

## Heat capacity of nitric acid by molecular dynamics

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Corrosion due to nitric acid in concentrated mediums is an active domain of investigations in nowadays-nuclear fuel reprocessing plants<sup>1</sup>. However, the complexity of the medium, due to the presence of strong electrolytes and thus heavy deviations from ideal behavior, hinders the determination of species activities required to predict speciation of the system<sup>2</sup>. Empirical models exist in the literature<sup>3</sup>, but require the use of, sometimes many, adjustable parameters. Theoretically, species activity can be derived knowing the free enthalpy of the system, thus we aim to compute nitric acid-water mixtures free enthalpy. First, we investigate reproducing by molecular dynamics the heat capacity of pure nitric acid, and then of the binary mixture.

**Keywords:** molecular dynamics, nitric acid, free enthalpy, thermodynamics

### References

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