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Ab initio analysis of the BCN, NBC and CNB fragments formation ROBERT JARA, VLADIMIR MAKAROV, GERARDO MORELL, BRAD WEINER — The Laser Ablation technique applied to the synthesis of nanostructured materials produce unique compositions, with correspondingly unique physical and chemical properties. In order to do smart utilization of this method, fundamental understanding of the precursor formation and incorporation mechanisms for the growth of different materials is crucial. Particularly important is to know what fragments are formed during the ablation process, in order to understand its dynamic evolution and eventual incorporation in the synthesized material. In connection to the synthesis of Boron Carbonitride, we have focused our attention on the dynamic evolution of the primary reactions upon BCN ablation using the *ab initio* method (Gaussian-98 software pack). The results (including the formation energy, direct and inverse rate constants, etc.) were estimated by considering the elementary reactions as bimolecular reactions: reactions between atoms, and atoms with diatomic molecules. The temperature dependence of the dissociation rate constant of three-atomic fragments by different channels was also analyzed using the RRKM theory. It was found that BCN and NBC are the most thermodynamically stable fragments. This theoretical analysis helps understand the strong tendency for BCN to grow stoichiometrically under a variety of experimental conditions.

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