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Supplementary Information for *The destruction of $^3HeT^+$ in collisions with tritium: A dynamical study*

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The present Supplementary Information contains:

- Table 1 with the parameters for the ABC calculation.
- Table 2 with the parameters for the QCT calculation.
- Figure 1 with the integral cross section as a function of the collision energy obtained with the three methods.
- Figure 2 with the integral cross sections for the T+^{3}HeT($v=0, j=0-5)^+ \rightarrow T_2^+ + ^3$He reaction obtained with the SQM method.
- Figure 3 with the integral cross sections for the T+^{3}HeT($v=0, j=0-5)^+ \rightarrow T_2^+ + ^3$He reaction obtained with the QCT method.
- Figure 4 with the rate constants for the T+^{3}HeT($v=0, j=0-5)^+ \rightarrow T_2^+ + ^3$He reaction obtained with the QCT method.
- Figure 5 with the rate constants for the T+^{3}HeT($v=0, j=0-5)^+ \rightarrow T_2^+ + ^3$He reaction obtained with the QCT method.
- Figure 6 with the thermal rate constants obtained from those for the for the T+^{3}HeT($v=0, j=0-5)^+ \rightarrow T_2^+ + ^3$He reaction obtained with the SQM and QCT methods.
- Figure 7 with the rotational distributions for the T+^{3}HeT($v=0, j=0)^+ \rightarrow T_2^+ + ^3$He reaction at $E_c = 10$ meV.
- Figure 8 with the final state-resolved differential cross sections at $E_c = 10$ meV for the T+^{3}HeT($v=0, j=0)^+ \rightarrow T_2^+ + ^3$He reaction.

Table 1 Values of the parameters for used in the ABC code for the calculation with $^3HeT^+$ (v=0, j=0) .

E_c range (eV)	j_{max}	E_{max} (eV)	ρ_{max} (a_0)	n_{sec}	J_{max}	Ω_{max}
$10^{-5}-10^{-4}$	30	1.4	150	3723	9	9
$10^{-4}-10^{-3}$	32	1.4	120	2973	15	10
$10^{-3}-10^{-2}$	32	1.4	80	1315	25	7
$10^{-2}-10^{-1}$	34	1.6	40	486	48	10

Table 2 Parameters for $^3HeT^+$ ($v=0$, $j=0$) used for the QCT calculations. Maximal impact parameter is in bohr and N_t represents the total number of trajectories.

E_c range (eV)	b_{max}	N_t
$10^{-5}-10^{-4}$	67.6 – 38.8	10000
$10^{-4}-10^{-3}$	38.8 – 22.4	10000
$10^{-3}-10^{-2}$	22.4 – 13.2	20000
$10^{-2}-10^{-1}$	13.2 – 10.3	20000
$10^{-1}-10^{0}$	13.2 – 8.7	30000

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⋆ Part of Festschrift Honouring Prof. N. Sathyamurthy's 75th birthday

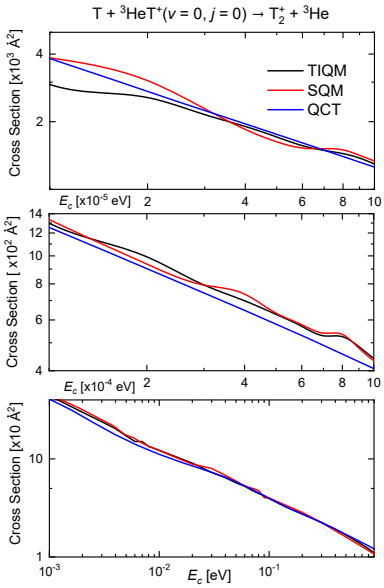

Fig. 1 Integral cross sections obtained with the TIQM (black), SQM (red) and QCT (blue) approaches for the T $+^3$HeT$^+(v=0, j=0) \rightarrow$ T$_2^+ +^3$He reaction separated in different log-scale decades for the energy: Top panel is between 10^{-5} and 10^{-4} eV; mid panel is between 10^{-4} and 10^{-3} eV and bottom panel is between 10^{-3} and 1 eV. Also notice factors for the cross sections in the y-axis.

