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$$HOSi^+ + e^- \rightarrow SiO + H \quad (1a)$$
$$\rightarrow Si + OH \quad (1b)$$
$$\rightarrow HSi + O \quad (1c)$$

Thermodynamic Data

$\Delta H^o_{298}(1a) \approx -344$ kJ mol^{-1}

$\Delta H^o_{298}(1b) \approx -163$ kJ mol^{-1}

$\Delta H^o_{298}(1c) \approx -25$ kJ mol^{-1}

Thermochemical data for $HOSi^+$ (and $HSiO^+$) were taken from Ref. [1], in which they were calculated from the proton affinity of SiO. The other enthalpies of formations were obtained from the NIST webbook and Ref. [3]. Reaction (1c) is almost thermoneutral, so small errors in the thermodynamic data to affect the viability of the process.

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
None			
Rate Coefficient Reviews and Evaluations			
$3.0 \times 10^{-7}(T/300)^{-0.5}$	10 – 300	UMIST database	
$3.0 \times 10^{-7}(T/300)^{-0.5}$		OSU website	
Branching Fraction Measurements			
None			
Branching Fraction Reviews and Evaluations			
(1a) = 0.5	10 – 300	UMIST database and OSU website	
(1b) = 0.5			
(1c) = 0.0			

Comments

Neither experimental studies nor theoretical computations were undertaken for the dissociative recombination of $HSiO^+$ or $HOSi^+$. Measurements could also be impeded by the difficulty to produce $HSiO^+$ and the existence of two isomers of this ion. In contrast to the isovalent HCO^+/HOC^+ system, the $HOSi^+$ ion is the more stable one (protonation on the oxygen atom of Si is energetically more favourable by 245 kJ/mol). In complete lack of data, the value of $3.0 \times 10^{-7}(T/300)^{-0.5}$ seems reasonable. Experimentally

determined values of the rate constant in the isovalent HCO^+ ion lie in the same range [4].

Based on the data on the isovalent ions HCO^+ (DCO^+), HN_2^+, and HCS^+ ions one could try to make a guess about the branching ratios. However, although the branching ratio of the H-atom abstraction is around 0.9 in HCO^+ [5] and HN_2^+ [6,7], the respective channel in HCS^+ [8] accounts for only 19 % of all dissociative recombination events. This is probably due to the presence or absence of favourable crossings between the ionic ground state and dissociative doubly-excited states of the intermediate neutral leading to the different products. State-of-the art theoretical calculations could be particularly valuable in predicting the branching fractions of the dissociative recombination of $HOSi^+$. In absence of any information it might be not the worst idea to expect the branching fraction of the H-atom abstraction (Reaction 1 (a)) of this species to lie between the ones for HCO^+, HN_2^+ and HCS^+, which would approximately be around 0.5 (the value already used in the models). It can then be assumed that Reaction 1(b) takes up the rest, since the almost thermoneutral reaction (1c) would mean a considerable rearrangement (H-migration from O to Si). Such rearrangements have been observed in DR processes, but are not likely to play a major role.

Preferred Values

Recommended rate constant:
$k = 3.0 \times 10^{-7}(T/300)^{-0.5} cm^3$ molecule^{-1} s^{-1}

Recommended branching fractions:
(1a) = 0.5
(1b) = 0.5
(1c) = 0.0

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