Title: **Numerical simulation study on the temperature dependence of the Arrhenius parameters and its relation with the kinetic compensation effect**

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SUMMARY

The original version of the Arrhenius equation does not take into account the temperature dependence of both the pre-exponential factor and the activation energy. However, a simple physical argument makes clear that this hypothesis (although valid indeed as an approximation) is not totally accurate. The two Arrhenius parameters are mutually interconnected, so that an increase of one of them with temperature leads to an increase of the other. This might be taken as a potential explanation of the widespread compensation effect, and the conditions under which this model results applicable have been explored by means of numerical simulations. An interesting parameter involved in them is T_{d}, the temperature corresponding to an activation energy that exactly doubles the value at 0 K. Provided that this magnitude does not differ much from one member of a homologous reaction series to another, there will be a linear E_{a} vs. $R \ln A$ (or $\Delta H^{\circ}_{\neq}$ vs. $\Delta S^{\circ}_{\neq}$) relationship, its slope being the isokinetic temperature, T_{ik} (when T = T_{ik} all the reactions of the series share the same rate constant). This physical model seems to be supported by the low values of parameter T_{d} obtained for chemical reactions involving proteins as reactants. Additionally, given that the random experimental errors provoke a shift in parameter T_{ik} toward the mean working temperature, this effect has been discounted in order to obtain the most probable (extrapolated) value of the isokinetic temperature for different reaction families selected from chemical bibliographic sources.

Keywords: isokinetic temperature, kinetic compensation effect, modified Arrhenius and Eyring equations, numerical simulations, temperature-dependent activation energy.