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Eu@C₈₈ Isomers: Calculated Relative Populations

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Relative populations of three energy-lowest IPR (isolated-pentagon-rule) isomers of Eu@C₈₈ are computed using the Gibbs energy based on characteristics from density functional theory and MP2 calculations (M06-2X/3-21G~SDD entropy term, and the MP2=FU/6-31G*~SDD or B2PLYPD=FU/6-31 + G*~SDD energetics). The calculations predict coexistence of three isomers, in agreement with extraction using a polar solvent, and offer a possible explanation why the Eu@C₂(27)-C₈₈ species should prevail with a non-polar solvent. Role of extraction solvents and catalysis is thus pointed out.

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Several Eu containing metallofullerenes have been observed¹⁻⁷ and calculated,⁸⁻¹² too. Their newest X-ray structural characterization includes⁵ one Eu@C₈₈ isomer, namely the species with the C₂ symmetry IPR (isolated-pentagon-rule) cage conventionally labeled 27, Eu@C₂(27)-C₈₈, thus further expanding the family of C₈₈ based endohedrals.^{13,14} There are 35 IPR satisfying topologies^{15,16} for the empty C₈₈ cages (observations found only one empty species¹⁵). In this study, the three energy-lowest Eu@C₈₈ isomers, including the observed Eu@C₂(27)-C₈₈ endohedral, are calculated for the first time in order to get a deeper insight into the isomeric system.

Traditionally, stabilities of nanocarbons have frequently been treated only in the terms of the potential energy. However, there are several examples¹⁷⁻²² that the entropic part of the Gibbs energy becomes important at high temperatures to such a degree that a structure which is not the potential-energy lowest can still become the most populated at higher temperatures. Moreover, other structures higher in potential energy can exhibit mutual stability interchanges with increasing temperature. The stability interchanges cannot be concluded just from the potential energies. Thus, stability calculations here are performed on the three IPR-based Eu@C₈₈ isomers, lowest in potential energy, in order to evaluate their relative equilibrium populations at synthetic temperatures consistently using both enthalpy and entropy parts of the Gibbs energy.

Calculations

The initial geometry optimizations were performed in a combined basis set: 3-21G basis²³ for C atoms and SDD basis²⁴ with the SDD effective core potential on Eu (coded here 3-21G~SDD), using density functional theory (DFT) approach, namely the M06-2X functional tested²⁵ as most reliable treatment in numerous situations (i.e., the unrestricted M06-2X/3-21G~SDD treatment). Moreover, the structures were further re-optimized using the standard 6-31G* basis sets²⁶ for C atoms, i.e., the M06-2X/6-31G*~SDD level.

Out of altogether 35 IPR satisfying C₈₈ cage topologies,^{15,16} three species lowest in potential energy were selected, first via calculations on empty dianion cages and then followed with the Eu containing endohedrals (Eu donates about two electrons to the cage). The selection points out three low-energy species: Eu@C_s(32)-C₈₈, Eu@C₁(18)-C₈₈, and Eu@C₂(27)-C₈₈.

Their inter-isomeric energetics was further refined using the advanced second order Møller-Plesset (MP2) perturbation treatment²⁷ with all electrons and the 6-31G*~SDD basis (MP2=FU/6-31G*~SDD) in the optimized M06-2X/6-31G*~SDD geometries. Moreover, a recent combination²⁸ of the DFT and MP2 approaches known as the B2PLYPD method with all electrons and the 6-31 + G*~SDD basis (B2PLYPD=FU/6-31+G*~SDD) was also employed. The spin state of the studied endohedrals is octet.

