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ON RELATIVE STABILITY REASONING FOR CLUSTERS OF DIFFERENT DIMENSIONS: AN ILLUSTRATION WITH THE C_{60}–C_{70} SYSTEM

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ABSTRACT

It has been shown that at the pressure conditions given by the establishment of equilibrium with graphite, the AM1 and MNDO methods predict that the C_{60} cluster is more highly populated than the C_{70} cluster. This conclusion also remains valid during the lowering of the energy term of C_{70} by slightly more than 400 kJ mol^{-1}. The relations between the cluster populations, pressure, temperature and the different degree of establishment of thermodynamic equilibrium conditions are discussed.

INTRODUCTION

It is about two years since the first observation of the considerable stability of pure carbon clusters C_{60} and C_{70} was reported by Kroto et al. [1]; this has become a topic where experiment and theory overlap. In a group of experimental studies [1–11], progress has been achieved in the determination of indirect structural evidence for these aggregates using lanthanum complexes [2] and, in the case of C_{60}, using UV spectra of its van der Waals' complexes with smaller species [11]. The enormous interest in these aggregates is connected with a number of conceptual problems of cluster chemistry and with the possible applications of these clusters, e.g. their role in interstellar space [1], possible application in catalysis [12] and their magnetic properties [13].

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Although the first theoretical studies on the C_{60} aggregate [14–18] preceded its observation, full-scale theoretical treatments [19–42] were not carried out until after this historical observation [1]. From the large amount of numerical information obtained, the most extensive computational studies are the MNDO [23] and AM1 [41] evaluations of the structures, energetics and vibrations of the clusters C_{60} and C_{70}, which open the way to the construction of partition functions and to thermodynamic considerations.

The observation of ref. 1 has indicated that, even after various numbers of collisions with helium carrier gas, the C_{60} cluster is systematically more highly populated than the C_{70} cluster. However, the straightforward relative stability reasoning for these clusters based on the heat of formation related to one C atom shows [23,41] just the opposite stability sequence; the C_{70} cluster is stabilized relative to the C_{60} cluster by a substantial 4 kJ mol^{-1} atom^{-1}. The prevailing belief in the relative reliability of the semiempirical quantum-chemistry methods used has initiated a more detailed examination of the problem of scales for the evaluation of the relative stabilities of clusters of different dimensions, with particular application to the C_{60}–C_{70} system. This is the subject of this paper.

COMPUTATIONAL OUTLINE

The structural optimizations [41] using the newest quantum-chemical semiempirical method AM1 [43] in the form of a computer program [44] confirmed the earlier conclusions [1,23] about the point groups of symmetry I_h and D_{5h} for the aggregates C_{60} and C_{70}, respectively (see Table 1). At this level, the primary characterization of the relative stability is given by the heat of formation at room temperature. The AM1 study [41] represents the first source of sets of harmonic vibration frequencies for the two carbon aggregates, which enable a reduction from room temperature to absolute zero temperature to be made, i.e. a transition to the heats of formation $\Delta H^{\ominus}_{f,0,60}$ and $\Delta H^{\ominus}_{f,0,70}$. For the following considerations it will be useful to introduce the quotient

$$z = \frac{\Delta H^{\ominus}_{\mathrm{f},0,60}}{60} - \frac{\Delta H^{\ominus}_{\mathrm{f},0,70}}{70} \tag{1}$$

Obviously, in the enthalpy scale, $z > 0$ means greater stability of C_{70}, whereas $z < 0$ means greater stability of C_{60}. From Table 1 it can be seen that the species C_{70} is enthalpy preferred in the AM1 method (i.e. the same conclusion as in the MNDO method [23]).

The knowledge of the structural and vibrational characteristics from the AM1 method enables an evaluation to be made [41] of the entropy parameters in terms of the rigid rotor and harmonic oscillator partition functions. Thus we move to the standard Gibbs energy scale in the consideration of

TABLE 1

Survey of AM1 energetics [a] of the $C_{60}(g)$ and $C_{70}(g)$ clusters

Species	Point group of symmetry	$\Delta H^{\ominus}_{f,0,n}$ [b]	$\Delta H^{\ominus}_{f,298,n}$ [b]	z [c]
$C_{60}(g)$	I_h	4087.0	4072.5	3.8168
$C_{70}(g)$	D_{5h}	4500.9	4484.8	

[a] In kJ mol^{-1} or kJ mol^{-1} $atom^{-1}$, according to ref. 41. [b] The heat of formation at 0 K or at room temperature ($n = 60$ or 70). [c] $z = \Delta H^{\ominus}_{f,0,60}/60 - \Delta H^{\ominus}_{f,0,70}/70$, when based on the MNDO $\Delta H^{\ominus}_{f,298,n}$ terms [23,41]; $z = 4.1421$ kJ mol^{-1} $atom^{-1}$.

stability. Nevertheless, it has been shown [41] that in this standard Gibbs energy scale the AM1 method prefers C_{70} to C_{60}. However, it has also been pointed out [37,39] that even the standard Gibbs energy is not fully adequate for the evaluation of the mutual stabilities of the two clusters, because the conventional standard state involved (1 atm pressure) is obviously very different from the real observation conditions.

