

# Topological Entropies of All 2907 Convex 4- to 9-atomic Polyhedral Clusters

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## ABSTRACT

The topological entropy  $H_S$  of all 2907 convex 4- to 9-atomic polyhedral clusters has been calculated from the point of different symmetrical positions of the atoms. It shows a general trend to drop with growing symmetry of clusters with many local exceptions. The topological entropy  $H_V$  of the same clusters has been calculated from the point of different valences (chemical bonds) of the atoms. It classifies the variety of clusters in more details. The relationships between the  $H_S$  and  $H_V$  entropies are discussed.

**Keywords:** Convex Polyhedral Clusters; Automorphism Group Orders; Symmetry Point Groups; Chemical Bonds; Topological Entropy

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## 1. Introduction

A general theory of convex polyhedra is given by Grünbaum<sup>[1]</sup>. In the series of papers we consider a special problem on the combinatorial variety of convex  $n$ -hedra rapidly growing with  $n$ . All combinatorial types of convex 4- to 12-hedra and simple (only 3 facets/edges meet at each vertex) 13- to 16-hedra have been enumerated and characterized by automorphism group orders (a.g.o.'s) and symmetry point groups (s.p.g.'s)<sup>[2]</sup>. Asymptotically, almost all  $n$ -hedra (and  $n$ -acra, *i.e.*  $n$ -vertex polyhedra, because of duality) seem to be combinatorially asymmetric (*i.e.* primitive triclinic). A method of naming any convex  $n$ -acron by a numerical code arising from the adjacency matrix of its edge graph has been suggested<sup>[3]</sup>. The combinatorial types of convex  $n$ -acra with the  $\min_n$  and  $\max_n$  names and some asymptotical (as  $n \rightarrow \infty$ ) relations between the latter have been found by Voytekhovskiy<sup>[4,5]</sup>. Here we consider the topological entropies as additional characteristics of convex  $n$ -acra.

Obviously, convex  $n$ -acra can also be interpreted as atomic clusters with atoms located in vertices and the edges considered as chemical bonds. It is interesting to know, if the topological entropy correlates with the a.g.o.'s of atomic clusters. If so, it can be taken as a continuous approximant of the discrete s.p.g.'s. On the other hand, there are convex  $n$ -acra with different numbers of edges, as a whole, and different valences of the vertices, in particular. It follows from the general theory of systems that their complexity mostly depends on relationships between the elements (*e.g.*, chemical bonds of the atoms) rather than on the number of the elements themselves (*e.g.*, the number of vertices equivalent under the automorphism group). Does the topological entropy effectively fix the complexity of the convex  $n$ -atomic clusters? The paper discusses these questions.

## 2. Statistical entropy and its properties

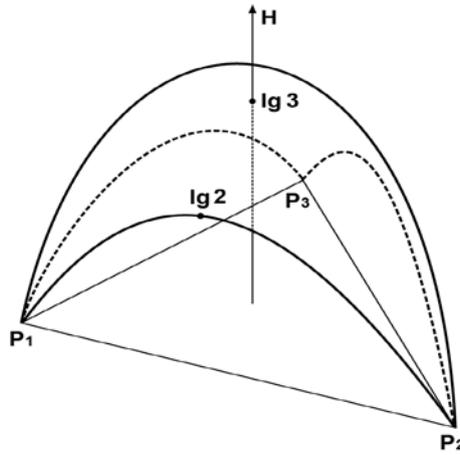
The concept of entropy has been suggested in thermodynamics by Clausius in 1865. Its statistical inter-

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pretation has been performed by Boltzmann in 1872. Afterwards, Shannon<sup>[6]</sup> and Halphen<sup>[7]</sup> have independently found the formula

$$H = - \sum_{i=1}^n p_i \log p_i$$

in the framework of the mathematical theory of communication and population statistics, respectively. In any case, this is the convolution of some distribution of probabilities  $p_i$  with an obvious restriction  $p_1 + \dots + p_n = 1$ . The  $H$  function is bounded by  $H_{\min} = 0$ , if one of  $p_i = 1$  (the others are 0's), and  $H_{\max} = \log n$ , if any  $p_i = 1/n$ . Its schematic graphs for two (arcs with  $H_{\max} = \lg 2$ ) and three (surface with  $H_{\max} = \lg 3$ ) probabilities are given over the barycentric diagram  $p_1 + p_2 + p_3 = 1$  in **Figure 1**. It is easy to see that small changes of the probabilities  $p_i$  at the corners of a diagram affect big changes of  $H$ , while the same changes of  $p_i$  in the central part of a diagram do not affect  $H$  that much.



