Additions & Corrections

Energy Efficiency in Chemical Reactions: A Comparative Study of Different Reaction Techniques

Mark J. Gronnow, Robin J. White, James H. Clark,* and Duncan J. Macquarrie (*Org. Process Res. Dev.* **2005**, *9*, 516–518).

In light of a recent review of our data we issue the following corrections to our paper. On page 517 of our original paper, Tables 1 and 2 should be replaced by the following tables where the reworked results are shown:

Table 1. Results of homogeneous Suzuki coupling

media	yield (%)	energy (kW/mol)
oil-bath dioxane	56.6	58303
oil-bath toluene	25.1	135458
microwave dioxane	40.7	491
microwave toluene	0	n/a
sc-CO ₂	11.5 (80)	1769565 (253750)

Table 2. Energy usage comparison of microwave and conventional heating for a variety of reactions

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reaction	yield (%) / corrected thermal (kW/mol)	yield (%)/ corrected microwave (kW/mol)
heterogeneous Suzuki Friedel-Crafts acylation Knoevenagel	28.6/1385 100/4.7 68.2/33.0	77.4/32.3 100/0.44 18.2/137

Despite the change in values, the conclusions previously published remain valid. Reactions which are traditionally slow under conventional heating show the greatest energy gain on transferring to microwave activation. These include many of the most widely used organic reactions.

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Eutectic Composition of a Chiral Mixture Containing a Racemic Compound

Yaling Wang,* Rosario LoBrutto, Robert W. Wenslow, and Ivan Santos [Org. Process Res. Dev. 2005, 9, 670–676].

Equations 18 and 19 on page 673 are incorrect. These equations were used in the paper qualitatively only, so the conclusions are not affected. However, these equations can be used to calculate eutectic constants, and incorrect equations will lead to wrong conclusions.

(e) Calculation of Eutectic ee in Dilute Solutions. Integration of eq 4 from temperatures T_1 to T_2 results in:

$$(\ln K_{\text{eu}})_{T_2} = (\ln K_{\text{eu}})_{T_1} + \int_{T_1}^{T_2} \frac{2[(\Delta H_S)_S - (\Delta H_S)_r]}{RT^2}$$
 (18)

From this equation, $K_{\rm eu}$ at T_2 can be calculated from $K_{\rm eu}$ at T_1 if the heat of solution for a pure enantiomer and the racemic compound are obtained. This indicates that the eutectic ee at T_2 can be calculated from the eutectic ee at T_1 (eqs 16 and 17).

Similarly, integration of eq 15 from temperatures T_1 to T_2 results in:

From this equation, K_{eu} at T_2 can be calculated from K_{eu} at

$$(\ln K_{\text{eu}})_{T_{2}} = (\ln K_{\text{eu}})_{T_{1}} + \int_{T_{1}}^{T_{2}} \left(\frac{2}{RT^{2}}\right) \times \left\{ (\Delta H_{f}^{(T_{m})_{S}})_{S} - (\Delta H_{f}^{(T_{m})_{r}})_{r} \right\} + \int_{T}^{(T_{m})_{S}} \left[(C^{s})_{S} - (C^{s})_{r} \right] dT + \left\{ \frac{1}{2} (\mu_{SS} - \mu_{RS}) \right\}$$

$$(19)$$

 T_1 if melting temperatures, enthalpy of fusions, and heat capacities for a pure enantiomer and the racemic compound are measured (ignoring the small differences between intermolecular homochiral and heterochiral interactions). Therefore, the eutectic ee at T_2 can be calculated from the eutectic ee at T_1 .

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