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$CH(^2\Pi) + NH_3$	→ $H_2CNH + H$	**(1)**	$\Delta H_r^{298} = -243.8$ kJ mol^{-1}
	→ $CH_2 + NH_2$	**(2)**	$\Delta H_r^{298} = +29.4$ kJ mol^{-1}
	→ $CH_3 + NH$	**(3)**	$\Delta H_r^{298} = -47.6$ kJ mol^{-1}
	→ $HCN + H_2 + H$	**(4)**	$\Delta H_r^{298} = -197.4$ kJ mol^{-1}
	→ $HCNH_2 + H$	**(5)**	$\Delta H_r^{298} = -89.5$ kJ mol^{-1}

The enthalpies of reaction are those given by Blitz et al. (4). See also Baulch et al. (*).

Rate Coefficient Data ($k = k_1 + k_2 + k_3 + k_4 + k_5$)

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	
Rate Coefficient Measurements (k)			
$(8.6 \pm 0.6) \times 10^{-11} \exp\{(230 \pm 30)/T\}$	297 – 677	Zabarnick, Fleming, Lin, 1989	(1)
$(7.2 \pm 1.7) \times 10^{-11} \exp\{(317 \pm 13)/T\}$	300 – 1300	Becker, et al 1993	(2)
$1.69 \times 10^{-10} (T/298\ K)^{-0.56} \exp(-28/T)$	23 – 295	Bocherel *et al*., 1996	(3)
$(1.5 \pm 0.05) \times 10^{-10}$	298	Blitz et al. 2012	(4a)
$(1.25 \pm 0.2) \times 10^{-10}$	298	Blitz et al. 2012	(4b)
Branching Ratios			
From their combined experimental and theoretical study, Blitz et al (4) inferred that ca. 96% of the reaction proceeds to $H_2CNH + H$ (that is, by channel (1)), Approximately 4% may proceed via channel (3).			
Reviews and Evaluations			
$k_1 = 1.69 \times 10^{-10} (T/300\ K)^{0.41} \exp(-19.0/T)$	23 – 1300	UMIST/UDFA database	
no values given		OSU website	

Comments

Refs. (1), (2) and (3): all these studies used the reliable pulsed photolysis / laser-induced fluorescence (PP/LIF) method. They yield very similar values for k_1 at 298 K. By extension the low T measurements reported in (3) can be considered reliable. The expression for the temperature-dependence of the overall rate coefficient given in the UMIST/UDFA data base appears to be based on these three studies and is similar to that given in ref. (3).

In ref. (4), Blitz et al. measured the rate coefficient at 298 K both by the PP/LIF method (4a) and by observing the rise in the LIF signals from the H atom product (4b). Both results are in good agreement with the earlier values at 298 K.

However, the main purpose of the study of Blitz et al. was to determine the branching ratios for this reaction. Their calculations (ab initio, transition state theory, and master equation) indicated that channel (1) is dominant. The experiments showed that the H atom yield from the reaction is 0.89 ± 0.07

Preferred Values

Rate coefficients (10 – 300 K)

$k(300\ K) = 1.6 \cdot 10^{-10}$ cm^3 molecule^{-1} s^{-1}
$k(10\ K) = 1.9 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}
$k(T) = 1.6 \times 10^{-10} (T/300)^{-0.05}$ cm^3 molecule^{-1} s^{-1}

Branching ratios

$k_1 / (k_1 + k_2 + k_3 + k_4 + k_5) = 0.95 \pm 0.05$
$k_3 / (k_1 + k_2 + k_3 + k_4 + k_5) = 0.05 \pm 0.05$

Reliability

$F_0 = 1.2$ g = 2

Comments on Preferred Values

Given the good agreement between the experimental values at 298 K, the estimate of 20% certainty seems generous. The wider uncertainty at 10 K reflects the fact that the measurements in (3) only go down to 25 K and it is not clear if k_1 will continue to increase below 25 K.

References

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