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Symmetric molecules under extreme conditions. The minimum Shannon entropy hypothesis in predicting probable structures

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Abstract. More and more chemical substances become an object of chemical research. This list include molecules formed and/or existing under extreme conditions (unusual pressures, irradiations, encapsulation etc.). Molecules with symmetric structure in such conditions often dominate over their non-symmetric isomers or related species. To discriminate symmetric and, hence, more probable chemical structures, Shannon entropy is used as a structural descriptor in mathematical chemistry. In this essay, we hypothesise about high probability formation of symmetric molecules with low Shannon entropies and exemplify the considerations with cases from fullerenes, oxygen allotropes, and aromatic hydrocarbon radicals, whereby Shannon entropy combines the roles of structural and stochastic descriptors.

1 Introduction

There is a regular situation in chemical research when organic chemist in one synthesis produces several isomeric compounds with different yields. Then the latter must be rationalised in terms of conventional approaches of physical chemistry. For this purpose, the total energies of the isomers are computed and compared, and usually they correlate with the yields: the lower energy, the higher yield in the chemical process. This is how the *minimum energy principle* works in chemical practice in the simplest mode. It is generally equivalent to the calculation and comparison of heat effects of the alternative reaction paths [1]. Despite some simplicity, this mode works also well for predicting ratios of the isomers formed in complex natural environments, *e.g.* interstellar medium [2–4]. Using this principle, we keep in mind that, being a restatement of the second law of thermodynamics, it works strictly for closed thermodynamic systems. Thus, guiding with an analogy, we treat molecular ensembles as the closed ones (or separated molecules are considered as isolated systems).

There is a number of cases to be reckoned with, when the abovementioned simple approach fails. Then one needs to scrutinise reaction mechanisms, compute and assess activation parameters for the alternative outcomes of chemical reactions under study (to name a few, refs [5–8]). Both their thermodynamic and kinetic parameters are addressed to modern quantum chemical methods for their *a priori* assessment [9–13].

However, no one must forget that real chemical reactions are more complex than their idealised models used in physical organic chemistry. If the last ones do not explain the observed reaction products and/or their yields, it becomes necessary to account other features of real chemical processes—the flows and external impacts (solvation and aggregation effects, pressure, irradiations, external electric fields etc.). When most factors are accounted in the detailed models, we leave the applicability area of the minimum energy principle meeting open systems, but let us return to the area.

Even considering some simple cases, it is difficult to reconcile theory and experiment when sometimes we observe thermodynamically unfavourable isomers. The reason may lie on surface and deal with lower stability of the thermodynamically favoured reaction products toward the further chemical transformations. Indeed, it is regularly expected that the favoured chemical structure correspond to the deep minimum of the potential energy surface (PES), *i.e.* moving on the surface from this minimum in any direction requires overcoming high activation barriers. However, there are cases when further conversions of the formed thermodynamically favourable product are associated with lower energy barriers as compared with unfavourable compounds, also formed in the chemical reaction. If the mentioned transformation is very fast, the experimentalist detects only the unfavourable product, but it is still possible to isolate and separately study alternative products of a chemical reaction (*e.g.* in low-temperature experiments; as an example, we mention the works from our experience on the reaction of fullerene C_{70} with ozone [14–16]). Computationally, the depicted issue may be resolved if considering most of the possible paths of product degradation.

What should chemists do to predict most probable structures without complicating the reaction model? A common practice includes assessing the reactivity and stability of the synthesised molecules in addition to their

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formation thermodynamics. This mode utilises global reactivity indices, *e.g.* HOMO–LUMO gaps, charge separation, hardness, and polarizability [17–21]. In the last case, the *minimum polarizability principle* was formulated. It states that thermodynamic stability in the isomeric series correlates with mean polarizability of the molecules [22]. In contrast to its fundamental sibling, the minimum-polarizability principle has a quality of correlation and may be violated [23–26]. Nevertheless, it was used for analysing various chemical compounds [24, 27–31] and demonstrated high efficiency in the (astro)chemistry of fullerenes, polycyclic aromatic hydrocarbons and organic compounds, whereby it assisted in rationalising the reaction outcomes harder understandable in terms of thermodynamics [24,31–33].

Going further in complementing energy with considerations of other parameters, we come to the proposition: can we break away from physical-chemical parameters and use only structural descriptors? We mean here those ones, which are calculated based on the topology of the molecules, *i.e.* they are deduced from the corresponding molecular graphs and quantitatively assess the presence of cycles, branching, molecular size, symmetry *etc*. [34–38]. Topological descriptors allow discriminating most stable isomers from the large sets of isomeric fullerenes [39–49]. The approaches utilising Shannon entropy (information entropy) as a structural descriptor well reflect molecular symmetry and other topological features of molecules and other chemical objects [50–73]. Shannon entropy and derived values are promising for automated classifications of molecules [35, 51, 54, 56, 57], solids [58–63], and chemical reactions [37, 64–68]. Furthermore, their relevance to physicochemical properties and processes is regularly discussed [55, 57, 59, 67, 69–71].

Previously, we applied Shannon entropy to fullerenes [72] and carbon allotropes [73] to computational separating synthesisable structures from the entire sets of the possible ones. In the present work, we discuss those results and some current calculations in the context of state-of-art experimental and theoretical works. We focus on the relevance of the title descriptor to chemical structures, which formation is hardly rationalised only in terms of energy.

2 Basic definitions and remarks

The detailed protocols for calculating Shannon entropy of chemical objects could be found in previous tutorial review [65]. Here we just highlight the key points. To be treated within this approach, the molecule is represented as a *molecular graph*, which vertices and edges correspond respectively to the atoms and chemical bonds of the molecule. In other words, the molecule is presented as the set of vertices and edges. Additionally, the vertices of this graph must be coloured depending on the type of chemical element. Further, theoreticians may operate with all of them or preferably only with the vertices or bonds. However, both—connectivity of the vertices and their elemental attributions—are necessary for elucidating the inequivalent vertices of the graph. When we perform such a sortation, we obtain the molecule divided into non-intersecting subsets of the vertices, which are also called *atom types* in structural chemistry. Inside the subset, the vertices are equivalent and correspond to the equivalent atoms or reaction sites of the molecule. In crystallography, when solid (its elementary cell) is similarly treated, it is said that the equivalent vertices form the orbit [74]. In general case, the vertices within one subset are connected with the same symmetry operations, *i.e.* the reflections about the symmetry planes/centres and rotations around the symmetry axes translates vertices of one atomic type into themselves [74].