**Figure 1.** The graph of  $H(p_1, p_2, p_3)$ . Hereinafter in nites, as decimal logarithms are used.

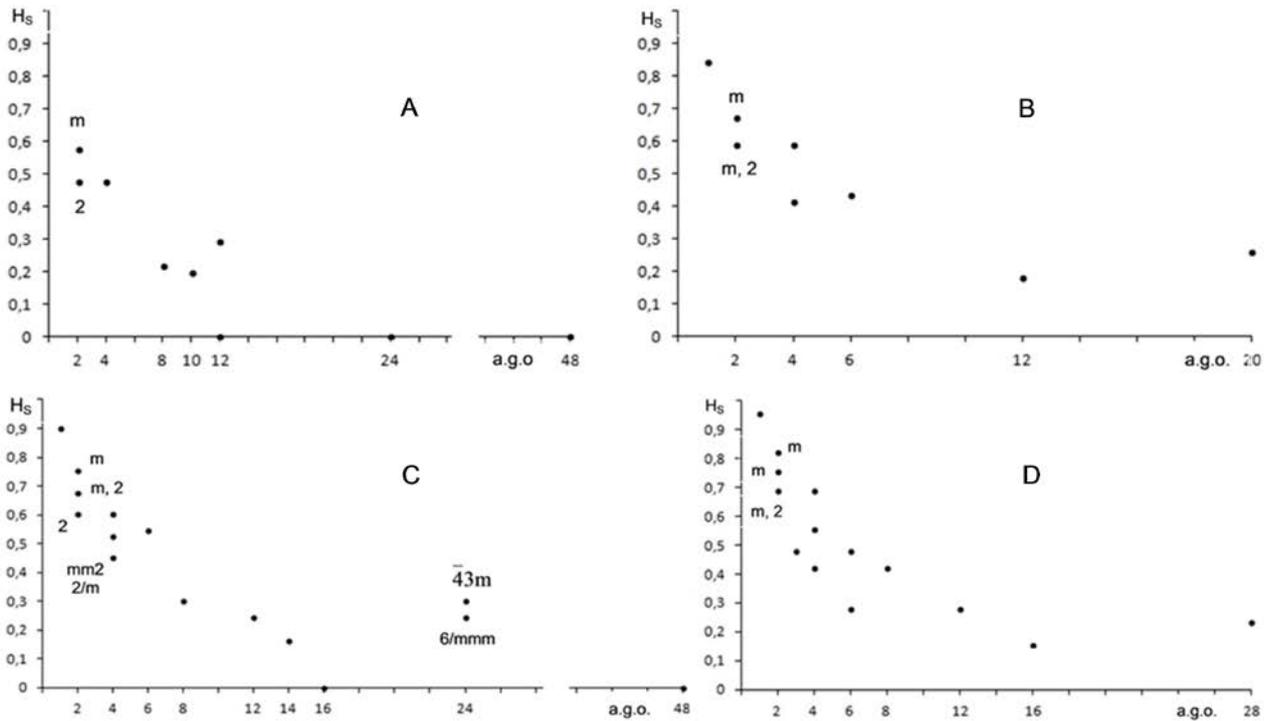
### 3. Entropy $H_S$ of convex $n$ -acra