In the optimized M06-2X/3-21G~SDD geometries, the harmonic vibrational analysis was carried out with the analytical force-constant matrix as input for the vibrational partition function. Moreover, the first ten electronic excitation energies were evaluated by means of the time-dependent (TD) DFT response theory²⁹ at the M06-2X/6-31G*~SDD level, namely for the construction³⁰ of the electronic partition functions. The computations are carried out with the Gaussian 16 program package.³¹

Relative concentrations (mole fractions) x_i of m isomers can be expressed^{32,33} through their partition functions q_i and the enthalpies at the absolute zero temperature $\Delta H_{0,i}^o$ (in other words, the ground-state energies—the relative potential energies corrected for the vibrational zero-point energies) by a compact formula:

$$x_i = \frac{q_i \exp[-\Delta H_{0,i}^o/(RT)]}{\sum_{j=1}^m q_j \exp[-\Delta H_{0,j}^o/(RT)]}, \quad [1]$$

where R is the gas constant and T the absolute temperature. Equation 1 is an exact formula that can be directly derived^{32,33} from the standard Gibbs energies of the isomers, supposing the conditions of the inter-isomeric thermodynamic equilibrium. Rotational-vibrational partition functions are to be constructed using the conventional rigid rotator and harmonic oscillator (RRHO) approximation. No frequency scaling is applied as it is not significant³⁴ for the x_i values at high temperatures. Finally, the chirality contribution³⁵ was included accordingly (for an enantiomeric pair its partition function q_i is doubled). Although the temperature region where fullerene or metallofullerene electric-arc synthesis takes place is not well known, the recent observations³⁶ supply some arguments to expect it around or above 1500 K. Thus, the computed results, produced by the program described elsewhere,³³ are discussed here focusing on the temperature region.³⁶

Actually, a modified^{20,37} RRHO approach for description of the encapsulate motions is in fact considered here, following experimental findings³⁸ from NMR spectra on endohedral symmetries. The observed cage symmetries are actually a result of large amplitude

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motions exhibited by the encapsulated atom(s), especially so at elevated temperatures (unless the motions are restricted by cage derivatizations³⁹). One can expect that if the encapsulate is relatively free then, at sufficiently high temperatures, its behavior in different cages will bring about the same contribution to the partition functions. However, such uniform contributions would then cancel out in Equation 1. This simplification is called^{20,37} free, fluctuating, or floating encapsulate model (FEM) and requires (in the case of a mono-metallofullerene) two steps. In addition to removal of the three lowest vibrational frequencies (belonging to the metal motions in the cage), the symmetries of the cages should be treated as the highest (topologically) possible, which reflects averaging effects of the large amplitude motions. For example, for the Eu@C₂(27)-C₈₈ isomer based on the C₂; 27 IPR cage, C₂ symmetry is employed within the FEM scheme though its static symmetry^{40,41} (i.e., after the geometry optimization) is just C₁. Generally speaking, the FEM treatment gives a better agreement^{20,37} with the available observed data compared to the conventional RRHO approach, and it is therefore also applied here.

Results and Discussion

Table I reports the Eu@C₈₈ isomeric separation energetics computed at the three selected levels (presented are just the differences in the potential energy without the zero-point vibrational energies). The lowest-energy Eu@C₈₈ isomer is the species with the C_s; 32 cage, being rather closely followed by the endohedrals with the C₁; 18 and C₂; 27 cages (Fig. 1). The energetics is relatively similar at the three computational levels considered. The MP2 and B2PLYPD methods are actually the most advanced approaches ever used with metallofullerenes.¹¹ For the two originally symmetric cages, their symmetry is after the geometry optimization reduced to just C₁.

Table II presents some selected computed characteristics for the three energy-lowest Eu@C₈₈ isomers. The calculated closest contacts between Eu and the cages fall within a similar interval of values as found previously¹⁰⁻¹² for other endohedrals encapsulating Eu. The M06-2X/6-31G* ~ SDD computed closest Eu-C contacts are on average longer by some 0.03 Å compared to the M06-2X/3-21G ~ SDD values. The values of lowest vibrational frequencies presented in Table II are in agreement with the generally known nearly-free motions of encapsulates in metallofullerenes (that help to recreate the cage symmetries in the NMR spectra). The M06-2X/3-21G ~ SDD computed Mulliken atomic charges on Eu predict that the metal donates almost exactly two electrons to the cage. The charges fall within a similar narrow interval of values found previously¹⁰⁻¹² with other Eu-encapsulating endohedrals.