The Shannon entropy (h) of N-atomic molecule is calculated as:

$$h = -\sum_{j=1}^{n} \frac{N_j}{N} \log_2 \frac{N_j}{N} \qquad (1)$$

where n is the number of atom types (orbits) in the molecule and N_j are their populations, herewith $\sum_{j=1}^{n} \frac{N_j}{N} = 1$. Equation (1) allows expressing the Shannon entropy of the molecule in bit atom^{-1}.

The relevance of Shannon entropy to the point symmetry of the molecules was discussed previously in general and in the context of the selected classes of carbon-rich compounds [51–55, 72]. Higher symmetries of the molecules are associated with lower Shannon entropies. Indeed, the highly symmetric molecules are divided into a fewer number of atom types, which have higher populations as compared with the case of the low-symmetry molecules [51]. These factors (low n and large N_j) decrease resulting h values according to Equation (1). Obviously, for reasonable comparison, Shannon entropy should be applied to the related compounds. Thus, the correlations of h with rotational symmetry number (σ) were obtained for some classes of fullerene oligomers and polycyclic aromatic hydrocarbons [52, 53, 72]. The molecules with the same point symmetries may differ in h values due to the differences in other aspects of their chemical structure.

In cheminformatics, Shannon entropy plays a role of a structural descriptor describing the topological complexity of the molecule [34, 50]. Symmetric species within the present approach are accordingly considered simple and *vice versa*: diminishing symmetry increases h values and marks the molecules as complex [65]. It is noteworthy that complexity is a fuzzy concept in natural sciences and elsewhere [75], and molecular complexity, being its special case, inherits in this fuzziness. It means that in other approaches for assessing molecular complexity (*e.g.* the concept of algorithmic complexity), the situation may be turned over that makes symmetric molecules indicated as complex [50, 76].

Shannon entropy should not be confused with thermodynamic one, though they are often compared ([70] and refs therein). The h values characterise structural complexity, whereas the thermodynamic entropy is the function of the state of matter composed as the sum of translational, rotational, and vibrational contributions. These quantities are symbate in series of isomeric and related compounds and antibate with the rotational symmetry number [67, 72].

3 Shannon entropy of the selected classes of molecules

3.1 Fullerenes

Fullerenes are the polyhedral molecules constructed with carbon atoms, which form condensed 5- and 6-membered cycles [76]. Nowadays, they are rigorously studied both in fundamental and applied aspects. Numerous fullerene derivatives have been synthesised by the moment and the mechanisms of the reactions underlying these syntheses have been revealed [77, 78].

However, the formation mechanism of fullerenes themselves is known in a lapidary manner and still have blind spots. For example, the most known fullerene formation mechanism has been proposed and developed in the works of Irle and Morokuma [79, 80] (there are other mechanistic studies on fullerene, which we do not consider because they relate to specific experimental conditions or many pre-computational assumptions, see refs [81, 82] as examples). It has been theoretically justified with the molecular dynamics simulations elucidating the key steps of assembling fullerenes under the conditions of arc-discharge fullerene synthesis (>2000 °C, helium atmosphere). The mechanism includes (*i*) the destruction of graphite that leads to the formation of the C_2 molecules; (*ii*) their nucleation resulting in the ring condensation with energetic preference of pentagons and hexagons; (*iii*) arising curvature, especially in the regions with pentagons condensed with the surrounded hexagons; and (*iv*) cage closure. However, the molecular dynamics simulations from refs [79, 80] reveal the formation of giant fullerenes–not most abundant C_{60} and C_{70}. The latter's formation was guessed due to top-down processes of shrinking giant fullerenes and later computationally confirmed [83]. The research on revealing the details of the mentioned mechanism and its alternatives are continued [84–90]. Anyway, molecular dynamics does not see the C_{60} and C_{70} molecules abundant and they still need to "be looked for" among the simulation products.

The relevant thermodynamic data, both experimental and computational, do not throw the light. Indeed, the heats of formation and total energies indicate the C_{70} fullerene as thermodynamically more stable and, hence, more preferable than C_{60} (Table 1) but in arc-discharge syntheses, it is not the major fullerene product and accompanies C_{60} with the C_{60}:C_{70} ratio varied from 50:1 to 5:1 [91–93].

Table 1. Thermodynamic and Shannon-entropy properties of the two most abundant fullerenes*

Fullerene	$\Delta_f H°$ (kcal mol^{-1})	$\Delta(E/n)$ (kcal mol^{-1})	h (bit atom^{-1})
C_{60} (I_h)	604.68±3.11	–17.33	0.000
C_{70} (D_{5h})	612.9±5.50	–18.18	2.236

* The $\Delta_f H°$ are heats (enthalpies) of formation that were calorimetrically measured in [94]. The values denote the total energies per atom of the fullerene molecules relative to C_{20}, the most unstable fullerene; $\Delta(E/n) = E(C_n)/n - E(C_{20})/20$; these estimates were computationally obtained with reliable DFT method PBE/3ζ [95]. Hereinafter, the Shannon entropies (h) were calculated according to Equation (1).

Quantum chemistry allows restoring the whole picture on the total energies as a function of the fullerene size. As we previously found with the reliable density-functional theory method (DFT) [95], this parameter descends approaching to the total energy per atom of graphite monolayer. When constructing the mentioned dependence, we analysed 2486 fullerene molecules and hoped finding some extrema corresponding to C_{60} and C_{70}. And we did not succeed (Figure 1) (note that minimum energy principle well works within the isomeric fullerene series [96]).

Let us now consider only structural features of fullerenes. To describe their complexity, we used the Shannon entropies calculated *via* Equation (1) [72]. The corresponding decompositions of the molecules over the atom types are shown in Figure 2. The C_{60} molecule has one of the highest point symmetries, *viz.* icosahedral I_h, so that all atoms of this molecule are equivalent and its Shannon entropy is zero. Notably, it was found the only zero-*h* molecule among the sorted 2079 fullerene structures. Thus, in terms of the approach, the buckminsterfullerene is the exclusive compound of the whole fullerenes family.

