

References

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ETUDES ON CONVEX POLYHEDRA.

5. TOPOLOGICAL ENTROPIES OF ALL 2907 CONVEX 4- TO 9-VERTEX POLYHEDRA

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Abstract

The topological entropy H_s of all 2907 convex 4- to 9-vertex polyhedra has been calculated from the point of different symmetrical positions of the vertices. It shows a general trend to drop with growing symmetry of polyhedra with many local exceptions. The topological entropy H_v of the same polyhedra has been calculated from the point of different valences of the vertices. It classifies the variety of polyhedra in more detail. The relationships between the H_s and H_v are discussed.

Synopsis

The paper discusses the relationships between the entropies H_s and H_v calculated for all 2907 convex 4- to 9-vertex polyhedra from the point of different symmetrical positions and valences of their vertices, respectively.

Key words

Convex polyhedra, automorphism group orders, symmetry point groups, valences, topological entropy.

1. Introduction

A general theory of convex polyhedra is given in (Grünbaum, 1967). In the series of papers we consider a special problem on the combinatorial variety of convex n -hedra rapidly growing with n . In Voytekhovskiy & Stepenshchikov (2008) and Voytekhovskiy (2014) 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). 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 in

Voytekhovskiy (2016). 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 in Voytekhovskiy (2017 *a, b*). 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.*, valences of the vertices) 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 interpretation has been performed by Boltzmann in 1872. Afterwards, Shannon (1948) and Halphen (1957) 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 Fig. 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.

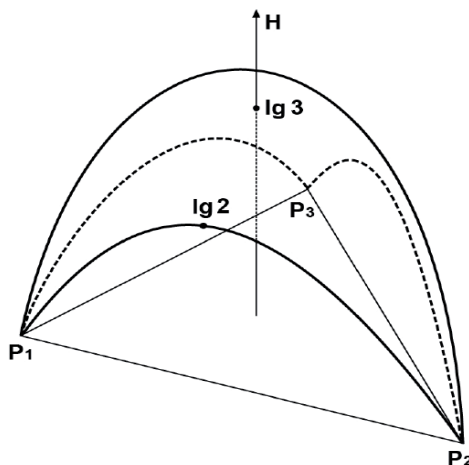


Figure 1. The graph of $H(p_1, p_2, p_3)$. Hereinafter in nites, as decimal logarithms are used.

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-acra.** 4: $\bar{4}3m$ (tetrahedron). **5-acra.** 14: $4mm$ (tetragonal pyramid), 23: $\bar{6}m2$ (trigonal bipyramid). **6-acra.** 1122: m , 15: $5m$ (pentagonal pyramid), 222: 2 , $mm2$, 6: $\bar{6}m2$ (trigonal prizm), $m\bar{3}m$ (octahedron). **7-acra.** 1111111: 1 , 11122: m , 1222: 2 , m , $mm2$, 124: $mm2$, 133: $3m$, 16: $6mm$, 25 $\bar{10}m2$. **8-acra.** 11111111: 1 , 111122: m , 112222: 2 , m , 1124: $mm2$, 1133: $3m$, 2222: 2 , $mm2$, 17: $7m$, 224: $mm2$, $2/m$, 26: $\bar{3}m$, $\bar{6}m2$, $6/mmm$, 44: mmm , $\bar{4}2m$, $\bar{4}3m$, 8: $\bar{8}2m$, $m\bar{3}m$. **9-acra.** 111111111: 1 , 1111122: m , 1112222: m , 122222: 2 , m , $mm2$, 1224: $mm2$, 144: $mm2$, $4mm$, 18: $8mm$, 27: $\bar{14}m2$, 333: 3 , $3m$, 36: $3m$, $\bar{6}m2$. The data have been used to calculate the entropy H_S (Fig. 2).

