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## Dedicated to Costică MUSTĂTA on his 60th anniversary

### PERIODIC 4.7 CAGES

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Abstract. A constructive procedure for 4,7 trivalent cages and their corresponding fused periodic cages are given. A counting theorem for these structures is formulated in terms of a general THE T counter and of a periodic description. The trival to 1,1 and 1 = 10 counter and the trible line and the trival to 1,1 and 1 = 10 counter and the trible line and trible l

# structure (2). From (d), 12 grants are deleted to obtain (e) and never at a '(W) and identifying notbulent by use it is a structure of the entractures (d) and (f) are capped by

Pure carbon cages, with the best studied spherical fullcrenes and capped tubulenes, represent novel allotropes of the carbon, generically called nanostructures. 1.5 Carbon is unique by the variety of its stable forms: chains, rings and cages, involving two, three and four coordination.

A polyhedron having ν vertices, α edges and f faces, obeys the Euler's theorem:

$$v - e + f = \chi(S) \tag{1}$$

with  $\chi(S)$  being the Euler's characteristic of the closed smooth surface S on which the polyhedron is embedded. Formula is useful for checking the consistency of an assumed structure. In this respect, other two results, also due to Euler, are recalled:

$$\sum_{d} dv_{d} = 2e \tag{2}$$

$$\sum_{s=0}^{\infty} s f_s = 2e$$
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where  $v_d$  and  $f_s$  denote vertices of degree (i.e., valency) d and s sided faces, respectively.

It is generally agreed that introduction of a small-sized cycle into a map (i.e., a lattice) covering a closed surface will produce a positive local curvature (and implicitly a strain, correlated with increased energy - when the system is a chemical one). Contrarily, a larger-sized cycle will bear a negative curvature. The total Gaussian curvatures  $^{8.9}$  k on a surface S represent a topological invariant (Gauss-Bonnet theorem):

$$\int_{S} kdA = 2\pi \chi(S) \tag{4}$$

For S being the sphere,  $\chi(S)$  is 2 while for the torus and cylinder is 0.

An Euler characteristic per site can be formulated as:6,10

where summation runs over all f-fold cycles surrounding the vertex i. Thus, the combinatorial curvature CK can be given in terms of Xi:

$$CK = \frac{1}{y} \sum_{ij} \chi_i$$
(6)

This paper proposes a way of building 4,7 trivalent cages and their corresponding fused periodic cages, for which a counting theorem is formulated in terms of a general and of a periodic counter.

Construction of 4,7 Cages

A cage built up only of 4-fold and 7-fold faces can be obtained in the following way: A tube TUHPH [9,4]. (i.e., a covering consisting of 6, 4, 6, 4-fold faces, disposed as bracelets, and next joined to form a tube, embedded on the cylinder - Figure 1, a) is cut as shown in (b) and next joined by a twist-coupling TW1 procedure (c). In the next step (d) 7-fols faces (12 points) are added at the two ends of the structure (c). From (d), 12 points are deleted to obtain (e) and next, by a TW3 and identifying the opposite points (i.e., deleting 6 points) results in structure (f). Finally, the structures (d) and (f) are capped by adding one point at each of their open ends to give the target structures CA, 4,7, (26 points) and CB, 4,7, (44 points).

Fulleroid cages of 5,7 type were reported in ref. 12. Vision 12. So one soon solution arrived eleber TUHPH (9,4), (a) (36 points)

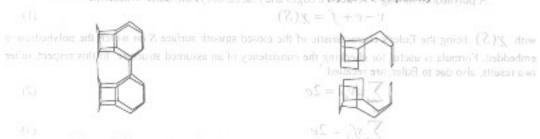


Figure 1. Construction algorithm for the 4,7 trivalent cages of series A and B.

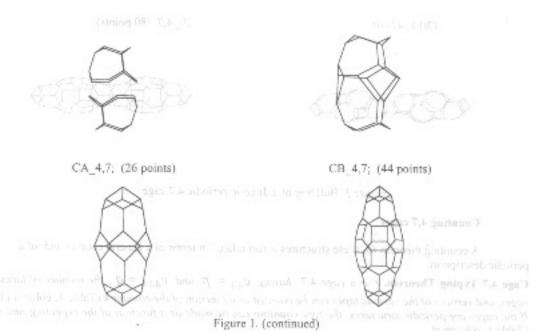
(c) (b\_TW1; 30 points)

(d) (c+12; 42 points)

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The first terms of the series A and B, illustrated in Figure 1 are 4,7 cages embedded on the sphere. As a consequence, they can be depicted by their Schlegel projection (Figure 2).