The Mulliken-charge calculation at the M06-2X/3-21G ~ SDD level deserves a more general comment. The Mulliken charges from the 3-21G ~ SDD basis, unlike the 6-31G* ~ SDD values, are known⁹ to give a good agreement with the available observed charges⁴³ for metallofullerenes. Moreover, there are also general methodological arguments⁴⁴ why larger basis sets should not be used with the Mulliken charges (as they can produce truly unreasonable values). Interestingly, an approximative analysis⁴⁵ supports⁴⁶ the charges from the 3-21G basis, too. Anyhow, it is not possible⁴⁷ to define uniquely charges on individual atoms—in fact there are

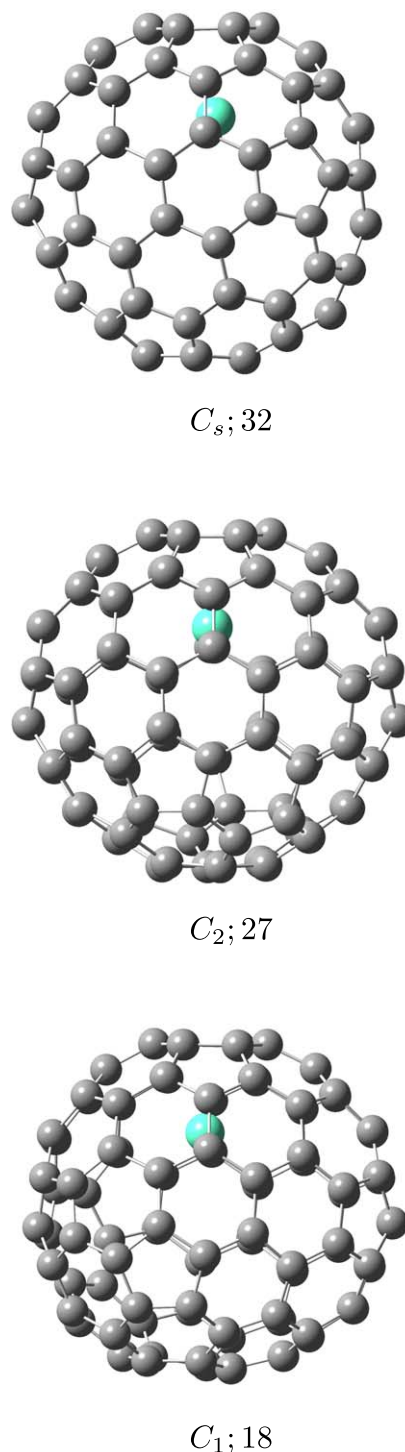


Figure 1. M06-2X/6-31G*~SDD optimized structures of the three lowest-energy Eu@C₈₈ isomers (Eu is always located just below the top ring).

Table I. Eu@C₈₈ relative potential energies $\Delta E_{pot,rel}$ calculated in the M06-2X/6-31G* ~ SDD optimized structures.

Species	$\Delta E_{pot,rel} / \text{kcal.mol}^{-1}$		
	M06-2X/6-31G* ~ SDD	MP2=FU/6-31G* ~ SDD	B2PLYPD=FU/6-31 + G* ~ SDD ^b
C ₂ ; 27 ^a	4.26	3.47	3.85
C ₁ ; 18 ^a	3.23	0.04	1.61
C _s ; 32 ^a	0.0	0.0	0.0

a) See Fig. 1. b) In the B3LYP-D3/6-31G* ~ SDD optimized geometry.⁴²

Table II. The selected characteristics of the Eu@C₈₈ isomers—the closest Eu-C contact^a r_{Eu-C} , the Mulliken charge^b on Eu q_{Eu} , the lowest vibrational frequency^b ω_{low} , and the lowest electronic excited state^c Ω_{low} .