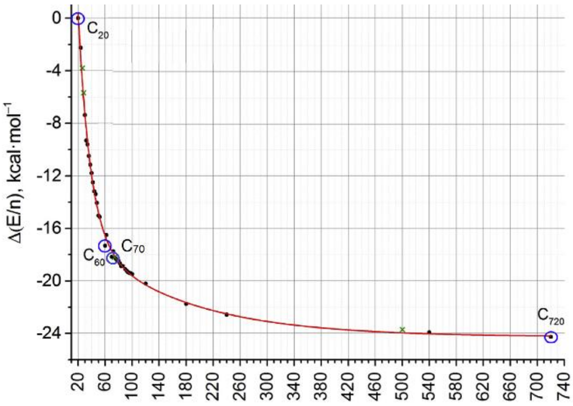

Fig. 1. Relative total energy per atom of fullerenes *vs* fullerene size (number of atoms in the molecule). Points correspond to quantum chemical computations of the lowest-energy fullerene isomers for each *n*. Red line is an approximation fit. Points of thermodynamically most stable and most unstable fullerenes in studied series, C_{20} (C_i or D_{3d}) and C_{720} (I_h), are circled as well as the most abundant C_{60} (I_h) and C_{70} (D_{5h}). Taken from ref [95] © 2018 Elsevier.

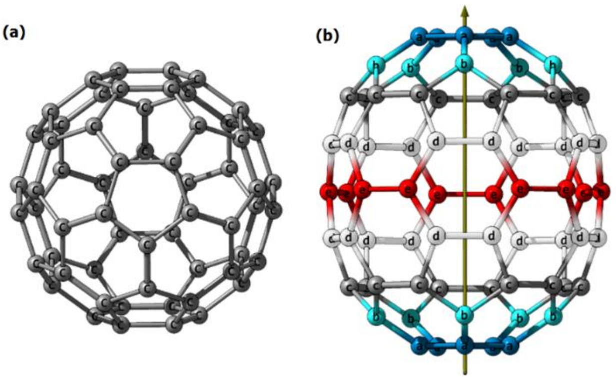

Fig. 2. Fullerenes (*a*) C_{60} and (*b*) C_{70}. Different colours in the C_{70} molecule denote the atoms of different atom types *a*–*e*. Taken from ref [55] © 2024 EDP Sciences.

The C_{70} molecule has lower symmetry D_{5h} and is partitioned over 5 atom types (Figure 2). Its partition formula is 3×10 + 2×20; the substitution of these values into Equation (1) leads to h = 2.236 bit atom^{-1}. This structure is more complex in terms of information-theoretic approach and, therefore, less abundant. Furthermore, only 14 fullerenes have Shannon entropies lying in the range [$h(C_{60})$, $h(C_{70})$]. This is less than 1% of the studied structures [72]. These fullerenes are synthetically achievable. To be honest, the sortation is not perfect because synthesised fullerenes are also presented out of this range. Nevertheless, we assumed that lower Shannon entropy of chemical structure is associated with higher likelihood of its formation.

3.2 Oxygen allotropes

Though oxygen does not possess a variety of allotropic forms, we studied the known all-oxygen molecules in terms of the information-theoretic approach [73]. We operated with the structures that correspond to the PES minima [97] and in addition to the experimental ones (Figure 3). Similar to the fullerene case, we indicated the range between the abundant forms of molecular oxygen, dioxygen O_2 ($D_{\infty h}$) and open isomer of ozone O_3 (C_{2v}) with h values, equal to 0.000 and 0.918 bit atom^{-1}. This range also involved three other structures: (*i*) the cyclic form of ozone O_3 (D_{3h}); (*ii*) chair-like molecule O_6 (D_{3d}); (*iii*) and cubic O_8 (D_{4h}). All of them are synthesised or synthesisable.

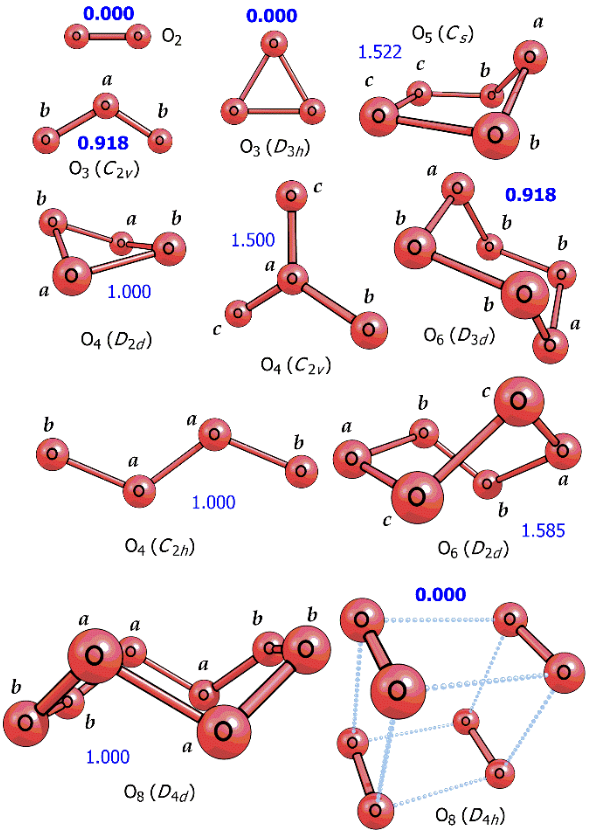

Fig. 3. Oxygen allotropes with their point symmetry groups. Inequivalent atoms are lettered, except the structures with the same atoms. The Shannon entropies (bit atom^{-1}) are shown in bold for the structures having $h \in [h(O_2), h(\text{open } O_3)]$ and plain otherwise. Adopted from ref [73] © 2015 Elsevier.

