Influence of minor impurities of acetone on soot formation in acetylene shock wave pyrolysis

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Acetylene is an unique species that plays a key role in the formation of polyaromatic hydrocarons (PAH) and soot. However, many existing kinetic models can not satisfactorily describe the experimental results on the soot formation during the pyrolysis of acetylene behind shock waves. We analyzed the possibility that such a discrepancy was caused by a minor impurity of acetone inevitably contained in commercially available acetylene [1,2] which influence was previoulsy reported ambiguously [3,4]. Soot volume fraction time profiles in 3% C_2H_2 + Ar mixture at shock tube conditions $T = 1700$–2300 K and $P = 3.5$–4.5 bar was observed and modeled.

It was shown that in the presence of only 0.5 mol % acetone impurity in acetylene (i.e. 150 ppm in studied mixture) the values of the soot volume fraction observed in shock tube experiments at given time $\tau = 0.5$–1.5 ms can increase by several orders of magnitude, as fast acetone decomposition at elevated temepatures releases CH_3 radical providing pathways for propargyl C_3H_3 and benzene ring formation thus accelerating subsequent PAH and soot growth. The effect is exceptionally strong in considered case of realtively low pressures when the soot formation occurs slowly and soot yield at the end of shock tube working time amount to less than one percent.

The importance of controlled acetylene purification was emphasized.

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