Rukhovich, A. D.
On the growth rate of the number of fullerenes. (English. Russian original) [Zbl 1419.52012]

A mathematical fullerene is a 3-dimensional simple convex polyhedron with all faces being either pentagons or hexagons. The Euler formula implies that the number of pentagonal faces of every fullerene is exactly 12. The author finds asymptotics of the number of fullerenes with a given number \( k \) of hexagonal faces (denoted by \( \varphi(k) \)), the number of fullerenes with at most \( k \) hexagonal faces (denoted by \( \Phi(k) \)), and the number of fullerenes which have a pair of neighboring pentagons and at most \( k \) hexagonal faces (denoted by \( \hat{\Phi}(k) \)). Fullerenes are considered up to combinatorial equivalence.

Among other results, the author proves that

\[
\begin{align*}
\Phi(k) &= \frac{809 \cdot \pi^{10} \cdot k^{10}}{2^{17} \cdot 3^{18} \cdot 5^{4} \cdot 7^{11}} + O(k^9), \\
\liminf_{k \to \infty} \frac{\varphi(k)}{k^9} &= \frac{809}{2^{115} \cdot 3^{13} \cdot 5^2}, \\
\limsup_{k \to \infty} \frac{\varphi(k)}{k^9} &= \frac{809}{2^{15} \cdot 3^{13} \cdot 5^2} \zeta(9), \\
\hat{\Phi}(k) &= \frac{809 \cdot \sqrt{3} \cdot \pi^9 \cdot k^9}{2^{14} \cdot 3^{18} \cdot 5^3 \cdot 7} + O(k^8).
\end{align*}
\]

The proofs are based on a result on the weighted number of oriented triangulations of a two-sphere with vertices of degree at most 6 and exactly 2\( k \) triangles obtained in [P. Engel and P. Smillie, Geom. Topol. 22, No. 5, 2839–2864 (2018; Zbl 1393.52012)].

One of the results obtained by the author disproves a conjecture on the number of IPR-fullerenes, those without a pair of pentagons sharing a common edge, formulated in [J. Cioslowski, J. Math. Chem. 52, No. 1, 1–5 (2014; Zbl 1282.92029)].

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MSC:
52B10 Three-dimensional polytopes
57R18 Topology and geometry of orbifolds
05C30 Enumeration in graph theory

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mathematical fullerene; convex polyhedron; simple polyhedron; IPR-fullerene; asymptotics

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References:

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