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Sublimation entropy and dissociation constants prediction by quantitative evaluation of molecular mobility in crystals

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One of the main problems in attempts to predict binding constants of molecules (or free energies of their binding) is a correct evaluation of configurational entropy of binding. Such an evaluation is possible by molecular dynamics simulation methods, but such simulations require a lot of computational time. We have developed an alternative approach which allows a fast calculation of the binding entropy from summarizing the available data on sublimation of crystals. Our method is based on an evaluation of the mean amplitude of those movements which are restricted in the bound molecule (e.g., in a crystal), but not restricted in its "free" state (e.g., in vapor). To this end, we use experimental data on sublimation enthalpy, pressure of saturated vapor, and structural characteristics of the molecule in question. The resulting average amplitude ($0.17 \pm 0.01 \text{ \AA}$) of molecular movements in crystals was used to predict sublimation entropies and dissociation constants for sublimation of many molecular crystals, as well as the standard entropy of binding of molecules by these crystals under standard conditions (pressure: 1 atmosphere, temperature: 25 degrees centigrade). The results of these predictions are in rather close agreement with experimental values. This work has been supported by the RSF grant 14-24-00157.

Biography

Alexei Finkelstein done his PhD in biophysics, Moscow PhysTech., 1976, DSc biophysics, Moscow University 1991. Author of >250 scientific papers and books "Protein Physics", (five Russian, two english and two chinese editions), and "physics of protein molecules" (in Russian). citation index by google scholar about 8400, hirsch index about 42. Since 1970, member and since 1999, head of protein physics laboratory at the institute of protein research, RAS. Since 1998, full professor of the Moscow University. Awards from FIRCA, INTAS, CASP, HHMI (3 times), RFBR, RSF, moscow grant, etc. State Prize of Russia in Science (1999), elected to the Russian Academy of Sciences (2008).

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