The above formula allows us to characterize the topology of convex  $n$ -acra in different ways. For example, let us define the entropy  $H_S$  from the point of different symmetrical positions of the vertices. In this case, for any  $n$ -acron, numbers  $n_i$  of vertices in different symmetrical positions and, afterwards, the probabilities  $p_i = n_i/n = n_i/\sum n_i$  should be calculated. It follows from the above that, for given  $n$ ,  $H_{S,\max}$  is attained by  $n$ -acra with any two vertices non-equivalent under the automorphism group, for example, by combinatorially asymmetric  $n$ -acra (*i.e.* those, which cannot be transformed to symmetric convex  $n$ -acra by the continuous transformations),  $n \geq 7$ . At the same time,  $H_{S,\min}$  is attained by vertex-transitive  $n$ -acra. These include regular (Platonic) and semi-regular (Archimedean) polyhedra, as well as the infinite series of prisms and antiprisms. They have even number  $n \geq 4$  of vertices, precisely: 4, 6, 8, 12, 20 for Platonic solids, 12 (2 times), 24 (4 times), 30, 48, 60 (4 times), 120 for Archimedean solids, and any even  $n \geq 6$  for prisms and antiprisms (cube and octahedron are topologically equivalent to a tetragonal prism and a trigonal antiprism, respectively). The further question is how  $H_S$  depends on a.g.o.'s and s.p.g.'s of  $n$ -acra with growing  $n$ . The edge graphs of all 2907 convex 4- to 9-acra and their a.g.o. and s.p.g. statistics (**Table 1**) have been extracted from [2].

The lexicographically ordered sequences of the vertices numbers in different symmetry positions for all convex 4- to 9-acra and related s.p.g.'s are as follows. **4-acron.** 4:  $\overline{4}3m$  (tetrahedron). **5-acra.** 14:  $4mm$  (tetragonal pyramid), 23:  $\overline{6}m2$  (trigonal bipyramid). **6-acra.** 1122:  $m$ , 15:  $5m$  (pentagonal pyramid), 222: 2,  $mm2$ , 6:  $\overline{6}m2$  (trigonal prism),  $m\overline{3}m$  (octahedron). **7-acra.** 1111111: 1, 111122:  $m$ , 1222: 2,  $m$ ,  $mm2$ , 124:  $mm2$ , 133:  $3m$ , 16:  $6mm$ , 25:  $\overline{10}m2$ . **8-acra.** 11111111: 1, 111122:  $m$ , 11222: 2,  $m$ , 1124:  $mm2$ , 1133:  $3m$ , 2222: 2,  $mm2$ , 17:  $7m$ , 224:  $mm2$ ,  $2/m$ , 26:  $\overline{3}m$ ,  $\overline{6}m2$ ,  $6/mmm$ , 44:  $mmm$ ,  $\overline{4}2m$ ,  $\overline{4}3m$ , 8:  $\overline{8}2m$ ,  $m\overline{3}m$ . **9-acra.** 111111111: 1, 1111122:  $m$ , 111222:  $m$ , 12222: 2,  $m$ ,  $mm2$ , 1224:  $mm2$ , 144:  $mm2$ ,  $4mm$ , 18:  $8mm$ , 27:



lences of vertices of  $n$ -acra:  $p_i = v_i/n$ . For example, there are 7 combinatorially asymmetric 7-acra (**Table 1**) of the same entropy  $H_S = H_{\max} = \lg 7$ . But almost all of them are unique as for valences of their vertices<sup>[3]</sup> (**Figure 3**): 232, 3211, 331 (two 7-acra), 412, 43, and 511. Hereinafter each sequence records the numbers  $v_i$  of  $i$ -valent vertices from  $v_3$  to  $v_{\max}$ . Obviously, the entropy  $H_V$  differs for the six classes. In the same way, the combinatorially asymmetric 8-acra (140 in total, **Table 1**) can be divided into 31 classes (see Figures in [2]). But, as 0's and permutations of the indexes  $v_i$  do not change  $H_V$ , combinatorially asymmetric 8-acra can be divided into 12 classes of different  $H_V$ .



**Figure 2.** Entropy  $H_S$  of convex 4- to 6-acra (A, 10 in total), 7-acra (B, 34), 8-acra (C, 257), and 9-acra (D, 2606) vs. a.g.o. The s.p.g.'s are given to the dots if they do not follow from the **Table 1**.

