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Interactive comment on "A new modeling tool for the diffusion of gases in ice or amorphous binary mixture in the polar stratosphere and the upper troposphere" *by* C. A. Varotsos and R. Zellner

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The authors considered the preexponential factor D0 and the activation energy E involved in the Arrhenius expression, i.e., Eq(1), of the diffusion coefficients for HCl, CH3OH, HCOOH and CH3COOH in ice as measured by Livingston et al (2002) and by Nehme (2006). Despite the large variation of the D0-value by several orders of magnitude, the authors interestingly find (see the Fig.2) that when plotting the logarithm of D0 versus E, a straight line results. It is argued that this finding stems from a thermodynamical model that interconnects the Gibbs activation energy for the diffusion process with the bulk properties, see Eq(7). The essence of the justification given in

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the manuscript goes as follows: On the basis of the afore mentioned thermodynamical model, explicit expressions –see Eqs(8) and (9)- are derived that interrelate the activation entropy and the activation enthalpy with the bulk elastic and expansivity data. These two expressions show that the ratio of the activation entropy and the activation enthalpy depends solely on bulk properties, thus being the same for different diffusants. This, in connection with the fact that D0 varies exponentially with the activation entropy –see Eq(6)- explains why lnD0 versus the activation energy (enthalpy) is a straight line, i.e, Fig2. The manuscript is well written and presents original results because –to the best of my knowledge- it is the first time that a linear relation between lnD0 and the activation entropy holds for various diffusants in ice. In addition, a well founded explanation of the latter finding is provided. Moreover, since it has been recently recognized that H20 ice particles play an important role in the polar stratosphere, the content of the manuscript perfectly fits the aims of the journal. Summarizing, the paper is of very good quality, hence I believe that it certainly merits publication in this journal.

Reference Livingston, F. E., Smith, J. A., and George, S. M.: General trends for bulk diffusion in ice and surface diffusion on ice, J. Phys. Chem. A, 106, 6309–6318, 2002. Nehme, R.: Diploma-thesis, University of Duisburg-Essen, edited by: Behr, P., Nehme, R., Zellner, R., in preparation, 2006.

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