



On the Clausius formulation of the second law in stationary chemical networks through the theorems of the alternative

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(Submitted on 1 Apr 2012 (v1), last revised 14 Jun 2012 (this version, v2))

In this article the Gordan theorem is applied to the thermodynamics of a chemical reaction network at steady state. From a theoretical viewpoint it is equivalent to the Clausius formulation of the second law for the out of equilibrium steady states of chemical networks, i.e. it states that the exclusion (presence) of closed reactions loops makes possible (impossible) the definition of a thermodynamic potential and vice versa. On the computational side, it reveals that calculating reactions free energy and searching infeasible loops in flux states are dual problems whose solutions are alternatively inconsistent. The relevance of this result for applications is discussed with an example in the field of constraints-based modeling of cellular metabolism where it leads to efficient and scalable methods to afford the energy balance analysis.

Subjects: **Statistical Mechanics (cond-mat.stat-mech)**; Biological Physics (physics.bio-ph); Chemical Physics (physics.chem-ph); Molecular Networks (q-bio.MN)

Cite as: [arXiv:1204.0178](#) [cond-mat.stat-mech]
(or [arXiv:1204.0178v2](#) [cond-mat.stat-mech] for this version)

Submission history

From: Daniele De Martino [[view email](#)]

[v1] Sun, 1 Apr 2012 08:25:54 GMT (110kb,D)

[v2] Thu, 14 Jun 2012 07:59:08 GMT (43kb,D)

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