The lexicographically ordered sequences of the numbers of the vertices with different valences for convex 4- to 9-acra and related s.p.g.'s have been extracted from [2] and are as follows. **4-acron.** 4:  $\bar{4}3m$  (tetrahedron). **5-acra.** 23:  $\bar{6}m2$  (trigonal bipyramid), 41:  $4mm$  (tetragonal pyramid). **6-acra.** 06:  $m\bar{3}m$  (octahedron), 222:  $mm2$ , 24:  $mm2$ , 321:  $m$ , 42: 2, 501:  $5m$  (pentagonal pyramid), 6:  $\bar{6}m2$  (trigonal prizm). **7-acra.** 052:  $\bar{10}m2$ , 133:  $3m$ , 151:  $m$ , 2221: 2, 2302:  $mm2$ , 232: 1,  $mm2$ , 2401:  $mm2$ , 25: 2,  $mm2$ , 3031:  $3m$ , 313:  $m$ , 3211: 1,  $m$ , 331: 1,  $m$ , 412: 1, 2, 4201:  $m$ ,  $mm2$ , 43: 1, 2,  $m$ ,  $3m$ , 511: 1,  $m$ , 6001:  $6mm$ , 61:  $m$ ,  $mm2$ .

**8-acra.** 044:  $\bar{4}2m$ , 0602:  $6/mmm$ , 062:  $mm2$ , 08:  $\bar{8}2m$ , 1331:  $m$ , 1412:  $m$ , 143: 1,  $m$ , 1511: 1,  $m$ , 161: 1,  $m$ , 206:  $\bar{3}m$ , 2141:  $mm2$ , 2222: 2,  $mm2$ , 22301:  $m$ , 224: 1, 2,  $m$ ,  $mm2$ , 23111: 1, 2321: 1,  $m$ , 24002:  $mm2$ , 2402: 1,  $mm2$ , 24101: 1, 242: 1, 2,  $m$ ,  $2/m$ , 2501: 1,  $m$ ,  $mm2$ , 26: 2,  $m$ ,  $\bar{6}m2$ , 3113:  $m$ , 31211: 1, 3131: 1,  $m$ , 3212: 1,  $m$ , 32201: 1,  $m$ , 323: 1,  $m$ , 33011: 1, 3311: 1, 34001:  $m$ , 341: 1,  $m$ , 4004:  $\bar{4}3m$ , 4022: 1,  $mm2$ , 40301:  $m$ , 404: 1,  $mm2$ ,  $\bar{4}2m$ , 4121: 1,  $m$ , 4202: 1, 2, 42101: 1,  $m$ , 422: 1, 2,  $m$ ,  $mm2$ , 4301: 1,  $m$ ,  $3m$ , 44: 1, 2,  $m$ ,  $mmm$ ,  $\bar{4}2m$ , 503: 1,  $m$ ,  $3m$ , 5111: 1, 52001:  $m$ , 521: 1,  $m$ , 602: 2,  $m$ , 6101: 1, 62: 1, 2,  $m$ ,  $mm2$ , 70001:  $7m$ , 701:  $m$ , 8:  $mm2$ ,  $m\bar{3}m$ .

**9-acra.** 036:  $\bar{6}m2$ , 0441:  $mm2$ , 0522:  $mm2$ , 054:  $m$ ,  $4mm$ , 0603:  $\bar{6}m2$ , 0621: 1,  $mm2$ , 07002:  $\bar{14}m2$ , 072: 2,  $mm2$ , 0801:  $mm2$ , 09:  $\bar{6}m2$ , 1251:  $m$ , 1332: 1, 135: 1,  $m$ , 1413:  $m$ , 14211: 1,  $m$ , 1431: 1,  $m$ , 15102:  $m$ , 1512: 1,  $m$ , 15201: 1,  $m$ , 153: 1,  $m$ , 16011: 1,  $m$ , 1611: 1,  $m$ , 17001:  $m$ , 171: 1,  $m$ , 2142: 2,  $m$ , 21501:  $m$ , 216:  $m$ , 2223: 2,  $m$ , 22311: 1,  $m$ , 224001: 2, 2241: 1,  $m$ ,  $mm2$ , 2304:  $mm2$ , 23121: 1,  $m$ , 23202: 2,  $m$ , 232101: 1,  $m$ , 2322: 1, 2,  $m$ ,  $mm2$ , 23301: 1,  $m$ , 234: 1, 2,  $m$ ,  $mm2$ , 240201: 2, 2403: 1,  $m$ , 241011: 1, 24111: 1, 242001: 1,

