Topological Properties of Circumcoronenes

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The regular-hexagon-shaped benzenoid hydrocarbons: B_1 = benzene (C_6H_6), B_2 = coronene ($C_{24}H_{12}$), B_3 = circumcoronene ($C_{54}H_{18}$), B_4 = circumcircumcoronene ($C_{150}H_{30}$), etc. possess unique topological properties. General expressions for the most important of such properties (number of fundamental structural invariants, number of Kekulé and Clar structures, number of aromatic sextets, Wiener and Szeged indices, spectral moments) are given, including a number of results that are communicated here for the first time. Cyclic conjugation in circumcoronenes is analyzed by means of its energy-effect, and found to agree with the predictions of Clar's aromatic sextet theory only in the case of B_1 and B_2.