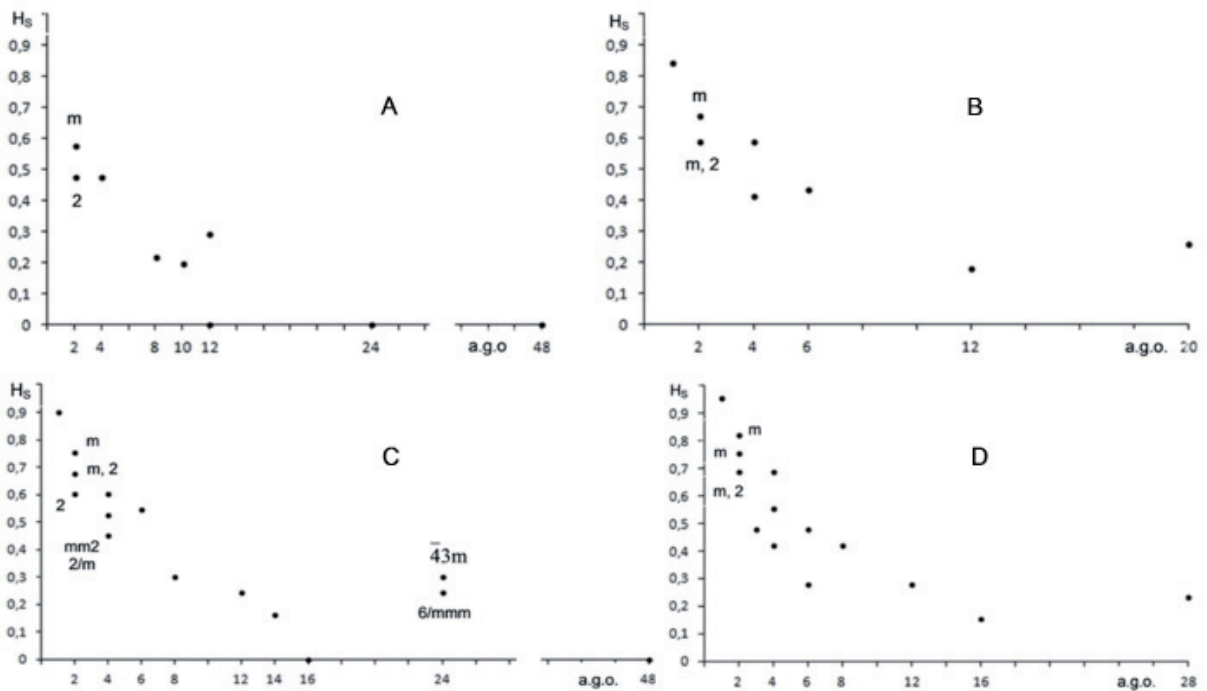


Figure 2. Entropy H_S of convex 4- to 6-acra (A, 10 in total), 7-acra (B, 34), 8-acra (C, 257), and 9-acra (D, 2606) vs. a.g.o. The s.p.g.'s are given to the dots if they do not follow from the Table 1.

The entropy H_S shows the general trend: the higher a.g.o., the lower H_S . But, there are a lot of local exceptions. The two 5-acra contradict to the trend. Some n-acra with the same a.g.o.'s (and even s.p.g.'s) have different H_S , while some n-acra with the same H_S have different s.p.g.'s (and even a.g.o.'s). Moreover, some n-acra with higher a.g.o.'s also have higher H_S . For given n, an equation $H_S = const$ is solvable over the p_1, \dots, p_n , if and only if $const = 0$ or $\lg n$. For the case $0 < const < \lg n$, it is not (*i.e.*, infinitely many points lie on the isoline $H = const$, see Fig. 1). In a discrete case, there is a finite number of probabilistic distributions $p_i = n_i / n$ for given n, and, therefore, a finite number of H_S values, which can be calculated in advance. In this case, for given H_S , related probabilities can be found. It is impossible, if n is not fixed. For example, the probabilities (3/6, 3/6)

for a 6-acron and (4/8, 4/8) for an 8-acron give the same H_S . For given n , the same H_S values are possible for n -acra with different s.p.g.'s and even a.g.o.'s mainly depending on whether the vertices lie on the planes and / or axes of symmetry.

