Determining free energy

<http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2674374/#c7>

book

<http://link.springer.com/book/10.1007%2F978-94-007-7606-7>

Maths

<http://pubs.acs.org/doi/full/10.1021/jp037421y>

The exact free energies,*fi*=−*kBT* ln[left angle bracket]*hi*[right angle bracket], were computed by numerically integrating Eq. [3](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2674374/#d3) over the potential given by Eq. [6](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2674374/#d6).

⟨*hi*⟩=∫*d****r*** *e^(*−*βU*(***r***)*hi*(***r***))/∫*d****r*** *e^(*−*βU*(***r***)),

(3)

*U*(*x*,*y*)=−3 exp(−(*x*−1)^2+*y^*2)−3 exp((*x*+1)^2+*y^*2)+15 exp(−8/25(*x^*2+*y^*2+20(*x*+*y*)^2))+32/625(*x^*4+*y^*4)+2/5exp(−2−4*y*).

(6)

Potential

<http://www.science.uva.nl/~bolhuis/tps/content/exercise.pdf>

http://en.wikipedia.org/wiki/Potential\_energy\_surface

<http://scitation.aip.org/content/aip/journal/jcp/128/24/10.1063/1.2916718>

Uncertainty

Noé, F 2008, 'Probability distributions of molecular observables computed from Markov models', *Journal Of Chemical Physics*, 128, 24, p. 244103, Academic Search Complete, EBSCO*host*, viewed 7 December 2014.