Bul. Ştiinţ. Univ. Baia Mare Ser. B,
Matematică-informatică, Vol XIV (1998), Nr. 1, 103-110

Dedicated to Professor Iulian Coroian on his 60th anniversary

A NEW METHOD FOR ORDERING THE VERTICES OF MOLECULAR GRAPHS

Zoiţa BERINDE and Vasile BERINDE

Abstract. In this paper a new algorithm,GAMA, for intramolecular ordering of molecular graphs is described.The algorithm is then applied for ordering acyclic connected graphs (trees) as well as cyclic molecular graphs.
A set of ten cyclic compact graphs has been considered in order to compare the results obtained by means of our algorithm, on one hand, to those obtained by means of others well-known procedures, IVEC [9] and MOLCEN [10], on the other hand. To define this new algorithm we use the concept of weighted electronic distance (d.e.p.) introduced in [6].