The Energy of a Graph and its Size Dependence.
An Improved Monte Carlo Approach

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Z. Naturforsch. 56 \textbf{a}, 342–346 (2001); received April 2, 2001

In an earlier work [Gutman et al., Chem. Phys. Lett. 297, 428 (1998)] the average energy $\langle E \rangle$ of graphs with \textit{n} vertices and \textit{m} edges was examined, in particular its dependence on \textit{n} and \textit{m}. The quantity $\langle E \rangle$ was computed from a set of randomly, but not uniformly, constructed $(n, m)$-graphs. We have now improved our method by constructing the $(n, m)$-graphs uniformly, so that every $(n, m)$-graph has equal probability to be generated. Differences between the old and new approaches are significant only in the case of graphs with a small number of edges.

Key words: Energy (of Graph); Total $\pi$-electron Energy; Random Graphs; Monte Carlo Methods.