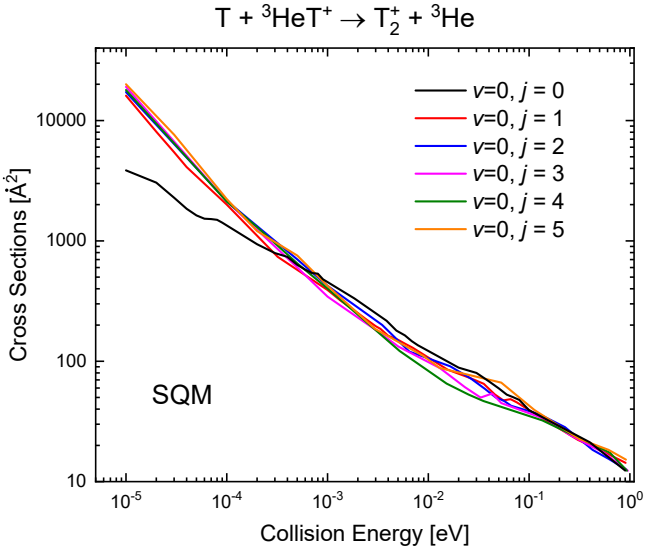

Fig. 2 Integral cross sections obtained with the SQM approach for the T $+^3$HeT$^+(v=0, j=0-5) \rightarrow$ T$_2^+ +^3$He reactions.

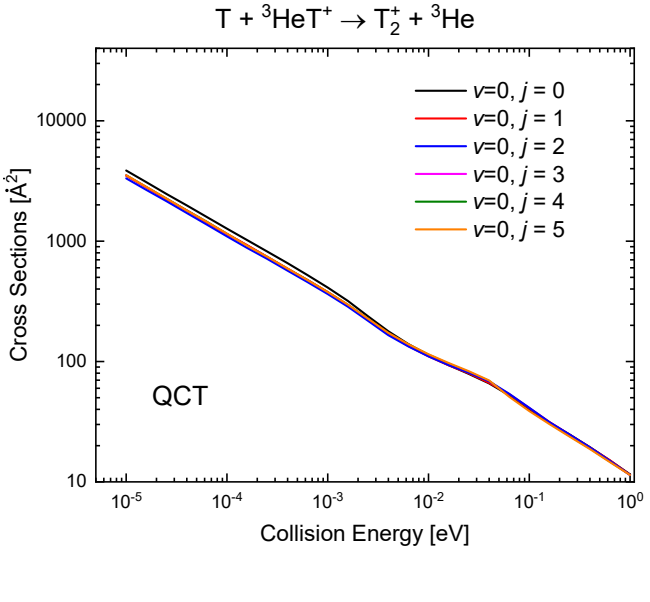

Fig. 3 Same as Figure 2 obtained with the QCT approach.

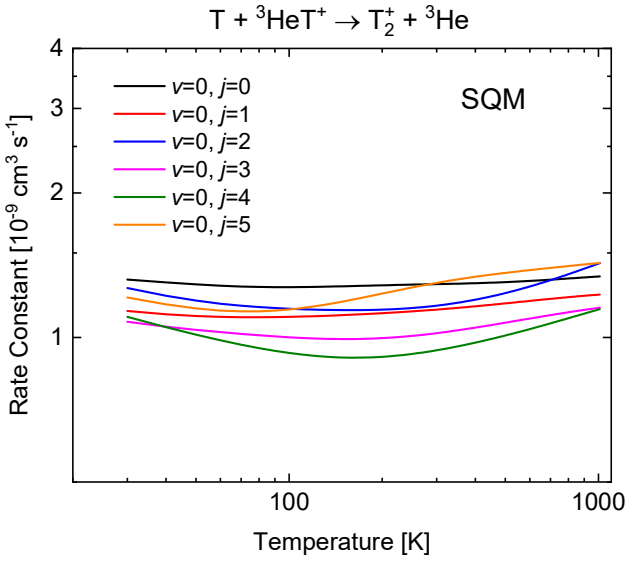

Fig. 4 Rate constants for the T $+^3$HeT$^+(v=0, j=0-5) \rightarrow$ T$_2^+ +^3$He reactions obtained from the SQM cross sections shown in Figure 2.

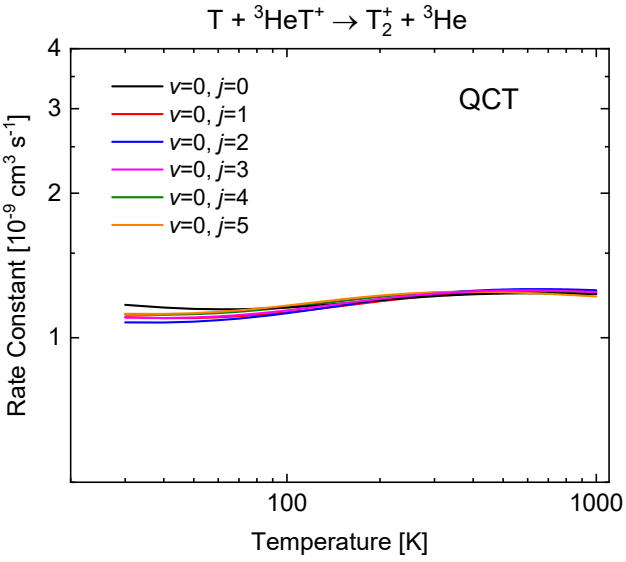

Fig. 5 Rate constants for the T $+^3$HeT$^+(v=0, j=0-5) \rightarrow$ T$_2^+ +^3$He reactions obtained from the QCT cross sections shown in Figure 3.

