Pressure plays important role in many chemical processes. It is known to drastically alter the chemical reactivity of chemical compounds. The effect of high pressure was examined during the compression simulations. The simulations were conducted as follows: twenty-seven molecules of CH3CXS representing a bulk system, where X = H, F, Cl, CH3, CF3 and NH2 were compressed at the constant rate of 10 GPa/ps until the target pressure of 30 GPa. The results indicated all but NH2 species participated in wide range of oligomerization reactions. The initiation reaction was dimerization reaction though a formation of a C-S bond between two nearby monomer MeCXS molecules. The pressure at which the dimerization reaction for each species was only dependent on the substituent functional group X. Energy decomposition analysis (EDA) was used to establish a trend between computed properties of MeCXS monomer molecules and its dimerization reaction pressures.