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ERRATUM

Multipole electrostatic model for MNDO-like techniques with minimal valence *spd*-basis sets

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In the paper, an erroneous conversion factor was used for the DFT and MP2 electrostatic potentials (ESP). As a consequence, Figs. 3–8 (detailed ESP of the test molecules) and Figs. 10 and 11 (correlation plots between multipole and DFT/MP2 ESP) contain systematic errors.

If the correct values are used, the agreement between the multipole and DFT/MP2 ESPs is enhanced significantly for all test molecules (Figs. 3–8). Only $SPCl_2$ remains a problem: the absolute ESP values for the DFT/MP2 calculations and their multipole/numerical counterparts still differ significantly, and the pairs of curves still show slightly different shapes.

For the 434 ESP points on the (symmetrized) molecular surfaces, the correlation coefficient, Carbo and Hodgkin indices improve to 0.952, 0.952, 0.938 for AM1* multipole versus B3LYP/6-31G(d) and 0.953, 0.953, 0.935 for AM1* multipole versus MP2/6-31G(d), respectively. The linear regression equations (in kcal mol^{-1} e^{-1}) change accordingly to

$$\begin{aligned} \mathrm{ESP_{DFT}} &= 0.8742 \times \mathrm{ESP_{AM1*}} - 0.0537 \\ &\text{with } r^2 = 0.907,\ \sigma = 3.55, \\ &\text{and MUE} = 2.52, \end{aligned} \tag{1}$$

$$\begin{aligned} \mathrm{ESP_{MP2}} &= 0.8940 \times \mathrm{ESP_{AM1*}} - 0.0672 \\ &\text{with } r^2 = 0.908,\ \sigma = 3.61, \\ &\text{and MUE} = 2.52. \end{aligned} \tag{2}$$

The online version of the original article can be found at http://dx.doi.org/10.1007/s00214-005-0657-9.

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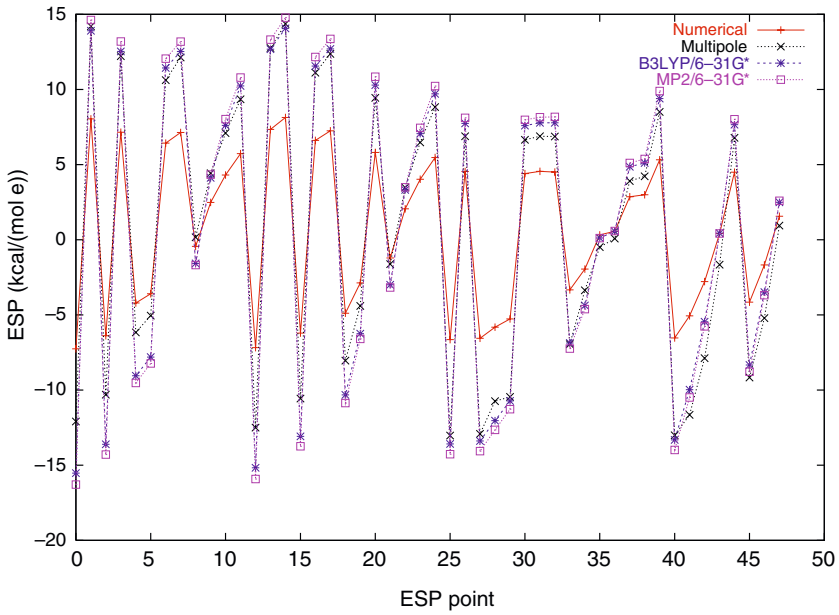

