We say that edges *e* and *f* of a plane graph *G* are in relation *opposite, e op f,* if they are opposite edges of an inner face of *G*. Note that the relation *co* is defined in the whole graph while *op* is defined only in faces. Using the relation *op* we can partition the edge set of *G* into *opposite edge strips, ops*. An *ops* is a quasi-orthogonal cut *qoc*, since *ops* is not transitive.

Let *G* be a connected graph and s_1, s_2, ..., s_k be the *ops* strips of *G*. Then the *ops* strips form a partition of $E(G)$. The length of *ops* is taken as maximum. It depends on the size of the maximum fold face/ring F_{max}/R_{max} con-

sidered, so that any result on Omega polynomial will have this specification.

Denote by $m(G,s)$ the number of *ops* of length *s* and define the Omega polynomial as:[33–40]

$$\Omega(G,x) = \sum_s m(G,s) \cdot x^s \quad (2)$$

Its first derivative (in $x = 1$) equals the number of edges in the graph:

$$\Omega'(G,1) = \sum_s m(G,s) \cdot s = e = |E(G)| \quad (3)$$

On Omega polynomial, the Cluj-Ilmenau index,[23] $CI = CI(G)$, was defined:

$$CI(G) = \left\{ [\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)] \right\} \quad (4)$$

Formulas to calculate Omega polynomial and CI index in three infinite networks, designed on the ground of BT_48, BC_48 and BC_96 units, are presented in Table 4. Formulas were derived from the numerical data calculated on cuboids of (k,k,k) dimensions by the Nano Studio software.[19] Omega polynomial was calculated at $R_{max}[8]$ and $R_{max}[12]$, respectively; examples are given in view of an easy verification of the general formulas. Also, formulas for the number of atoms, edges and rings (R[6], R[8] and R[12]) are included in this table. Note that Omega polynomial description is an alternative to the crystallographic description and can be useful in understanding the topology of these networks.

6. Conclusions

Polybenzene, described in O'Keeffe *et al.*[1] as an embedding of a 6.8^2 net in the infinite periodic minimal *D*-surface and denoted here (as the repeating unit) BT_48, was predicted to be stable for an eventual laboratory synthesis. Two other structures: BC_48 (also described by O'Keeffe *et al.*) and BC_96, a structure designed by us following the same steps used for BT_48, also represent embeddings of the benzene-patch, but now in the periodic

Table 4. Omega polynomial and net parameters in polybenzene networks.

Net	Omega Polynomial
BT_48	R$_{max}$[8]

$$\Omega(BT\_48) = 18k^2 X^2 + 6k(k-1)X^{2k} + 6kX^{4k} + \sum_{s=1}^{k-1} 12kX^{4s}$$

$$\Omega'(1) = 12k^2(3k+2) = |E(G)| = edges$$

$$CI(G) = 8k^2(162k^4 + 216k^3 + 61k^2 + 3k - 13)$$

$$atoms = 24k^2(k+1) = |V(G)|$$

$$R[6] = 4k^3; \ R[8] = 6k^3 - 3k^2 + 3k$$

R$_{max}$[12]

$$\Omega(BT\_48) = 6X^{2k(2k+1)} + 3X^{4k^2(k+1)} + \sum_{s=1}^{k-1} 12X^{2s(2k+1)}$$

$$\Omega'(1) = 12k^2(3k+2) = |E(G)| = edges$$

$$CI(G) = 8k(6k^2 + 2k - 1)(26k^3 + 24k^2 + 6k + 1)$$

$$R[12] = 4k^3$$

Examples	R$_{max}$[8]

$k=5$; $\Omega(G) = 450X^2 + 60X^4 + 60X^8 + 120X^{10} + 60X^{12} + 60X^{16} + 30X^{20}$;

CI=25955400; atoms=3600; edges=5100; R(6)=500; R(8)=690

$k=6$; $\Omega(G) = 648X^2 + 72X^4 + 72X^8 + 252X^{12} + 72X^{16} + 72X^{20} + 36X^{24}$;

CI=74536992; atoms=6048; edges=8640; R(6)= 864; R(8)= 1206

R$_{max}$[12]

$k=5$; $12X^{22} + 12X^{44} + 12X^{66} + 12X^{88} + 6X^{110} + 3X^{600}$;

CI= 24683160; R[12]= 500.