2, m, 2421: 1, 2, m, 250002: mm2, 25002: 1, mm2, 250101: 1, 2502: 1, 2, m, 25101: 1, m, 252: 1, 2, m, 260001: mm2, 2601: 1, 2, m, mm2, 27: 1, 2, m, mm2, 3033: m, 3m, 3051: 1, m, 31221: 1, m, 31302: 1, 313101: 1, 3132: 1, 31401: 1, m, 315: 1, m, 32031: 1, m, 32112: 1, m, 321201: 1, m, 3213: 1, m, 322011: 1, m, 32211: 1, m, 323001: 1, m, 3231: 1, m, 33021: 1, m, 33102: 1, m, 331101: 1, 3312: 1, m, 33201: 1, m, 333: 1, m, 3, 3m, 340011: 1, m, 34011: 1, m, 341001: 1, m, 3411: 1, m, 35001: 1, m, 351: 1, m, 40212: 2, 402201: mm2, 4023: 2, m, 40311: 1, m, 404001: 4mm, 4041: 1, 2, m, mm2, 41022: m, 4104: 1, m, 41121: 1, m, 41202: 1, m, 412101: 1, 4122: 1, 2, m, mm2, 41301: 1, m, 414: 1, 2, m, mm2, 4203: 1, 2, m, mm2, 42111: 1, 422001: 1, 2, m, 4221: 1, 2, m, mm2, 43002: 1, 2, 430101: 1, m, 4302: 1, 2, m, 43101: 1, m, 432: 1, 2, m, mm2, 440001: 1, m, mm2, 4401: 1, 2, m, mm2, 45: 1, 2, m, 4mm, 50031: m, 5013: 1, m, 50211: 1, m, 503001: m, 5031: 1, m, 5112: 1, m, 51201: 1, m, 513: 1, m, 52011: 1, m, 521001: 1, m, 5211: 1, m, 53001: 1, m, 531: 1, m, 6021: 1, 2, m, 6102: 1, 2, m, 61101: 1, 612: 1, 2, m, 620001: m, mm2, 6201: 1, 2, m, 63: 1, 2, m, 3m,  $\bar{6}m2$ , 7011: 1, m, 71001: 1, m, 711: 1, m, 800001: 8mm, 8001: m, mm2, 81: 1, m, mm2.

The data have been used to calculate the entropy  $H_V$  (**Figure 3**). The main feature of  $H_V$  is that it classifies the variety of convex 4- to 9-acra in more details than  $H_S$  with  $H_S \geq H_V$  for any  $n$  and s.p.g.

