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Estimation of thermodynamic properties of carbonate minerals for applicative purposes

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Carbonates are key minerals in many fields, including geochemistry, biology, geology, and medical sciences. Despite their broad relevance, very few works reported thermodynamic data for these compounds. When experimental thermodynamic data are not available (e.g. for solid solutions, nonstoichiometric compositions, hydrates, etc.) or when they appear questionable in some sense, the development of predictive approaches becomes crucial. Indeed, having comprehensive tools to predict thermodynamic properties could allow drawing stability diagrams, questioning the conditions of formation of minerals and better understanding their evolution. Based on additive "building blocks" method, relying on a polyhedral approach [1], we propose in this work to apply the predictive *ThermAP* (*Applied Predictive Thermodynamics*) approach, first used for apatite compounds [2], to carbonate minerals.

This method aims to adequately predict properties such as the standard enthalpy of formation (ΔH°_{f}), Gibbs free energy (ΔG°_{f}), and entropies (S°) for carbonate minerals at T = 298 K. In a first stage, we applied this additive model to simple carbonate phases implying divalent cations, and determined the enthalpy, free energy and entropy contribution of each constituting ion by thoroughly comparing final outcomes (ΔH°_{f}, ΔG°_{f}, S°) with robust literature data. Good agreement was found between the estimated and literature data, with small relative errors, allowing us to validate and extend this study to monovalent cations, more complex solid solutions, and hydrated phases.

Using this *ThermAP* strategy makes it possible to estimate such thermodynamic properties for any carbonate mineral containing elements such as Ca, Mg, Sr, Ba, Mn, Fe, Co, Ni, Cu, Zn, Cd and Pb. Furthermore, this approach may enrich thermodynamic databases such as *Thermoddem*, or be used to feed speciation tools for thermochemical calculations, such as the PHREEQC software [3], to broaden its use in geochemical modeling.

Ultimately, our goal is to draw a "*periodic table*" of recommended thermodynamic values for carbonate minerals, as was done previously for apatites, and possibly expand the approach to $T > 298$ K.

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[2] Drouet C, The Journal of Chemical Thermodynamics 136 (2019) 182-189.

[3] PHREEQC, version 3, U.S. Geological Survey