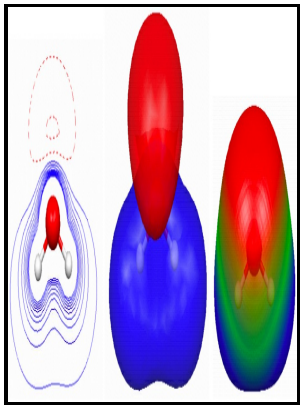
Molecular electrostatic potentials - concepts and applications

Elsevier - Mixed QM/MM molecular electrostatic potentials



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Molecular Electrostatic Potentials, Volume 3

Bloom, Yi An, Steven E. For example, in the perfluoroarene-arene interactions utilized in crystal engineering, the present results suggest that this strong interaction arises primarily from the direct interaction of the fluorines with the non-fluorinated ring, not π-polarization.

Electric potential

Similarly, for aniline the additive ESP overestimates the ESP above the ring, as was apparent in. Simplified analytic expressions for the molecular electrostatic potential.

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Electrostatic Potential Minimum of the Aromatic Ring as a Measure of Substituent Constant

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