Octaoxygen O_8 (D_{4h}) clusters were synthesised as building blocks of the high-pressure ε-phase of solid oxygen [98]. Elusive cyclic ozone structure O_3 (D_{3h}) was strongly evidenced in experimental study [99] whereby equilateral triangle O_3 was found centred over the magnesium atoms on the MgO (111) surface annealed above 1450 °C. Quantum chemical studies that justify possible existence of cyclic O_3 have been conducted more than 50 years [100]. We would like to mention here the works focusing on the recommendations about the stabilisation of cyclic O_3: in complexes with metals [101] and water molecules [102], inside the fullerene cages [73, 103, 104], and as isotopologues containing heavy ^{18}O isotopes [105]. Spectroscopic differentiation of the cyclic and open forms of ozone is also computationally scrutinised [106].

Very recently, the evidence for existing O_6 molecules in the hypothetical oxygen-helium compound HeO_3 has been reported (Figure 4) [107]. It is assessed to be stable at ~1.9 TPa according to DFT computations. In this work, the chair-like structure was predicted for hexaoxygen. The theoretical analysis [73] indicates two O_6 isomers, *viz.* twisted O_6 (D_{2d}) and chair-like O_6 (D_{3d}) forms with the respective h values 1.585 and 0.918 bit atom^{-1}. Thus, only the last structure, more symmetric and having lower Shannon entropy, fits within the range between the two most abundant oxygen forms. Note that O_6 (D_{3d}) is also favoured over O_6 (D_{2d}) in terms of energy in 2.58 kcal mol^{-1} (the CCSD/cc-pVTZ computations) [97].

Thus, Shannon entropy acts as a good index for sorting achieved and highly likely achievable all-oxygen structures.

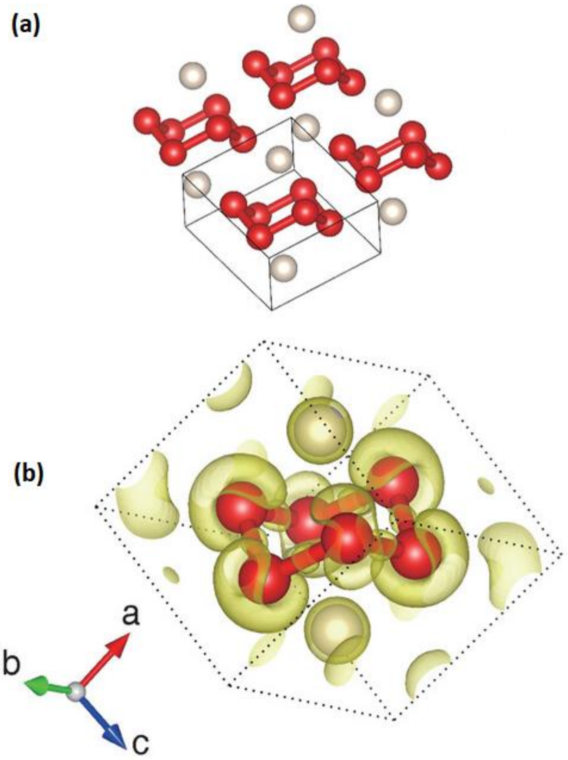

Fig. 4. The modelled crystal structure of HeO_3 (*a*) and the corresponding 3D plot of electronic localization function (*b*). Adopted from ref [104] © 2025 The Authors, Wiley-VCH GmbH; CC BY 4.0 License.

3.3 Aromatic hydrocarbon radicals

Astrochemistry is rapidly developed interdisciplinary field that deduces evolution of complex matter in the universe based on astronomical observations and their analysis with state-of-art physical and spectroscopic techniques [108]. One of the branch of this field deals with the molecules abundant in the interstellar and circumstellar media (molecular clouds, hot cores and corinos, circumstellar envelops *etc.*), and aromatic hydrocarbons and their derivatives are one of most abundant organic compounds in space [109]. Previously [119], we studied molecular complexity of interstellar molecules in terms of Shannon entropy.

According to the Cologne Database for Molecular Spectroscopy (CDMS) [111, 112], the list of the derivatives of hydrocarbons, detected in interstellar media, includes aromatic benzene C_6H_6, indene C_9H_8, naphthalene $C_{10}H_8$, acenaphthylene $C_{12}H_8$, pyrene $C_{16}H_{10}$, coronene $C_{24}H_{12}$, and unsaturated hydrocarbon cyclopentadiene C_5H_6 (see also some original works [113–119]). These molecules are collected in Figure 5 with their symmetries. The latter vary from low C_S for C_5H_6 and C_9H_8 to high D_{6h} for C_6H_6 and $C_{24}H_{12}$. The Shannon entropies in this set vary in the range 1.000…3.970 bit atom^{-1} (Table 2). We highlight that Shannon entropy generally does not depend on molecular size. Indeed, larger hydrocarbons may obtain lower h estimates (*e.g.* compare $C_{16}H_{10}$ *vs* $C_{12}H_8$).

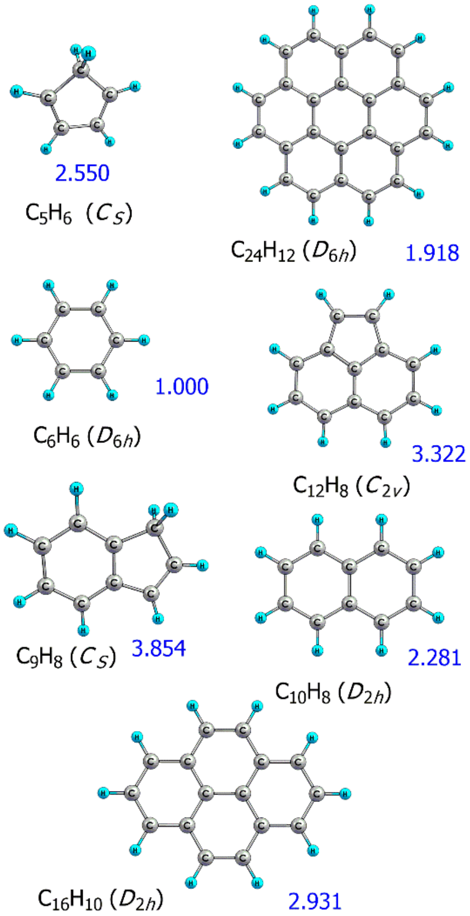

Fig. 5. Aromatic hydrocarbon currently detected in interstellar and circumstellar media as cyano-derivatives [111]. Hereinafter, the h values are shown in bit atom^{-1}.