Species	$r_{Eu-C} / \text{\AA}$	q_{Eu}	$\omega_{low} / \text{cm}^{-1}$	$\Omega_{low} / \text{cm}^{-1}$
C ₂ ; 27	2.649/ 2.677	1.977	39.8	11 509
C ₁ ; 18	2.618/ 2.650	1.986	36.3	12 013
C _s ; 32	2.579/ 2.607	1.984	37.1	11 270

a) M06-2X/3-21G~SDD / M06-2X/6-31G*~SDD terms. b) M06-2X/3-21G ~ SDD terms. c) M06-2X/6-31G* ~ SDD terms. d) See Fig. See Fig. 1.

numerous other definitions in addition to the (most common) Mulliken charges and each of them contains an element of arbitrariness. However, it is not really possible to say generally which approach provides the best atomic charges. Each concept offers distinct advantages and each suffers from disadvantages. A unique universal definition which would satisfy all requirements is in fact rather unlikely^{44,47} to be ever constructed. Thus, the choice ultimately rests with a reasonable applicability for a particular situation. With metallofullerenes, it should be rational to apply such calculational treatments that can reasonably well reproduce charge terms derived from observations.

Figure 2 presents the main output of this study—temperature development of the relative concentrations of the three energy-lowest Eu@C₈₈ isomers in a wide temperature region for both

advanced inter-isomeric energetics. Qualitatively speaking, the MP2 and B2PLYPD approaches produce similar pictures for the relative isomeric populations (the B2PLYPD method can be considered²⁸ more advanced and more reliable). Anyhow, the calculations prediction a coexistence of two comparable major isomers and one minor species. However, this is in agreement with the isomeric population observed in the experiments of Shinohara et al.² On the other hand, Lu et al.⁵ isolated and X-ray identified only one species. A reason could be rooted in the used extraction solvents—either dimethylformamide² DMF, generally recommended for metallofullerene extraction,^{2,48,49} or carbon disulfide⁵ CS₂, differing in their polarity^{48,49} (though catalytic effects² (Ni) represent another factor). The solubility^{48,50} of metallofullerenes can be related to their polarity—and polarity to the calculated dipole moments. Incidentally, the M06-2X/3-21G ~ SDD dipole moments of Eu@C₂(27)-C₈₈, Eu@C₁(18)-C₈₈, and Eu@C_s(32)-C₈₈ are 0.2783, 1.0008, and 1.6317 D, respectively. Hence, the dipole moments suggest that Eu@C₂(27)-C₈₈ should have better solubility in non-polar CS₂ than the other two species. This reasoning offers an explanation why the relative populations in Fig. 2 do not agree with the solitary isolation⁵ of Eu@C₂(27)-C₈₈.

Frequently, there are stability similarities when encapsulating different metals, however, with about the same charge transfer to the cage, e.g.¹⁰ This similarity is related to the fact that metallofullerenes are not formed via some new covalent bond but rather stabilized by just an ionic bond.^{51–53} Unfortunately, the C₈₈ cages are still rare^{13,14,54,55} and mostly are employed by clusterfullerenes^{56,57} (like the C_s(32)-C₈₈ cage treated here) so that an analysis of such similarities is yet not possible.

In addition to the influence of different extraction solvents,^{2,48,49,58,59} there are differences in the applied metal source that could be related to kinetic and catalytic aspects,⁶⁰ i.e., to different degrees to which the

