# Reply to Comment on "Computational Investigation of $SO_3-NH_{3-n}X_n$ ($n = 0-3$; X = F, Cl) Interactions"

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It is known that when interacting with ionic as well as neutral electrophiles, nitrogen trifluoride, $NF_3$ may behave as a bifunctional Lewis base, able to form N- and F-coordinated isomers of comparable stability. Nevertheless, although the bifunctional Lewis base of $NF_3$ species exists, the effect of the successive fluorine and chlorine substitution on the nitrogen atom, with respect to $SO_3-NH_3$, has been reported in ref 1.

Grandinetti et al.[2] have suggested that the coordination of $NF_3$ to $SO_3$ may occur not only by nitrogen, as suggested by us, but also by fluorine. The aim of our published work is the study of the stability and the effect of the fluorine and chlorine substitution on the nitrogen atom, with respect to the well-known prototypical donor−acceptor complex $H_3N-SO_3$. In our paper, it is clear that we do not reject the possible coordination of $NF_3$ to $SO_3$ by fluorine atom.

## References and Notes

(1) Solimannejad, M.; Boutalib, A. *J. Phys. Chem. A* **2004**, *108*, 10342.
(2) Antoniotti, P.; Borocci, S.; Grandinetti, F. *J. Phys. Chem. A* **2005**, *109*, 2410.

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