Fast Analytical Evaluation of Intermolecular Electrostatic Interaction Energies Using the Pseudoatom Representation of the Electron Density.

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This paper is dedicated to the memory of Professor Philip Coppens (1930-2017)

Abstract   Previously reported (Volkov, A., Koritsanszky T. S. & Coppens, P. (2004). *Chem. Phys. Lett.* **391**, 170–175) Exact Potential and Multipole Moment Method (EP/MM) for evaluation of intermolecular electrostatic interaction energies using the nuclei-centered pseudoatom representation of electron densities is significantly improved in terms of both speed and accuracy by replacing the numerical quadrature integration of the Exact Potential with a fully-analytical technique. The resulting approach, incorporated in the XDPROP module of the software package XD, has been tested on several molecular systems ranging in size from water-water to dodecapeptide-dodecapeptide dimers using electron densities constructed via the University at Buffalo Aspherical Atom Databank. The improved hybrid method provides electrostatic interaction energies within 0.1 kJ/mol from the exact value for all benchmark systems. The running time per dimer is under 12 seconds on a 2012 central processing unit (2.8 GHz AMD Opteron 6348) and under 4 seconds on a relatively modern processor (2.8 GHz Intel Xeon E3-1505M v5), even for a dodecapeptide-dodecapeptide system.