Reply to Comment on "Tunneling Abstraction Reactions of Tritium Atoms with HD and with Mixtures of H_2 and D_2 in Superfluid and Normal-Fluid ³He⁻⁴He Media at 1.3 K^{*1}

Yasuyuki Aratono,^{*,†} Takuro Matsumoto,[‡] Toshiyuki Takayanagi,[†] Takayuki Kumada,[†] Kenji Komaguchi,[§] and Tetsuo Miyazaki^{†,‡}

Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki-ken 319-1195, Japan, Department of Applied Chemistry, School of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan, and Faculty of Engineering, Hiroshima University, Higashi Hiroshima 739-8527, Japan

Received: November 1, 1999

Due to an unfortunate mistake in calculating the partition functions in our computational code, the calculated thermal rate constants were found to be incorrect. The correct values are presented here in Table 3. Also, Figure 5 should be replaced accordingly.

The statement that the adiabatic barrier height for the THD transition state is larger than that for TDH is found to be wrong. The latter is slightly larger than the former.

Nevertheless, we would like to emphasize that the conclusions of the paper are unchanged. We would like to thank Dr. Srinivasan and Prof. Truhlar for pointing out the quantitative

[†] Japan Atomic Energy Research Institute.

[‡] Nagoya University.

§ Hiroshima University.

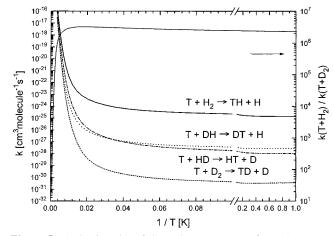


Figure 5. Arrhenius plot of thermal rate constants for $T + H_2$, D_2 , and HD in the temperature range 10-300 K.

TABLE 3: Thermal Rate Constants k(T) Calculated with the Reduced Dimensionality Theory (in Units of cm³ molecule⁻¹ s⁻¹)

	,			
<i>T</i> /K	$T+H_2$	$T+D_2 \\$	T + DH	T + HD
300	2.8(-16)	2.9(-17)	2.6(-17)	9.6(-17)
200	1.8(-18)	6.4(-20)	8.3(-20)	4.1(-19)
100	3.2(-22)	1.9(-25)	2.0(-24)	1.1(-23)
50	4.4(-24)	4.3(-29)	8.8(-27)	1.5(-26)
10	2.3(-25)	4.4(-31)	3.8(-28)	2.9(-28)
5	1.7(-25)	3.3(-31)	3.0(-28)	1.3(-28)
1.3	1.4(-25)	3.5(-31)	2.8(-28)	1.1(-28)

disagreement in the calculated rate constants between our results and earlier computational results. We regret that we did not cite the paper by Truhlar and co-workers.²

(1) J. Phys. Chem. A. 1998, 102, 1501.

(2) J. Phys. Chem. 1983, 87, 3415.

^{*} To whom all correspondence should be addressed: Fax: +81-29-282-5927. E-mail: aratono@popsvr.tokai.jaeri.go.jp.