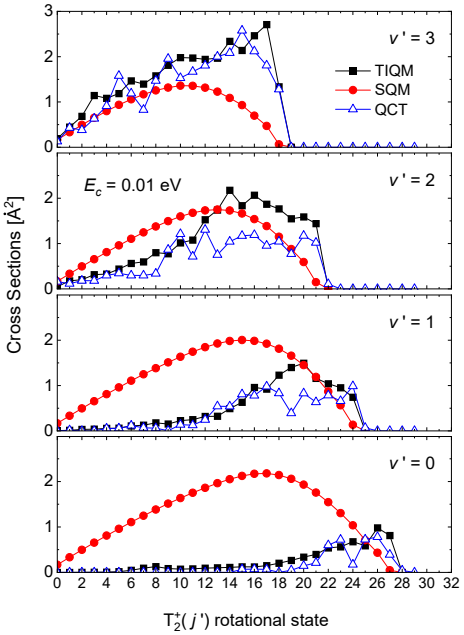

Fig. 7 Rotational distributions (measured in Å^2) at $E_c = 1 \times 10^{-1}$ calculated with the TIQM (black squares), SQM (red circles) and QCT (blue triangles) approaches for the T $+^3$HeT$^+(v=0, j=0) \rightarrow$ T$_2^+(v'=0-3, j')+^3$He reaction.

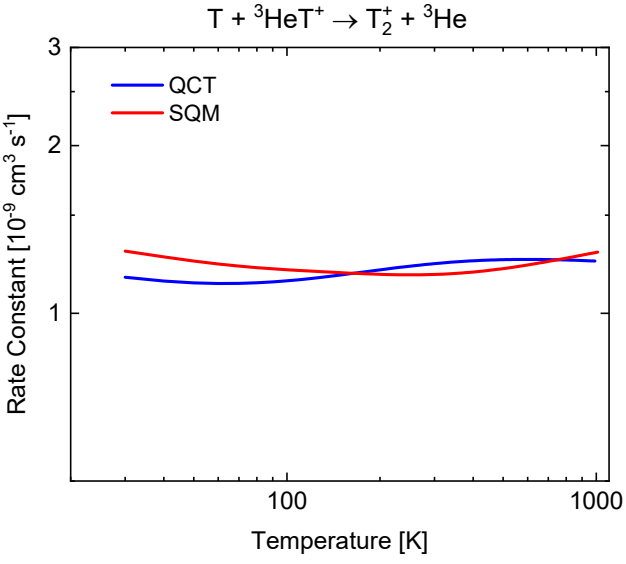

Fig. 6 Comparison between the thermal rate constants obtained from those for the T $+^3$HeT$^+(v=0, j=0-5) \rightarrow$ T$_2^+ +^3$He reactions obtained from the QCT (blue) and QCT (red) rate constants shown in Figures 5 and 4, respectively, by means of the expression $k(T) = e^{-E_j/KT} k_j(T) / \sum_j e^{-E_j/KT}$, where j stands for the corresponding $v=0, j=0-5$ rovibrational state.

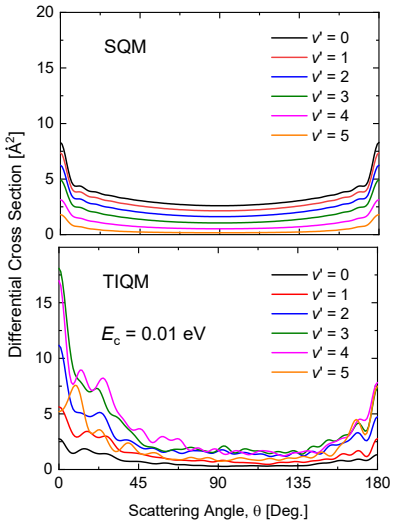

Fig. 8 Final vibrational state solved differential cross sections for the T $+^3$HeT$^+(v=0, j=0) \rightarrow$ T$_2^+(v'=0-5)+^3$He reaction at $E_c = 0.01$, obtained with the SQM (top panel) and TIQM (bottom panel) approaches .