For a more detailed evaluation of the effect of pressure on the mutual proportions of the C_{60} and C_{70} populations, let us consider a simple model in an ideal gas phase formed only by these two clusters (i.e. until further notice, let us ignore the existence of other $C_n(g)$ clusters (cf. refs. 45–47)). The process

$$C_{60}(I_h;\ g) = \tfrac{6}{7}C_{70}(D_{5h};\ g) \tag{2}$$

is characterized by the equilibrium constant in terms of the equilibrium partial pressures of its components

$$K_p = \frac{p_{70}^{6/7}}{p_{60}} \tag{3}$$

This constant can be evaluated from the AM1 information [41]. If the total pressure of this two-component gas phase is now introduced, p_{60} and p_{70} can be studied as a function of this pressure. In particular, it is also possible to introduce a total pressure $\overline{P}_{60-70}$ at which the two partial pressures p_{60} and p_{70} are equal (and, hence, equal to $\overline{P}_{60-70}/2$); obviously it is

$$\overline{P}_{60-70} = 2K_p^{-7} \tag{4}$$

At every value of total pressure in this gas phase in the interval $(\overline{P}_{60-70};\ \infty)$, the relative population of C_{70} is higher than that of C_{60} (i.e. $p_{70} > p_{60}$). In the pressure interval $(0;\ \overline{P}_{60-70})$ the opposite is true ($p_{60} > p_{70}$).

Out of all the values of the total pressure, a definite value is that of the saturated gas phase formed by C_{60} and C_{70} in equilibrium with graphite (P^{sat}_{60-70}). For its determination it is necessary to consider the heterogeneous equilibria

$$nC(s) = C_n(g)\ (n = 60 \text{ or } 70) \tag{5}$$

whose equilibrium constants are as follows

$$\ln K_{\mathrm{p},n} = \ln p_n^{\mathrm{sat}} = \Delta\Phi^{\ominus}_{\mathrm{f},T,n}/R - \Delta H^{\ominus}_{\mathrm{f},0,n}/R/T \tag{6}$$

where $\Delta\Phi^{\ominus}_{\mathrm{f},T,n}$ is the thermodynamic potential of formation of the C_n(g) aggregate, and R and T have their usual meanings. Then it is possible to determine P^{sat}_{60-70}

$$P^{\mathrm{sat}}_{60-70} = p^{\mathrm{sat}}_{60} + p^{\mathrm{sat}}_{70} \tag{7}$$

on the basis of the AM1 description [41] of the C_{60} and C_{70} clusters and the data given for graphite [46].

A saturated vapour represents a physically well-defined, unambiguous situation and hence it is useful in the examination of the problem of the mutual stabilities of the two clusters at these particular conditions. This problem, of course, is solved by calculation of the p^{sat}_{60} and p^{sat}_{70} pressures. However, from a methodical point of view it seems useful to elucidate the limits within which it is possible to vary the energy term without changing the relative stability sequence of the two clusters. For simplicity let us consider that the $\Delta H^{\ominus}_{\mathrm{f},0,60}$ term is fixed and that the $\Delta H^{\ominus}_{\mathrm{f},0,70}$ term is variable, being characterized by the quantity introduced in eqn. (1)

$$\Delta H^{\ominus}_{\mathrm{f},0,70} = \tfrac{7}{6}\Delta H^{\ominus}_{\mathrm{f},0,60} - 70z \tag{8}$$

Let us now look for a threshold value z_{th} at which the partial pressures of the two clusters above graphite are equal ($p^{\mathrm{sat}}_{60} = p^{\mathrm{sat}}_{70}$). Obviously, for every $z > z_{\mathrm{th}}$ the population of C_{70} in the saturated vapour will be higher than that of C_{60}, whereas for every $z < z_{\mathrm{th}}$ the C_{60} population will be higher. The combination of eqns. (1) and (6) gives

$$z_{\mathrm{th}} = \tfrac{1}{70}\left[\tfrac{1}{6}\Delta H^{\ominus}_{\mathrm{f},0,60} + T\left(\Delta\Phi^{\ominus}_{\mathrm{f},T,60} - \Delta\Phi^{\ominus}_{\mathrm{f},T,70}\right)\right] \tag{9}$$

At saturation conditions, i.e. in equilibrium with graphite, the C_{60} cluster will be more highly populated than C_{70} for every $\Delta H^{\ominus}_{\mathrm{f},0,70}$ value from the interval $(\tfrac{7}{6}\Delta H^{\ominus}_{\mathrm{f},0,60} - 70z_{\mathrm{th}};\infty)$. On the other hand, for every $\Delta H^{\ominus}_{\mathrm{f},0,70}$ value from the interval $(-\infty;\tfrac{7}{6}\Delta H^{\circ}_{\mathrm{f},0,60} - 70z_{\mathrm{th}})$ the C_{70} cluster will be more highly populated at saturation conditions.