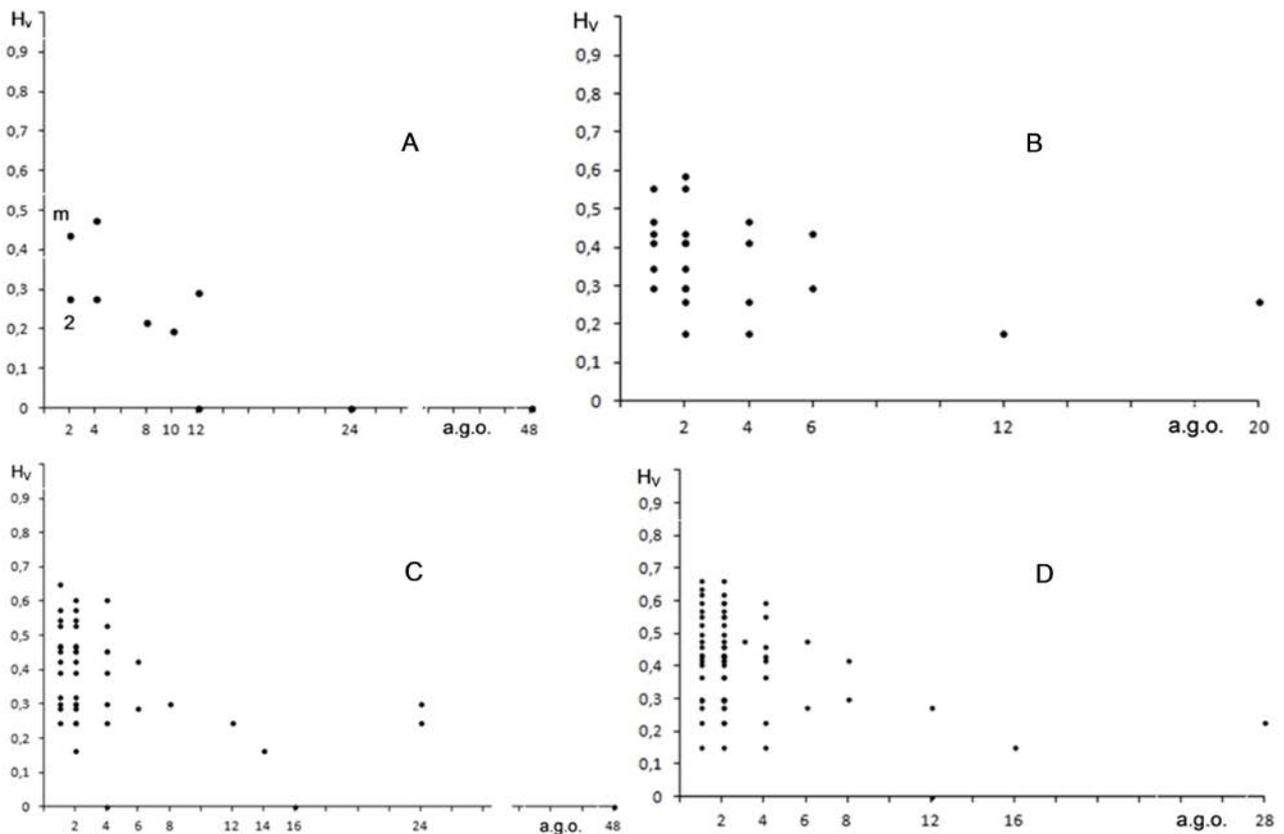


Figure 3. Entropy  $H_V$  for the same classes of convex  $n$ -acra as in Figure 2.

## 5. Discussion

The relationships between the entropies  $H_S$  and  $H_V$  in a general case can be formulated in two statements.

**Statement 1.**  $H_S \geq H_V$  for any convex  $n$ -acron, *i.e.* for any  $n$  and s.p.g.

**Proof.** First of all, the statement is true for all convex 4- to 9-acra (**Table 2**).  $H_S > H_V$  mostly for  $n$ -acra of low symmetry, while  $H_S = H_V$  mostly for  $n$ -acra of high symmetry with the transition classes of a.g.o.'s from 2 to 12. Careful consideration of  $n$ -acra has allowed to establish the following. Let us take any  $n$ -acron with vertices of different symmetry positions. Obviously, vertices equivalent under the automorphism group have the same valences. The question is if the non-equivalent vertices have different valences or not.  $H_S =$



quite well characterized by s.p.g.'s. The second one should distinguish n-acra of the same s.p.g. and different numbers of edges, for example, the overwhelming majority of combinatorially asymmetric n-acra for given  $n \geq 7$ . To do this, the topological entropy  $H_V$  is suggested, which considers the valences of vertices of n-acra. It classifies the variety of convex 4- to 9-acra in more details. It is proved that  $H_V$  can reach 0 as minimum (for example, for regular and semi-regular polyhedra, as well as the infinite series of prisms and antiprisms), but never  $\lg n$  as maximum, because there are no convex n-acra with all vertices of different valences. It is also proved that  $H_S \geq H_V$  for any convex n-acron, *i.e.* for any  $n$  and s.p.g.  $H_S = H_V$  if the vertices non-equivalent under the automorphism group also have different valences, and  $H_S > H_V$  if not.

## Conflict of interest

No conflict of interest was declared by the author.