Table 2. Symmetry, partition and Shannon entropy of the selected hydrocarbons and their radicals

Molecule	Partition over atom types	h (bit atom^{-1})
Hydrocarbons from CDMS [111]		
C_5H_6 (C_S)	1×1 + 5×2	2.550
C_6H_6 (D_{6h})	2×6	1.000
C_9H_8 (C_S)	1×2 + 15×2	3.970
$C_{10}H_8$ (D_{2h})	1×2 + 4×4	2.281
$C_{12}H_8$ (C_{2v})	10×2	3.322
$C_{16}H_{10}$ (D_{2h})	3×2 + 5×4	2.931
$C_{24}H_{12}$ (D_{6h})	2×6 + 2×12	1.918
Hydrocarbon radicals from work [120]		
C_5H_5 (D_{5h})	2×5	1.000
C_9H_7 (C_{2v})	2×1 + 7×2	3.125
$C_{13}H_9$ (D_{3h})	1×1 + 3×3 + 2×6	2.401
$C_{15}H_9$ (C_{2v})	4×1 + 10×2	3.752
$C_{17}H_9$ (C_{2v})	4×1 + 11×2	3.854
$C_{17}H_{11}$ (C_1)	28×1	4.807
$C_{19}H_{11}$ (C_{2v})	4×1 + 13×2	4.040
Helicenes [REFs]		
$C_{18}H_{12}$ (C_2)	15×2	3.907
$C_{22}H_{14}$ (C_2)	18×2	4.170

In the sets made up with the same-symmetry structures, the Shannon entropy increases with the number of atoms in the molecule [72]. In the CDMS set, this tendency is revealed when comparing C_S-, D_{2h}-, and D_{6h}-symmetry hydrocarbons.

We pay attention to recent study [120] explored the stability of different molecules C_nH_m with wide-range varied numbers n and m using the criteria, taken from the theory of the stability of nanoclusters. The favourability of the C_nH_m molecules was ranked using several energetic values that accounted the conversion of the molecules into their far and closest analogues $C_{n\pm k}H_{m\pm l}$ (before such ranking in ref [120], all structures were confirmed as corresponding to the PES minima). Hydrocarbon molecules, which conversion is associated with positive energy descriptors (*i.e.* their conversion requires energy costs), were considered magic and highly probable structures [120]. Surprisingly, in addition to expected hydrocarbons, some aromatic hydrocarbon radicals also titled as magic (Figure 6). It is noteworthy that these structures are mostly symmetric (only $C_{17}H_{11}$ has symmetry C_1). The stability of the radicals is comparable to that of regular hydrocarbons though their molecules bear unpaired electrons. Obviously, high symmetry favours the delocalisation of the unpaired electrons over a high number of the sites and, hence, stabilises the aromatic radical [121–124]. Note that C_9H_7 and $C_{13}H_9$ radicals are detected in Titan's atmosphere [125–127] and $C_{13}H_9$ is known as stable radical with rich chemistry [128].

Shannon entropy reflects the symmetry in the radical set taken from [120]. The h values vary from 1.000 for C_5H_5 (D_{5h}) to 4.807 bit atom^{-1} for $C_{17}H_{11}$ (C_1) (Table 2). Comparing the radicals' estimates with the h-range for CDMS hydrocarbons (1.000…3.970 bit atom^{-1}), we find that only $C_{17}H_{11}$ (C_1) and $C_{16}H_{11}$ (C_{2v}) do not get into. The other aromatic hydrocarbon radicals enter it, so that they may be considered as highly probable structures for interstellar detection.

Another challenge of modern astrochemistry deals with non-planar polycyclic aromatic hydrocarbons. Spiral-shaped molecules of helicenes are such of that (Figure 7). Their molecules are favoured in terms of minimum polarizability principle and disfavoured in terms of energy [24, 31]. In laboratory experiments simulating circumstellar conditions, [4]helicene and [5]helicene were detected as the main products of the reactions between aromatic radicals and vinylacetylene under inert helium atmosphere [129, 130].

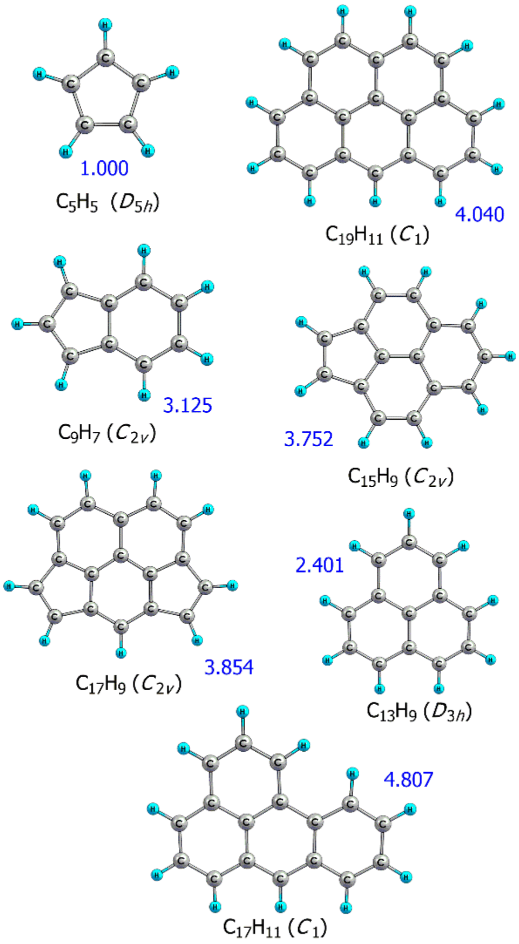

Fig. 6. Hydrocarbon radicals favoured in terms of the approach of work [120].

