INTRODUCTION

Fundamentally chemistry is concerned with issues of bonding. Chemists are used to discussions of molecular properties and of reaction chemistry with Lewis structures. The drawbacks of the Lewis structures are well recognized. Frequently, the *formal* charges indicated by the Lewis structures are completely inadequate as representations of the *actual* bonding situation. The topological electron density analysis pioneered by Bader [1] provides a powerful method to study bonding as it is based solely on the total electron density distribution.

We have written programs for the graphical analysis of molecular electron density distributions that combine information about the electron density and its gradient at the same time. The gradient vector field plays a central role in the topological theory of **Atoms in Molecules** (AIM) for the definition of atomic basins and molecular graphs. We combined a presentation of the gradient vector field (line shape, line density) with an illustration of the magnitude of the electron density (color coding). We recently employed this new method in a study of stabilized carbenium ions [2]. Here, the method is described and results are presented of an application of this analysis to the study of cation dinitrogen interactions in various systems RN_2^+.

METHOD

Structures were optimized at the MP2(full)/6-31G* theoretical level using ***Gaussian92*** [3] and the MP2(full)/6-31G* wave functions of the optimized structures were written to wfn-files. These provide the input for the computations of electron density functions in real Cartesian space. For comparison between the RHF/6-31G* and MP2(full)/6-31G* theoretical levels, electron density functions were also calculated based on the RHF/6-31G* wave functions for CH_3NN^+, HNN^+ and N_2. The program ***CCExtreme*** uses these electron density functions to find the coordinates of the critical points between the atoms and the ring critical points for cyclic molecules. The critical point information is stored in a file fname.crt. The program ***CCShumaker*** then converts the crt-file to a form readable by the program ***CCSchuss*** and creates fname.shu. ***CCSchuss*** uses the information in the wfn- and shu-files and creates fname.gvf. This gvf-file contains a two-dimensional position vector, information on the gradient vector lines and the magnitude of the electron density at every point along the gradient path. ***CCGVF*** displays the color-coded gradient vector fields based on the gvf-file data.