Atmos. Chem. Phys. Discuss., 13, C4824–C4825, 2013
www.atmos-chem-phys-discuss.net/13/C4824/2013/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "A theoretical model on the formation mechanism and kinetics of highly toxic air pollutants from halogenated formaldehydes reacted with halogen atoms" *by* Y. M. Ji et al.

Anonymous Referee #2

Received and published: 16 July 2013

The manuscript entitled "A Theoretical Model on the Formation Mechanism and Kinetics of Air Highly Toxic Pollutions from Halogenated Formaldehydes Reacted with Halogen Atoms" by Ji et al. presents a systematic study on reaction mechanisms and kinetics between various halogenated formaldehydes with F, Cl and Br atoms, respectively. While such reactions are very important for the protection of ozone in the atmospheric community, there are only limited experimental data to analyze their mechanisms and kinetics. The results in this paper, therefore, are very important for the air protection field. Some of their theoretical results match the available experiments very well,

which validate their calculation techniques to evaluate reaction pathways and kinetics. Two different reaction mechanisms (Hydrogen abstraction and halogen addition) are carefully compared through the thermodynamic and kinetic calculations. Moreover, the systems under study certainly represent an important class of atmospheric reactions relevant for the readership of ACP. Their comprehensive studies supply the theoretical foundations for the understanding of these reactions. Therefore, the work deserves publication in ACP after some revisions:

1. The manuscript should be carefully checked with respect to the use of English language. There are some grammatical errors in the paper, especially the usage of the article and plural.

2. The authors have compared two reaction mechanisms: hydrogen abstraction and X addition. They should make it clear which mechanism is preferred for the reactions in the abstract.

3. I suggest the authors to change '3.2.1' section into '3.3' section.

4. In the last section, the authors analysed the effect of the altitude. In the supplement, the authors mentioned that the effect of the altitude is considered through the relationship between the altitude and the temperature. I suggest the authors to clarify such consideration in the manuscript. Since the calculated results are very important for their conclusions, could author move Table S10 into the paper?

5. In Table 1, 'OH-addition pathway' should be 'X-addition pathway'.

6. In Fig. 2, the author should make it clear in the caption which reaction mechanism is used to calculate the relationship between the rate constants and 1000/T. And in the last image, kBr+BrCHO is missing.

7. The caption 'Fig. 4' should be 'Scheme 1'.

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 18205, 2013.