

# REFINED DATA ON O<sub>2</sub> DISSOCIATION RATE MEASURED BY O-ARAS BEHIND SHOCK WAVES\*

N. S. Bystrov<sup>1</sup>, A. V. Emelianov<sup>2</sup>, A. V. Eremin<sup>3</sup>, and P. I. Yatsenko<sup>4</sup>

**Abstract:** The formation of atomic oxygen in high-temperature gas flows affects both the thermodynamic state of the gas and the kinetics of proceeding chemical processes. During hypersonic and space flights, there is still a significant lack of understanding of the phenomena of flow around high-speed vehicles. One of the main reactions occurring in the bow shock zone is the dissociation of molecular oxygen into O atoms. Experimental studies of the kinetics of O<sub>2</sub> dissociation were carried out by various methods; however, the O<sub>2</sub> dissociation rate constants in modern combustion mechanisms still differ by orders of magnitude. Therefore, the clarification of these values is a very urgent task. In this work, precision measurements of the rate constant of oxygen dissociation performed by the ARAS (atomic resonance absorption spectroscopy) method in the temperature range of 2600–5000 K behind the reflected shock waves were carried out which made it possible to noticeably refine the previous data. The best fit to the present experimental data is given by the expression  $k = 1.34 \pm 0.4 \cdot 10^{14} \exp(-(53620 \pm 2620)/T)$  cm<sup>3</sup>/(mole·s).

**Keywords:** shock tube; atomic resonance absorption spectroscopy; molecular oxygen; dissociation rate constant

**DOI:** 10.30826/CE23160102

**EDN:** RIRHHL

## Acknowledgments

The support of this study by the grant DFG-RFBR SCHU 1369/24-2 is gratefully acknowledged.

## References

- Gimelshein, F., and I. J. Wysong. 2019. Validation of high-temperature air reaction and relaxation models using emission data. *J. Thermophys. Heat Tr.* 33:606–616. doi: 10.2514/1.T5555.
- Candler, G. V. 2019. Rate effects in hypersonic flows. *Annu. Rev. Fluid Mech.* 51:379–402. doi: 10.1146/annurev-fluid-010518-040258.
- Watt, W. S., and A. L. Myerson. 1969. Atom formation rates behind shock waves in oxygen. *J. Chem. Phys.* 51:1638–1643. doi: 10.1063/1.1672225.
- Jerig, L., K. Thielen, and P. Roth. 1991. High-temperature dissociation of oxygen diluted in argon or nitrogen. *AIAA J.* 29:1136–1139. doi:10.2514/3.10714.
- Generalov, N. A., and S. A. Losev. 1966. Vibrational, excitation, and decomposition of molecular oxygen and carbon dioxide behind shock waves. *J. Quant. Spectrosc. Ra.* 6:101–125. doi: 10.1016/0022-4073(66)90066-5.
- Naudet, V., S. Abid, and C. E. Paillard. 1999. A high temperature chemical kinetic study of the O<sub>2</sub> dissociation and the O atoms recombination by ARAS. *J. Chim. Phys.* 96:1123–1145. doi: 10.1051/jcp:1999203.
- Thielen, K., and P. Roth. 1983. Stollwellenuntersuchungen zum Start der Reaktion CO + O<sub>2</sub>. *Ber. Bunsen. Phys. Chem.* 87:920–925. doi: 10.1002/bbpc.19830871017.
- Breshears, W. D., and P. F. Bird. 1971. Density gradient measurements of O<sub>2</sub> dissociation in shock waves. *J. Chem. Phys.* 55:4017–4026. doi: 10.1063/1.1676695.
- Camac, M., and A. Vaughan. 1961. O<sub>2</sub> dissociation rates in O<sub>2</sub>–Ar mixtures. *J. Chem. Phys.* 34:460–470. doi: 10.1063/1.4757209.
- Schexnayder, C. J., Jr., and J. S. Evans. 1961. Measurements of the dissociation rate of molecular oxygen. NASA TR-R-108. 18 p.
- Wray, K. L. 1962. Shock-tube study of the coupling of the O<sub>2</sub>–Ar rates of dissociation and vibrational relaxation. *J. Chem. Phys.* 37:1254–1263. doi: 10.1063/1.1733273.
- Ibraguimova, L. B., A. L. Sergievskaya, and O. P. Shatalov. 2013. Dissociation rate constants for oxygen at temperatures up to 11 000 K. *Fluid Dyn.* 48(4):550–555. doi: 10.1134/S0015462813040145.
- Owen, G., D. F. Davidson, and R. K. Hanson. 2016. Measurements of oxygen dissociation using laser absorption. *J. Thermophys. Heat Tr.* 30(2):274–278. doi: 10.2514/1.T4506.

\*This paper is based on the work that was presented at the 10th International Symposium on Nonequilibrium Processes, Plasma, Combustion, and Atmospheric Phenomena (NEPCAP), October 3–7, 2022, Sochi, Russia.

