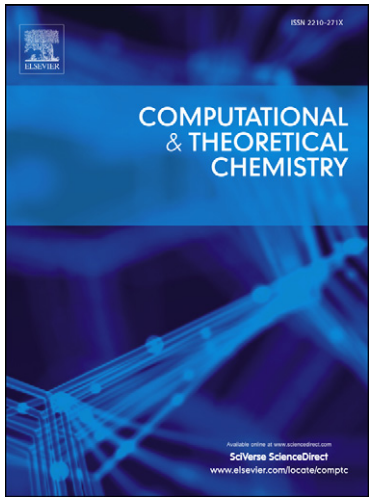

Atomic charge and atomic dipole fluxes during stretching displacements in small molecules

Tiago Quevedo Teodoro, Roberto Luiz Andrade Haiduke

PII: S2210-271X(12)00587-7
DOI: http://dx.doi.org/10.1016/j.comptc.2012.11.017
Reference: COMPTC 959

To appear in: *Computational & Theoretical Chemistry*

Received Date: 18 September 2012
Revised Date: 9 November 2012
Accepted Date: 9 November 2012

Please cite this article as: T.Q. Teodoro, R.L.A. Haiduke, Atomic charge and atomic dipole fluxes during stretching displacements in small molecules, *Computational & Theoretical Chemistry* (2012), doi: http://dx.doi.org/10.1016/j.comptc.2012.11.017

Atomic charge and atomic dipole fluxes during stretching displacements in small molecules

Tiago Quevedo Teodoro* and Roberto Luiz Andrade Haiduke

tiagoquevedo@iqsc.usp.br

haiduke@iqsc.usp.br

Phone 55-16-3373-8280

FAX 55-16-3373-9975

Departamento de Química e Física Molecular

Instituto de Química de São Carlos, Universidade de São Paulo

Av. Trabalhador São-carlense, 400 - CP 780

13560-970 - São Carlos, SP, Brazil

Abstract

First, the convergence in values of dynamic quantities such as atomic charge flux and atomic dipole flux that take place in stretching displacements is investigated in this work by means of calculations with three basis sets (cc-pVDZ, cc-pVTZ and cc-pVQZ) and different theoretical methods (HF, MP2, MP4(SDQ) and CCSD). The charges were obtained from QTAIM, Mulliken and NPA formalisms while atomic dipoles are only calculated from QTAIM. We studied a group of simple diatomic and triatomic molecules with diverse chemical bonding character: HF, HCl, LiH, NaH, NaCl, LiF, NaF, BF, AlF, BeO, MgO, CO, ClF, HCN, HNC, OCS, CO_2 and CS_2. The data obtained indicate that these dynamic quantities show well-behaved convergence patterns except by those from Mulliken for some triatomic systems with increasing basis set size. Some relevant dependence of QTAIM fluxes was observed in HF and HNC when small basis sets are used but the results still converge when larger basis sets are employed. Moreover, charge fluxes from QTAIM are in nice accordance with chemical arguments while the other formalisms exhibit results that are not plausible in some cases. The most remarkable ones are noticed in highly ionic diatomic systems, which should present negligible charge flux values during bond stretching displacements around equilibrium geometries.

Keywords*:* Charge flux; Atomic dipole flux; Convergence; Basis set; Electron correlation