Finally, it should be noted that, provided the presence of other clusters in the gas phase does not affect the values of the equilibrium constants $K_{\mathrm{p},n}$ from eqn. (6), the above-mentioned conclusions remain valid in the presence of further clusters. If we were interested in the populations of these further clusters, eqn. (6) would also have to be calculated for them. For the presentation of the populations of the individual clusters it is useful to write the expression in terms of their mole fractions

$$x_i = \frac{p_i^{\mathrm{sat}}}{\sum\limits_j p_j^{\mathrm{sat}}} \tag{10}$$

where the summation is carried out over all the clusters considered.

RESULTS AND DISCUSSION

From the above reasoning it is already obvious that the evaluation of the mutual stabilities of clusters represents a relatively subtle problem. Conventionally this evaluation has been made using the potential energy term or, in the case of some semiempirical methods of quantum chemistry, using the heat of formation at room temperature or, even better, at the absolute zero temperature related to a single particle. This procedure has also been applied to the relative stability of the C_{60} and C_{70} clusters. As can be seen from Table 1, using the $\Delta H^{\ominus}_{f,0,n}/n$ scale the C_{70} cluster is stabilized relative to the C_{60} cluster (in the AM1 method) by about 3.82 kJ mol^{-1} $atom^{-1}$ (if the reduction from room temperature to absolute zero based on the AM1 frequencies [41] is used in the case of the MNDO results [23], then this preference of C_{70} is about 4.14 kJ mol^{-1} $atom^{-1}$). A more rigorous approach will also take into account the entropy term, which will enable a transition to be made to the standard Gibbs energy scale.

If isomeric clusters are considered, then the comparison of their stabilities will be correct at this level. If, however, clusters of different dimensions are treated, then a problem arises with the pressure. The relative populations are pressure dependent to such an extent that certain pressure changes can even cause a reversal in the stability sequence. (The finding [41] that the C_{70} cluster continues to be preferred when the standard Gibbs energy related to 1 atom is used is, in itself, insignificant with respect to the interpretation of the observation.) An indication of the pressure at which such reversal takes place in the $C_{60}(g)$–$C_{70}(g)$ system is given by the $\bar{P}_{60-70}$ quantity from Table 2, which shows that this occurs at substantially lower pressures than those chosen for the standard state of the gas phase. Below this $\bar{P}_{60-70}$ pressure limit the C_{60} cluster becomes relatively more stable in accordance with the observation in ref. 1. However, the experiment in ref. 1 provides no quantitative information about the pressure conditions. The evaluation of

TABLE 2

AM1 characterization[a] of C_{60}–C_{70} gas-phase population interplay

T (K)	P^{sat}_{60-70} (atm)	$\bar{P}_{60-70}$ (atm)	z_{th}[b] (kJ mol^{-1} $atom^{-1}$)	
298	1.950×10^{-706}	4.276×10^{-275}	9.672	(9.997)
500	1.175×10^{-418}	3.724×10^{-162}	9.656	(9.981)
1000	4.074×10^{-208}	3.557×10^{-79}	9.680	(10.006)
2000	1.585×10^{-104}	5.508×10^{-38}	9.855	(10.181)
3000	1.084×10^{-70}	1.795×10^{-24}	10.10	(10.421)
4000	3.999×10^{-54}	9.312×10^{-18}	10.39	(10.718)
5000	1.910×10^{-44}	9.121×10^{-14}	10.74	(11.066)

[a] See text for the meaning of P^{sat}_{60-70}, $\bar{P}_{60-70}$ and z_{th}. [b] The value based on the MNDO $\Delta H^{\ominus}_{f,298,60}$ term [23,41] is given in parentheses.

