

Abstract Submitted
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Formation of SiO^+ and CS^+ cations by radiative association¹

JAMES BABB, ITAMP, Center for Astrophysics | Harvard & Smithsonian, ROBERT FORREY, Penn State U., BRENDAN MCLAUGHLIN, Queen's U. Belfast — Rate constants for the formation of SiO^+ by radiative association are calculated using accurate molecular data. The ab initio potential curves and transition dipole moment functions were obtained using the multi-reference configuration interaction approach with the Davidson correction (MRCI+Q) and aug-cc-pCV5Z basis sets. The rate constants include both direct and indirect (inverse rotational predissociation) formation processes. The indirect processes are evaluated for conditions of local thermodynamic equilibrium (LTE) and also in the non-LTE limit of zero radiation temperature and atomic density. Phenomenological rate constants for SiO^+ formation in realistic astrophysical environments are expected to lie between these limiting cases. We compare the results for SiO^+ with those for the isoelectronic system CS^+ , for which we have calculated the molecular data similarly to that for SiO^+ .

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