4. Entropy H_V of convex n -acra

It seems that the entropy H_S characterizes a 'disorder' more than a 'complexity' of n -acra. The first parameter is quite well characterized by s.p.g.'s. From this point of view, combinatorially asymmetric n -acra are maximum disordered, while n -acra with $H_S = 0$ are maximum ordered. At the same time, there are n -acra with the same s.p.g.'s, but vertices of different valences. We presume them to be of different complexity, which is not fixed by H_S . To distinguish between them, we suggest the entropy H_V considering different valences 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 (Voytekhovskiy, 2016, Fig. 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 Figs in Voytekhovskiy & Stepenshchikov, 2008). 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 .

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 (Voytekhovskiy & Stepenshchikov, 2008) 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 prism). **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: $3m$, 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 (Fig. 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.

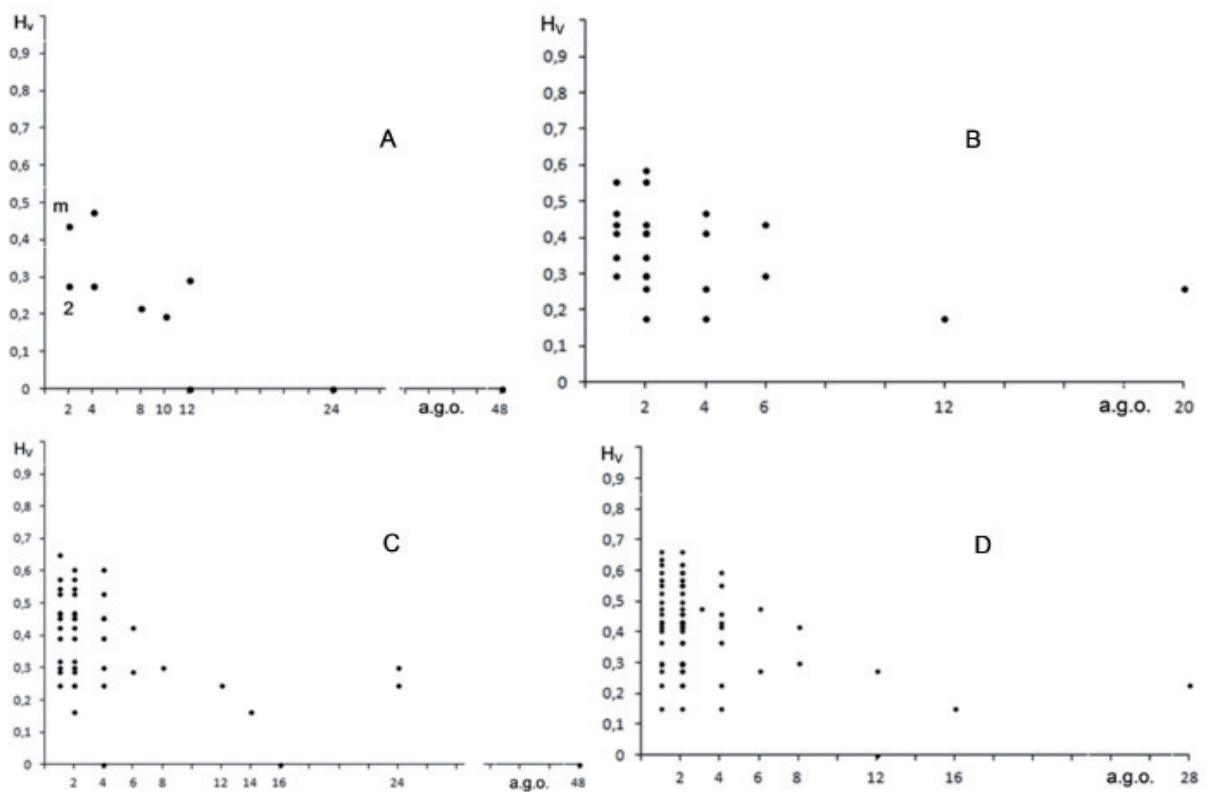


Figure 3. Entropy H_V for the same classes of convex n -acra as in Fig. 2.