TABLE 3

The mole fractions of the $C_n(g)$ clusters in their equilibrium ideal gas mixture above graphite obtained [a] for the original z value [b] and the threshold values z_{th} [c]

T	x_n(%)						
(K)	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=60$	$n=70$
298	100.0	2.23×10^{-18}	1.34×10^{-13}	9.42×10^{-41}	8.39×10^{-42}	3.91×10^{-587} 3.91×10^{-587}	5.65×10^{-659} 3.91×10^{-587}
500	100.0	1.23×10^{-9}	3.41×10^{-6}	1.19×10^{-22}	4.26×10^{-23}	5.56×10^{-350} 5.56×10^{-350}	1.11×10^{-392} 5.56×10^{-350}
1000	99.4	3.58×10^{-3}	6.24×10^{-1}	2.46×10^{-9}	2.61×10^{-9}	6.42×10^{-177} 6.42×10^{-177}	2.33×10^{-198} 6.42×10^{-177}
2000	43.8	2.11	54.1	3.49×10^{-3}	6.30×10^{-3}	2.08×10^{-92} 2.08×10^{-92}	1.89×10^{-103} 2.08×10^{-92}
3000	15.8	7.29	76.4	1.50×10^{-1}	3.19×10^{-1}	3.16×10^{-65} 3.16×10^{-65}	7.03×10^{-73} 3.16×10^{-65}
4000	9.52	12.7	74.9	8.72×10^{-1}	1.99	5.71×10^{-52} 5.71×10^{-52}	5.57×10^{-58} 5.71×10^{-52}
5000	7.16	17.5	67.4	2.35	5.56	2.94×10^{-44} 2.94×10^{-44}	2.54×10^{-49} 2.94×10^{-44}

[a] Thermodynamic data: $n=1$–5 (ref. 46); $n=60,70$ (AM1 calculations). [b] Upper line for the z value (see Table 1). [c] Lower line for the z_{th} values (see Table 2).

the situation under saturation conditions, i.e. equilibrium with graphite solid phase is rather exceptional (for this purpose, graphite is thermodynamically described by the data of ref. 46). Table 2 (P^{sat}_{60-70}) shows that the pressures at which the heterogeneous equilibrium is established lie substantially lower than the point of reversion $\bar{P}_{60-70}$. (How low these pressures are can be seen when the partial pressures are replaced by the volume concentrations of the particles; for example, the partial pressure of 10^{-22} atm corresponds to 245 particles per 1 m^3 at $T = 3000$ K.) Obviously, although the pressure–temperature conditions of the experiment in ref. 1 are not yet clear, a proper consideration of the pressure factor [37,39] offers a possibility of introducing conformity between theoretical and observed data in spite of the apparent discrepancy shown in Table 1 using the heat of formation.

Table 3 shows that a certain relative proportion of cluster populations with different dimensions is maintained within a relatively wide interval of the energy term. So, for example, at saturation conditions $C_{70}(g)$ is less stable than $C_{60}(g)$ at the temperatures 298 and 3000 K, not only for the original [41] AM1 value $\Delta H^{\ominus}_{f,0,70} = 4501$ kJ mol^{-1}, but also for any value of the interval (4091;∞) and (4061;∞) kJ mol^{-1} respectively. This means that the theory predicts $C_{60}(g)$ to be more stable at saturation conditions even if the energy of C_{70} is decreased by, for example, 400 kJ mol^{-1}. If we consider that the value of 400 kJ mol^{-1} is one order of magnitude greater than the expected possible error [43] of the AM1 method, we can take this prediction of theory to be very reliable.

CONCLUDING REMARKS

This entire computational study is based on the presumption that thermodynamic equilibrium is established to at least a partial degree. No kinetic aspects, for example, rates of cluster growth or decomposition or interconversion of particular clusters, are treated here. From this purely thermodynamic point of view it is possible to differentiate three levels of thermodynamic equilibrium: (i) the establishment of equilibrium between isomers of a particular cluster, (ii) the establishment of (i) and also equilibria between clusters of various dimensions, and (iii) the establishment of (ii) and also equilibrium with the corresponding condensed phase. The application of the nozzle expansion technique has, so far, provided no way of testing the degree of establishment of the equilibria (i)–(iii). It must be expected that, in general, such experiments will be rather far from the conditions of thermodynamic equilibrium (cf., for example, refs. 48–50). However, the basic problems concern not only the degree of thermodynamic equilibrium, but also the kinds of motions which exist in larger clusters and their theoretical description, and the transferability of the results which are valid for the clusters treated as particles in the gas phase into the condensed phase, etc. [48–53].

With regard to the results of this study it can be speculated that the historical experiment [1] effectively succeeded in realizing a rather unique, kinetically convenient mechanism (inclusive of the special, adequate temperature–pressure regime) which led to a considerable production of the C_{60} and C_{70} clusters; however, it is quite possible that the experiment was rather far from the conditions of thermodynamic equilibria (i)–(iii) in all its phases. In particular, it must be noted that after cooling in the nozzle the C_{60} and C_{70} populations formed can be stabilized by convenient kinetic factors (cf. ref. 3) which efficiently prevent the attainment of the respective equilibrium conditions. This fact indicates the necessity for developing a theory of non-equilibrium cluster populations, although this aim appears to be rather distant with respect to the present approaches.

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