Erratum to: Computational prediction of selectivities in nonreversible and reversible hydroformylation reactions catalyzed by unmodified rhodium-carbonyls

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The original version of this article unfortunately contained a mistake. The last two terms of Eqs. (1) and (2) are not correct. Equations (1) and (2) should read, respectively:

$$B : L = k_B : k_L = \sum k_B[C] : \sum k_L[C] = \sum e^{-\Delta G_B^\ddagger/RT} : \sum e^{-\Delta G_L^\ddagger/RT} \approx \sum e^{-\Delta E_B^\ddagger/RT} : \sum e^{-\Delta E_L^\ddagger/RT} \quad (1)$$

and

$$b : b' = k_b : k_{b'} = \sum e^{-\Delta G_b^\ddagger/RT} : \sum e^{-\Delta G_{b'}^\ddagger/RT} \approx \sum e^{-\Delta E_b^\ddagger/RT} : \sum e^{-\Delta E_{b'}^\ddagger/RT} \quad (2)$$

The online version of the original article can be found at <http://dx.doi.org/10.1007/s00894-010-0864-8>.

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