

## Accepted Manuscript

Thermochemistry of the simplest metal organic frameworks: Formates  $[M(HCOO)_2] \cdot xH_2O$  (M = Li, Mg, Mn, Co, Ni, and Zn)

G.P. Nagabhushana, Radha Shivaramaiah, Alexandra Navrotsky

PII: S0021-9614(17)30355-5  
DOI: <https://doi.org/10.1016/j.jct.2017.09.030>  
Reference: YJCHT 5229

To appear in: *J. Chem. Thermodynamics*

Received Date: 4 April 2017  
Revised Date: 18 September 2017  
Accepted Date: 24 September 2017

Please cite this article as: G.P. Nagabhushana, R. Shivaramaiah, A. Navrotsky, Thermochemistry of the simplest metal organic frameworks: Formates  $[M(HCOO)_2] \cdot xH_2O$  (M = Li, Mg, Mn, Co, Ni, and Zn), *J. Chem. Thermodynamics* (2017), doi: <https://doi.org/10.1016/j.jct.2017.09.030>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



**Thermochemistry of the simplest metal organic frameworks:****Formates  $[M(\text{HCOO})_2] \cdot x\text{H}_2\text{O}$  (M = Li, Mg, Mn, Co, Ni, and Zn)**

G.P. Nagabhushana, Radha Shivaramaiah, and Alexandra Navrotsky\*

Peter A. Rock Thermochemistry Laboratory and NEAT ORU,

University of California Davis

Davis CA 95616

**Abstract**

The simplest organic-inorganic hybrid material, with the smallest organic moiety, is a metal formate with divalent cations connected by formate anions. These metal formates have shown enormous potential for applications, particularly in gas storage and recently as anodes in lithium ion battery materials. Since formic acid is produced industrially on a large scale, metal formates could become very significant from an economic point of view. We report the enthalpies of formation of this important class of materials, measured using acid solution calorimetry. The formation enthalpies calculated from the respective metal chlorides/oxides and formic acid are negative for all the samples, with the energetic stability decreasing in the order  $\text{Mg} > \text{Zn} > \text{Mn} > \text{Co} > \text{Ni} > \text{Li}$ . Thus these materials show thermodynamic stability with respect to their oxides and should persist for long times when used in applications/devices.

**Key words:** Metal Formates, Acid solution calorimetry, Formation Enthalpy, LIB, Anode materials

Download English Version:

<https://daneshyari.com/en/article/6659878>

Download Persian Version:

<https://daneshyari.com/article/6659878>

[Daneshyari.com](https://daneshyari.com)