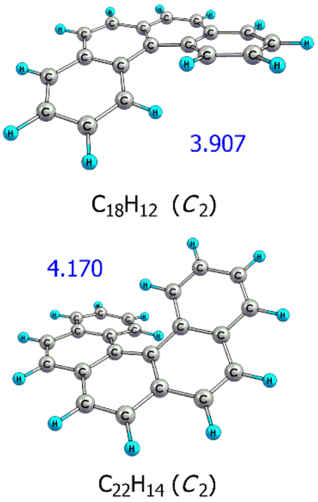

Fig. 7. Two helicenes proposed for detection under interstellar and circumstellar conditions.

Regardless of the size, all helicenes belong to the C_2-symmetry molecules [53]. According to the calculated Shannon entropies of the two mentioned helicenes (Table 2), only [4]helicene is favoured in terms of the approach, as its estimate of the structural complexity, equal to 3.907 bit atom^{-1}, fits into the CDMS aromatic hydrocarbon range (h = 1.000…3.970 bit atom^{-1}).

3.4 Some minor cases

At the end of this section, we mention two minor examples from experimental and computational chemistries. The first one deals with the isomerisation of highly functionalised fullerene fluorides $C_{60}F_{36}$, which formally requires moving one F atom to a neighbouring addition site (Figure 8). The interconversion

$$C_{60}F_{36}\ (C_1) \leftrightarrow C_{60}F_{36}\ (C_3) \tag{2}$$

occurs under their high-temperature synthesis [131] or slowly when stored under ambient atmosphere at room temperatures [132]. Reaction (2) is an isomerisation only formally because its two-stage bimolecular mechanism was computationally justified [133]. Thermodynamically, the C_3 isomer is ~1.67 kcal mol^{-1} more stable than the C_1 one, and the isomers reveal indistinguishably equal mean polarizabilities, 88.8 Å^3 (calculated with DFT method PBE/3ζ [134]). The title approach indicates the favourability of the spontaneous movement of the original molecular system, $C_{60}F_{36}$ (C_1), toward the state with higher symmetry. When converted, the Shannon entropy decreases from 6.585 to 5.000 bit atom^{-1} (see Table 3).

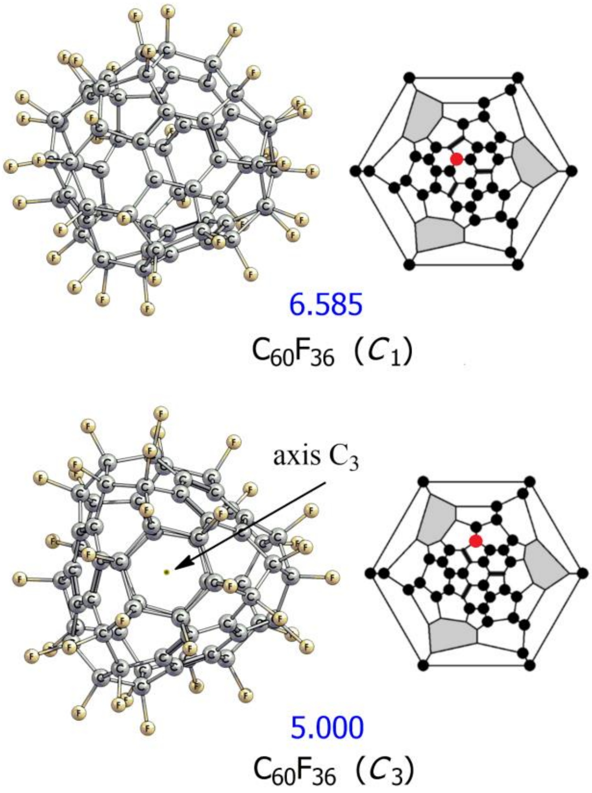

Fig. 8. Two interconvertible isomeric fullerene fluorides $C_{60}F_{36}$ and their Schlegel diagrams showing in red the peripatetic fluorine atom.

Table 3. Symmetry, partition and Shannon entropy of the selected molecules and clusters

Molecule	Partition over atom types	*h* (bit atom^{-1})
Fullerene fluorides		
$C_{60}F_{36}$ (C_1)	96×1	6.585
$C_{60}F_{36}$ (C_3)	32×3	5.000
Boron nanoclusters		
B_{39} (O_h)	1×1 + 1×6 + 1×8 + 1×24	2.585
B_{49} (C_1)	49×1	5.615

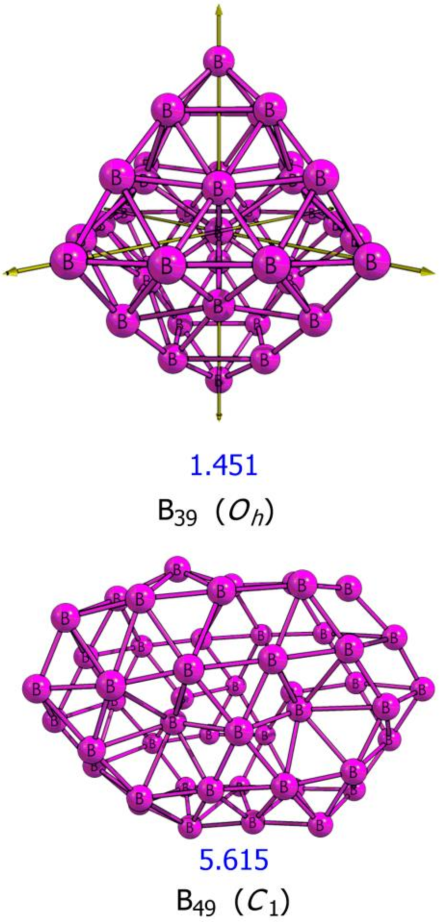

Fig. 9. Two boron nanoclusters B_{39} (O_h) (with the symmetry axes) and B_{49} (C_1).

Mono-element nanoclusters is another case, which could be used for revealing the regularities. In addition to carbon, boron also possesses diverse crystalline and nanosized forms and their theoretical studies are among hot topics of computational nanoscience [135, 136]. In work [136], the authors applied the computational protocols similar to their work on the C_nH_m molecules [120] for selecting magic B_n nanoclusters, which combine the correspondence to the PES minima and stability toward the conversion into the closest analogues. They concluded that the symmetry of magic structures is generally higher than that of the ordinary neighbours.