Fig. 3 Water: ESP on the symmetrized solvent-accessible surface

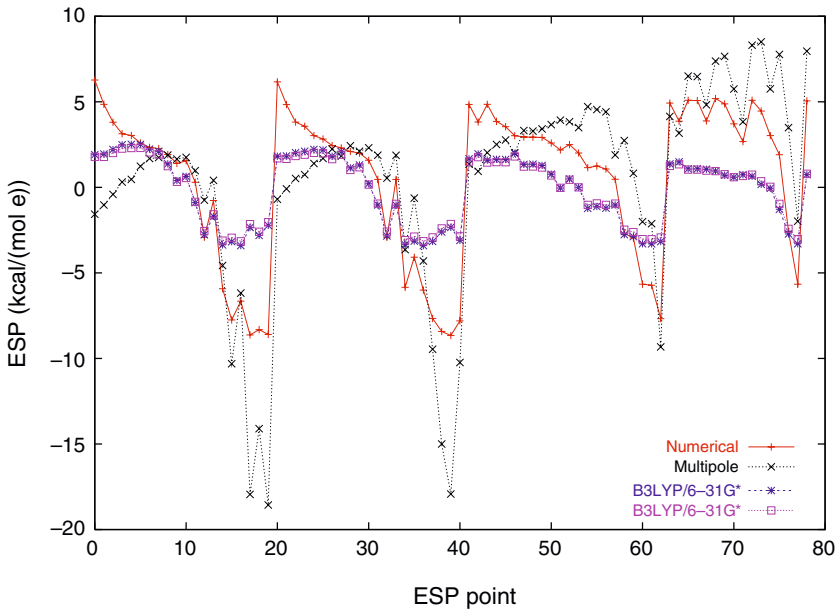

Fig. 4 $SPCl_3$: ESP on the symmetrized solvent-accessible surface

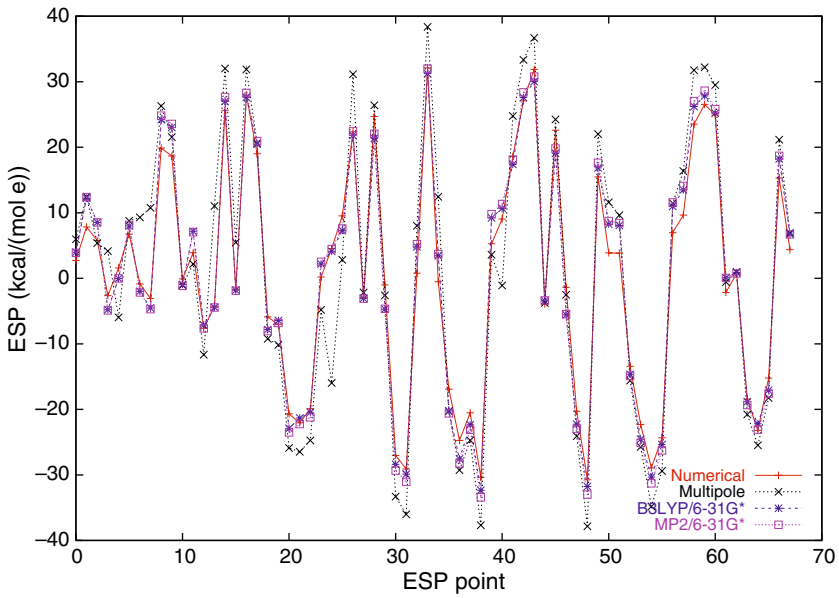

Fig. 5 Cysteine: ESP on the solvent-accessible surface

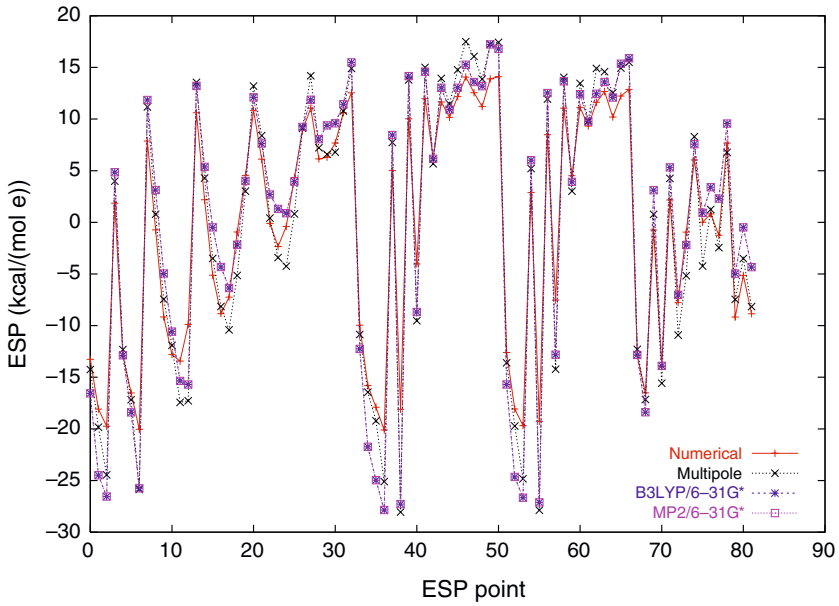

Fig. 6 Cytosine: ESP on the symmetrized solvent-accessible surface

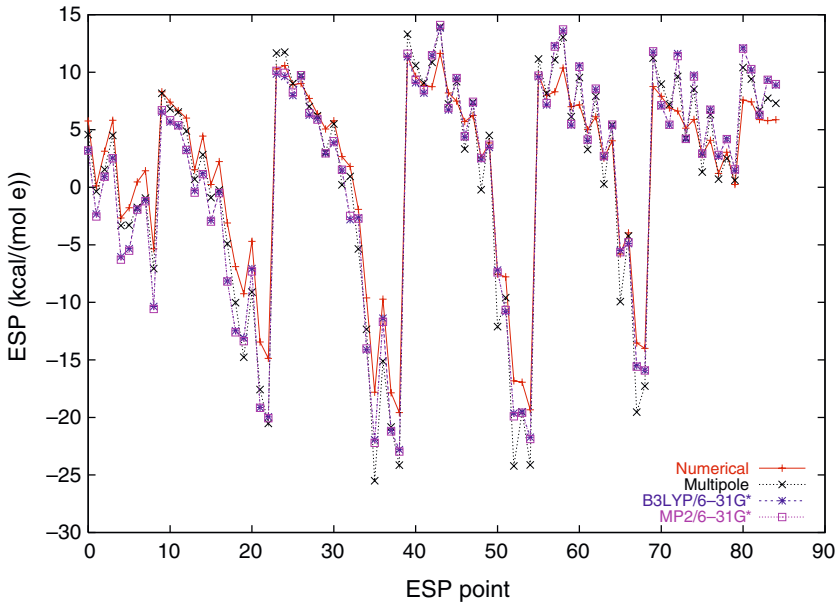