$k=6$; $12X^{26} + 12X^{52} + 12X^{78} + 12X^{104} + 12X^{130} + 6X^{156} + 3X^{1008}$;

CI= 71009232; R[12]= 864.

BC_48	R$_{max}$[8]

$$\Omega(BC\_48) = 12kX + 12k(k+1)X^2 + 3k(k-1)(2k-1)X^4 + \sum_{s=1}^{k-1} 24kX^{(2+4s)}$$

$$\Omega'(1) = 12k^2(6k-1) = |E(G)| = edges$$

$$CI(G) = 4k(1296k^5 - 432k^4 + 4k^3 - 24k^2 + 32k - 3)$$

$$atoms = 48k^3 = |V(G)|$$

$$R[6] = (2k)^3; \ R[8] = 12k^2(k-1)$$

R$_{max}$[12]

$$\Omega(BC\_48) = (6k-3)X^{(2k)^2} + 6X^{(2k)^3}$$

$$\Omega'(1) = 12k^2(6k-1) = |E(G)| = edges$$

$$CI(G) = 96k^4(50k^2 - 19k + 2)$$

$$R[12] = 6k(2k^2 - 2k + 1)$$

Examples	R$_{max}$[8]

$k=5$; $60X + 360X^2 + 540X^4 + 120X^6 + 120X^{10} + 120X^{14} + 120X^{18}$

CI=75601140; atoms=6000; edges=8700; R(6)= 1000; R(8)= 1200.

$k=6$; $72X + 504X^2 + 990X^4 + 144X^6 + 144X^{10} + 144X^{14} + 144X^{18} + 144X^{22}$

CI= 228432312; atoms=10368; edges=15120; R(6)=1728; R(8)=2160.

R$_{max}$[12]

$k=5$; $27X^{100} + 6X^{1000}$; CI= 69420000; R[12]=1230.

$k=6$; $33X^{144} + 6X^{1728}$; CI= 210014208; R[12]=2196.

Net	Omega Polynomial
BC_96	$R_{max}[8]$

$$\Omega(BC\_96) = 36kX^2 + 12k(k-1)X^3 + 3(k-1)(k^2-k+8)X^4 + 24(k-1)X^8 +$$
$$12k^2X^{4k} + \sum_{s=0}^{k-3} 24(k-s-2)(X^{10+6s} + X^{14+6s})$$
$$\Omega'(1) = 12k^2(9k+1) = |E(G)| = edges$$
$$CI(G) = 12k(972k^5 + 216k^4 - 16k^3 - 4k^2 + 3k + 1)$$
$$atoms = 24k^2(3k+1) = |V(G)|$$
$$R[6] = 4k(5k-3); \ R[8] = 12k^3; \ R[12] = 6k(k-1)^2$$

Examples	$R_{max}[8]$

$k=5$; $\Omega(G) = 180X^2 + 240X^3 + 336X^4 + 96X^8 + 72X^{10} + 72X^{14} + 48X^{16} + 348X^{20} + 24X^{22} + 24X^{26}$

$CI=190224960$; atoms=9600; edges=13800; R[6]= 2200; R[8]=1500.

$k=6$; $\Omega(G) = 216X^2 + 360X^3 + 570X^4 + 120X^8 + 96X^{10} + 96X^{14} + 72X^{16} + 72X^{20} + 48X^{22} + 432X^{24} + 48X^{26} + 24X^{28} + 24X^{32}$

$CI=564093144$; atoms=16416; edges=23760; R[6]= 3888; R[8]=2592

minimal *P*-surface. We gave here a rational structure construction of the units of these networks. Their stability, relative to C_{60} but also to diamonds (D_5 and D_6), was calculated, at HF level of theory. The results confirmed the stability evaluation of O'Keeffe *et al.* for their polybenzene-structures and shown a similar stability for BC_96, at least as stable as C_{60}. A Graph-theoretical description, in terms of Omega polynomial, of the three infinite networks was also presented.