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## Appendix 1

Consider the sequences of numbers  $v_i$  of different valences for convex 5- to 9-acra (related  $H_V$  are in parentheses) ordered by the algorithm to follow: ...  $p \dots q \dots (H_1) \rightarrow \dots p-1 \dots q+1 \dots (H_2)$ , where  $1 \leq p \leq q$ .

**5-acra.** 23 (0,292)  $\rightarrow$  14 (0,217).

**6-acra.** (Hereinafter 0's and permutations of  $v_i$  are omitted in the sequences as they do not affect  $H_V$ .)  
222 (0,477)  $\rightarrow$  123 (0,439)  $\rightarrow$  24 (0,276)  $\rightarrow$  15 (0,196)  $\rightarrow$  6 (0).

**7-acra.** The main trend: 1222 (0,587)  $\rightarrow$  1123 (0,555)  $\rightarrow$  223 (0,469)  $\rightarrow$  133 (0,436)  $\rightarrow$  124 (0,415)  $\rightarrow$  34 (0,297)  $\rightarrow$  25 (0,260)  $\rightarrow$  16 (0,178); offshoot: 124 (0,415)  $\rightarrow$  115 (0,346).

**8-acra.** The main trend: 11123 (0,649)  $\rightarrow$  1223 (0,574)  $\rightarrow$  1133 (0,545)  $\rightarrow$  233 (0,470)  $\rightarrow$  224 (0,452)  $\rightarrow$  134 (0,423)  $\rightarrow$  44 (0,301)  $\rightarrow$  35 (0,287)  $\rightarrow$  26 (0,244)  $\rightarrow$  17 (0,164)  $\rightarrow$  8 (0); offshoots: 2222 (0,602)  $\rightarrow$  1223 (0,574); 1133 (0,545)  $\rightarrow$  1124 (0,527)  $\rightarrow$  1115 (0,466); and 134 (0,423)  $\rightarrow$  125 (0,391)  $\rightarrow$  116 (0,319).

**9-acra.** The main trend: 11223 (0,661)  $\rightarrow$  2223 (0,595)  $\rightarrow$  1233 (0,569)  $\rightarrow$  333 (0,477)  $\rightarrow$  234 (0,461)  $\rightarrow$  144 (0,419)  $\rightarrow$  135 (0,407)  $\rightarrow$  45 (0,298)  $\rightarrow$  36 (0,276)  $\rightarrow$  27 (0,230)  $\rightarrow$  18 (0,152)  $\rightarrow$  9 (0); offshoots: 11223 (0,661)  $\rightarrow$  11133 (0,636)  $\rightarrow$  11124 (0,620); 1233 (0,569)  $\rightarrow$  1224 (0,553)  $\rightarrow$  1134 (0,528)  $\rightarrow$  1125 (0,499)  $\rightarrow$  1116 (0,435); 234 (0,461)  $\rightarrow$  225 (0,432); and 135 (0,407)  $\rightarrow$  126 (0,369)  $\rightarrow$  117 (0,297).

The above sequences could be ordered in different ways. We have followed the rule of a "slow down" to include as many sequences in the main trends, as possible. With no exception, the above algorithm causes  $H_1 > H_2$ . To prove the inequality in a general case (for any  $1 \leq p \leq q$  and  $n$ ), we should show that

$$-(p/n) \ln(p/n) - (q/n) \ln(q/n) > -[(p-1)/n] \ln[(p-1)/n] - [(q+1)/n] \ln[(q+1)/n].$$

If  $p \rightarrow 1$ , then  $[(p-1)/n] \ln[(p-1)/n] \rightarrow 0$ . Hence, for  $p = 1$  we get an obvious inequality  $(q+1) (1+1/q)^q > 1$ . For  $2 \leq p \leq q$  we should prove the inequality

$$p^p / (p-1)^{p-1} < (q+1)^{q+1} / q^q = f(q) .$$

Consider  $f(q)$  as a continuous function and use a logarithmic derivative

$$df/dq = \ln(1+1/q) \times (q+1)^{q+1} / q^q > 0 .$$

That is,  $f(q)$  grows with the growing arguments  $q = p, p + 1, p + 2, \text{ etc.}$

