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

Harald Fripertinger, Ivan Gutman^a, Adalbert Kerber^b, Axel Kohnert^b, and Dušica Vidović^a

Institut für Mathematik, Karl Franzens Universität Graz, Heinrichstraße 36, A-8010 Graz, Austria ^a Faculty of Science, University of Kragujevac, P. O. Box 60, YU-34000 Kragujevac, Yugoslavia ^b Lehrsuhl II für Mathematik, Universität Bayreuth, D-95440 Bayreuth, Germany

Reprint requests to Prof. I. G.; Fax: +381 34 335040; E-mail: gutman@knez.uis.kg.ac.yu

Z. Naturforsch. 56 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 n vertices and m edges was examined, in particular its dependence on n and 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 π -electron Energy; Random Graphs; Monte Carlo Methods.