

## Reply to the Comment by R. D. Sharma

Sharma's criticism of RBD's work can be summarized as follows:

1. Sharma's earlier work has already examined the ro-vibrational distributions for the  $N(^4S) + O_2$  reaction and, therefore, RBD's work is superfluous.
2. Because of the choice of initial conditions used in RBD's work, the results are irrelevant for thermochemical modeling of the upper atmosphere.
3. The initial conditions used in RBD's calculations do not correspond to the experiment with which the results are compared.

The first criticism is invalid because it does not appear that RBD and Sharma had the same goals in mind, as explained below. We do, however, regret that we failed to cite Sharma's earlier work in our paper.

The second criticism is not valid. Sharma assumes that the ultimate goal of our work was to provide information for atmospheric modeling. Most of the discussion in the paper deals with energy disposal in these reactions and how potential surface topology plays a role in the efficient channeling of collision energy into internal energy of the products. We could have chosen any initial conditions at all to investigate this. We chose rotational temperatures close to those observed in the upper atmosphere simply because that makes the results more interesting. However, this should not be construed as an attempt to model the chemistry of the upper atmosphere. Nowhere in the paper do we claim the latter to be our goal.

Due to his misperception as to the true goal of our work, Sharma takes exception to Figures 1 and 3. The main message conveyed by Figure 1 is explained in the first paragraph of Section 3. This has to do with the adherence of this reaction to the propensity rules proposed by Polanyi. Figure 3, which Sharma finds irrelevant, also conveys a similar message regarding energy disposal. This is clearly stated at the end of the third paragraph of Section 3. The difference between Figure 3 and 4, discussed in the fourth paragraph of Section 4, also has to do with energy disposal, not thermochemical modeling of the upper atmosphere.

The main thrust of the third criticism is that RBD chose a rotational temperature of 1000 K to determine the rotational distributions of  $O_2$  in their calculations whereas the experimental conditions almost certainly corresponded to a much lower temperature. This criticism is valid. However, the favorable comparison of our results with those of Duff, which were presumably carried out with a lower  $O_2$  rotational temperature, clearly indicates that the results are fairly insensitive to this parameter. The comparisons also make it clear that the oscillatory behavior of  $\sigma_{v'}$  observed in the experiments cannot be reproduced by QCT calculations on the Duff surfaces. Sharma further points out in this comparison, RBD combines the  $O_2$  ( $v = 0,1$ ) cross-sections in an unspecified manner. For Mr. Sharma's benefit, we provide the following equation, which can be derived easily from background material found in any undergraduate Physical Chemistry textbook:

$$\sigma_{v'} = \sum_v \sigma_v^v e^{-(\epsilon_v - \epsilon_0)/k_B T},$$

where  $v$  and  $v'$  are the vibrational quantum number of the reagent and the product, respectively, the  $\epsilon_v$  are the vibrational energy levels of the reagent,  $k_B$  is Boltzmann's constant and  $T$  is the temperature in Kelvins (298 K in our work). The small differences between our results and those of Duff indicate the quite small contributions made by the  $O_2(v = 1)$  cross-sections after being weighted by the Boltzmann factor.