# Reaction Dynamics with Silane

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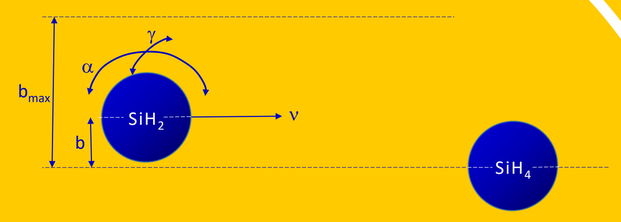
## Introduction

The Quantemol Database (QDB) aims to solve one of the most challenging and recurring problems when modelling plasmas – the lack of data on the key reactions that drive plasma processes. The project aims to address this problem by providing a platform for the provision, exchange, and validation of chemistry datasets [1]. Where the experimental data for the reactions is lacking, it must be calculated theoretically, and here we discuss a general method we use to complete the datasets for complex systems.

## Method

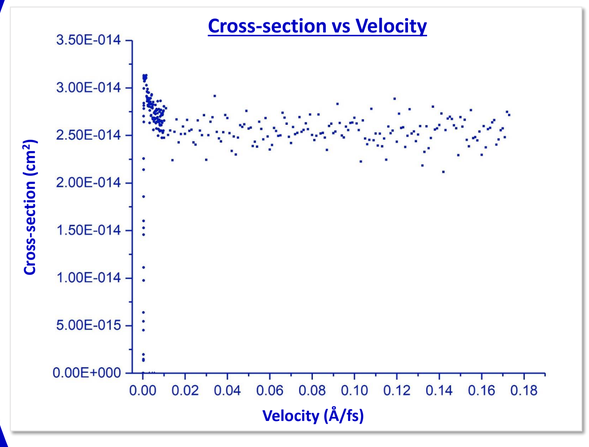


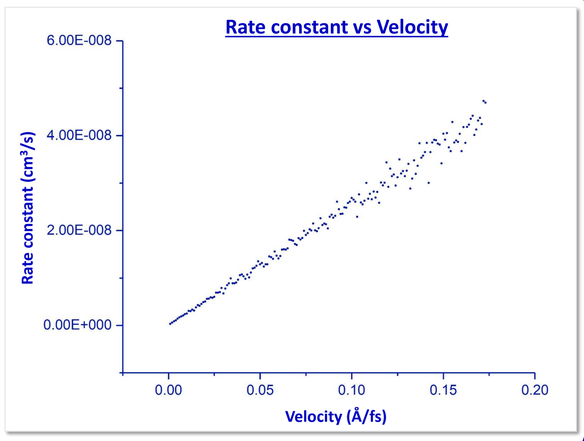

$$\sigma = \pi b_{max}^2 \frac{N}{N_{tot}} \quad [2] \qquad k_v = v\sigma_{(v)} \quad [3] \qquad v = \sqrt{\frac{8RT}{\pi M}}$$

σ – cross-section; ν – velocity; M – mass
k – rate constant; T – temperature
N – number of successful reactions
$N_{tot}$ – total number of reactions

## Results

At simulation temperatures of 300 K the rate constant was calculated to be **8.42 x10$^{-10}$ cm$^3$ s$^{-1}$**, which compares well to the literature value of **3.80 x10$^{-10}$ cm$^3$ s$^{-1}$** (10 Torr, 293 K)[4]

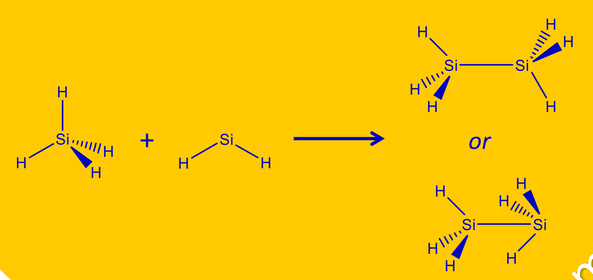



However at 650 K, the calculated rate constant is **1.21 x10$^{-9}$ cm$^3$ s$^{-1}$**, which compares poorly to the literature value of **5.4 x10$^{-11}$ cm$^3$ s$^{-1}$**. (10 Torr, 662 K)[4]

## Computational details

15,500 calculations were performed with the deMon DFTB code [5]. The z-matrix was randomised for each iteration, altering *b*, two angles and four dihedral angles.




Multiple isomers?

## Conclusion

While the calculated and literature results for the rate constant for $SiH_2 + SiH_4 \rightarrow Si_2H_6$ at 300 K are of the same order of magnitude, reproducing the same accuracy at 650 K proved problematic, with a difference of $10^2$. In order to calculate meaningful data for population of the QDB, it is necessary to understand why this difference arises in order to obtain results which are accurate at plasma conditions.

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[1] J. Tennyson *et al*, *Plasma Sources Sci. Technol.*, 2017, **26**, 055014. [2] K. Sakimoto, *J. Phys. B: At. Mol. Opt. Phys.*, 2004, **37**, 2255 – 2276. [3] A. Kupperman and E. F. Greene, *J. Chem. Educ.*, 1968, **45**, 361. [4] R. Becerra *et al*, *J. Chem. Soc., Faraday Trans.*, 1995, **91**, 2723 – 2732. [5] A.M. Koster *et al*, deMon2k, V.5, *The deMon developers*, Cinvestav, Mexico City, 2018.