

Abstract Submitted
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Formation of SiO by radiative association: the impact of resonances¹ ROBERT C. FORREY, Penn State University, BRENDAN M. MCLAUGHLIN, Queen's University Belfast, JAMES F. BABB, Harvard-Smithsonian Center for Astrophysics, PHILLIP C. STANCIL, University of Georgia — Detailed quantum chemistry calculations within the MRCI+Q approximation are presented using an aug-cc-pV6Z (AV6Z) basis set, for the potential energy curves and transition dipole moments between low lying molecular states of singlet spin symmetry for the SiO molecule. The high quality molecular data are used to obtain radiative association cross sections and rate coefficients for collisions between ground state Si and O atoms. Quantal methods are used and compared with semiclassical results. We find that the resonance features present in the quantum mechanical cross sections play a significant role, enhancing the rate coefficients at low temperatures by several orders of magnitude. These new molecular formation rates will therefore have important implications for applications in astrophysics.

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