

OPEN PROBLEMS IN MATHEMATICAL CHEMISTRY

PROBLEM 1

THE "EXPLODED MOLECULE" CONJECTURE

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Consider the lowest electronic state for each possible nuclear configuration of an arbitrary neutral molecule or of a family of molecular fragments of at least three nuclei. Within the Born–Oppenheimer approximation, for each fixed nuclear configuration, the electronic energy E_e is taken as the total energy E_t minus the nuclear repulsion energy E_n . That is to say, $E_e = E_t - E_n$.

It is conjectured that the electronic energy E_e reaches its absolute maximum value for configurations in which all the nuclei are pairwise infinitely separated, i.e. for so-called "exploded molecule" configurations. A collection of relevant references follows.

References

- [1] E.H. Lieb and B. Simon, *J. Phys.* B11(1978)L537.
- [2] P.G. Mezey, *Int. J. Quant. Chem.* 29(1986)85.
- [3] P.G. Mezey, *Potential Energy Hypersurfaces* (Elsevier, Amsterdam, 1987) Ch. 5.
- [4] G.A. Arteca and P.G. Mezey, *Phys. Rev.* A35(1987)4044.
- [5] T. Hoffmann-Ostenhof and J.D. Morgan III, *J. Chem. Phys.* 75(1981)843.

Note: Solutions to this and other problems published in this series should be addressed to Professor P.G. Mezey. It is anticipated that valid solutions to problems appearing in our series will be published in future issues of the *Journal of Mathematical Chemistry*.