Let us show that the above inequality takes place even for the minimum argument  $q = p, \text{ i.e.}$

$$p^p / (p-1)^{p-1} < (p+1)^{p+1} / p^p \quad \text{or} \quad 1 < (p+1)^{p+1} (p-1)^{p-1} / p^{2p} = f(p) .$$

Again, consider  $f(p)$  as a continuous function and use a logarithmic derivative

$$df/dp = \ln(1-1/p^2) \times (p+1)^{p+1} (p-1)^{p-1} / p^{2p} < 0 .$$

That is,  $f(p)$  drops with the growing arguments  $p = 2, 3, 4, \text{ etc.}$  Indeed,  $f(2) = 1,6875$ ,  $f(3) = 1,404\dots$ ,  $f(4) = 1,287\dots$ ,  $f(5) = 1,223\dots$ ,  $f(6) = 1,182\dots$

Nevertheless, if  $p \rightarrow \infty$ , then

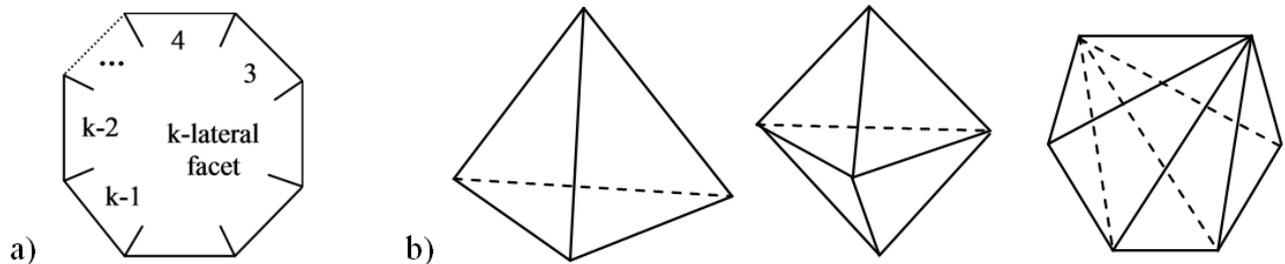
$$\lim f(p) = \lim (p+1)^{p+1} (p-1)^{p-1} / p^{2p} = \lim (1+1/p)^p (1-1/p)^p [1+2/(p-1)] = e \times e^{-1} \times 1 = 1 .$$

That is,  $f(p)$  tends to 1 from above, *i.e.*  $f(p) > 1$  for any  $p$ . Thus,  $H_1 > H_2$  for any  $1 \leq p \leq q$  and  $n$ .

## Appendix 2

Assume that a convex polyhedron exists with all the facets being different (*i.e.* of different number of edges). Let us consider its Schlegel diagram on a facet with a maximum number of edges ( $k$ -lateral facet, **Figure 4a**). More precisely, let us consider how its corona (*i.e.* a set of facets touching it edge-to-edge) is built. After  $(k-1)$ -,  $(k-2)$ - ... 4-, and 3-lateral facets being attached to  $k$ -lateral one in any order, 3 more edges are free. And we can conclude that our initial assumption that all facets are different is wrong. Obviously, in the above case, 3 same (*i.e.* of the same number of edges), or 2 and 1, or 3 different facets can be attached to them. As any (*i.e.* 3- to  $k$ -lateral) facet is used, 4 same, or 3 and 2, or 3 pairs of same facets will result on a polyhedron.

Assume that not all  $k-3$  types of the facets are submitted in the corona. Then, after the facets of each type being attached by one to  $k$ -lateral facet, more than 3 edges are free. To complete the corona, one should choose more than 3 facets from their less than before  $(k-3)$  variety. Obviously, both reasons may not reduce the frequency of occurrence of the facets in the corona: 4 same, or 3 and 2, or 3 pairs of same facets. Finally, because of the duality, any convex  $n$ -acron has at least 4, or 3 and 2, or 3 pairs of vertices of same valences. The limit cases are: a tetrahedron, a trigonal dipyramid, and a 6-acron of  $mm2$  s.p.g. (**Figure 4b**).



**Figure 4.** The Schlegel diagram on a  $k$ -lateral facet. b) The limit convex 4-, 5-, and 6-acra. See text.