MOLECULE CHEMISTRY IN SUPERNOVA EJECTA: INSIGHTS FROM PRESOLAR SiC GRAINS.

P. Hoppe[1] and E. Zinner[2]. [1]Max Planck Institute for Chemistry, Particle Chemistry Dep., 55128 Mainz, Germany. E-mail: peter.hoppe@mpic.de. [2]Laboratory for Space Sciences and Physics Dep., Washington University, St. Louis, MO 63130, USA.

Introduction: Primitive Solar System materials contain small quantities of presolar grains that formed in the winds of evolved stars or in the ejecta of stellar explosions [1]. Of particular importance are SiC grains from Type II supernovae (SNeII), the X grains, characterized by isotopically light Si [2], and the "unusual" and C (subsequently designated U/C) grains, characterized by heavy Si [3-5]. Many of the isotopic signatures of these grains can be satisfactorily reproduced by ad hoc SN mixing models. In this approach, matter from different layers in a SNII [e.g., 6] is mixed in variable proportions. With ad hoc SN mixing, however, it is not possible to explain the isotope data of Fe in X grains [7] and of S in U/C grains [3-5]. While it can not be completely ruled out that predictions for certain isotope abundances in current SN models [6] are in error, it is more likely that the problems with Fe and S point towards element fractionation processes during or prior to SiC formation. Here we will explore the possible role of molecule chemistry in SN ejecta in this respect.

S and Fe in Supernova Grains: The U/C grains have isotopically light S [3-5]. Because Si- and S-isotopic signatures (i.e., heavy or light Si and S) correlate very well in the interior of SNeII [6], ad hoc mixing models fail to account for heavy Si together with light S. Most X grains have higher than solar $^{57}Fe/^{56}Fe$ but solar $^{54}Fe/^{56}Fe$ [7]. The light Si of X grains requires significant contributions from the Si/S zone, which should lead to higher than solar $^{54}Fe/^{56}Fe$ in X grains, contrary to observation.

Discussion: Models based on chemical kinetics predict formation of various molecules in the ejecta of massive SNe [8]. Molecules such as CO and SiO have been observed in the ejecta of SN1987A [9]. According to the models by [8], 13-34% of the ejected matter is in the form of molecules. The molecule inventory depends strongly on the degree of mixing. If H from the outer SN layers mixes with matter from interior layers, then H_2, H_2O, OH, N_2, O_2, CO, CO_2, SO, and SiO dominate. If no mixing occurs, O_2, SiS, and CO dominate. In this latter case about 25% of all molecules are SiS that formed in the Si/S zone. Ad hoc SN mixing shows that it is possible to produce heavy Si even if matter from the Si/S zone is admixed. If SiS molecules from the Si/S zone are incorporated efficiently by the growing SiC grains, while elemental S or other S molecules are not, it would be possible to condense SiC grains with light S and heavy Si. The Fe-isotopic signature of X grains requires preferential trapping of Fe from the He/C and He/N zones. According to the models of molecule chemistry in SN ejecta by [8], some $(FeS)_2$ dust precursors form in the Si/S zone which may prevent Fe from the Si/S zone to be trapped by the growing SiC X grains. Clearly, more detailed work is needed to follow up on these ideas.

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