Just as a final example in this essay, we compare two magic boron nanoclusters B_{39} (O_h) and B_{49} (C_1) as the extreme cases of possible symmetries (Figure 9). The first cluster belongs to one of the highest symmetry point groups and therefore obtains lower Shannon entropy as compared with the second one having no symmetry elements (Table 3). Both nanoclusters are open-shell, *i.e.* they bear the odd numbers of electrons. Thermodynamically, B_{49} (C_1) is more stable than B_{39} (O_h): their total energies equal respectively –674.727 and –674.735 a.u. per atom. However, the fragmentation energies and second energy difference (the discrete analogue of the second derivative of the energy) of these nanoclusters indicate the favourability of the high-symmetry structure: compare these values 2.046 and 7.551 eV for B_{39} (O_h); and 0.181 and 6.235 eV for B_{49} (C_1) (the above energy values are performed with DFT method PBE0/Def2-TZVPP [136]). Thus, Shannon entropy reaffirms the symmetric structure, which is favoured in terms of several energy parameters (contrasting only with the thermodynamic stability).

4 Discussion

4.1 Formulation of the hypothesis

We demonstrated the favourability of symmetric molecules formed in specific conditions, unusual for typical laboratory chemistry. We do not pretend on the generality of our conclusions and this favourability should be treated as a tendency, which may be violated. In our works, Shannon entropy is used to estimate the symmetry of the molecules. For deeper understanding the relations between this structural descriptor and symmetry features, we refer the readers to our previous works scrutinising this aspect [51–53, 65, 72]. Here, it is necessary to keep in mind that different molecules may belong to the same symmetry point-group [65]. When treating the molecules within the information-theoretic approach, the symmetry operations fade into background—their result becomes crucial: the partition of the atoms of the molecule over the atom types. The larger symmetry of the molecule, the lower number of the atom types and higher their populations [51]. Commonly, the related molecules with the same structural pattern and different size exhibit the same symmetry but different Shannon entropy [72]. Thus, the latter is more suitable for distinguishing the molecules that the symmetry itself.

The higher molecular symmetry, the lower Shannon entropy of the molecule. The last criterion may be used for discriminating most probable chemical structures. The idea is quite simple and include two steps: (*i*) calculating the range of *h* values typical for the synthesised structures and (*ii*) selecting chemical structures possessing the Shannon entropies fitting into the range. Based on the examples above, we see that it appropriately works and, therefore, we hypothesise that *the molecules with low Shannon entropies are formed with high probability under extreme conditions*.

4.2 The physical interpretation

The structure, scilicet the partition over atom types, of low-*h* molecules is more homogeneous as compared with their high-*h* counterparts. Thus, under extremal syntheses and conditions, the molecules with more uniform chemical structure are preferably formed. Let us try to depict the reasons for this.

Under high pressures, temperatures or irradiations, the electrons in atoms and molecules occupy higher levels [137, 138], so that the systems become electronically excited. These high levels may be degenerated, so that electrons populating them are "indistinguishable"—in contrast to the ground state. The electron density is being uniformed that makes the reaction sites exposing the same reactivity, instead of diversified one as in the ground state. Further, the atoms in very close states assumedly conserve the uniformity and "harden" in a symmetric structure.

The above proposition does not seem crazy in the context of the phenomenon of plasma crystals [139–147]. Complex plasmas may naturally self-organise themselves into stable ordered structures, *e.g.* concentric spheres [142–144], layered clusters [145, 146], tubes or helices [147]. Fullerenes, our first example of this work, are synthesised under plasma conditions regardless of the mode of its generation [148]. As the mechanism of their formation is still under discussion, its alternatives are proposed. For example, the concept of plasma crystal is invoked for such alternative [149]. Indeed, in the macroscopic model systems, the stabilised multi-shell clusters occur in plasma, *viz.* concentric spheres or multi-shell polyhedral ensembles (Figure 10). In the context of the fullerene formation, this aspect is interesting because the fullerene synthesis is always accompanied with the formation of carbon nano-onions [150], a class of carbon allotropes, which structure is made up with concentric fullerene cages composed in a Russian-doll manner [47, 151–153]. Herewith, the parts of carbon nano-onion are the polyhedra differing in size, but having the same symmetry and structural pattern, *e.g.* all cages of nano-onion $C_{60}@C_{240}@C_{540}$ keep the I_h symmetry. It is assumed that similar self-assembling the symmetric structures at the atomic level precedes the formation of other abovementioned species.

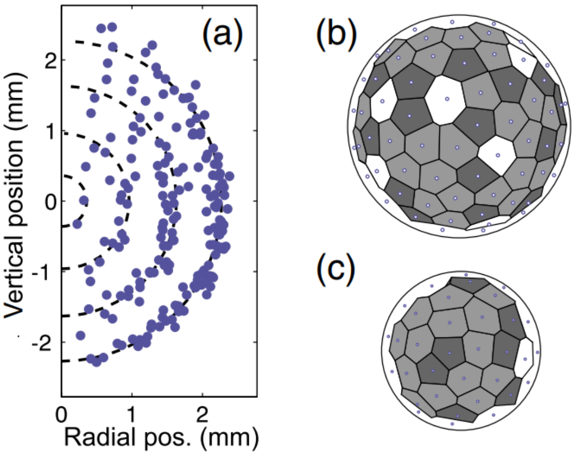

Fig. 10. A 190-particle cluster. (*a*) Its shell structure is disclosed by projecting all particles into the (ρ,z)-plane irrespective of their angular position with regard to the z axis. (*b*) Bottom view of Coulomb ball shows the arrangement of the particles (small circles) in the shells $M = 4$ and (*c*) $M = 3$ superimposed by the Voronoi cell analysis. Hexagons are shaded light grey and pentagon dark grey. Taken from ref [142] © 2004 American Physical Society.

If we accept the above considerations, we may say that extremal conditions convert atoms to such uniform states, in which they expose almost the same reactivity, or in other words, this uniformity is a response of matter to extremal conditions.