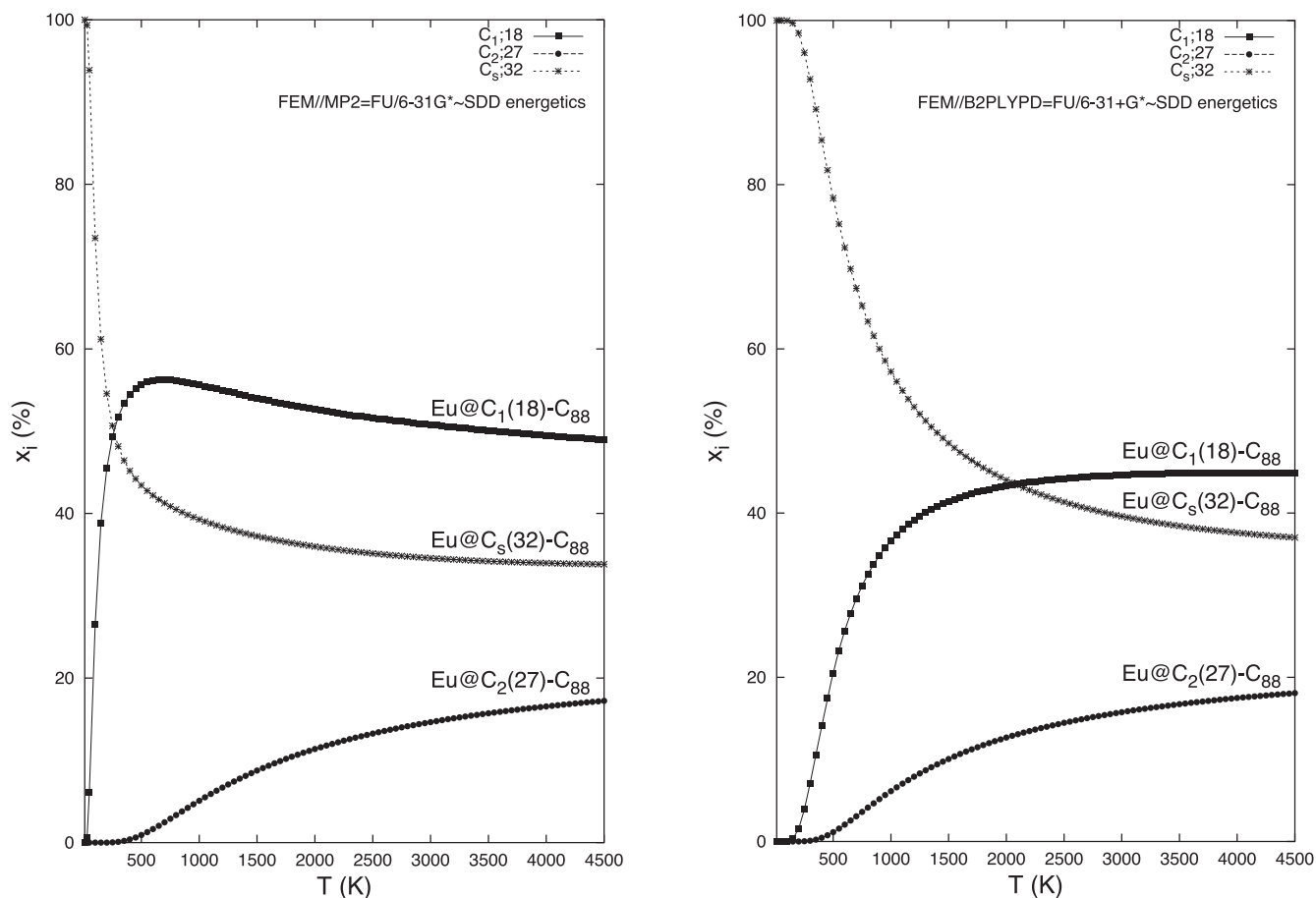


Figure 2. The relative populations of the Eu@C₈₈ isomers based on the FEM treatment with the MP2=FU/6-31G*~SDD (left) and B2PLYPD=FU/6-31+G*~SDD (right) energetics.

expected inter-isomeric thermodynamic equilibrium could be achieved in the synthesis. Finally, the inter-isomeric energetics in the whole family of Eu-nanocarbons^{8–12,61–64} could in future be treated even with the MP4 approach in order to further analyze computational predictions for fullerene systems.^{46,65}

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