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A drug delivery model: 5-fluorouracil intercalated into montmorillonite investigated to the Hartree-Fock level

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Molecular mechanics calculations, based on equations such as the one below, are used to investigate a colorectal cancer drug, 5-fluorouracil, intercalated into a clay, montmorillonite. This combination is currently being considered as a drug delivery system. The swelling of clays has been studied since the 1930s and is still not fully understood. *Spartan' 14* is used for the calculations. Semi-empirical and *ab initio* basis set scaling is also examined since there are roughly 300 atoms involved in the full model.

$$EB_{ij} = 143.9325 \frac{k_{ij}}{2} \Delta r_{ij}^2 \left(1 + c \Delta r_{ij} + \frac{7}{12} c^2 \Delta r_{ij}^2 \right)$$

Biography

John H Summerfield has completed his PhD in Physical Chemistry from Oregon State University (1994). His teaching responsibilities include teaching Physics for non-science students, General Chemistry, Physical Chemistry and Organic Chemistry (lab). His specialties/research interests are in computer models of lithium ion batteries and computer models of clays as a drug delivery method.

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