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SEMINARI CHIMICI

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Titolo

Rate theory: past, present and future

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A brief history is presented, outlining the development of rate theory during the past century. Starting from Arrhenius[1], we follow especially the formulation of transition state theory by Wigner and Eyring[2]. Parallel to the development of rate theory in the Chemistry community, Kramers[3] published in 1940 a seminal paper on the relation between Einstein's theory of Brownian motion and rate theory. The relationship between Kramers' approach and that of the Chemists will be discussed and described. Although classical rate theory reached a high level of maturity, its quantum analog leaves the theorist with serious challenges to this very day. A definite quantum TST has not been formulated to date although some very useful approximate quantum rate theories have been invented (see e.g. Ref. 4). The successes and challenges facing quantum rate theory are outlined. We end with a discussion of some of the open problems facing rate theory at this point in time.

1. S. Arrhenius, Z. Phys. Chem. (Leipzig) **4**, 226 (1889).
2. H. Pelzer and E. Wigner, Z. Phys. Chem. Abt. B **15**, 445 (1932); E. Wigner, Z. Phys. Chem. Abt. B **19**, 203 (1932); H. Eyring, J. Chem. Phys. **3**, 107 (1935); E. Wigner, Trans. Faraday Soc. **34**, 29 (1938); H. Eyring, Trans. Faraday Soc. **34**, 41 (1938).
3. H. Kramers, Physica (Amsterdam) **7**, 284 (1940)
4. E. Pollak and P. Talkner, Chaos **15**, 026116 (2005)