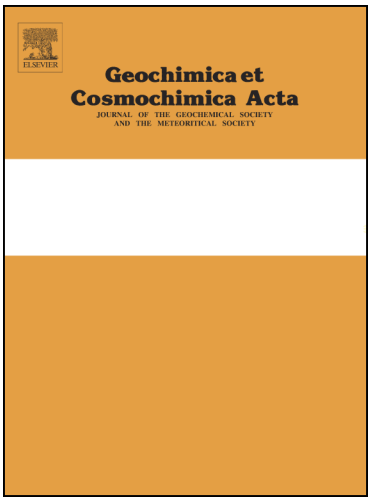

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Graphite Grain-Size Spectrum and Molecules from Core-Collapse Supernovae

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Abstract

Our goal is to compute the abundances of carbon atomic complexes that emerge from the C+O cores of core-collapse supernovae. We utilize our chemical reaction network in which every atomic step of growth employs a quantum-mechanically guided reaction rate. This tool follows step-by-step the growth of linear carbon chain molecules from C atoms in the oxygen-rich C+O cores. We postulate that once linear chain molecules reach a sufficiently large size, they isomerize to ringed molecules, which serve as seeds for graphite grain growth. We demonstrate our technique for merging the molecular reaction network with a parallel program that can follow 10^{17} steps of C addition onto the rare seed species. Due to radioactivity within the C+O core, abundant ambient oxygen is unable to convert C to CO, except to a limited degree that actually facilitates carbon molecular ejecta. But oxygen severely minimizes the linear-carbon-chain abundances. Despite the tiny abundances of these linear-carbon-chain molecules, they can give rise to a small abundance of ringed-carbon molecules that serve as the nucleations on which graphite grain growth builds. We expand the C+O-core gas adiabatically from 6000K for 10^9 s when reactions have essentially stopped. These adiabatic tracks emulate the actual expansions of the supernova cores. Using a standard model of 10^{56} atoms of C+O core ejecta having O/C=3, we calculate standard ejection yields of graphite grains of all sizes

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