Fig. 7 Sarin: ESP on the solvent-accessible surface

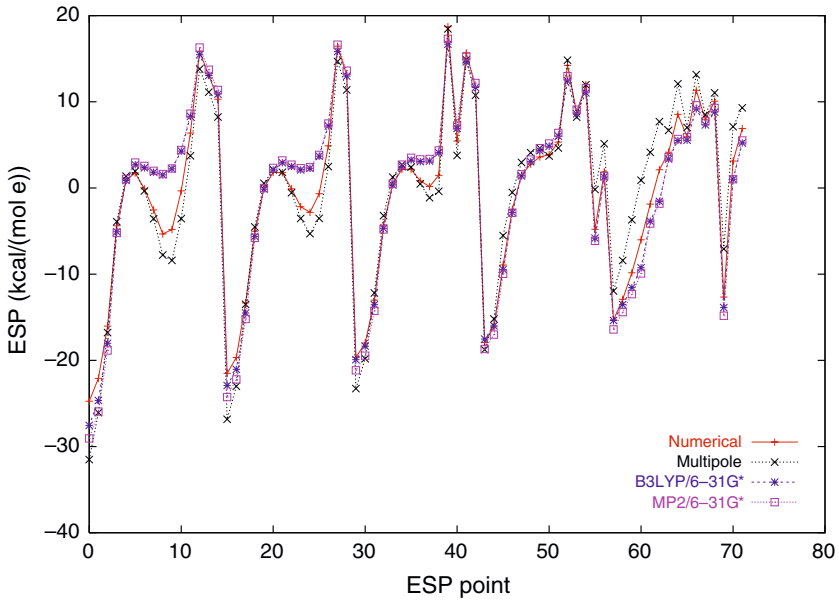

Fig. 8 $MoCp_2Cl_2$: ESP on the symmetrized solvent-accessible surface

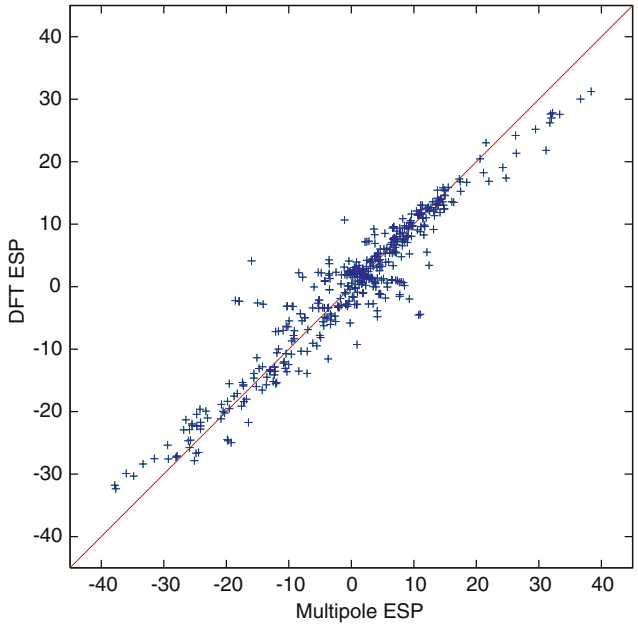

Fig. 10 Multipole Versus DFT ESP (ESP points all test molecules included)

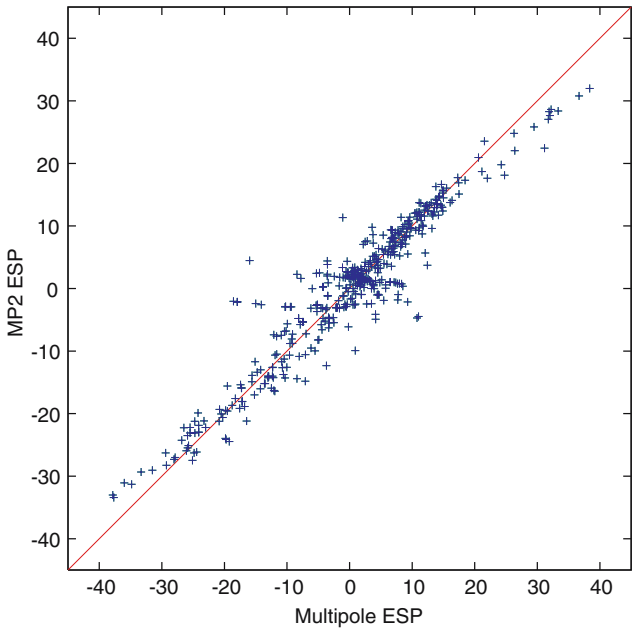

Fig. 11 Multipole Versus MP2 ESP (ESP points of all test molecules inclued)