<sup>1</sup>Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation, [bystrovns.jiht@gmail.com](mailto:bystrovns.jiht@gmail.com)

<sup>2</sup>Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation, [aemelia@ihed.ras.ru](mailto:aemelia@ihed.ras.ru)

<sup>3</sup>Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation, [eremin@jiht.ru](mailto:eremin@jiht.ru)

<sup>4</sup>Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation, [mr.pavlik@gmail.com](mailto:mr.pavlik@gmail.com)

14. Streicher, J.W., A. Krish, R.K. Hanson, K.M. Hanquist, R.S. Chaudhry, and I.D. Boyd. 2020. Shock-tube measurements of coupled vibration–dissociation time-histories and rate parameters in oxygen and argon mixtures from 5000 K to 10 000 K. *Phys. Fluids* 32:076103. doi: 10.1063/5.0012426.
15. Baulch, D.L., D.D. Drysdale, J. Duxbury, and S.J. Grant. 1976.  $\text{HO}_2 + M \rightarrow \text{O} + \text{O} + M$ . *Evaluated kinetic data for high temperature reactions: Homogeneous gas phase reactions of the  $\text{O}_2-\text{O}_3$  system, the  $\text{CO}-\text{O}_2-\text{H}_2$  system, and of sulphur-containing species*. Butterworths. 3:11–32.
16. Drakon, A.V., A.V. Emelianov, A.V. Eremin, and P.I. Yatsenko. 2017. Study of trifluoromethane dissociation within wide pressure and temperature ranges by molecular resonance absorption spectroscopy. *High Temp.* 55:239–45. doi: 10.7868/S0040364417020041.
17. Bystrov, N.S., A.V. Emelianov, A.V. Eremin, and P.I. Yatsenko. 2018. Direct measurements of rate coefficients for thermal decomposition of  $\text{CF}_3\text{I}$  using shock-tube ARAS technique. *J. Phys. D Appl. Phys.* 51(18):184004. doi: 10.1088/1361-6463/aab8e5.
18. Bystrov, N., A. Emelianov, A. Eremin, B. Loukhovitski, A. Sharipov, and P. Yatsenko. 2020. Experimental study of high temperature oxidation of dimethyl ether, *n*-butanol and methane. *Combust. Flame* 218:121–133. doi: 10.1016/j.combustflame.2020.04.003.
19. Bystrov, N., G. Capriolo, A. Emelianov, A. Eremin, P. Yatsenko, and A. Konnov. 2021. High-temperature oxidation of propanol isomers in the mixtures with  $\text{N}_2\text{O}$  at high Ar dilution conditions. *Fuel* 287(3):119499. 11 p. doi: 10.1016/j.fuel.2020.119499.
20. Alekseev, V.A., N. Bystrov, A. Emelianov, A. Eremin, P. Yatsenko, and A.A. Konnov. 2022. High-temperature oxidation of acetylene by  $\text{N}_2\text{O}$  at high Ar dilution conditions and in laminar premixed  $\text{C}_2\text{H}_2 + \text{O}_2 + \text{N}_2$  flames. *Combust. Flame* 238(4):111924. doi: 10.1016/j.combustflame.2021.111924.
21. Glarborg, P., J.A. Miller, B. Ruscic, and S.J. Klippenstein. 2018. Modeling nitrogen chemistry in combustion. *Prog. Energ. Combust.* 67:31–68. doi: 10.1016/j.pecs.2018.01.002.
22. Bystrov, N.S., A.V. Emelianov, A.V. Eremin, and P.I. Yatsenko. 2019. Eksperimental'noe issledovanie reaktsii *n*-butanola s kislorodom za udarnymi volnami ARAS metodom [Experimental study of reaction of *n*-butanol with oxygen behind shock waves using ARAS method]. *Fiziko-khimicheskaya kinetika v gazovoy dinamike* [Physical-Chemical Kinetics in Gas Dynamics] 20(1). 15 p. doi: 10.33257/PhChGD.20.1.799.
23. Mulvihill, C.R., S.A. Alturaifi, and E.L. Petersen. 2021. A shock-tube study of the  $\text{N}_2\text{O} + M = \text{N}_2 + \text{O} + M$  ( $M = \text{Ar}$ ) rate constant using  $\text{N}_2\text{O}$  laser absorption near 4.6  $\mu\text{m}$ . *Combust. Flame* 224:6–13. doi: 10.1016/j.combustflame.2020.10.040.

Received April 21, 2022

## Contributors

**Bystrov Nikita S.** (b. 1995) — PhD student, research scientist, Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation; [bystrovns.jiht@gmail.com](mailto:bystrovns.jiht@gmail.com)

**Emelianov Alexander V.** (b. 1959) — Candidate of Science in physics and mathematics, senior research scientist, Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation; [aemelia@ihed.ras.ru](mailto:aemelia@ihed.ras.ru)

**Eremin Alexander V.** (b. 1946) — Doctor of Science in physics and mathematics, professor, chief research scientist, Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation; [eremin@jiht.ru](mailto:eremin@jiht.ru)

**Yatsenko Pavel I.** (b. 1993) — Candidate of Science in physics and mathematics, senior research scientist, Joint Institute for High Temperatures of the Russian Academy of Sciences, 13-2 Izhorskaya Str., Moscow 125412, Russian Federation; [mr.pav1kk@gmail.com](mailto:mr.pav1kk@gmail.com)