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The reaction kinetics of amino radicals with sulfur dioxide - DTU Orbit (08/11/2017)

The reaction kinetics of amino radicals with sulfur dioxide

Application of the laser photolysis-laser-induced fluorescence method to the reaction NH₂+SQ₁ in argon bath gas yields pressure-dependent, third-order kinetics which may be summarized as $k = (1.49 \pm 0.15) \times 10^{-34} \, (\text{T}/298 \, \text{K})^{-0.83} \, \text{cm}^6$ molecule⁻² s⁻¹ over 292-555K, where the uncertainty is the 95% confidence interval and includes possible systematic errors. The quenching of vibrationally excited NH₂ is consistent with a high-pressure limit for NH₂+SO₂ of $(1.62 \pm 0.25) \times 10^{-11} \, \text{cm}^3$ molecule⁻¹ s⁻¹ over the temperature range 295-505K, where again the 95% confidence interval is shown. *Ab* initio analysis yields a H₂N-SO₂ dissociation enthalpy of 73.5 kJ mol⁻¹, and comparison with RRKM theory and the exponential down model for energy transfer yields $<\Delta E>_{\text{down}} = 350 \, \text{cm}^{-1}$ for Ar at room temperature.

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