First order Derivatives of Thermodynamic Functions under Assumption of no Chemical Changes

L. Jäntschi[1]* and S. D. Bolboacă[2]

[1]*Department of Physics and Chemistry, Technical University of Cluj-Napoca, Romania*
[2]*Department of Medical Informatics and Biostatistics, Iiuliu Haţieganu" University of Medicine and Pharmacy Cluj-Napoca, Romania*

*Author for correspondence e-mail: lorentz.jantschi@gmail.com

The total differentials of a function *f* of several variables are the sum of all partial differentials [1]. In the absence of chemical changes, all state thermodynamic parameters are total differentials and depend on two variables (Table 1).

Table 1. Differentials of thermodynamic parameters

$dE = T \cdot dS - p \cdot dV + \Sigma_i \cdot \mu_i \cdot dn_i$	in the presence of chemical changes
$dn_i = 0$ for each *i*	provided that no chemical chnages
$dE = T \cdot dS - p \cdot dV$	in the presence of chemical changes

E = internal energy; S = entropy; V = volume; n = number of particles

Identifying the heat from reversible process $dQ_{rev} = T \cdot dS$ and mechanical work in the form of that from quasi-static processes $dw_{cvs} = -p \cdot dV$, these two thermodinamic quantities (dQ and dw) became total differentials. The condensed collection of the Bridgman's thermodynamic equations [2] was used as starting point in this study. A series of codification schemas were developed and implemented in order to obtain all first order partial derivatives [3] (Table 2).

Table 2. Gradients after pressure (*p*), volume (*V*) and temperature (*T*) of an unknown function (*f*)

Variable			$\left.\frac{\partial f}{\partial x}\right\|_{z=ct} = \left.\frac{\partial f}{\partial x}\right\|_{y=ct} + \left.\frac{\partial f}{\partial y}\right\|_{x=ct} \cdot \left.\frac{\partial y}{\partial x}\right\|_{z=ct}$	$\left.\frac{\partial f}{\partial z}\right\|_{x=ct} = \left.\frac{\partial f}{\partial y}\right\|_{x=ct} \cdot \left.\frac{\partial y}{\partial z}\right\|_{x=ct}$	Order
z	x	y	fxz = fxy + fyx·yxz	fzx = fyx·yzx	f = E
p	T	V	**fpV = fpT + fTp·TpV**	**fVp = fTp·TVp**	**6**
p	V	T	**fpT = fpV + fVp·VpT**	**fTp = fVp·VTp**	**5**
T	p	V	**fTV = fTp + fpT·pTV**	**fVT = fpT·pVT**	**2**
T	V	p	**fTp = fTV + fVT·VTp**	**fpT = fVT·VpT**	**4**
V	p	T	**fVT = fVp + fpV·pVT**	**fTV = fpV·pTV**	**1**
V	T	p	**fVp = fVT + fTV·TVp**	**fpV = fTV·TpV**	**3**

The results of the implementation are available at the following URL: http://l.academicdirect.org/Chemistry/ChemPhys/. The inputs of the application are state parameters, process differentials, thermodynamic equations and gradients. The first order partial derivatives, counting a number of two-hundred and forty equations, are displayed as the output. The transformation of an interactive interrogation is conducted in our lab in order to allow selecting the function, the variable and the constant before generation of the thermodynamic equation first order derivatives.

References

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2. P. W. Bridgman, Physical Review, 3, 1914, 273-281.
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