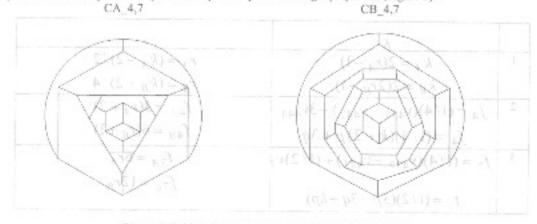


Figure 2. Schlegel projection of the monomeric 4,7 cages

In a further step, two uncapped units (see Figure 3 ) are joined by identifying their opposite edges to give a periodic 4,7 cage (in our example B<sub>2</sub>\_4,7).

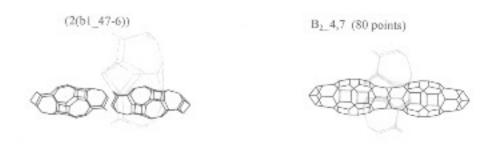


Figure 3. Building of a dimeric periodic 4,7 cage

## Counting 4,7 cages

A counting theorem for these structures is formulated in terms of a general counter and of a periodic description:

Cage 4.7 Typing Theorem. For a cage 4.7 having  $e_{44} = p$  and  $v_{444} = q$ , the number of faces, edges, and vertices of the various tapes can be counted as a function of the counter k (Table 1, column k). If the cages are periodic structures, the type counting can be made as a function of the repeating unit r (Table 1, column r).

Table 1. Periodic Cages 4.7 There I entired at how motified how A sorres and to among units off and a sorrest and a standard of the year and a standard of the year and a standard of the year.

K	p
$k_A = 2(r_A - 1)$	$r_A = (k_A + 2)/2$
$k_B = 2(2r_B - 1)$	$r_B = (k_B + 2)/4$
$f_4 = (1/4)(v_{477} - v_{447}) + 3v_{444}$	$f_{4A} = 3(r_A + 2)$
$f_4 = (1/4)(k+2)p+3q$	$f_{4B} = 6(r_B + 1)$
$f_7 = (1/4)(v_{477} + v_{447}) + (1/2)v_7$	$f_{7A} = 6r_A$
$f_7 = (1/2)(3p - 3q + kp)$	$f_{7B} = 12r_B$
	$k_B = 2(2r_B - 1)$ $f_4 = (1/4)(v_{477} - v_{447}) + 3v_{444}$ $f_4 = (1/4)(k+2)p + 3q$ $f_7 = (1/4)(v_{477} + v_{447}) + (1/2)v_7$

In a further step, 100 andapper cans (see a joing 3) care or need my mee or one or a manufact A 2 care can are example 35 - 4 71

4		$e_{44} = p$ $e_{47} = (4+k)$	r) p		$e_{47A} = 2(r_A + 1)p$
27.6	$e_{77} = 4$	p - (15/2)q	+(5/	4) pk	$e_{47B} = 2(2r_B + 1)p$
	0	81 - 5	Œ.	(8)	$e_{77A} = (3/2)p - (15/2)q + (5/2)pr_A$ $e_{77B} = (3/2)p - (15/2)q + 5pr_B$
\$150 1500		$9V_{444} = q$ $V_{447} = 2p - q$ $V_{7} = (k + 4)q$	3q	24	$v_{447} = 2p - 3q$
7860	81	$v_{777} = kp/$			$v_{477A} = 2(r_A + 1)p - 3q$ $v_{477B} = 2(2r_B + 1)p - 3q$ $v_{777A} = (r_A - 1)p$
6		6 36			$\nu_{777B} = (2r_B - 1)p$
002.0	×1	5p - 5q + (3	5	<b>€</b> 62	$N_A = 3p(r_A + 1) - 5q$ 00 - 3 $N_B = 3p(2r_B + 1) - 5q$ 00 - 8
-nSF	$k_m$ :	$= k_A + k_B$ $= 2(r_A + 2r_L)$	(-1)	84	$r_A = (1/2)k_m - 2r_B + 1$ $r_B = ((1/2)k_m - r_A + 1)/2$
en 0-	$f_{7m} = (1$	$1/4$ ) $(k_m + 2)$ $(3p - 3e)$	$q + k_m$	p)	$f_{4m} = f_{4A} + f_{4B} - 6$ $f_{7m} = f_{7A} + f_{7B}$
020	$N_m = 6$	p = 5q + (3	(2) pk	m-2	$N_m = N_A + N_B - 8(r_A + r_B - 1)$ $N_m = r_A N_{1A} + r_B N_{1B} - 8(r_A + r_B - 1)$

The above theorem is demonstrated by construction (see also ref. 6). It also hold in mixed cages, (Table 1, entries 7 to 9). Table 2 includes the counting results for some cages 4.7. It is easily seen that these cages have predominant negative curvature (column CK, Table 2).