4.3 The probabilistic interpretation

Shannon entropy (as its thermodynamic analogue) has a probabilistic interpretation [154]. This feature is used in studies on physical [155] and physicochemical processes [156]. In these applications, Equation (2) treats N_j/N as the probability of the j-th outcome of the event in a system, or probability of its j-th state [70]. When the number of outcomes is low or the some of those are highly probable, the Shannon entropy goes down indicating the decrease in the uncertainty in the system. Such systems are then considered as highly probable and ordered: a smaller Shannon entropy associated with a higher likelihood of the state of the system was previously postulated for physical [155, 156] but rarely invoked in chemistry. However, this physical interpretation seems transferrable to our molecular cases.

If we accept this interpretation, the question arises about the probabilistic nature of chemical processes, which are usually ruled with thermodynamic and activation energy considerations (Figure 11). It seems that there is a range of conditions, in which energy considerations cease to be decisive. Such conditions arise when the reacting atoms or molecules obtain the energies much higher than the activation barriers of the competing reaction paths. In other words, the molecular system has more than enough energy to overcome any activation barrier. At the first glance, this situation must result in the equiprobable formation of the products of both reaction paths. However, we hypothesise that in the described uncertain situation, the molecular system move toward the more ordered state, which is not obligatorily associated with the lower activation barrier.

Thus, we hypothesise about the tendency of molecular systems to diminishing the Shannon entropy, in the extreme case. There is trivial solution for such minimisation that correspond to the case of the ensemble composed only by the atoms [68], *i.e.* containing no chemical structures. Obviously, other solutions are more important for solving the problem of finding probable chemical species.

4.4 The information-theoretic interpretation

In our works, we treat Shannon (information) entropy mostly as a structural descriptor (see reviews [65, 70]). This universal value has several interpretations including original one [157]. The latter is contextualised in mathematical chemistry in terms of information processing, as Equation (1) provides (*i*) the lower bound of the resources required for coding the structure of the molecule; and (*ii*) the upper bound of the information, which can be coded by the considered molecule (these estimates imply distinguishing the inequivalent atoms in the molecule) [65].

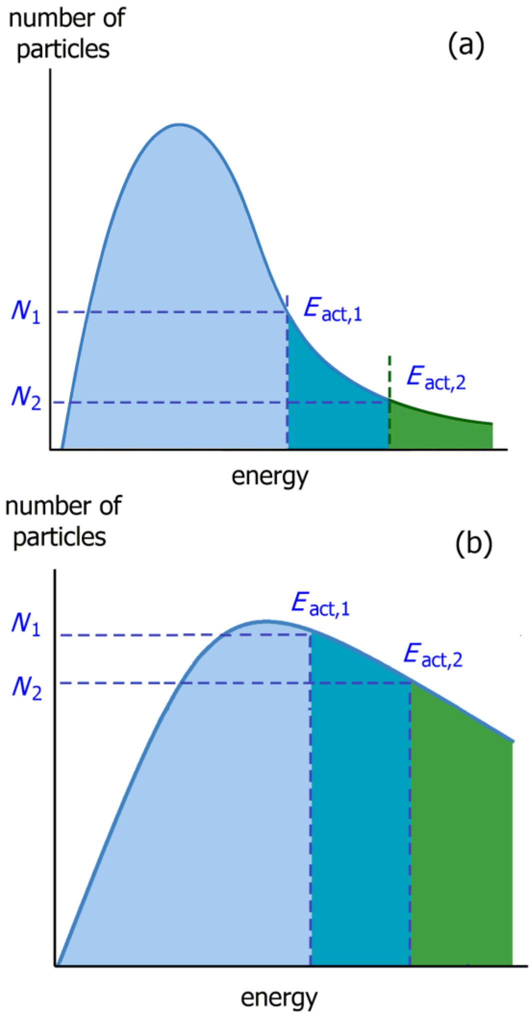

Fig. 11. The energy *vs* number of particles profile of a molecular system, in which two reactions with activation energies $E_{act,1} < E_{act,2}$ proceed. The corresponding number of the molecules with energies $E \geq E_{act,i}$ are designated as N_i. (*a*) Under the standard conditions $N_1 > N_2$ and reaction 1 is therefore more probable. (*b*) The molecules bear the energy excess, so that N_i are increased as compared with the first case and $N_1 \sim N_2$. Colour codes of the reaction probability in the profile: purple—none of the reactions, turquoise—only reaction 1, green—both reactions.

In this aspect, we just mention novel philosophical modes considering traditional objects of natural science through the prism of quantum mechanics, information processing, recursivity and contingency [158–163]. Some of them consider information as an independent manifestation of objective reality, which is not reducible to energy and matter. We are cautious with such approaches, so as not to engage in unnecessary speculations. Nevertheless, we would like to point the following.

In a very general manner, matter is interpreted as the way of embodying information [164–166]. Some investigators go further and match these two concepts [166]. We deduce from these works the necessity of revealing the regularities of information evolution—these are currently poorly elaborated. Nevertheless, the related themes of symmetry—information relations are used in crystallography for structural classifications and phase transition studies [58–63, 167, 168].

5 Conclusion

We have studied different chemical structures to reveal the preference of low-Shannon entropy species, which indicate the high symmetry. These molecules usually dominate over their low-symmetry analogues under extreme conditions (unusual pressures, irradiations, encapsulation etc.). The chemical structures of the symmetric molecules consist of the non-numerous highly populated groups of equivalent atoms (atom types), and this uniformity often plays the role of stabilising factor. Additionally, we tried to make general rationalising the favourability of the symmetric molecules in line with other approaches dealing with uncertainties in chemical behaviour of molecular systems, so that Shannon entropy combines the properties of structural and stochastic descriptors.

Once chemistry was defined as a science about the structural organisation of matter, which really exists in $1\times10^{\pm6}$ days in the temperature and pressure ranges $300\times10^{\pm3}$ K and $1\times10^{\pm3}$ [169]. Currently, chemists go far beyond these limits and discover novel compounds, which previously considered unstable or even exotic. To reveal the diversity of chemical structures at the range of conditions, becoming wider and wider, novel approaches are developed. Among those, we consider the information-theoretic approach in a format of hypothesis as a tool to complement ones, based on energy and molecular parameters.

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