Dicarbon formation in collisions of two carbon atoms

JAMES BABB, ITAMP, Center for Astrophysics | Harvard & Smithsonian, RYAN SMYTH, BRENDA MCLAUGHLIN, ITAMP & Queen’s U. Belfast — Radiative association cross sections and rates are computed, using a quantum approach, for the formation of C₂ molecules (dicarbon) during the collision of two ground state C(3P) atoms. We find that transitions originating in the C 1Π_g, 3Π_g, and 5Π_u states are the main contributors to the process. The results are compared and contrasted with previous results obtained from a semi-classical approximation. New ab initio potential curves and transition dipole moment functions have been obtained for the present work using the multi-reference configuration interaction approach with the Davidson correction (MRCI+Q) and aug-cc-pCV5Z basis sets. Applications of the current computations to various astrophysical environments and laboratory studies are briefly discussed focusing on these rates. We discuss recent calculations on collisions of a carbon atom and a carbon ion.

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