From Experimentally Determined Enthalpies of Sublimation to the Validation of a Force Field for MD Simulations on Sulfur- and Halogen-Containing Active Pharmaceutical Ingredients

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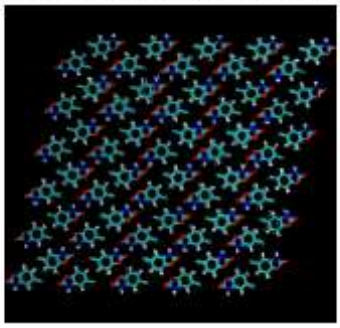
Molecular dynamics simulations provide a powerful tool to investigate many aspects of solid-state pharmaceuticals (e.g., crystallization, solubility, stability, polymorphism, phase transitions).[1-4] A pre-condition for the application of these methods is, however, the development of suitable force fields, which must be validated against reliable structural and energetic data. This work describes the determination of the enthalpies of sublimation of sulfanilamide, sulfapyridine, chlorzoxazone, clioquinol and triclosan by Calvet-drop microcalorimetry and their application in the development of a general purpose OPLS-AA based force field, to study sulfur- and halogen-containing APIs.



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