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 (Tabl. 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. $H_S = H_V$ if so, $H_S > H_V$ if not. In the latter case, decrease in the variety of valences is resulted in reduction of H_V (if compared with H_S) in accordance with the general properties of the entropy H .

Table 2. Relationships between H_S and H_V for convex 4- to 9-acra. Note: $>$ means $H_S > H_V$ for all n-acra in the class; $=$ means $H_S = H_V$ for all n-acra in the class; \geq means both types of n-acra are in the class.

п.г.а.	т.г.с.	V		4		5		6		7					8						9																			
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28	$\bar{14}m2$																																							
48	$m\bar{3}m$																																							

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 ... q ... (H_1) → ... p-1 ... q+1 ... (H_2), where $1 \leq p \leq q$. **5-acra.** 23 (0,292) → 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) → 123 (0,439) → 24 (0,276) →

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 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 $q = p$, *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 .

Statement 2. Entropy H_v never reaches maximum $\lg n$.

Proof. We should prove that there are no n -acra with all vertices of different valences. Actually, even more strict statement takes place: any convex n -acron has at least 4, or 3 and 2, or 3 pairs of vertices of the same valences.

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, Fig. 4 a). 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. (Fig. 4 b).

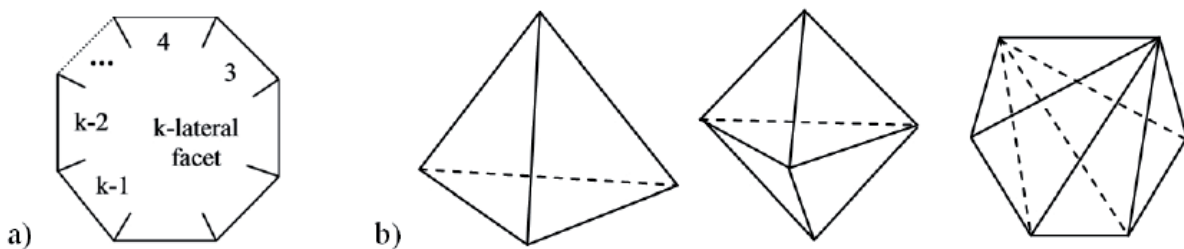


Figure 4. a) The Schlegel diagram on a k -lateral facet. b) The limit convex 4-, 5-, and 6-acra. See text.

6. Conclusions

It follows from general considerations that the topological entropy H_S is hardly interpreted in initial terms (in our case, a.g.o.'s and s.p.g.'s of convex n -acra even for given n). The H_S value fixes any n -acron on a scale between $H_{S,\min} = 0$ and $H_{S,\max} = \lg n$. But, small changes of the probabilities p_i at the corners of a field of definition (Fig. 1) affect big changes of H_S , while the same changes of p_i in the central part of the field of definition do not affect H_S that much. $H_{S,\max} = \lg n$ is attained by, for example, combinatorially asymmetric convex n -acra (for $n \geq 7$). $H_{\min} = 0$ is attained by, for example, regular and semi-regular n -acra (all the cases are enumerated) as well as the infinite series of prisms and antiprisms (for even $n \geq 4$). Between the two bounds, the entropy H_S of convex 4- to 9-acra shows a general trend: the higher a.g.o., the lower H_S . But, there are a lot of exceptions. For given n , the $0 < H_S < \lg n$ values do not allow us to know a.g.o.'s (the more so s.p.g.'s) of n -acra.

The entropy H_s characterizes a ‘disorder’ rather than a ‘complexity’ of convex n-acra. The first one is 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.

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ETUDES ON CONVEX POLYHEDRA. 6. CONVEX 0-POLYHEDRA

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Abstract

New tools to describe a convex polyhedron and their links to the recent theory of crystal morphology are discussed in the paper. Zero-polyhedra, *i.e.* those with a 0 determinant of adjacency matrices of edge graphs, are found to prevail among convex