The cutting-coupling procedure above suggested could be important in the follerence synthesis, where mourrpletely formed cages, were observed. They may join together to from cuprarodecolar assorphites. If the joining units are identical, it reachts in a pure polymeric structure, or, is confinemented scores, is considered structure. If the units are different the reaching structure, we all of a co-polymer. The forming and can also be compile, consisting may of ourse frage (Figure 4, as or mixed 5.2 days (Figure 4.

4		111		12 -				s in Some Cages 4.7.					
	Cage	R	10	4	2:0	644	$e_{4,7}$	67.7	Vita	P4.4.7	V422	P2.7.7	CK
	14 - 201			-		6	-	9	2	6	18	0	1.154
	E = 39 C3A <sub>2_A</sub> N = 44,	2		12		6	36	24	2	V 6	30	6	0.273
	E = 66 $C3A_{3=4,2}$				No. of					2.0 -	- (cal)		
	N = 62; E = 93	4	3_	150	18	6	48	39	1.2	6	42	12	-0.097
	C3A <sub>4_4,7</sub> N = 80; E = 120	. 6	4	18	24	6	60	54	2	6	54	18	-0.387
	C3B_4,7 N = 44;	1/2	F		12		36	24	2	6	30	6	0.273
6	C3B <sub>2-4.7</sub>			189			60	54	2	6	54	18	-0.300
	E = 120 C3B <sub>3_4,7</sub>			24			84	84		1 4 + 1 5 6 -			-0.517
	B = 174			1000									
H	$C3AB_{-4,7}$ () N = 62; E = 93	4		15	1.8	6	48	3.0	2	6	42	12	-0.097
9	C3AAB <sub>-4.7</sub> C3ABA <sub>-4.7</sub>	6	.)8-	18	24	6	60			6 6			-0.300
	N = 80; E = 120	1)8	Zh.	$\Lambda^{84}$	+ 1	Apr	- m.Y.						
10	C3ABB_4,3 N = 98; E = 147	8	-	21	30	6	72	69	2	6	66	24	-0.429

## Perspectives

The cutting-coupling procedure above suggested could be important in the fullerene synthesis, where incompletely formed cages were observed. They may join together to form supramolecular assemblies.<sup>13</sup> If the joining units are identical, it results in a pure polymeric structure, or, in mathematical sense, a periodic structure.<sup>14</sup> If the units are different, the resulting structure is called a co-polymer. The joining unit can also be variable, consisting e.g., of pure 7 rings (Figure 4, a) or mixed 5,7 rings (Figure 4, b).

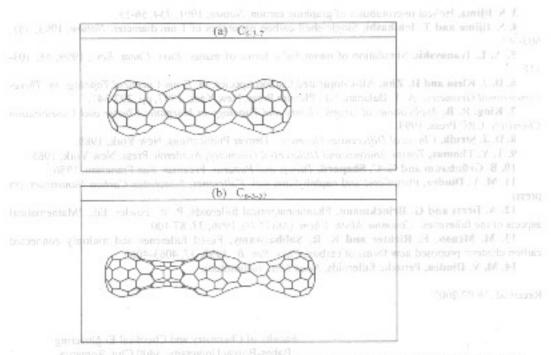


Figure 4. Periodic fullerenes with the repeating unit r = 3 and joining units 7 (a) and 5,7 (b).

#### Conclusions

Pure 4,7 trivalent cages were built up by using small segments of the tubular HPH net and appropriate cutting-joining operations. Such transformations could be plausible routes in the fate of the vaporized graphite.

Counting of the constitutive components of the 4,7 cages was accomplished in terms of a general counter and of a periodic description.

The novel class of periodic fullerenes, announced here, showed a heat of formation lower than the parent spherical fullerenes, <sup>14</sup> deserving more attention in theoretical studies and experimental research.

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