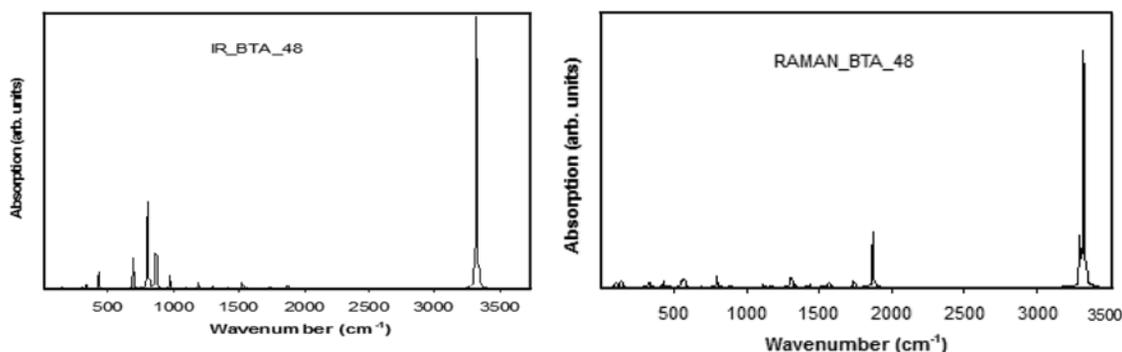# 7. Appendix.

Vibrational spectra of BTA_48 and BCZ_48 units.
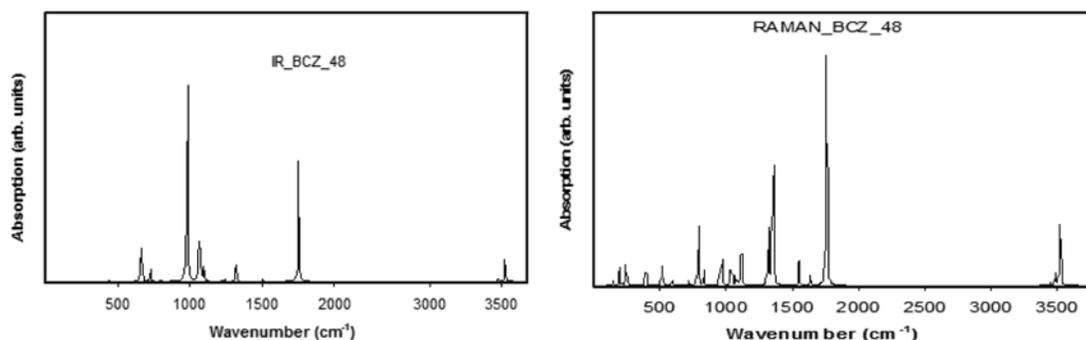

Figure w. IR and Raman spectra of BTA_48 unit

Figure w. IR and Raman spectra of BCZ_48 unit

8. Acknowledgements

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Povzetek

O'Keeffe et al., so več benzene opisali kot vpetost v 6.8² mreže v neskončno periodično minimalno D-površino z eno vrsto ogljikovih atomov in napovedali, da imajo le-ti bistveno nižje atomske energije kot C_{60}, ki v nanoznanostih služi kot referenčna struktura. Prav tako so opisali 6.8² mreže vgrajene v periodične minimalne P-površine. V tem članku predstavimo konstrukcijo racionalne strukture za tri benzenske enote (tretja tukaj opisana je prvič predstavljena v literaturi) in ustrezna omrežja. Njihovo stabilnost smo glede na C_{60} in tudi glede na diamante (D_5 in D_6) izračunali na ravni Hartree-Fock teorije. Rezultati so potrdili že znane stabilnostne izračune in kažejo na možno uporabno teh struktur v eksperimentalnih študijah. Predstavili smo tudi graf-teoretični opis teh neskončnih omrežij s pomočjo Omega polinomov.